



Full wwPDB EM Validation Report ⓘ

Dec 14, 2024 – 09:45 PM EST

PDB ID : 1Q5C
EMDB ID : EMD-1052
Title : S-S-lambda-shaped TRANS and CIS interactions of cadherins model based on fitting C-cadherin (1L3W) to 3D map of desmosomes obtained by electron tomography
Authors : He, W.; Cowin, P.; Stokes, D.L.
Deposited on : 2003-08-06
Resolution : 30.00 Å (reported)
Based on initial model : 1L3W

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

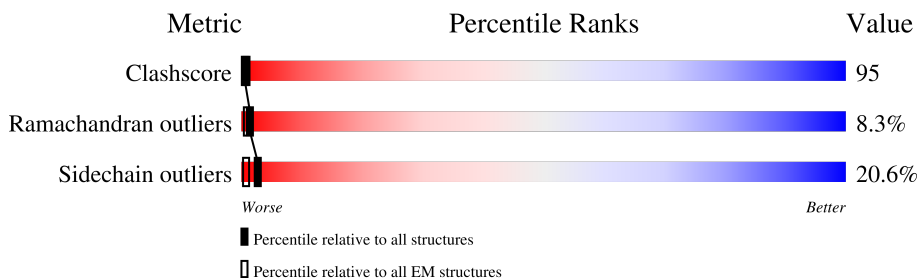
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 30.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	880	
1	B	880	
1	C	880	
1	D	880	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	801	-	-	X	-
2	NAG	A	805	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	806	X	-	X	-
2	NAG	A	807	-	-	X	-
2	NAG	A	809	-	-	X	-
2	NAG	A	810	-	-	X	-
2	NAG	A	902	X	-	X	-
2	NAG	A	903	X	-	-	-
2	NAG	A	904	-	-	X	-
2	NAG	B	801	-	-	X	-
2	NAG	B	805	X	-	X	-
2	NAG	B	806	X	-	X	-
2	NAG	B	807	-	-	X	-
2	NAG	B	809	-	-	X	-
2	NAG	B	810	-	-	X	-
2	NAG	B	902	X	-	X	-
2	NAG	B	903	X	-	-	-
2	NAG	B	904	-	-	X	-
2	NAG	C	801	-	-	X	-
2	NAG	C	805	X	-	-	-
2	NAG	C	806	X	-	X	-
2	NAG	C	807	-	-	X	-
2	NAG	C	809	-	-	X	-
2	NAG	C	810	-	-	X	-
2	NAG	C	902	X	-	X	-
2	NAG	C	903	X	-	-	-
2	NAG	C	904	-	-	X	-
2	NAG	D	801	-	-	X	-
2	NAG	D	805	X	-	X	-
2	NAG	D	806	X	-	X	-
2	NAG	D	807	-	-	X	-
2	NAG	D	809	-	-	X	-
2	NAG	D	810	-	-	X	-
2	NAG	D	902	X	-	X	-
2	NAG	D	903	X	-	-	-
2	NAG	D	904	-	-	X	-
3	NDG	A	811	-	-	X	-
3	NDG	B	811	-	-	X	-
3	NDG	D	811	-	-	X	-

2 Entry composition [i](#)

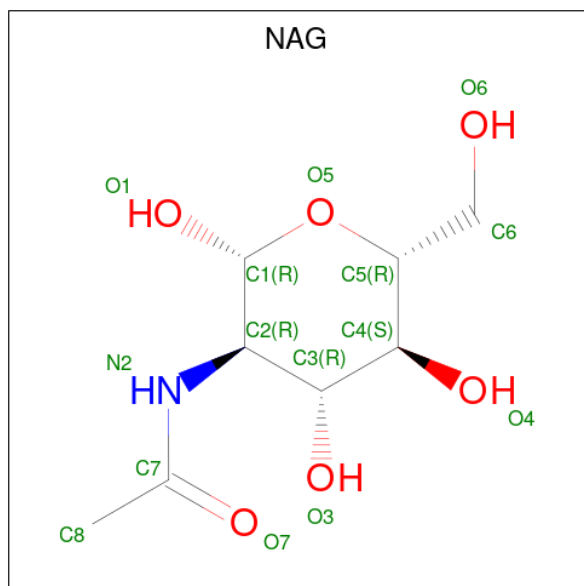
There are 4 unique types of molecules in this entry. The entry contains 17652 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called EP-cadherin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	540	Total	C	N	O	S	0	0
			4191	2635	695	850	11		
1	B	540	Total	C	N	O	S	0	0
			4191	2635	695	850	11		
1	C	540	Total	C	N	O	S	0	0
			4191	2635	695	850	11		
1	D	540	Total	C	N	O	S	0	0
			4191	2635	695	850	11		

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	

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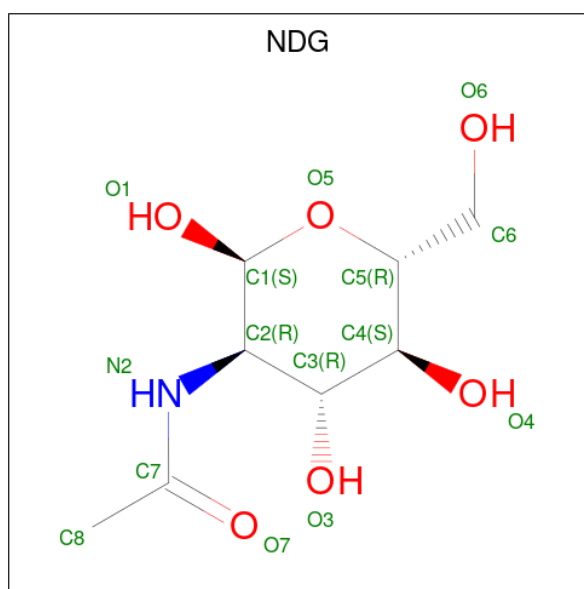
Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 3 is 2-acetamido-2-deoxy- α -D-glucopyranose (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	

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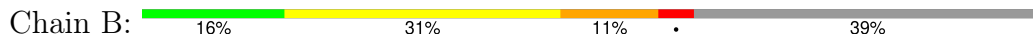
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Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	A	12	Total	Ca	0
			12	12	
4	B	12	Total	Ca	0
			12	12	
4	C	12	Total	Ca	0
			12	12	
4	D	12	Total	Ca	0
			12	12	

- Molecule 1: EP-cadherin



SER	LEU	Y507	P442	V381	A317	G251	Y187	Q101	K33	ASN	MET
LEU	LEU	S508	R443	V382	T318	T252	T188		V34	PHE	GLY
LEU	LEU	S509		K382	T319	T253	T189		V35	SER	LYS
LEU	PHE	Y510	T446	D384	T320	G254	V190	R105	ARG	LYS	THR
LEU	LEU	Y511	M447	N385	V321	G255	V191	P106	HIS	CYS	THR
LEU	LYS		C448	T322	G256	G257	Q192	F108	ARG	LYS	LEU
ARG	LYS	L512	D449	T323	V323	A257	A193	T109	SER	THR	LEU
LYS	ARG	S514	Q450	V388	E324	G258	T194	Q110	GLY	ARG	ASN
ASN	ALA	D515	N451			G259	D195	Q111	GLY	LYS	ALA
ASP	PRO	D516				G260	L196	D111	GLU	HIS	SER
GLU	HIS	A516	P452	N391	N327	G261	E197	V112	ALA	LEU	VAL
VAL	VAL	O517		G392		R262	G198		N45	GLY	TRP
LYS	VAL	N518	L457	N393	P330	G263	A199	S116	P46	SER	LEU
ARG	ARG	N519	T458	L394	F331	G264	A199	V117	ARG	TYR	LEU
PRO	PRO	N520	T459	D395	F332	G265	G200	E119	VAL	ASP	CYS
ASN	ARG	Q521	I459	R396	V333	E265	L201	R118	GLY	VAL	GLY
LEU	SER	E522	D461	S397	P334	G266	V203	E119	SER	GLY	LEU
LEU	SER	L523		E398	T332	G267	V202		G49	ASP	LEU
LEU	ASN	Y523		S398	A335	G267	V203	V127	LYS	LYS	CYS
ASP	PRO	Y524	I464	E399	V336	F268		M128	F51	SER	CYS
TRP	ASP	Y525	F465	E399	S337	F269	I208	M128	R52	PRO	ARG
GLY	GLU	Y526	P466	V400	R338	G270	I209	A129	VAL	VAL	PHE
GLY	ASP		N467	V401	R338	G271	I209	V130	LEU	ARG	GLN
SER	ILE	ASP	N467	N402	V339	G272	Q210	S131	THR	THR	VAL
ARG	GLY	Y529	T468	N403	D340	T272	I211	A132	VAL	VAL	VAL
ASN	ASN	Y469	V469	V341	T273	D274	T212	T133	PHE	LEU	VAL
PHE	ASP	S530	N404	N405	S342	G275	D213	D134	PRO	PRO	PRO
ARG	ASP	S531	R470	T405	E343	G276	A214		GLY	ASP	SER
LYS	ILE	C532	V471	Y406	D344	E277	G215	D137	THR	GLY	ILE
LEU	ASP	E533	K472	T407	S344	G278	D216	M138	HIS	THR	ASN
LEU	PHE	Y534	V473	V408	L345	S277	D216	I139	THR	VAL	ALA
ALA	GLU		S474	I409	S346	N278	N217		THR	VAL	ALA
ASP	ASN		L475	M410	R347	Q279			GLY	LEU	ASP
MET	LEU	Y537	L475	M410	R347	G280	I220	L142	LEU	VAL	VAL
TYR	ASP	K538	S476	L411	G348	G281	F221		LYS	LYS	SER
GLY	GLU	C539	S476	V412	E349	L281	D222	L146	ARG	ARG	GLY
GLY	ALA	Q540	H477	T413	R350	G282	P223		D67	LYS	CYS
ASP	ASP	GLU	G478	T413	K350	T283	K224	I150	VAL	LYS	LYS
ASP	ASN	LYS	S479	D414	I351	T284	T225	L151	ARG	LYS	PRO
ASP	GLY	LYS	D480	D415	L352	G285	G226	K152	D1	GLY	LEU
ASP	GLY	LEU	L481	G416	S353	K286	Y226	E157	W2	HIS	PHE
PRO	PRO	VAL	T482	V417	L354	G287	T227	Q153	V3	LYS	LYS
THR	THR	GLY	W483	S418		G287	T227	D154	I4	ASP	SER
ALA	ALA	GLY	K484	V419	D358	L288	A228	P155	S77	SER	SER
PRO	PRO	PHE	A485	G420	A485	G289	L229	E156	H78	THR	ALA
PRO	PRO	ASP	E486	T421	D360	F290	V230	P231	S79	LYS	GLU
TYR	TYR	LEU	L487	G422	K361	G291	P231	E157	K8	PHE	TYR
ASP	ASP	PRO	D488	T423	Q382	L292	E232		R80	THR	TYR
LEU	LEU	ILE	S489	G424	Q383	G293	M233	P160	V81	THR	ILE
SER	SER	LEU	K490	T425	L364		E234	M161	E11	ILE	PHE
LEU	GLN	LEU	G491	L426	Q385	V296	T235	F162	R83	SER	SER
VAL	VAL	VAL	T492	L427	K366	G297	G236	F163	N84	THR	VAL
PHE	PHE	ILE	S493	L428	L367	L298	F237	T164	P16	THR	VAL
ASP	ASP	ARG	M494	H429	S368	Q299	E238	I165	G85	TRP	ASN
GLY	GLY	GLY	L495	V430	F369	I300	V239		S86	ASP	ARG
TYR	TYR	GLY	L496	L431	F370	T301	Q240	T169	P87	ALA	ARG
GLY	GLY	ASP	L497	D432	L331		G170	G170	V88	ARG	GLU
SER	SER	VAL	S497	V433	K372	P307	R241	V171	E89	GLY	LEU
LEU	LEU	LEU	Q498	N434	M373	G308	L242		Q23	ILE	GLU
ALA	ALA	ARG	T499	D435	D374	S309	S243	L174	P91	LYS	GLY
PRO	PRO	LEU	Q500	D435	P375		V244		M92	HIS	GLY
ASP	ASP	LEU	Q501	D436	P375	S310	G245	L175	E93	SER	ARG
ILE	ILE	LEU	L502	G437	A376	V311	T245	G176	N27	THR	LYS
ALA	ALA	MET	K503	P438	R377	L312	L247	I175	I94	THR	ARG
ALA	ALA	PHE	K504	V439	V378		D248	G176	R30	ASN	LEU
SER	SER	ARG	K504	V439	V378		D248	G176	I96	ILE	GLY
LEU	LEU	ASN	G505	P440	L379	S315	M249	R181	F31	ALA	LYS
LEU	LEU	ASP	D506	G441	T260	G316	P250	F186	D100	VAL	VAL

- Molecule 1: EP-cadherin





4 Experimental information

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of tilted images used	Not provided	
Resolution determination method	Not provided	
CTF correction method	no CTF correction. Imaging at underfocus 0.4 micron with CM200FEG microscope at 50,000 magnification	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1200	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	500	Depositor
Magnification	68276	Depositor
Image detector	GENERIC GATAN	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDG, NAG, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.70	8/4276 (0.2%)	1.39	77/5839 (1.3%)
1	B	0.70	8/4276 (0.2%)	1.39	78/5839 (1.3%)
1	C	0.70	8/4276 (0.2%)	1.39	78/5839 (1.3%)
1	D	0.70	8/4276 (0.2%)	1.39	78/5839 (1.3%)
All	All	0.70	32/17104 (0.2%)	1.39	311/23356 (1.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	4
1	C	0	4
1	D	0	4
All	All	0	16

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	335	ALA	CA-CB	-8.37	1.34	1.52
1	A	335	ALA	CA-CB	-8.36	1.34	1.52
1	D	335	ALA	CA-CB	-8.34	1.34	1.52
1	C	335	ALA	CA-CB	-8.29	1.35	1.52
1	B	539	CYS	CB-SG	8.15	1.96	1.82
1	A	539	CYS	CB-SG	8.15	1.96	1.82
1	C	539	CYS	CB-SG	8.14	1.96	1.82
1	D	539	CYS	CB-SG	8.13	1.96	1.82
1	A	223	PRO	CG-CD	7.02	1.73	1.50
1	B	223	PRO	CG-CD	7.00	1.73	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	223	PRO	CG-CD	7.00	1.73	1.50
1	D	223	PRO	CG-CD	6.98	1.73	1.50
1	D	523	THR	N-CA	-6.25	1.33	1.46
1	B	523	THR	N-CA	-6.25	1.33	1.46
1	C	523	THR	N-CA	-6.22	1.33	1.46
1	A	523	THR	N-CA	-6.22	1.33	1.46
1	B	522	LEU	N-CA	-5.99	1.34	1.46
1	C	522	LEU	N-CA	-5.98	1.34	1.46
1	A	522	LEU	N-CA	-5.98	1.34	1.46
1	D	18	PRO	N-CD	5.97	1.56	1.47
1	C	18	PRO	N-CD	5.95	1.56	1.47
1	D	522	LEU	N-CA	-5.95	1.34	1.46
1	B	18	PRO	N-CD	5.94	1.56	1.47
1	A	18	PRO	N-CD	5.90	1.56	1.47
1	A	530	CYS	CB-SG	5.51	1.91	1.82
1	C	530	CYS	CB-SG	5.49	1.91	1.82
1	D	530	CYS	CB-SG	5.49	1.91	1.82
1	B	530	CYS	CB-SG	5.46	1.91	1.82
1	C	499	THR	CA-CB	5.04	1.66	1.53
1	B	499	THR	CA-CB	5.02	1.66	1.53
1	A	499	THR	CA-CB	5.02	1.66	1.53
1	D	499	THR	CA-CB	5.01	1.66	1.53

All (311) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	520	PRO	CA-C-N	-13.29	87.95	117.20
1	B	520	PRO	CA-C-N	-13.27	88.00	117.20
1	C	520	PRO	CA-C-N	-13.27	88.00	117.20
1	A	520	PRO	CA-C-N	-13.25	88.04	117.20
1	D	235	ILE	N-CA-C	12.74	145.39	111.00
1	D	290	PHE	N-CA-C	12.74	145.39	111.00
1	A	290	PHE	N-CA-C	12.73	145.38	111.00
1	C	235	ILE	N-CA-C	12.73	145.38	111.00
1	B	235	ILE	N-CA-C	12.73	145.37	111.00
1	C	290	PHE	N-CA-C	12.73	145.37	111.00
1	B	290	PHE	N-CA-C	12.72	145.35	111.00
1	A	235	ILE	N-CA-C	12.71	145.32	111.00
1	B	374	ASP	N-CA-C	11.61	142.35	111.00
1	A	374	ASP	N-CA-C	11.60	142.32	111.00
1	C	374	ASP	N-CA-C	11.60	142.33	111.00
1	D	374	ASP	N-CA-C	11.60	142.33	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	17	PHE	C-N-CD	-11.54	95.21	120.60
1	C	17	PHE	C-N-CD	-11.54	95.22	120.60
1	A	17	PHE	C-N-CD	-11.53	95.24	120.60
1	D	17	PHE	C-N-CD	-11.53	95.25	120.60
1	B	398	SER	N-CA-C	11.37	141.71	111.00
1	D	398	SER	N-CA-C	11.38	141.71	111.00
1	A	398	SER	N-CA-C	11.37	141.69	111.00
1	C	398	SER	N-CA-C	11.36	141.66	111.00
1	B	465	PRO	C-N-CD	-11.04	96.31	120.60
1	C	465	PRO	C-N-CD	-11.04	96.31	120.60
1	D	465	PRO	C-N-CD	-11.04	96.32	120.60
1	A	465	PRO	C-N-CD	-11.01	96.38	120.60
1	D	222	ASP	CB-CG-OD2	10.09	127.38	118.30
1	C	222	ASP	CB-CG-OD2	10.06	127.36	118.30
1	B	222	ASP	CB-CG-OD2	10.04	127.33	118.30
1	A	222	ASP	CB-CG-OD2	10.02	127.31	118.30
1	A	236	GLY	N-CA-C	-9.99	88.13	113.10
1	B	236	GLY	N-CA-C	-9.99	88.14	113.10
1	D	236	GLY	N-CA-C	-9.97	88.17	113.10
1	B	230	VAL	C-N-CD	-9.97	98.66	120.60
1	C	236	GLY	N-CA-C	-9.97	88.18	113.10
1	C	230	VAL	C-N-CD	-9.94	98.72	120.60
1	D	230	VAL	C-N-CD	-9.94	98.74	120.60
1	A	230	VAL	C-N-CD	-9.94	98.74	120.60
1	A	374	ASP	CB-CA-C	-9.66	91.08	110.40
1	B	376	ALA	N-CA-C	9.66	137.09	111.00
1	C	374	ASP	CB-CA-C	-9.66	91.08	110.40
1	B	374	ASP	CB-CA-C	-9.66	91.08	110.40
1	D	374	ASP	CB-CA-C	-9.66	91.08	110.40
1	C	376	ALA	N-CA-C	9.65	137.07	111.00
1	D	376	ALA	N-CA-C	9.65	137.07	111.00
1	A	376	ALA	N-CA-C	9.65	137.05	111.00
1	B	522	LEU	CA-CB-CG	-9.38	93.73	115.30
1	A	522	LEU	CA-CB-CG	-9.38	93.74	115.30
1	D	522	LEU	CA-CB-CG	-9.37	93.75	115.30
1	C	522	LEU	CA-CB-CG	-9.36	93.78	115.30
1	A	520	PRO	N-CA-C	9.31	136.31	112.10
1	C	520	PRO	N-CA-C	9.31	136.30	112.10
1	A	223	PRO	N-CA-C	-9.30	87.92	112.10
1	B	520	PRO	N-CA-C	9.30	136.27	112.10
1	A	221	PHE	C-N-CA	-9.29	98.46	121.70
1	B	221	PHE	C-N-CA	-9.29	98.47	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	221	PHE	C-N-CA	-9.29	98.46	121.70
1	C	223	PRO	N-CA-C	-9.30	87.93	112.10
1	D	221	PHE	C-N-CA	-9.29	98.46	121.70
1	D	223	PRO	N-CA-C	-9.30	87.93	112.10
1	B	223	PRO	N-CA-C	-9.29	87.94	112.10
1	D	481	LEU	N-CA-C	-9.29	85.92	111.00
1	B	481	LEU	N-CA-C	-9.28	85.95	111.00
1	D	520	PRO	N-CA-C	9.28	136.23	112.10
1	C	481	LEU	N-CA-C	-9.28	85.96	111.00
1	A	481	LEU	N-CA-C	-9.26	85.99	111.00
1	D	481	LEU	CA-CB-CG	-8.76	95.14	115.30
1	B	481	LEU	CA-CB-CG	-8.76	95.15	115.30
1	A	481	LEU	CA-CB-CG	-8.76	95.16	115.30
1	C	481	LEU	CA-CB-CG	-8.74	95.19	115.30
1	D	289	ASP	C-N-CA	-8.44	100.61	121.70
1	B	289	ASP	C-N-CA	-8.43	100.63	121.70
1	C	289	ASP	C-N-CA	-8.43	100.64	121.70
1	A	289	ASP	C-N-CA	-8.42	100.65	121.70
1	C	516	ALA	N-CA-C	-8.36	88.42	111.00
1	A	516	ALA	N-CA-C	-8.35	88.45	111.00
1	B	516	ALA	N-CA-C	-8.35	88.45	111.00
1	D	516	ALA	N-CA-C	-8.35	88.46	111.00
1	C	222	ASP	C-N-CD	-8.20	102.56	120.60
1	A	222	ASP	C-N-CD	-8.20	102.56	120.60
1	B	222	ASP	C-N-CD	-8.19	102.58	120.60
1	D	222	ASP	C-N-CD	-8.19	102.58	120.60
1	B	290	PHE	CA-C-N	-8.19	99.19	117.20
1	A	290	PHE	CA-C-N	-8.18	99.20	117.20
1	D	290	PHE	CA-C-N	-8.18	99.21	117.20
1	C	290	PHE	CA-C-N	-8.17	99.22	117.20
1	B	46	PRO	C-N-CD	-8.05	102.89	120.60
1	A	46	PRO	C-N-CD	-8.03	102.94	120.60
1	D	46	PRO	C-N-CD	-8.03	102.94	120.60
1	C	46	PRO	C-N-CD	-8.02	102.95	120.60
1	C	233	ASN	N-CA-C	7.88	132.27	111.00
1	A	233	ASN	N-CA-C	7.87	132.26	111.00
1	D	233	ASN	N-CA-C	7.86	132.22	111.00
1	B	233	ASN	N-CA-C	7.86	132.21	111.00
1	D	336	VAL	N-CA-C	7.81	132.09	111.00
1	A	336	VAL	N-CA-C	7.81	132.09	111.00
1	B	336	VAL	N-CA-C	7.80	132.05	111.00
1	C	522	LEU	C-N-CA	-7.80	102.21	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	522	LEU	C-N-CA	-7.79	102.23	121.70
1	C	336	VAL	N-CA-C	7.79	132.03	111.00
1	D	522	LEU	C-N-CA	-7.79	102.23	121.70
1	B	522	LEU	C-N-CA	-7.78	102.25	121.70
1	A	362	GLN	N-CA-C	-7.73	90.13	111.00
1	D	362	GLN	N-CA-C	-7.73	90.14	111.00
1	C	362	GLN	N-CA-C	-7.72	90.16	111.00
1	B	362	GLN	N-CA-C	-7.72	90.17	111.00
1	C	234	GLU	N-CA-C	-7.60	90.48	111.00
1	A	234	GLU	N-CA-C	-7.60	90.48	111.00
1	B	234	GLU	N-CA-C	-7.58	90.55	111.00
1	D	234	GLU	N-CA-C	-7.57	90.56	111.00
1	A	234	GLU	C-N-CA	7.43	140.28	121.70
1	D	234	GLU	C-N-CA	7.41	140.22	121.70
1	C	234	GLU	C-N-CA	7.40	140.21	121.70
1	B	234	GLU	C-N-CA	7.40	140.20	121.70
1	C	521	GLN	C-N-CA	-7.39	103.22	121.70
1	A	521	GLN	C-N-CA	-7.39	103.23	121.70
1	B	521	GLN	C-N-CA	-7.37	103.28	121.70
1	D	521	GLN	C-N-CA	-7.36	103.30	121.70
1	A	277	SER	N-CA-C	-7.21	91.53	111.00
1	D	277	SER	N-CA-C	-7.20	91.56	111.00
1	B	277	SER	N-CA-C	-7.19	91.59	111.00
1	C	277	SER	N-CA-C	-7.19	91.59	111.00
1	C	337	SER	N-CA-C	-7.19	91.59	111.00
1	D	337	SER	N-CA-C	-7.19	91.60	111.00
1	A	337	SER	N-CA-C	-7.18	91.62	111.00
1	B	337	SER	N-CA-C	-7.17	91.64	111.00
1	D	503	LYS	N-CA-C	7.03	129.97	111.00
1	C	503	LYS	N-CA-C	7.02	129.94	111.00
1	B	503	LYS	N-CA-C	7.01	129.92	111.00
1	A	503	LYS	N-CA-C	7.00	129.90	111.00
1	A	523	THR	N-CA-CB	-6.95	97.10	110.30
1	B	523	THR	N-CA-CB	-6.94	97.11	110.30
1	C	523	THR	N-CA-CB	-6.93	97.12	110.30
1	D	523	THR	N-CA-CB	-6.93	97.14	110.30
1	A	492	THR	N-CA-C	6.78	129.31	111.00
1	C	492	THR	N-CA-C	6.77	129.27	111.00
1	D	492	THR	N-CA-C	6.76	129.26	111.00
1	B	492	THR	N-CA-C	6.76	129.24	111.00
1	D	448	CYS	CA-CB-SG	-6.71	101.93	114.00
1	A	448	CYS	CA-CB-SG	-6.69	101.96	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	448	CYS	CA-CB-SG	-6.68	101.97	114.00
1	B	448	CYS	CA-CB-SG	-6.68	101.98	114.00
1	D	476	SER	N-CA-C	6.59	128.78	111.00
1	C	476	SER	N-CA-C	6.58	128.78	111.00
1	A	476	SER	N-CA-C	6.58	128.77	111.00
1	D	398	SER	C-N-CA	-6.58	105.24	121.70
1	A	398	SER	C-N-CA	-6.58	105.25	121.70
1	C	398	SER	C-N-CA	-6.58	105.25	121.70
1	B	398	SER	C-N-CA	-6.57	105.26	121.70
1	B	476	SER	N-CA-C	6.57	128.75	111.00
1	B	491	GLY	N-CA-C	6.55	129.47	113.10
1	D	491	GLY	N-CA-C	6.53	129.44	113.10
1	A	491	GLY	N-CA-C	6.53	129.41	113.10
1	C	525	VAL	N-CA-C	-6.53	93.38	111.00
1	C	491	GLY	N-CA-C	6.51	129.38	113.10
1	D	525	VAL	N-CA-C	-6.51	93.42	111.00
1	A	525	VAL	N-CA-C	-6.50	93.45	111.00
1	B	525	VAL	N-CA-C	-6.49	93.47	111.00
1	B	335	ALA	N-CA-C	-6.33	93.90	111.00
1	A	335	ALA	N-CA-C	-6.33	93.91	111.00
1	C	335	ALA	N-CA-C	-6.33	93.91	111.00
1	D	335	ALA	N-CA-C	-6.33	93.92	111.00
1	C	532	CYS	N-CA-C	6.32	128.06	111.00
1	D	532	CYS	N-CA-C	6.31	128.03	111.00
1	A	532	CYS	N-CA-C	6.30	128.00	111.00
1	B	532	CYS	N-CA-C	6.29	127.98	111.00
1	C	234	GLU	CA-C-N	-6.28	103.38	117.20
1	B	234	GLU	CA-C-N	-6.28	103.39	117.20
1	D	234	GLU	CA-C-N	-6.28	103.39	117.20
1	A	234	GLU	CA-C-N	-6.24	103.46	117.20
1	B	222	ASP	N-CA-C	6.16	127.64	111.00
1	A	222	ASP	N-CA-C	6.16	127.63	111.00
1	A	235	ILE	CA-C-N	-6.16	103.89	116.20
1	D	222	ASP	N-CA-C	6.16	127.62	111.00
1	C	222	ASP	N-CA-C	6.15	127.62	111.00
1	D	235	ILE	CA-C-N	-6.14	103.92	116.20
1	B	235	ILE	CA-C-N	-6.14	103.92	116.20
1	C	235	ILE	CA-C-N	-6.14	103.92	116.20
1	C	397	GLU	C-N-CA	-6.14	106.36	121.70
1	A	397	GLU	C-N-CA	-6.14	106.36	121.70
1	B	397	GLU	C-N-CA	-6.13	106.38	121.70
1	D	397	GLU	C-N-CA	-6.12	106.40	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	503	LYS	CB-CA-C	-6.11	98.19	110.40
1	B	18	PRO	CA-N-CD	-6.10	102.96	111.50
1	B	503	LYS	CB-CA-C	-6.09	98.22	110.40
1	C	18	PRO	CA-N-CD	-6.09	102.97	111.50
1	C	503	LYS	CB-CA-C	-6.09	98.22	110.40
1	A	503	LYS	CB-CA-C	-6.08	98.24	110.40
1	D	18	PRO	CA-N-CD	-6.08	102.99	111.50
1	A	18	PRO	CA-N-CD	-6.08	102.99	111.50
1	D	502	LEU	N-CA-C	6.07	127.38	111.00
1	C	502	LEU	N-CA-C	6.06	127.36	111.00
1	B	502	LEU	N-CA-C	6.05	127.33	111.00
1	A	502	LEU	N-CA-C	6.05	127.33	111.00
1	A	2	TRP	N-CA-C	-6.03	94.71	111.00
1	D	2	TRP	N-CA-C	-6.03	94.73	111.00
1	B	2	TRP	N-CA-C	-6.01	94.76	111.00
1	C	2	TRP	N-CA-C	-6.01	94.76	111.00
1	D	374	ASP	C-N-CD	5.98	140.95	128.40
1	A	222	ASP	N-CA-CB	5.97	121.35	110.60
1	C	374	ASP	C-N-CD	5.97	140.94	128.40
1	D	222	ASP	N-CA-CB	5.96	121.33	110.60
1	A	374	ASP	C-N-CD	5.96	140.91	128.40
1	C	222	ASP	N-CA-CB	5.95	121.30	110.60
1	B	374	ASP	C-N-CD	5.94	140.88	128.40
1	B	222	ASP	N-CA-CB	5.94	121.29	110.60
1	C	364	ILE	N-CA-C	-5.92	95.00	111.00
1	A	364	ILE	N-CA-C	-5.92	95.03	111.00
1	D	364	ILE	N-CA-C	-5.91	95.04	111.00
1	B	364	ILE	N-CA-C	-5.91	95.05	111.00
1	D	382	ASN	N-CA-C	-5.84	95.22	111.00
1	C	376	ALA	CA-C-N	-5.84	104.35	117.20
1	B	382	ASN	N-CA-C	-5.84	95.24	111.00
1	A	376	ALA	CA-C-N	-5.83	104.36	117.20
1	D	376	ALA	CA-C-N	-5.83	104.37	117.20
1	A	382	ASN	N-CA-C	-5.83	95.27	111.00
1	C	382	ASN	N-CA-C	-5.83	95.27	111.00
1	B	376	ALA	CA-C-N	-5.81	104.42	117.20
1	B	471	TYR	N-CA-C	5.74	126.50	111.00
1	C	471	TYR	N-CA-C	5.73	126.47	111.00
1	D	471	TYR	N-CA-C	5.72	126.45	111.00
1	A	471	TYR	N-CA-C	5.72	126.45	111.00
1	B	481	LEU	CA-C-N	-5.70	104.65	117.20
1	C	481	LEU	CA-C-N	-5.70	104.65	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	481	LEU	CA-C-N	-5.70	104.66	117.20
1	D	481	LEU	CA-C-N	-5.70	104.67	117.20
1	D	374	ASP	C-N-CA	-5.67	98.17	122.00
1	C	374	ASP	C-N-CA	-5.67	98.19	122.00
1	B	374	ASP	C-N-CA	-5.67	98.21	122.00
1	A	374	ASP	C-N-CA	-5.66	98.21	122.00
1	A	403	ASN	N-CA-C	-5.64	95.78	111.00
1	B	403	ASN	N-CA-C	-5.63	95.80	111.00
1	D	403	ASN	N-CA-C	-5.63	95.80	111.00
1	C	403	ASN	N-CA-C	-5.63	95.81	111.00
1	B	221	PHE	CA-C-N	5.58	129.48	117.20
1	A	221	PHE	CA-C-N	5.57	129.46	117.20
1	D	505	GLY	N-CA-C	5.57	127.03	113.10
1	C	505	GLY	N-CA-C	5.57	127.03	113.10
1	C	221	PHE	CA-C-N	5.56	129.43	117.20
1	D	221	PHE	CA-C-N	5.56	129.43	117.20
1	B	505	GLY	N-CA-C	5.55	126.98	113.10
1	D	502	LEU	CB-CA-C	-5.54	99.67	110.20
1	A	505	GLY	N-CA-C	5.54	126.95	113.10
1	B	502	LEU	CB-CA-C	-5.54	99.68	110.20
1	A	502	LEU	CB-CA-C	-5.53	99.69	110.20
1	C	502	LEU	CB-CA-C	-5.53	99.69	110.20
1	D	157	GLU	C-N-CD	-5.47	108.56	120.60
1	A	157	GLU	C-N-CD	-5.47	108.57	120.60
1	C	157	GLU	C-N-CD	-5.47	108.57	120.60
1	B	157	GLU	C-N-CD	-5.45	108.60	120.60
1	B	519	ASN	N-CA-C	5.37	125.49	111.00
1	D	519	ASN	N-CA-C	5.36	125.48	111.00
1	C	519	ASN	N-CA-C	5.35	125.44	111.00
1	A	519	ASN	N-CA-C	5.34	125.42	111.00
1	A	405	THR	N-CA-C	5.32	125.36	111.00
1	C	405	THR	N-CA-C	5.32	125.36	111.00
1	B	405	THR	N-CA-C	5.32	125.35	111.00
1	D	405	THR	N-CA-C	5.32	125.35	111.00
1	C	367	LEU	CA-CB-CG	-5.31	103.08	115.30
1	D	367	LEU	CA-CB-CG	-5.30	103.10	115.30
1	B	367	LEU	CA-CB-CG	-5.29	103.12	115.30
1	A	367	LEU	CA-CB-CG	-5.28	103.15	115.30
1	B	521	GLN	N-CA-C	-5.21	96.94	111.00
1	D	521	GLN	N-CA-C	-5.21	96.94	111.00
1	C	521	GLN	N-CA-C	-5.20	96.95	111.00
1	A	521	GLN	N-CA-C	-5.20	96.95	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	290	PHE	O-C-N	5.20	131.01	122.70
1	A	290	PHE	O-C-N	5.19	131.00	122.70
1	A	520	PRO	C-N-CA	5.18	134.65	121.70
1	B	290	PHE	O-C-N	5.17	130.98	122.70
1	C	532	CYS	N-CA-CB	-5.17	101.29	110.60
1	B	520	PRO	C-N-CA	5.17	134.62	121.70
1	C	290	PHE	O-C-N	5.17	130.97	122.70
1	C	520	PRO	C-N-CA	5.17	134.61	121.70
1	D	532	CYS	N-CA-CB	-5.16	101.31	110.60
1	A	532	CYS	N-CA-CB	-5.15	101.33	110.60
1	D	520	PRO	C-N-CA	5.14	134.54	121.70
1	B	18	PRO	CA-CB-CG	-5.13	94.26	104.00
1	B	532	CYS	N-CA-CB	-5.13	101.37	110.60
1	A	18	PRO	CA-CB-CG	-5.12	94.27	104.00
1	B	339	VAL	N-CA-C	5.12	124.83	111.00
1	D	18	PRO	CA-CB-CG	-5.12	94.27	104.00
1	C	339	VAL	N-CA-C	5.12	124.82	111.00
1	C	522	LEU	N-CA-C	-5.12	97.18	111.00
1	A	522	LEU	N-CA-C	-5.12	97.19	111.00
1	B	522	LEU	N-CA-C	-5.12	97.19	111.00
1	A	339	VAL	N-CA-C	5.11	124.81	111.00
1	D	522	LEU	N-CA-C	-5.11	97.21	111.00
1	D	339	VAL	N-CA-C	5.10	124.77	111.00
1	C	18	PRO	CA-CB-CG	-5.09	94.32	104.00
1	A	16	PRO	C-N-CA	-5.07	109.02	121.70
1	C	16	PRO	C-N-CA	-5.07	109.03	121.70
1	B	16	PRO	C-N-CA	-5.07	109.03	121.70
1	D	16	PRO	C-N-CA	-5.06	109.06	121.70
1	C	470	PRO	N-CA-C	5.03	125.19	112.10
1	C	332	PHE	N-CA-C	-5.03	97.42	111.00
1	D	332	PHE	N-CA-C	-5.03	97.42	111.00
1	B	470	PRO	N-CA-C	5.03	125.17	112.10
1	A	332	PHE	N-CA-C	-5.03	97.42	111.00
1	C	221	PHE	N-CA-C	5.03	124.57	111.00
1	B	332	PHE	N-CA-C	-5.03	97.43	111.00
1	B	221	PHE	N-CA-C	5.02	124.56	111.00
1	A	221	PHE	N-CA-C	5.02	124.55	111.00
1	A	539	CYS	N-CA-C	5.02	124.55	111.00
1	D	470	PRO	N-CA-C	5.02	125.15	112.10
1	B	539	CYS	N-CA-C	5.01	124.54	111.00
1	D	539	CYS	N-CA-C	5.01	124.54	111.00
1	D	221	PHE	N-CA-C	5.01	124.53	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	539	CYS	N-CA-C	5.01	124.52	111.00

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	PHE	Sidechain
1	A	18	PRO	Mainchain
1	A	222	ASP	Mainchain
1	A	520	PRO	Mainchain
1	B	17	PHE	Sidechain
1	B	18	PRO	Mainchain
1	B	222	ASP	Mainchain
1	B	520	PRO	Mainchain
1	C	17	PHE	Sidechain
1	C	18	PRO	Mainchain
1	C	222	ASP	Mainchain
1	C	520	PRO	Mainchain
1	D	17	PHE	Sidechain
1	D	18	PRO	Mainchain
1	D	222	ASP	Mainchain
1	D	520	PRO	Mainchain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4191	0	4089	796	0
1	B	4191	0	4081	863	0
1	C	4191	0	4078	1116	0
1	D	4191	0	4082	1111	0
2	A	182	0	168	93	0
2	B	182	0	168	90	0
2	C	182	0	169	92	0
2	D	182	0	169	92	0
3	A	28	0	24	9	0
3	B	28	0	24	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	28	0	24	8	0
3	D	28	0	24	9	0
4	A	12	0	0	0	0
4	B	12	0	0	0	0
4	C	12	0	0	0	0
4	D	12	0	0	0	0
All	All	17652	0	17100	3289	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 95.

All (3289) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ILE:HB	1:D:2:TRP:CE2	1.18	1.70
1:C:87:PRO:HG3	1:D:43:ALA:CB	1.22	1.65
1:C:87:PRO:CG	1:D:43:ALA:CB	1.77	1.61
1:C:87:PRO:HG3	1:D:43:ALA:CA	1.16	1.58
1:D:464:ILE:HD12	1:D:465:PRO:CD	1.29	1.58
1:C:81:VAL:HG21	1:D:45:ASN:CB	1.32	1.55
1:C:87:PRO:CA	1:D:43:ALA:HB2	1.12	1.55
1:C:81:VAL:CG2	1:D:45:ASN:CB	1.80	1.54
1:A:24:ILE:CB	1:D:2:TRP:CE2	1.91	1.54
1:B:83:GLU:HB2	1:C:25:LYS:CD	1.10	1.54
1:B:464:ILE:HD12	1:B:465:PRO:CD	1.30	1.54
1:C:464:ILE:HD12	1:C:465:PRO:CD	1.30	1.54
1:A:464:ILE:HD12	1:A:465:PRO:CD	1.30	1.53
1:C:81:VAL:HG12	1:D:43:ALA:CB	1.33	1.53
1:C:83:GLU:HA	1:D:41:GLN:CD	1.24	1.53
1:C:81:VAL:CG1	1:D:43:ALA:HB3	1.40	1.52
1:B:31:PHE:HE1	1:D:75:VAL:CG1	1.22	1.50
1:C:1:ASP:HA	1:D:89:GLU:CD	1.21	1.48
1:B:83:GLU:CB	1:C:25:LYS:CD	1.87	1.48
1:B:33:LYS:N	1:C:25:LYS:HE2	1.26	1.47
1:A:24:ILE:CB	1:D:2:TRP:NE1	1.77	1.46
1:C:27:ASN:HD22	1:D:93:GLU:CB	1.26	1.46
1:A:1:ASP:N	1:B:94:ILE:HD11	1.18	1.45
1:C:32:ASN:H	1:D:75:VAL:CG2	1.24	1.45
1:C:79:HIS:CA	1:D:39:THR:HG21	1.24	1.45
1:C:87:PRO:CG	1:D:43:ALA:HA	1.38	1.43
1:B:31:PHE:N	1:C:30:ARG:HB2	1.31	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:464:ILE:CD1	1:C:465:PRO:HD2	1.50	1.42
1:C:79:HIS:HA	1:D:39:THR:CG2	1.09	1.41
1:A:2:TRP:CE2	1:B:80:ALA:CB	1.76	1.41
1:B:464:ILE:CD1	1:B:465:PRO:HD2	1.50	1.40
1:A:464:ILE:CD1	1:A:465:PRO:HD2	1.50	1.40
1:D:464:ILE:CD1	1:D:465:PRO:HD2	1.50	1.40
1:C:85:GLY:CA	1:D:42:GLY:N	1.83	1.38
1:B:31:PHE:HA	1:C:30:ARG:CA	1.54	1.38
1:C:81:VAL:CG2	1:D:45:ASN:HB2	0.91	1.37
1:C:83:GLU:HA	1:D:41:GLN:NE2	1.06	1.37
1:C:87:PRO:CD	1:D:43:ALA:HA	1.55	1.37
1:B:89:GLU:HA	1:D:1:ASP:CB	1.34	1.36
1:C:87:PRO:CA	1:D:43:ALA:CB	2.02	1.36
1:A:9:VAL:C	1:D:30:ARG:HD3	1.44	1.35
1:B:31:PHE:HA	1:C:30:ARG:N	1.38	1.35
1:C:1:ASP:N	1:D:28:LYS:HD3	1.37	1.34
1:A:90:GLU:HB3	1:B:3:VAL:C	1.46	1.33
1:C:83:GLU:CA	1:D:41:GLN:NE2	1.90	1.33
1:A:2:TRP:CD2	1:B:80:ALA:HB2	1.29	1.33
1:B:31:PHE:CE1	1:D:75:VAL:CG1	2.12	1.33
1:B:31:PHE:CE1	1:D:75:VAL:HG11	1.64	1.33
1:C:1:ASP:CA	1:D:89:GLU:CD	1.96	1.32
1:B:89:GLU:CA	1:D:1:ASP:CB	1.87	1.32
1:A:24:ILE:HB	1:D:2:TRP:NE1	1.02	1.32
1:C:90:GLU:HB3	1:D:79:HIS:O	1.28	1.31
1:C:1:ASP:O	1:D:28:LYS:NZ	1.63	1.31
1:C:87:PRO:CB	1:D:43:ALA:CB	2.09	1.31
1:C:27:ASN:ND2	1:D:93:GLU:CB	1.91	1.31
1:C:81:VAL:HG22	1:D:45:ASN:ND2	1.42	1.30
1:C:32:ASN:N	1:D:75:VAL:HG21	1.43	1.30
1:C:79:HIS:CB	1:D:44:ASP:OD1	1.81	1.29
1:C:85:GLY:HA2	1:D:42:GLY:N	1.40	1.28
1:C:32:ASN:N	1:D:75:VAL:CG2	1.92	1.27
1:A:2:TRP:CE2	1:B:80:ALA:HB2	0.95	1.27
1:A:4:ILE:CA	1:B:91:PRO:N	1.97	1.26
1:C:84:ASN:HB2	1:D:74:TYR:CE1	1.44	1.25
1:B:89:GLU:HA	1:D:1:ASP:CG	0.94	1.24
1:C:28:LYS:O	1:D:75:VAL:HG13	1.07	1.24
1:C:28:LYS:O	1:D:75:VAL:CG1	1.86	1.24
1:A:4:ILE:HA	1:B:91:PRO:N	1.20	1.23
1:A:91:PRO:N	1:B:3:VAL:HG22	1.51	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:GLU:HB2	1:C:25:LYS:CG	1.53	1.23
1:B:30:ARG:C	1:C:30:ARG:HB2	1.58	1.23
1:C:4:ILE:CG2	1:D:87:PRO:HG2	1.69	1.23
1:C:87:PRO:N	1:D:43:ALA:HB2	1.52	1.22
1:B:33:LYS:H	1:C:25:LYS:CE	1.52	1.22
1:C:90:GLU:OE1	1:D:53:ILE:CD1	1.85	1.22
1:A:2:TRP:CD2	1:B:80:ALA:CB	2.04	1.22
1:A:4:ILE:HA	1:B:90:GLU:C	1.59	1.22
1:C:1:ASP:HA	1:D:89:GLU:OE2	1.37	1.21
1:C:85:GLY:CA	1:D:42:GLY:CA	1.77	1.21
1:C:540:GLN:O	1:C:540:GLN:CD	1.79	1.21
1:B:86:SER:CA	1:D:90:GLU:HG3	1.62	1.20
1:C:87:PRO:CG	1:D:43:ALA:CA	1.85	1.20
1:C:84:ASN:HB2	1:D:74:TYR:CZ	1.43	1.20
1:B:540:GLN:O	1:B:540:GLN:CD	1.79	1.19
1:A:540:GLN:O	1:A:540:GLN:CD	1.79	1.19
1:C:31:PHE:HB2	1:D:95:THR:CG2	1.72	1.19
1:C:90:GLU:CA	1:D:79:HIS:H	1.53	1.19
1:B:32:ASN:HB2	1:C:29:ASP:OD2	1.41	1.19
1:B:83:GLU:N	1:C:25:LYS:HD3	1.56	1.19
1:C:84:ASN:CB	1:D:74:TYR:CE1	2.15	1.19
1:C:31:PHE:CB	1:D:95:THR:HG23	1.72	1.18
1:C:79:HIS:HB2	1:D:44:ASP:OD1	1.40	1.18
1:B:31:PHE:HE2	1:C:26:SER:O	1.25	1.18
1:D:450:GLN:HG2	1:D:532:CYS:O	1.43	1.18
1:C:450:GLN:HG2	1:C:532:CYS:O	1.43	1.18
1:D:8:LYS:H	1:D:8:LYS:HD2	1.04	1.18
1:D:540:GLN:O	1:D:540:GLN:CD	1.79	1.18
1:C:89:GLU:OE1	1:D:78:SER:OG	1.56	1.17
1:D:474:SER:HB2	1:D:512:LEU:HG	1.25	1.17
1:A:482:THR:HG23	1:A:499:THR:CG2	1.75	1.17
1:A:469:TYR:CG	1:A:470:PRO:HD2	1.81	1.16
1:B:89:GLU:CA	1:D:1:ASP:HB2	1.41	1.16
1:B:482:THR:HG23	1:B:499:THR:CG2	1.75	1.16
1:D:423:THR:HB	2:D:810:NAG:C7	1.76	1.16
1:D:482:THR:HG23	1:D:499:THR:CG2	1.75	1.16
1:B:423:THR:HB	2:B:810:NAG:C7	1.76	1.16
1:B:469:TYR:CG	1:B:470:PRO:HD2	1.81	1.16
1:B:83:GLU:CB	1:C:25:LYS:HD2	1.55	1.16
1:C:87:PRO:CD	1:D:43:ALA:CA	2.16	1.16
1:A:338:ARG:HD3	1:A:352:ILE:HG22	1.26	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:ASP:N	1:D:88:VAL:HG12	1.61	1.16
1:C:482:THR:HG23	1:C:499:THR:CG2	1.75	1.16
1:D:234:GLU:H	1:D:235:ILE:HG23	1.08	1.16
1:C:35:TYR:O	1:D:45:ASN:ND2	1.76	1.15
1:D:338:ARG:HD3	1:D:352:ILE:HG22	1.26	1.15
1:B:234:GLU:H	1:B:235:ILE:HG23	1.08	1.15
1:C:469:TYR:CG	1:C:470:PRO:HD2	1.81	1.15
1:A:450:GLN:HG2	1:A:532:CYS:O	1.43	1.15
1:D:469:TYR:CG	1:D:470:PRO:HD2	1.80	1.15
1:C:83:GLU:CA	1:D:41:GLN:CD	2.11	1.15
1:C:91:PRO:CB	1:D:37:SER:OG	1.93	1.15
1:B:31:PHE:CA	1:C:30:ARG:N	2.08	1.14
1:C:87:PRO:CB	1:D:43:ALA:HB1	1.72	1.14
1:C:87:PRO:CB	1:D:43:ALA:HB2	1.75	1.14
1:B:450:GLN:HG2	1:B:532:CYS:O	1.43	1.14
1:C:423:THR:HB	2:C:810:NAG:C7	1.76	1.14
1:A:423:THR:HB	2:A:810:NAG:C7	1.76	1.13
1:C:8:LYS:H	1:C:8:LYS:HD2	1.04	1.13
1:B:30:ARG:C	1:C:30:ARG:CB	2.16	1.13
1:C:403:ASN:HB2	2:C:902:NAG:H83	1.30	1.13
1:A:9:VAL:C	1:D:30:ARG:CD	2.18	1.13
1:B:32:ASN:CB	1:C:29:ASP:OD2	1.96	1.13
1:C:81:VAL:HG23	1:D:45:ASN:HB2	1.28	1.13
1:C:84:ASN:CB	1:D:74:TYR:CZ	2.23	1.13
1:B:84:ASN:OD1	1:C:26:SER:CA	1.85	1.12
1:B:89:GLU:CA	1:D:1:ASP:CG	1.90	1.12
1:C:93:GLU:OE2	1:D:85:GLY:HA2	1.43	1.12
1:C:27:ASN:ND2	1:D:93:GLU:HB3	1.58	1.12
1:C:79:HIS:CA	1:D:39:THR:CG2	1.84	1.12
1:D:32:ASN:HD21	1:D:83:GLU:HB2	0.98	1.12
1:A:8:LYS:H	1:A:8:LYS:HD2	1.04	1.12
1:B:154:ASP:C	2:B:801:NAG:H82	1.70	1.12
1:C:31:PHE:HB2	1:D:95:THR:HG21	1.32	1.12
1:D:403:ASN:HB2	2:D:902:NAG:H83	1.30	1.12
1:B:89:GLU:N	1:D:1:ASP:HB2	1.65	1.11
1:B:301:THR:HG21	2:B:805:NAG:H82	1.29	1.11
1:A:403:ASN:HB2	2:A:902:NAG:H83	1.30	1.11
1:C:31:PHE:HB3	1:D:75:VAL:HG22	1.23	1.11
1:C:338:ARG:HD3	1:C:352:ILE:HG22	1.26	1.11
1:A:154:ASP:C	2:A:801:NAG:H82	1.70	1.11
1:B:83:GLU:H	1:C:25:LYS:HD3	0.97	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:ASP:C	2:D:801:NAG:H82	1.70	1.11
1:A:1:ASP:N	1:B:94:ILE:CD1	2.13	1.11
1:A:90:GLU:HB3	1:B:3:VAL:CA	1.70	1.10
1:B:222:ASP:O	1:B:222:ASP:OD1	1.69	1.10
1:C:474:SER:HB2	1:C:512:LEU:HG	1.25	1.10
1:B:83:GLU:CG	1:C:25:LYS:HD2	1.82	1.10
1:A:90:GLU:HG3	1:B:3:VAL:HG23	1.24	1.10
1:A:222:ASP:OD1	1:A:222:ASP:O	1.69	1.10
1:A:234:GLU:H	1:A:235:ILE:HG23	1.08	1.10
1:B:474:SER:HB2	1:B:512:LEU:HG	1.25	1.09
1:C:90:GLU:OE2	1:D:53:ILE:CG2	2.00	1.09
1:C:91:PRO:CA	1:D:37:SER:OG	1.81	1.09
1:A:227:THR:HG21	2:A:807:NAG:C8	1.82	1.09
1:C:86:SER:N	1:D:42:GLY:HA3	0.97	1.09
1:C:222:ASP:OD1	1:C:222:ASP:O	1.69	1.09
1:B:86:SER:CA	1:D:90:GLU:CA	2.30	1.09
1:C:154:ASP:C	2:C:801:NAG:H82	1.70	1.09
1:C:227:THR:HG21	2:C:807:NAG:C8	1.82	1.09
1:D:482:THR:HG23	1:D:499:THR:HG22	1.09	1.09
1:A:9:VAL:CA	1:D:30:ARG:HD3	1.83	1.09
1:C:482:THR:HG23	1:C:499:THR:HG22	1.09	1.09
1:A:32:ASN:HD21	1:A:83:GLU:HB2	0.98	1.09
1:B:227:THR:HG21	2:B:807:NAG:C8	1.82	1.08
1:C:32:ASN:HD21	1:C:83:GLU:HB2	0.98	1.08
1:D:227:THR:HG21	2:D:807:NAG:C8	1.82	1.08
1:C:234:GLU:H	1:C:235:ILE:HG23	1.08	1.08
1:A:474:SER:HB2	1:A:512:LEU:HG	1.25	1.08
1:B:8:LYS:H	1:B:8:LYS:HD2	1.04	1.08
1:C:31:PHE:CB	1:D:95:THR:CG2	2.29	1.08
1:D:222:ASP:OD1	1:D:222:ASP:O	1.69	1.08
1:D:301:THR:HG21	2:D:805:NAG:H82	1.29	1.08
1:B:33:LYS:N	1:C:25:LYS:CE	2.13	1.08
1:A:301:THR:HG21	2:A:805:NAG:H82	1.29	1.07
1:C:31:PHE:CE2	1:D:74:TYR:N	2.21	1.07
1:C:87:PRO:HA	1:D:43:ALA:HB2	1.11	1.07
1:C:90:GLU:OE1	1:D:53:ILE:HD13	0.90	1.07
1:C:301:THR:HG21	2:C:805:NAG:H82	1.29	1.07
1:B:31:PHE:CA	1:C:30:ARG:HB2	1.85	1.07
1:A:290:PHE:HB2	1:A:292:LEU:N	1.69	1.07
1:B:335:ALA:HB1	3:B:811:NDG:O6	1.54	1.07
1:B:482:THR:HG23	1:B:499:THR:HG22	1.09	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:ASP:HA	1:D:75:VAL:HG11	1.31	1.07
1:C:450:GLN:CG	1:C:532:CYS:O	2.03	1.07
1:C:89:GLU:N	1:D:38:ILE:HG13	1.69	1.07
1:A:450:GLN:CG	1:A:532:CYS:O	2.02	1.06
1:C:81:VAL:HG22	1:D:45:ASN:CG	1.74	1.06
1:C:87:PRO:HD3	1:D:43:ALA:HA	1.32	1.06
1:C:290:PHE:HB2	1:C:292:LEU:N	1.69	1.06
1:B:450:GLN:CG	1:B:532:CYS:O	2.03	1.06
1:C:1:ASP:H2	1:D:88:VAL:CG1	1.66	1.06
1:A:337:SER:HA	1:A:427:ILE:HG23	1.38	1.06
1:B:290:PHE:HB2	1:B:292:LEU:N	1.69	1.06
1:C:4:ILE:HG22	1:D:87:PRO:HB2	1.38	1.06
1:C:485:ALA:O	1:C:486:GLU:HG2	1.54	1.06
1:A:482:THR:HG23	1:A:499:THR:HG22	1.09	1.06
1:A:485:ALA:O	1:A:486:GLU:HG2	1.55	1.06
1:B:403:ASN:HB2	2:B:902:NAG:H83	1.30	1.06
1:D:290:PHE:HB2	1:D:292:LEU:N	1.69	1.06
1:A:335:ALA:HB1	3:A:811:NDG:O6	1.54	1.06
1:B:338:ARG:HD3	1:B:352:ILE:HG22	1.26	1.06
1:D:469:TYR:CD1	1:D:470:PRO:HD2	1.91	1.06
1:A:24:ILE:CA	1:D:2:TRP:CE2	2.23	1.05
1:B:469:TYR:CD1	1:B:470:PRO:HD2	1.92	1.05
1:C:84:ASN:C	1:D:74:TYR:CE2	2.28	1.05
1:D:335:ALA:HB1	3:D:811:NDG:O6	1.54	1.05
1:D:450:GLN:CG	1:D:532:CYS:O	2.03	1.05
1:B:485:ALA:O	1:B:486:GLU:HG2	1.55	1.05
1:A:464:ILE:CD1	1:A:465:PRO:CD	2.20	1.05
1:B:337:SER:HA	1:B:427:ILE:HG23	1.38	1.05
1:C:81:VAL:HG21	1:D:45:ASN:CA	1.87	1.05
1:C:335:ALA:HB1	3:C:811:NDG:O6	1.54	1.05
1:A:3:VAL:HG22	1:B:78:SER:H	1.21	1.04
1:A:8:LYS:HE3	1:D:28:LYS:HG3	1.39	1.04
1:C:31:PHE:HE2	1:D:73:LYS:C	1.50	1.04
1:C:82:SER:CB	1:D:75:VAL:H	1.70	1.04
1:C:522:LEU:HD22	1:C:523:THR:HB	1.39	1.04
1:D:485:ALA:O	1:D:486:GLU:HG2	1.54	1.04
1:B:31:PHE:CE2	1:C:26:SER:O	2.09	1.04
1:B:84:ASN:ND2	1:D:91:PRO:HB2	1.71	1.04
1:C:31:PHE:CG	1:D:95:THR:HG23	1.92	1.04
1:C:87:PRO:HG3	1:D:43:ALA:HB1	1.17	1.04
1:C:90:GLU:OE2	1:D:53:ILE:HG21	1.57	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:GLU:CB	1:D:79:HIS:O	2.05	1.04
1:C:469:TYR:CD1	1:C:470:PRO:HD2	1.92	1.04
1:A:24:ILE:HA	1:D:2:TRP:CG	1.60	1.04
1:A:290:PHE:HB2	1:A:292:LEU:H	0.88	1.04
1:B:464:ILE:CD1	1:B:465:PRO:CD	2.20	1.04
1:C:87:PRO:CG	1:D:43:ALA:HB1	1.61	1.04
1:D:464:ILE:CD1	1:D:465:PRO:CD	2.20	1.04
1:D:522:LEU:HD22	1:D:523:THR:HB	1.39	1.04
1:A:469:TYR:CD1	1:A:470:PRO:HD2	1.92	1.04
1:C:482:THR:HG21	1:C:499:THR:H	1.23	1.04
1:C:81:VAL:HG11	1:D:45:ASN:H	1.21	1.03
1:A:482:THR:CG2	1:A:499:THR:N	2.22	1.03
1:C:464:ILE:CD1	1:C:465:PRO:CD	2.20	1.03
1:C:482:THR:CG2	1:C:499:THR:N	2.22	1.03
1:A:1:ASP:H2	1:B:94:ILE:HD11	1.20	1.02
1:B:84:ASN:OD1	1:C:26:SER:C	1.96	1.02
1:D:482:THR:CG2	1:D:499:THR:N	2.22	1.02
1:B:83:GLU:CB	1:C:25:LYS:HD3	1.76	1.02
1:A:482:THR:HG21	1:A:499:THR:H	1.23	1.02
1:C:90:GLU:N	1:D:79:HIS:N	2.07	1.02
1:C:450:GLN:HB2	1:C:533:GLU:HA	1.41	1.02
1:C:337:SER:HA	1:C:427:ILE:HG23	1.38	1.02
1:C:403:ASN:HB2	2:C:902:NAG:C8	1.90	1.02
1:B:482:THR:CG2	1:B:499:THR:N	2.22	1.02
1:C:81:VAL:HG22	1:D:45:ASN:HD22	1.02	1.02
1:C:90:GLU:N	1:D:79:HIS:H	1.54	1.02
1:C:290:PHE:HB2	1:C:292:LEU:H	0.88	1.02
1:A:432:ASP:OD2	1:A:464:ILE:HG22	1.60	1.01
1:C:1:ASP:N	1:D:88:VAL:CG1	2.21	1.01
1:C:81:VAL:CG1	1:D:44:ASP:H	1.73	1.01
1:B:403:ASN:HB2	2:B:902:NAG:C8	1.90	1.01
1:B:290:PHE:HB2	1:B:292:LEU:H	0.88	1.01
1:B:432:ASP:OD2	1:B:464:ILE:HG22	1.60	1.01
1:C:81:VAL:HG11	1:D:44:ASP:N	1.75	1.01
1:C:82:SER:HB3	1:D:75:VAL:H	1.23	1.01
1:A:24:ILE:HB	1:D:2:TRP:CZ2	1.96	1.01
1:A:522:LEU:HD22	1:A:523:THR:HB	1.39	1.01
1:B:274:ASP:O	1:B:278:ASN:HA	1.61	1.01
1:D:290:PHE:HB2	1:D:292:LEU:H	0.88	1.01
1:A:403:ASN:HB2	2:A:902:NAG:C8	1.90	1.01
1:C:79:HIS:CB	1:D:39:THR:CG2	2.37	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:GLU:OE1	1:D:78:SER:N	1.75	1.01
1:C:93:GLU:H	1:D:81:VAL:HG11	1.25	1.01
1:C:274:ASP:O	1:C:278:ASN:HA	1.61	1.01
1:D:274:ASP:O	1:D:278:ASN:HA	1.61	1.01
1:C:4:ILE:HG22	1:D:87:PRO:CB	1.90	1.00
1:B:31:PHE:N	1:C:30:ARG:CB	2.24	1.00
1:B:522:LEU:HD22	1:B:523:THR:HB	1.39	1.00
1:C:32:ASN:N	1:D:75:VAL:HG23	1.76	1.00
1:D:337:SER:HA	1:D:427:ILE:HG23	1.38	1.00
1:A:188:THR:HG23	1:A:208:ILE:HG12	1.43	1.00
1:A:274:ASP:O	1:A:278:ASN:HA	1.61	1.00
1:C:81:VAL:HG22	1:D:45:ASN:HB2	1.32	1.00
1:D:403:ASN:HB2	2:D:902:NAG:C8	1.90	1.00
1:A:523:THR:HG23	1:A:524:VAL:H	1.27	1.00
1:B:86:SER:HA	1:D:90:GLU:CA	1.39	1.00
1:C:432:ASP:OD2	1:C:464:ILE:HG22	1.60	1.00
1:C:523:THR:HG23	1:C:524:VAL:H	1.26	1.00
1:D:432:ASP:OD2	1:D:464:ILE:HG22	1.60	1.00
1:A:450:GLN:HB2	1:A:533:GLU:HA	1.41	0.99
1:C:1:ASP:H2	1:D:88:VAL:HG12	0.84	0.99
1:C:93:GLU:CB	1:D:81:VAL:HG11	1.92	0.99
1:B:31:PHE:HE2	1:C:26:SER:C	1.65	0.99
1:C:79:HIS:CB	1:D:39:THR:HG22	1.93	0.99
1:C:90:GLU:CB	1:D:79:HIS:H	1.74	0.99
1:C:188:THR:HG23	1:C:208:ILE:HG12	1.43	0.99
1:B:482:THR:HG21	1:B:499:THR:H	1.23	0.99
1:B:320:THR:HG21	2:B:807:NAG:N2	1.78	0.99
1:C:4:ILE:CG2	1:D:87:PRO:CG	2.41	0.99
1:D:188:THR:HG23	1:D:208:ILE:HG12	1.43	0.99
1:D:450:GLN:HB2	1:D:533:GLU:HA	1.41	0.99
1:D:482:THR:HG21	1:D:499:THR:H	1.23	0.99
1:B:523:THR:HG23	1:B:524:VAL:H	1.26	0.98
1:B:31:PHE:HA	1:C:30:ARG:CB	1.92	0.98
1:B:450:GLN:HB2	1:B:533:GLU:HA	1.41	0.98
1:A:482:THR:CG2	1:A:499:THR:H	1.76	0.98
1:A:10:SER:N	1:D:30:ARG:CD	2.27	0.98
1:C:2:TRP:H	1:D:89:GLU:HA	1.23	0.98
1:A:320:THR:HG21	2:A:807:NAG:N2	1.78	0.98
1:B:82:SER:HB3	1:C:27:ASN:HB3	1.44	0.98
1:C:1:ASP:N	1:D:28:LYS:CD	2.25	0.98
1:D:482:THR:CG2	1:D:499:THR:H	1.76	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:PRO:HA	1:D:79:HIS:CD2	1.96	0.98
1:C:482:THR:CG2	1:C:499:THR:H	1.76	0.98
1:B:30:ARG:O	1:C:30:ARG:HG3	1.64	0.97
1:C:320:THR:HG21	2:C:807:NAG:N2	1.78	0.97
1:D:523:THR:HG23	1:D:524:VAL:H	1.26	0.97
1:C:31:PHE:CG	1:D:95:THR:CG2	2.47	0.97
1:D:8:LYS:H	1:D:8:LYS:CD	1.74	0.97
1:B:366:LYS:HG3	1:B:367:LEU:H	1.28	0.97
1:B:86:SER:CA	1:D:90:GLU:CG	2.20	0.97
1:C:8:LYS:H	1:C:8:LYS:CD	1.74	0.97
1:B:188:THR:HG23	1:B:208:ILE:HG12	1.43	0.97
1:A:366:LYS:HG3	1:A:367:LEU:H	1.28	0.97
1:B:87:PRO:HG2	1:C:2:TRP:HB2	1.45	0.97
1:D:320:THR:HG21	2:D:807:NAG:N2	1.78	0.97
1:C:80:ALA:HB3	1:D:77:SER:HB3	1.45	0.97
1:D:366:LYS:HG3	1:D:367:LEU:H	1.28	0.97
1:C:4:ILE:HG23	1:D:87:PRO:HG2	1.45	0.96
1:C:81:VAL:HG22	1:D:45:ASN:CB	1.78	0.96
1:A:32:ASN:HD21	1:A:83:GLU:CB	1.79	0.96
1:C:27:ASN:HD22	1:D:93:GLU:HB2	0.80	0.96
1:C:87:PRO:HA	1:D:43:ALA:CB	1.77	0.96
1:B:235:ILE:CG1	1:B:287:GLY:HA2	1.96	0.96
1:C:32:ASN:HD21	1:C:83:GLU:CB	1.79	0.96
1:C:81:VAL:HG13	1:D:44:ASP:OD2	1.64	0.96
1:C:86:SER:HA	1:D:42:GLY:C	1.83	0.96
1:D:482:THR:HG21	1:D:499:THR:N	1.81	0.96
1:B:482:THR:CG2	1:B:499:THR:H	1.76	0.96
1:A:3:VAL:HG22	1:B:78:SER:N	1.79	0.96
1:A:227:THR:HG21	2:A:807:NAG:H83	1.48	0.96
1:A:235:ILE:CG1	1:A:287:GLY:HA2	1.96	0.96
1:A:482:THR:HG21	1:A:499:THR:N	1.81	0.96
1:C:81:VAL:CG1	1:D:44:ASP:N	2.27	0.96
1:B:31:PHE:CA	1:C:30:ARG:H	1.75	0.96
1:C:27:ASN:ND2	1:D:93:GLU:H	1.62	0.96
1:C:320:THR:HG21	2:C:807:NAG:HN2	1.31	0.96
1:B:83:GLU:HB2	1:C:25:LYS:HD2	0.96	0.95
1:C:31:PHE:HE2	1:D:74:TYR:N	1.59	0.95
1:C:235:ILE:CG1	1:C:287:GLY:HA2	1.96	0.95
1:A:24:ILE:HB	1:D:2:TRP:HE1	1.28	0.95
1:B:31:PHE:CB	1:C:30:ARG:H	1.79	0.95
1:C:88:VAL:HG12	1:D:94:ILE:HB	1.47	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:VAL:O	1:D:94:ILE:HD12	1.65	0.95
1:B:320:THR:HG21	2:B:807:NAG:HN2	1.31	0.95
1:C:81:VAL:HB	1:D:41:GLN:C	1.86	0.95
1:A:2:TRP:NE1	1:B:80:ALA:HB2	1.82	0.95
1:A:24:ILE:CA	1:D:2:TRP:CG	2.39	0.95
1:A:90:GLU:CB	1:B:3:VAL:C	2.35	0.95
1:B:86:SER:N	1:D:90:GLU:HG3	1.44	0.95
1:C:1:ASP:H2	1:D:28:LYS:HD3	0.96	0.95
1:A:2:TRP:C	1:B:92:MET:HB2	1.79	0.95
1:A:90:GLU:CG	1:B:3:VAL:HG23	1.96	0.95
1:B:227:THR:HG21	2:B:807:NAG:H83	1.48	0.95
1:B:31:PHE:HE1	1:D:75:VAL:HG11	0.78	0.94
1:D:235:ILE:CG1	1:D:287:GLY:HA2	1.96	0.94
1:C:87:PRO:CA	1:D:76:LEU:HD22	1.96	0.94
1:A:24:ILE:HA	1:D:2:TRP:CD1	2.02	0.94
1:A:290:PHE:CB	1:A:292:LEU:H	1.79	0.94
1:B:366:LYS:CG	1:B:367:LEU:H	1.80	0.94
1:B:482:THR:HG21	1:B:499:THR:N	1.81	0.94
1:A:1:ASP:H3	1:B:94:ILE:CD1	1.73	0.94
1:A:4:ILE:CA	1:B:90:GLU:C	2.33	0.94
1:C:87:PRO:C	1:D:76:LEU:HD22	1.88	0.94
1:A:89:GLU:OE1	1:B:2:TRP:HB3	1.65	0.94
1:C:289:ASP:O	1:C:290:PHE:HB3	1.67	0.94
1:D:366:LYS:CG	1:D:367:LEU:H	1.80	0.94
1:B:83:GLU:CA	1:C:25:LYS:HD3	1.97	0.94
1:C:91:PRO:CA	1:D:79:HIS:CD2	2.50	0.94
1:C:90:GLU:HB3	1:D:79:HIS:C	1.87	0.94
1:D:227:THR:HG21	2:D:807:NAG:H83	1.48	0.94
1:D:290:PHE:CB	1:D:292:LEU:H	1.79	0.94
1:A:8:LYS:H	1:A:8:LYS:CD	1.74	0.94
1:C:290:PHE:CB	1:C:292:LEU:H	1.79	0.94
1:D:32:ASN:HD21	1:D:83:GLU:CB	1.79	0.94
1:C:366:LYS:HG3	1:C:367:LEU:H	1.28	0.94
1:A:99:ILE:HG21	1:D:30:ARG:HH12	1.29	0.93
1:C:27:ASN:HD22	1:C:28:LYS:N	1.66	0.93
1:C:91:PRO:HB2	1:D:37:SER:OG	1.65	0.93
1:A:195:ASP:HB2	1:A:201:LEU:H	1.34	0.93
1:B:396:ARG:HH22	1:B:464:ILE:HB	1.33	0.93
1:C:352:ILE:HG13	1:C:388:VAL:HB	1.51	0.93
1:D:352:ILE:HG13	1:D:388:VAL:HB	1.51	0.93
1:B:227:THR:HG21	2:B:807:NAG:C7	1.99	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:PRO:HD3	1:D:43:ALA:CA	1.92	0.93
1:C:366:LYS:CG	1:C:367:LEU:H	1.80	0.93
1:A:27:ASN:HD22	1:A:28:LYS:N	1.66	0.93
1:C:32:ASN:ND2	1:C:83:GLU:HB2	1.83	0.93
1:C:227:THR:HG21	2:C:807:NAG:H83	1.48	0.93
1:C:464:ILE:HD12	1:C:465:PRO:HD2	0.94	0.93
1:A:366:LYS:CG	1:A:367:LEU:H	1.80	0.93
1:A:396:ARG:HH22	1:A:464:ILE:HB	1.33	0.93
1:B:27:ASN:HD22	1:B:28:LYS:N	1.66	0.93
1:A:1:ASP:HA	1:B:24:ILE:HG21	1.51	0.93
1:A:24:ILE:CB	1:D:2:TRP:CD1	2.52	0.93
1:A:24:ILE:CG2	1:D:2:TRP:NE1	2.32	0.92
1:B:290:PHE:CB	1:B:292:LEU:H	1.79	0.92
1:B:464:ILE:HD12	1:B:465:PRO:HD2	0.94	0.92
1:D:195:ASP:HB2	1:D:201:LEU:H	1.34	0.92
1:A:90:GLU:C	1:B:3:VAL:HG22	1.85	0.92
1:A:320:THR:HG21	2:A:807:NAG:HN2	1.31	0.92
1:A:446:THR:HG23	1:A:539:CYS:SG	2.09	0.92
1:A:464:ILE:HD12	1:A:465:PRO:HD2	0.94	0.92
1:B:32:ASN:CA	1:C:29:ASP:OD2	2.17	0.92
1:B:404:ASN:ND2	1:B:404:ASN:O	2.03	0.92
1:C:27:ASN:ND2	1:D:93:GLU:HB2	1.65	0.92
1:D:464:ILE:HD12	1:D:465:PRO:HD2	0.94	0.92
1:A:227:THR:HG21	2:A:807:NAG:C7	1.99	0.92
1:C:81:VAL:HB	1:D:41:GLN:CA	1.86	0.92
1:C:404:ASN:O	1:C:404:ASN:ND2	2.03	0.92
1:D:289:ASP:O	1:D:290:PHE:HB3	1.67	0.92
1:D:320:THR:HG21	2:D:807:NAG:HN2	1.31	0.92
1:B:403:ASN:HB2	2:B:902:NAG:C7	2.00	0.92
1:C:86:SER:N	1:D:41:GLN:O	2.01	0.92
1:D:27:ASN:HD22	1:D:28:LYS:N	1.66	0.92
1:D:446:THR:HG23	1:D:539:CYS:SG	2.10	0.92
1:B:31:PHE:CA	1:C:30:ARG:CB	2.48	0.92
1:A:32:ASN:ND2	1:A:83:GLU:HB2	1.84	0.92
1:C:88:VAL:HG22	1:D:76:LEU:HD23	1.47	0.92
1:C:195:ASP:HB2	1:C:201:LEU:H	1.34	0.92
2:C:805:NAG:H62	2:C:806:NAG:C7	2.00	0.92
1:D:227:THR:HG21	2:D:807:NAG:C7	1.99	0.92
1:D:396:ARG:HH22	1:D:464:ILE:HB	1.33	0.92
1:C:87:PRO:HD3	1:D:42:GLY:O	1.69	0.92
1:C:227:THR:HG21	2:C:807:NAG:C7	1.99	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:446:THR:HG23	1:C:539:CYS:SG	2.10	0.92
2:A:805:NAG:H62	2:A:806:NAG:C7	1.99	0.91
1:B:446:THR:HG23	1:B:539:CYS:SG	2.10	0.91
1:C:1:ASP:H3	1:D:88:VAL:HB	1.35	0.91
1:C:340:ASP:HA	1:C:429:HIS:HB3	1.53	0.91
1:D:32:ASN:ND2	1:D:83:GLU:HB2	1.84	0.91
1:A:403:ASN:HB2	2:A:902:NAG:C7	2.00	0.91
1:A:404:ASN:O	1:A:404:ASN:ND2	2.03	0.91
1:C:86:SER:H	1:D:74:TYR:HD2	1.16	0.91
1:C:517:GLN:O	1:C:519:ASN:N	2.03	0.91
1:D:335:ALA:CB	3:D:811:NDG:O6	2.18	0.91
1:B:234:GLU:N	1:B:235:ILE:HG23	1.86	0.91
1:A:335:ALA:CB	3:A:811:NDG:O6	2.18	0.91
1:B:83:GLU:H	1:C:25:LYS:CD	1.84	0.91
1:B:335:ALA:CB	3:B:811:NDG:O6	2.18	0.91
1:C:1:ASP:O	1:D:28:LYS:CE	2.19	0.91
1:A:340:ASP:HA	1:A:429:HIS:HB3	1.53	0.91
1:B:289:ASP:O	1:B:290:PHE:HB3	1.67	0.91
2:C:805:NAG:O5	2:C:806:NAG:H83	1.71	0.91
1:A:10:SER:N	1:D:30:ARG:HD3	1.86	0.91
1:C:90:GLU:CD	1:D:53:ILE:HG21	1.89	0.91
1:C:396:ARG:HH22	1:C:464:ILE:HB	1.33	0.91
1:C:403:ASN:HB2	2:C:902:NAG:C7	2.00	0.91
1:D:403:ASN:HB2	2:D:902:NAG:C7	2.00	0.91
1:B:83:GLU:CG	1:C:25:LYS:CD	2.45	0.91
2:B:805:NAG:H62	2:B:806:NAG:C7	2.00	0.91
1:A:289:ASP:O	1:A:290:PHE:HB3	1.67	0.90
1:B:31:PHE:CE2	1:C:26:SER:C	2.45	0.90
1:B:352:ILE:HG13	1:B:388:VAL:HB	1.51	0.90
1:B:378:TRP:HB2	1:B:379:LEU:HD23	1.53	0.90
1:A:378:TRP:HB2	1:A:379:LEU:HD23	1.53	0.90
1:B:30:ARG:C	1:C:30:ARG:CG	2.31	0.90
1:D:234:GLU:N	1:D:235:ILE:HG23	1.86	0.90
2:D:805:NAG:O5	2:D:806:NAG:H83	1.71	0.90
1:C:79:HIS:HB3	1:D:44:ASP:OD1	1.70	0.90
1:D:8:LYS:HD2	1:D:8:LYS:N	1.87	0.90
1:D:517:GLN:O	1:D:519:ASN:N	2.03	0.90
1:A:154:ASP:HB3	1:A:155:PRO:HD2	1.54	0.90
1:C:1:ASP:HA	1:D:89:GLU:OE1	1.68	0.90
1:C:87:PRO:CD	1:D:43:ALA:CB	2.48	0.90
2:D:805:NAG:H62	2:D:806:NAG:C7	1.99	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ILE:CB	1:D:2:TRP:CZ2	2.54	0.90
1:B:464:ILE:HD11	1:B:465:PRO:HD2	1.53	0.90
1:B:517:GLN:O	1:B:519:ASN:N	2.03	0.90
1:C:396:ARG:NH2	1:C:464:ILE:CG2	2.35	0.90
1:D:340:ASP:HA	1:D:429:HIS:HB3	1.53	0.90
1:D:404:ASN:O	1:D:404:ASN:ND2	2.03	0.90
1:C:374:ASP:O	1:C:375:PRO:C	2.06	0.90
1:C:378:TRP:HB2	1:C:379:LEU:HD23	1.53	0.90
1:A:396:ARG:NH2	1:A:464:ILE:CG2	2.35	0.90
2:A:805:NAG:O5	2:A:806:NAG:H83	1.71	0.90
1:B:154:ASP:HB3	1:B:155:PRO:HD2	1.54	0.90
1:C:234:GLU:N	1:C:235:ILE:HG23	1.86	0.90
1:A:234:GLU:N	1:A:235:ILE:HG23	1.86	0.90
1:C:335:ALA:CB	3:C:811:NDG:O6	2.18	0.90
1:C:90:GLU:OE2	1:D:53:ILE:HG23	1.72	0.89
1:B:396:ARG:NH2	1:B:464:ILE:CG2	2.35	0.89
1:B:518:ASN:O	1:B:520:PRO:HD3	1.72	0.89
1:A:523:THR:HG23	1:A:524:VAL:CG2	2.03	0.89
1:B:8:LYS:H	1:B:8:LYS:CD	1.74	0.89
1:B:195:ASP:HB2	1:B:201:LEU:H	1.34	0.89
1:C:8:LYS:HD2	1:C:8:LYS:N	1.87	0.89
1:C:81:VAL:CG2	1:D:45:ASN:HD22	1.85	0.89
1:D:449:ASP:H	1:D:532:CYS:HB3	1.37	0.89
1:A:338:ARG:HD3	1:A:352:ILE:CG2	2.02	0.89
1:C:93:GLU:H	1:D:81:VAL:CG1	1.86	0.89
2:B:805:NAG:O5	2:B:806:NAG:H83	1.71	0.89
1:C:371:ILE:CD1	1:C:381:VAL:HG11	2.03	0.89
1:C:518:ASN:O	1:C:520:PRO:HD3	1.72	0.89
1:D:154:ASP:HB3	1:D:155:PRO:HD2	1.54	0.89
1:D:523:THR:HG23	1:D:524:VAL:CG2	2.03	0.89
1:D:338:ARG:HD3	1:D:352:ILE:CG2	2.02	0.89
1:A:517:GLN:O	1:A:519:ASN:N	2.03	0.89
1:A:8:LYS:CE	1:D:28:LYS:HG3	2.03	0.89
1:D:464:ILE:HD12	1:D:465:PRO:HD3	1.53	0.89
1:D:518:ASN:O	1:D:520:PRO:HD3	1.72	0.89
1:A:4:ILE:HA	1:B:91:PRO:CD	1.94	0.89
1:A:8:LYS:HD2	1:A:8:LYS:N	1.87	0.89
1:B:464:ILE:HD12	1:B:465:PRO:HD3	1.53	0.89
1:A:221:PHE:HE1	1:A:315:SER:O	1.56	0.89
1:B:31:PHE:CA	1:C:30:ARG:CA	2.49	0.89
1:B:85:GLY:C	1:D:91:PRO:HD2	1.92	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:PHE:HE1	1:B:315:SER:O	1.56	0.89
1:C:154:ASP:HB3	1:C:155:PRO:HD2	1.54	0.89
1:D:221:PHE:HE1	1:D:315:SER:O	1.56	0.89
1:A:24:ILE:HG22	1:D:2:TRP:CD1	2.08	0.88
1:A:352:ILE:HG13	1:A:388:VAL:HB	1.51	0.88
1:B:449:ASP:H	1:B:532:CYS:HB3	1.37	0.88
1:C:318:THR:HG21	2:C:806:NAG:H5	1.55	0.88
1:B:371:ILE:CD1	1:B:381:VAL:HG11	2.03	0.88
1:C:89:GLU:OE1	1:D:78:SER:CB	2.21	0.88
1:A:449:ASP:H	1:A:532:CYS:HB3	1.37	0.88
1:B:8:LYS:HD2	1:B:8:LYS:N	1.87	0.88
1:C:31:PHE:HB3	1:D:75:VAL:CG2	2.02	0.88
1:C:81:VAL:HG13	1:D:40:GLY:H	1.38	0.88
1:C:464:ILE:HD12	1:C:465:PRO:HD3	1.53	0.88
1:C:486:GLU:HB2	1:C:495:LEU:HB2	1.56	0.88
1:D:396:ARG:NH2	1:D:464:ILE:CG2	2.35	0.88
1:A:3:VAL:HG23	1:B:91:PRO:HB3	1.55	0.88
1:C:338:ARG:HD3	1:C:352:ILE:CG2	2.02	0.88
1:B:523:THR:HG23	1:B:524:VAL:CG2	2.03	0.88
1:A:91:PRO:HA	1:B:1:ASP:O	1.73	0.88
1:A:374:ASP:O	1:A:375:PRO:C	2.06	0.88
1:B:338:ARG:HD3	1:B:352:ILE:CG2	2.02	0.88
1:C:464:ILE:HD11	1:C:465:PRO:HD2	1.53	0.88
1:C:482:THR:HG21	1:C:499:THR:N	1.81	0.88
1:D:378:TRP:HB2	1:D:379:LEU:HD23	1.53	0.88
1:A:464:ILE:HD11	1:A:465:PRO:HD2	1.53	0.88
1:C:449:ASP:H	1:C:532:CYS:HB3	1.37	0.88
1:A:343:GLU:HB3	1:A:433:VAL:HG21	1.55	0.88
1:A:486:GLU:HB2	1:A:495:LEU:HB2	1.56	0.88
1:C:483:TRP:CZ3	1:C:498:PRO:HG3	2.09	0.88
1:C:523:THR:HG23	1:C:524:VAL:CG2	2.03	0.88
1:B:483:TRP:CZ3	1:B:498:PRO:HG3	2.09	0.88
1:C:89:GLU:OE1	1:D:78:SER:CA	2.22	0.88
1:D:371:ILE:CD1	1:D:381:VAL:HG11	2.03	0.88
1:D:464:ILE:HD11	1:D:465:PRO:HD2	1.53	0.88
1:A:518:ASN:O	1:A:520:PRO:HD3	1.72	0.88
1:C:343:GLU:HB3	1:C:433:VAL:HG21	1.55	0.87
1:D:333:VAL:HB	1:D:334:PRO:HD3	1.56	0.87
1:D:483:TRP:CZ3	1:D:498:PRO:HG3	2.09	0.87
1:B:340:ASP:HA	1:B:429:HIS:HB3	1.53	0.87
1:B:257:ALA:O	1:B:273:THR:HG21	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:GLU:CD	1:D:53:ILE:HD13	1.95	0.87
1:C:440:PRO:CD	1:C:522:LEU:HD12	2.05	0.87
1:A:371:ILE:CD1	1:A:381:VAL:HG11	2.03	0.87
1:D:441:SER:OG	1:D:442:PRO:HD3	1.75	0.87
1:A:440:PRO:CD	1:A:522:LEU:HD12	2.05	0.87
1:C:257:ALA:O	1:C:273:THR:HG21	1.74	0.87
1:B:318:THR:HG21	2:B:806:NAG:H5	1.56	0.86
1:C:35:TYR:HD2	1:D:45:ASN:OD1	1.55	0.86
1:A:318:THR:HG21	2:A:806:NAG:H5	1.56	0.86
1:D:374:ASP:O	1:D:375:PRO:C	2.06	0.86
1:A:320:THR:HG21	2:A:807:NAG:C2	2.05	0.86
1:B:333:VAL:HB	1:B:334:PRO:HD3	1.56	0.86
1:B:343:GLU:HB3	1:B:433:VAL:HG21	1.55	0.86
1:C:81:VAL:CG1	1:D:45:ASN:H	1.87	0.86
1:C:221:PHE:HE1	1:C:315:SER:O	1.56	0.86
1:C:320:THR:HG21	2:C:807:NAG:C2	2.05	0.86
1:B:320:THR:HG21	2:B:807:NAG:C2	2.05	0.86
1:A:257:ALA:O	1:A:273:THR:HG21	1.74	0.86
1:B:486:GLU:HB2	1:B:495:LEU:HB2	1.56	0.86
1:C:333:VAL:HB	1:C:334:PRO:HD3	1.56	0.86
1:A:483:TRP:CZ3	1:A:498:PRO:HG3	2.09	0.86
1:B:374:ASP:O	1:B:375:PRO:C	2.06	0.86
1:C:82:SER:HB3	1:D:75:VAL:N	1.89	0.86
1:B:440:PRO:CD	1:B:522:LEU:HD12	2.05	0.86
1:B:441:SER:OG	1:B:442:PRO:HD3	1.75	0.86
1:A:99:ILE:HG21	1:D:30:ARG:NH1	1.90	0.86
1:A:441:SER:OG	1:A:442:PRO:HD3	1.75	0.86
1:C:91:PRO:CA	1:D:79:HIS:HD2	1.89	0.86
1:D:486:GLU:HB2	1:D:495:LEU:HB2	1.56	0.86
1:C:87:PRO:HD2	1:D:51:PHE:HB2	1.57	0.86
1:C:235:ILE:HG13	1:C:287:GLY:HA2	1.57	0.86
1:C:31:PHE:HE1	1:D:97:ASN:OD1	1.58	0.86
1:C:523:THR:HG23	1:C:524:VAL:N	1.90	0.86
1:A:440:PRO:HD2	1:A:522:LEU:HD12	1.58	0.85
1:C:441:SER:OG	1:C:442:PRO:HD3	1.75	0.85
1:B:464:ILE:HD12	1:B:465:PRO:N	1.91	0.85
1:A:464:ILE:HD12	1:A:465:PRO:HD3	1.53	0.85
1:D:440:PRO:CD	1:D:522:LEU:HD12	2.05	0.85
1:D:523:THR:HG23	1:D:524:VAL:N	1.90	0.85
1:B:483:TRP:HZ2	1:B:507:TYR:CE1	1.95	0.85
1:B:523:THR:HG23	1:B:524:VAL:N	1.90	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:GLY:CA	1:D:42:GLY:HA2	1.70	0.85
1:D:257:ALA:O	1:D:273:THR:HG21	1.74	0.85
1:A:235:ILE:HG13	1:A:287:GLY:HA2	1.58	0.85
1:C:91:PRO:HA	1:D:79:HIS:HD2	1.40	0.85
1:C:483:TRP:HZ2	1:C:507:TYR:CE1	1.95	0.85
1:D:423:THR:CB	2:D:810:NAG:C7	2.54	0.85
1:A:4:ILE:HG22	1:B:91:PRO:O	1.76	0.85
1:A:464:ILE:HD12	1:A:465:PRO:N	1.91	0.85
1:A:483:TRP:HZ2	1:A:507:TYR:CE1	1.95	0.85
1:C:451:ASN:N	1:C:533:GLU:O	2.10	0.85
1:D:318:THR:HG21	2:D:806:NAG:H5	1.56	0.85
1:D:343:GLU:HB3	1:D:433:VAL:HG21	1.55	0.85
1:B:483:TRP:HZ2	1:B:507:TYR:HE1	1.24	0.85
1:C:81:VAL:HG12	1:D:43:ALA:CA	2.07	0.85
1:C:90:GLU:CA	1:D:79:HIS:N	2.38	0.85
1:A:438:PRO:HB3	1:A:471:TYR:HE2	1.41	0.85
1:B:30:ARG:O	1:C:30:ARG:HA	1.77	0.85
1:C:31:PHE:O	1:D:73:LYS:HD3	1.77	0.85
1:C:87:PRO:HB3	1:D:43:ALA:HB1	1.56	0.85
1:D:464:ILE:HD12	1:D:465:PRO:N	1.91	0.85
1:D:483:TRP:HZ2	1:D:507:TYR:CE1	1.95	0.85
1:A:333:VAL:HB	1:A:334:PRO:HD3	1.56	0.85
1:A:423:THR:CB	2:A:810:NAG:C7	2.54	0.85
1:D:320:THR:HG21	2:D:807:NAG:C2	2.05	0.85
1:B:438:PRO:HB3	1:B:471:TYR:HE2	1.41	0.85
1:B:423:THR:CB	2:B:810:NAG:C7	2.54	0.84
1:B:375:PRO:HB3	1:B:400:TYR:CE2	2.12	0.84
1:C:423:THR:CB	2:C:810:NAG:C7	2.54	0.84
1:B:451:ASN:N	1:B:533:GLU:O	2.10	0.84
1:D:155:PRO:HB2	2:D:801:NAG:H81	1.60	0.84
1:B:230:VAL:O	1:B:324:GLU:N	2.11	0.84
1:B:235:ILE:HG13	1:B:287:GLY:HA2	1.58	0.84
1:C:438:PRO:HB3	1:C:471:TYR:HE2	1.41	0.84
1:A:523:THR:HG23	1:A:524:VAL:N	1.90	0.84
1:D:375:PRO:HB3	1:D:400:TYR:CE2	2.12	0.84
1:A:396:ARG:NE	1:A:432:ASP:HB2	1.93	0.84
1:C:1:ASP:H2	1:D:28:LYS:CD	1.86	0.84
1:C:375:PRO:HB3	1:C:400:TYR:CE2	2.12	0.84
1:D:396:ARG:NE	1:D:432:ASP:HB2	1.93	0.84
1:A:155:PRO:HB2	2:A:801:NAG:H81	1.59	0.84
1:C:230:VAL:O	1:C:324:GLU:N	2.11	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:440:PRO:HD2	1:C:522:LEU:HD12	1.59	0.84
1:D:230:VAL:O	1:D:324:GLU:N	2.11	0.84
1:A:423:THR:HB	2:A:810:NAG:N2	1.93	0.84
1:C:1:ASP:CA	1:D:89:GLU:OE2	2.16	0.84
1:C:1:ASP:CA	1:D:28:LYS:HD3	2.08	0.84
1:C:396:ARG:NE	1:C:432:ASP:HB2	1.93	0.84
1:A:375:PRO:HB3	1:A:400:TYR:CE2	2.12	0.83
1:A:147:SER:OG	1:A:167:ARG:HD2	1.78	0.83
1:C:464:ILE:HD12	1:C:465:PRO:N	1.92	0.83
1:D:438:PRO:HB3	1:D:471:TYR:HE2	1.41	0.83
1:A:423:THR:CB	2:A:810:NAG:N2	2.42	0.83
1:A:451:ASN:N	1:A:533:GLU:O	2.10	0.83
1:B:423:THR:CB	2:B:810:NAG:N2	2.42	0.83
1:A:87:PRO:O	1:B:2:TRP:CZ2	2.30	0.83
1:B:32:ASN:ND2	1:B:83:GLU:H	1.77	0.83
1:D:423:THR:CB	2:D:810:NAG:N2	2.42	0.83
1:B:32:ASN:CB	1:C:27:ASN:HA	2.07	0.83
1:B:448:CYS:O	1:B:452:PRO:HG3	1.79	0.83
1:C:448:CYS:O	1:C:452:PRO:HG3	1.79	0.83
1:D:448:CYS:O	1:D:452:PRO:HG3	1.78	0.83
1:A:230:VAL:O	1:A:324:GLU:N	2.11	0.83
1:C:423:THR:CB	2:C:810:NAG:N2	2.42	0.83
1:C:28:LYS:HD3	1:C:88:VAL:HG12	1.61	0.83
1:C:483:TRP:HZ2	1:C:507:TYR:HE1	1.24	0.83
1:B:396:ARG:NE	1:B:432:ASP:HB2	1.93	0.83
1:D:28:LYS:HD3	1:D:88:VAL:HG12	1.61	0.83
1:D:440:PRO:HD2	1:D:522:LEU:HD12	1.59	0.83
1:D:469:TYR:CG	1:D:470:PRO:CD	2.61	0.83
1:A:32:ASN:ND2	1:A:83:GLU:H	1.77	0.83
1:B:423:THR:HB	2:B:810:NAG:N2	1.93	0.83
1:B:446:THR:HG21	1:B:537:ILE:O	1.79	0.83
1:C:32:ASN:ND2	1:C:83:GLU:H	1.77	0.83
1:C:80:ALA:CB	1:D:39:THR:OG1	2.25	0.83
1:C:85:GLY:C	1:D:41:GLN:C	2.34	0.83
1:D:446:THR:HG21	1:D:537:ILE:O	1.79	0.83
1:A:289:ASP:O	1:A:289:ASP:OD2	1.97	0.82
1:B:154:ASP:HB3	2:B:801:NAG:HN2	1.44	0.82
1:B:482:THR:HG21	1:B:500:GLN:N	1.94	0.82
1:A:469:TYR:CG	1:A:470:PRO:CD	2.61	0.82
1:A:540:GLN:O	1:A:540:GLN:OE1	1.97	0.82
1:B:540:GLN:O	1:B:540:GLN:OE1	1.97	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:451:ASN:N	1:D:533:GLU:O	2.10	0.82
1:A:448:CYS:O	1:A:452:PRO:HG3	1.79	0.82
1:C:87:PRO:HD3	1:D:42:GLY:C	2.00	0.82
1:D:482:THR:HG21	1:D:500:GLN:N	1.94	0.82
1:C:482:THR:HG21	1:C:500:GLN:N	1.94	0.82
1:C:540:GLN:O	1:C:540:GLN:OE1	1.97	0.82
1:D:235:ILE:HG13	1:D:287:GLY:HA2	1.58	0.82
1:A:482:THR:HG21	1:A:500:GLN:N	1.94	0.82
1:B:469:TYR:CG	1:B:470:PRO:CD	2.61	0.82
1:D:423:THR:HB	2:D:810:NAG:N2	1.93	0.82
1:B:28:LYS:HD3	1:B:88:VAL:HG12	1.61	0.82
1:B:440:PRO:HD2	1:B:522:LEU:HD12	1.59	0.82
1:C:469:TYR:CG	1:C:470:PRO:CD	2.61	0.82
1:B:155:PRO:HB2	2:B:801:NAG:H81	1.59	0.82
1:B:234:GLU:H	1:B:235:ILE:CG2	1.92	0.82
1:B:277:SER:C	1:B:278:ASN:HD22	1.83	0.82
1:C:423:THR:HB	2:C:810:NAG:N2	1.93	0.82
1:D:483:TRP:HZ2	1:D:507:TYR:HE1	1.24	0.82
1:D:32:ASN:ND2	1:D:83:GLU:H	1.77	0.81
1:D:277:SER:C	1:D:278:ASN:HD22	1.83	0.81
1:D:289:ASP:O	1:D:289:ASP:OD2	1.97	0.81
1:A:3:VAL:N	1:B:78:SER:O	2.12	0.81
1:A:154:ASP:HB3	2:A:801:NAG:N2	1.95	0.81
1:C:155:PRO:HB2	2:C:801:NAG:H81	1.60	0.81
1:A:154:ASP:HB3	2:A:801:NAG:HN2	1.45	0.81
1:A:446:THR:HG21	1:A:537:ILE:O	1.79	0.81
1:B:289:ASP:O	1:B:289:ASP:OD2	1.97	0.81
1:C:85:GLY:CA	1:D:41:GLN:C	2.47	0.81
1:C:85:GLY:HA3	1:D:42:GLY:HA2	1.62	0.81
1:C:87:PRO:HG3	1:D:43:ALA:C	2.00	0.81
1:C:154:ASP:HB3	2:C:801:NAG:HN2	1.44	0.81
1:C:446:THR:HG21	1:C:537:ILE:O	1.79	0.81
1:A:483:TRP:HZ2	1:A:507:TYR:HE1	1.24	0.81
1:C:289:ASP:O	1:C:289:ASP:OD2	1.97	0.81
1:C:31:PHE:CE1	1:D:97:ASN:OD1	2.33	0.81
1:C:154:ASP:HB3	2:C:801:NAG:N2	1.95	0.81
1:B:496:LEU:HD21	1:B:509:ILE:HD13	1.63	0.81
1:D:154:ASP:HB3	2:D:801:NAG:N2	1.95	0.81
1:D:496:LEU:HD21	1:D:509:ILE:HD13	1.63	0.81
1:D:540:GLN:O	1:D:540:GLN:OE1	1.97	0.81
1:A:90:GLU:HB3	1:B:3:VAL:O	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:GLU:HB3	1:B:268:PHE:HE2	1.46	0.81
1:C:517:GLN:C	1:C:519:ASN:H	1.84	0.81
1:A:396:ARG:HH21	1:A:464:ILE:HG22	1.46	0.81
1:B:290:PHE:CE2	1:B:293:ARG:HB2	2.16	0.81
1:C:496:LEU:HD21	1:C:509:ILE:HD13	1.63	0.81
1:D:469:TYR:CD2	1:D:470:PRO:HD2	2.16	0.81
1:A:28:LYS:HD3	1:A:88:VAL:HG12	1.61	0.81
1:A:277:SER:C	1:A:278:ASN:HD22	1.84	0.81
1:B:469:TYR:CD2	1:B:470:PRO:HD2	2.16	0.81
1:C:290:PHE:CE2	1:C:293:ARG:HB2	2.16	0.81
1:A:486:GLU:O	1:A:494:MET:HA	1.81	0.81
1:B:30:ARG:C	1:C:30:ARG:HG3	1.96	0.81
1:B:127:VAL:HG13	1:B:128:MET:H	1.46	0.81
1:B:486:GLU:O	1:B:494:MET:HA	1.81	0.81
1:C:486:GLU:O	1:C:494:MET:HA	1.81	0.81
1:D:517:GLN:C	1:D:519:ASN:H	1.84	0.81
1:A:265:GLU:HB3	1:A:268:PHE:HE2	1.46	0.80
1:B:86:SER:N	1:D:91:PRO:HD2	1.96	0.80
1:B:154:ASP:HB3	2:B:801:NAG:N2	1.95	0.80
1:C:79:HIS:HB3	1:D:39:THR:HG22	1.63	0.80
1:C:84:ASN:HA	1:D:71:TYR:CD2	2.16	0.80
1:D:486:GLU:O	1:D:494:MET:HA	1.81	0.80
1:A:290:PHE:CE2	1:A:293:ARG:HB2	2.16	0.80
1:A:469:TYR:CD2	1:A:470:PRO:HD2	2.16	0.80
1:B:30:ARG:O	1:C:30:ARG:CG	2.29	0.80
1:A:517:GLN:C	1:A:519:ASN:H	1.84	0.80
1:C:432:ASP:OD2	1:C:464:ILE:CG2	2.30	0.80
1:A:127:VAL:HG13	1:A:128:MET:H	1.46	0.80
1:C:86:SER:CA	1:D:42:GLY:C	2.46	0.80
1:C:93:GLU:N	1:D:81:VAL:HG11	1.96	0.80
1:C:299:GLN:HG2	1:C:318:THR:HG23	1.62	0.80
1:D:265:GLU:HB3	1:D:268:PHE:HE2	1.46	0.80
1:D:406:TYR:CD1	2:D:808:NAG:H83	2.17	0.80
1:C:222:ASP:OD1	1:C:222:ASP:C	2.20	0.80
1:C:277:SER:C	1:C:278:ASN:HD22	1.84	0.80
1:A:396:ARG:HD3	1:A:431:LEU:C	2.02	0.80
1:B:517:GLN:C	1:B:519:ASN:H	1.84	0.80
1:C:265:GLU:HB3	1:C:268:PHE:HE2	1.46	0.80
1:C:540:GLN:O	1:C:540:GLN:CG	2.30	0.80
1:A:234:GLU:H	1:A:235:ILE:CG2	1.92	0.80
1:A:299:GLN:HG2	1:A:318:THR:HG23	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:THR:OG1	1:A:500:GLN:HG2	1.82	0.80
1:A:496:LEU:HD21	1:A:509:ILE:HD13	1.63	0.80
1:C:396:ARG:HH21	1:C:464:ILE:HG22	1.46	0.80
1:C:469:TYR:CD2	1:C:470:PRO:HD2	2.16	0.80
1:D:371:ILE:HD11	1:D:381:VAL:HG11	1.64	0.80
1:A:406:TYR:CD1	2:A:808:NAG:H83	2.17	0.80
1:C:1:ASP:H3	1:D:88:VAL:CB	1.95	0.80
1:D:234:GLU:H	1:D:235:ILE:CG2	1.92	0.80
1:A:232:GLU:HG3	1:A:290:PHE:N	1.98	0.79
1:A:290:PHE:HD2	1:A:293:ARG:H	1.28	0.79
1:B:155:PRO:C	1:B:157:GLU:H	1.86	0.79
1:B:232:GLU:HG3	1:B:290:PHE:N	1.98	0.79
1:B:406:TYR:CD1	2:B:808:NAG:H83	2.17	0.79
1:C:35:TYR:CD2	1:D:45:ASN:OD1	2.35	0.79
1:C:87:PRO:CD	1:D:43:ALA:HB2	2.12	0.79
1:C:234:GLU:H	1:C:235:ILE:CG2	1.92	0.79
1:D:396:ARG:HH21	1:D:464:ILE:HG22	1.46	0.79
1:B:396:ARG:HH21	1:B:464:ILE:HG22	1.46	0.79
1:B:396:ARG:HD3	1:B:431:LEU:C	2.03	0.79
1:C:1:ASP:CB	1:D:89:GLU:CD	2.37	0.79
1:C:83:GLU:OE1	1:D:41:GLN:NE2	2.12	0.79
1:D:449:ASP:HB3	1:D:532:CYS:H	1.47	0.79
1:D:540:GLN:O	1:D:540:GLN:CG	2.30	0.79
1:A:365:GLN:HG3	1:A:365:GLN:O	1.82	0.79
1:C:127:VAL:HG13	1:C:128:MET:H	1.46	0.79
1:D:290:PHE:CE2	1:D:293:ARG:HB2	2.16	0.79
1:A:523:THR:CG2	1:A:524:VAL:H	1.94	0.79
1:B:27:ASN:HD22	1:B:27:ASN:C	1.85	0.79
1:C:371:ILE:HD11	1:C:381:VAL:HG11	1.64	0.79
1:C:27:ASN:HD22	1:C:27:ASN:C	1.85	0.79
1:C:85:GLY:HA2	1:D:42:GLY:H	1.45	0.79
1:D:127:VAL:HG13	1:D:128:MET:H	1.46	0.79
2:D:904:NAG:H3	2:D:904:NAG:O7	1.82	0.79
1:A:7:ILE:HG23	1:D:27:ASN:OD1	1.83	0.79
1:A:195:ASP:HB3	1:A:200:GLY:HA3	1.65	0.79
1:C:406:TYR:CD1	2:C:808:NAG:H83	2.17	0.79
1:D:154:ASP:HB3	2:D:801:NAG:HN2	1.44	0.79
1:D:482:THR:OG1	1:D:500:GLN:HG2	1.82	0.79
2:D:809:NAG:H61	2:D:810:NAG:H62	1.65	0.79
1:A:24:ILE:CG1	1:D:2:TRP:CZ2	2.66	0.79
1:B:32:ASN:HB3	1:C:27:ASN:HA	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:ASP:HB3	1:B:532:CYS:H	1.47	0.79
1:C:27:ASN:ND2	1:D:93:GLU:N	2.30	0.79
1:C:154:ASP:CB	1:C:155:PRO:HD2	2.13	0.79
1:A:154:ASP:CB	1:A:155:PRO:HD2	2.13	0.79
1:A:301:THR:HG21	2:A:805:NAG:C8	2.12	0.79
1:A:485:ALA:O	1:A:486:GLU:CG	2.31	0.79
1:B:299:GLN:HG2	1:B:318:THR:HG23	1.63	0.79
2:B:904:NAG:H3	2:B:904:NAG:O7	1.82	0.79
1:C:485:ALA:O	1:C:486:GLU:CG	2.30	0.79
1:D:154:ASP:CB	1:D:155:PRO:HD2	2.13	0.79
1:D:299:GLN:HG2	1:D:318:THR:HG23	1.62	0.79
1:A:1:ASP:HA	1:B:24:ILE:HD13	1.63	0.79
1:A:222:ASP:OD1	1:A:222:ASP:C	2.20	0.79
1:C:396:ARG:HD3	1:C:431:LEU:C	2.03	0.79
1:A:432:ASP:OD2	1:A:464:ILE:CG2	2.30	0.78
1:A:540:GLN:O	1:A:540:GLN:CG	2.30	0.78
1:B:485:ALA:O	1:B:486:GLU:CG	2.31	0.78
1:A:238:GLU:HA	1:A:283:THR:HG22	1.66	0.78
1:B:154:ASP:CB	1:B:155:PRO:HD2	2.13	0.78
1:C:238:GLU:HA	1:C:283:THR:HG22	1.66	0.78
1:B:371:ILE:HD11	1:B:381:VAL:HG11	1.64	0.78
1:C:90:GLU:CB	1:D:79:HIS:N	2.45	0.78
1:D:232:GLU:HG3	1:D:290:PHE:N	1.98	0.78
1:B:222:ASP:OD1	1:B:222:ASP:C	2.20	0.78
1:C:232:GLU:HG3	1:C:290:PHE:N	1.98	0.78
1:D:396:ARG:HD3	1:D:431:LEU:C	2.03	0.78
1:A:24:ILE:CA	1:D:2:TRP:CD1	2.61	0.78
1:A:501:GLN:HG2	1:A:501:GLN:O	1.84	0.78
1:B:88:VAL:O	1:D:1:ASP:CB	2.32	0.78
2:B:809:NAG:H61	2:B:810:NAG:H62	1.65	0.78
1:D:432:ASP:OD2	1:D:464:ILE:CG2	2.30	0.78
1:C:155:PRO:C	1:C:157:GLU:H	1.86	0.78
2:C:809:NAG:H61	2:C:810:NAG:H62	1.65	0.78
1:A:155:PRO:C	1:A:157:GLU:H	1.86	0.78
1:A:156:GLU:HG3	1:A:160:PRO:HB3	1.66	0.78
1:A:524:VAL:CG2	2:A:904:NAG:H81	2.14	0.78
1:C:93:GLU:HB2	1:D:81:VAL:HG11	1.64	0.78
1:C:156:GLU:HG3	1:C:160:PRO:HB3	1.66	0.78
1:C:449:ASP:HB3	1:C:532:CYS:H	1.47	0.78
1:D:222:ASP:OD1	1:D:222:ASP:C	2.20	0.78
1:D:365:GLN:HG3	1:D:365:GLN:O	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:GLU:HG3	1:B:160:PRO:HB3	1.66	0.78
1:C:482:THR:OG1	1:C:500:GLN:HG2	1.82	0.78
1:D:155:PRO:C	1:D:157:GLU:H	1.86	0.78
2:A:904:NAG:O7	2:A:904:NAG:H3	1.82	0.78
1:B:432:ASP:OD2	1:B:464:ILE:CG2	2.30	0.78
1:B:482:THR:OG1	1:B:500:GLN:HG2	1.82	0.78
1:C:81:VAL:HG13	1:D:40:GLY:N	1.98	0.78
1:D:238:GLU:HA	1:D:283:THR:HG22	1.66	0.78
1:A:10:SER:HB2	1:D:30:ARG:HG3	1.64	0.78
1:A:449:ASP:HB3	1:A:532:CYS:H	1.47	0.78
1:B:238:GLU:HA	1:B:283:THR:HG22	1.66	0.78
1:B:523:THR:CG2	1:B:524:VAL:N	2.46	0.78
1:A:147:SER:OG	1:A:167:ARG:CG	2.32	0.77
1:A:371:ILE:HD11	1:A:381:VAL:HG11	1.64	0.77
1:B:524:VAL:CG2	2:B:904:NAG:H81	2.14	0.77
1:C:82:SER:N	1:D:41:GLN:O	2.17	0.77
1:D:27:ASN:HD22	1:D:27:ASN:C	1.85	0.77
1:B:290:PHE:HD2	1:B:293:ARG:H	1.28	0.77
1:B:335:ALA:HB1	3:B:811:NDG:H6	1.49	0.77
1:C:365:GLN:HG3	1:C:365:GLN:O	1.82	0.77
1:C:523:THR:CG2	1:C:524:VAL:H	1.94	0.77
1:A:2:TRP:CG	1:B:80:ALA:HB2	2.16	0.77
1:A:147:SER:OG	1:A:167:ARG:CD	2.32	0.77
1:C:524:VAL:CG2	2:C:904:NAG:H81	2.14	0.77
2:C:904:NAG:O7	2:C:904:NAG:H3	1.82	0.77
1:D:223:PRO:HD2	1:D:226:TYR:OH	1.85	0.77
1:D:485:ALA:O	1:D:486:GLU:CG	2.30	0.77
1:A:24:ILE:HG13	1:D:2:TRP:CZ2	2.19	0.77
1:A:223:PRO:HD2	1:A:226:TYR:OH	1.85	0.77
1:C:35:TYR:HD2	1:D:45:ASN:CG	1.86	0.77
1:D:194:THR:HB	1:D:198:GLY:HA2	1.66	0.77
1:D:524:VAL:CG2	2:D:904:NAG:H81	2.14	0.77
1:A:2:TRP:O	1:B:92:MET:HB2	1.83	0.77
1:C:86:SER:HA	1:D:42:GLY:O	1.84	0.77
1:C:195:ASP:HB3	1:C:200:GLY:HA3	1.65	0.77
1:C:223:PRO:HD2	1:C:226:TYR:OH	1.85	0.77
2:A:809:NAG:H61	2:A:810:NAG:H62	1.65	0.77
1:B:31:PHE:HZ	1:C:34:VAL:HG21	1.49	0.77
1:C:86:SER:HB3	1:D:76:LEU:HD11	1.66	0.77
1:C:90:GLU:OE2	1:D:36:TYR:C	2.17	0.77
1:C:194:THR:HB	1:C:198:GLY:HA2	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:PHE:HZ	1:D:296:TYR:HH	1.30	0.77
1:C:523:THR:CG2	1:C:524:VAL:N	2.46	0.77
1:D:195:ASP:HB3	1:D:200:GLY:HA3	1.65	0.77
1:A:27:ASN:HD22	1:A:27:ASN:C	1.85	0.77
1:A:290:PHE:HZ	1:A:296:TYR:HH	1.33	0.77
1:A:505:GLY:C	1:A:506:ASP:OD1	2.23	0.77
1:B:30:ARG:O	1:C:30:ARG:CB	2.31	0.77
1:B:362:GLN:O	1:B:364:ILE:HG23	1.85	0.77
1:C:81:VAL:HG11	1:D:45:ASN:N	1.99	0.77
1:A:194:THR:HB	1:A:198:GLY:HA2	1.67	0.77
1:A:432:ASP:CG	1:A:464:ILE:HG22	2.05	0.77
1:B:540:GLN:O	1:B:540:GLN:CG	2.30	0.77
1:A:196:LEU:HB2	1:A:199:ALA:HB3	1.67	0.76
1:B:86:SER:HA	1:D:90:GLU:HA	1.62	0.76
1:C:31:PHE:HA	1:D:73:LYS:NZ	2.00	0.76
1:C:432:ASP:CG	1:C:464:ILE:HG22	2.05	0.76
1:D:272:THR:HG22	1:D:273:THR:H	1.51	0.76
1:B:440:PRO:HB3	1:B:457:LEU:HD21	1.67	0.76
1:D:290:PHE:HD2	1:D:293:ARG:H	1.28	0.76
1:D:505:GLY:C	1:D:506:ASP:OD1	2.23	0.76
1:A:366:LYS:CG	1:A:367:LEU:N	2.48	0.76
1:B:195:ASP:HB3	1:B:200:GLY:HA3	1.65	0.76
1:B:505:GLY:C	1:B:506:ASP:OD1	2.23	0.76
1:C:186:GLU:O	2:C:801:NAG:O7	2.03	0.76
1:C:362:GLN:O	1:C:364:ILE:HG23	1.85	0.76
1:D:186:GLU:O	2:D:801:NAG:O7	2.03	0.76
1:D:368:SER:HG	1:D:370:PHE:HE1	1.33	0.76
1:B:365:GLN:O	1:B:365:GLN:HG3	1.82	0.76
1:B:366:LYS:CG	1:B:367:LEU:N	2.48	0.76
1:C:396:ARG:HH21	1:C:464:ILE:CG2	1.98	0.76
1:D:241:ARG:HE	1:D:281:ILE:HD12	1.51	0.76
1:A:90:GLU:N	1:B:2:TRP:HE3	1.83	0.76
1:B:186:GLU:O	2:B:801:NAG:O7	2.04	0.76
1:C:88:VAL:CG1	1:D:94:ILE:HB	2.15	0.76
1:C:505:GLY:C	1:C:506:ASP:OD1	2.23	0.76
1:D:440:PRO:HB3	1:D:457:LEU:HD21	1.67	0.76
1:A:186:GLU:O	2:A:801:NAG:O7	2.03	0.76
1:A:396:ARG:HH21	1:A:464:ILE:CG2	1.98	0.76
1:B:432:ASP:CG	1:B:464:ILE:HG22	2.05	0.76
1:A:24:ILE:CG2	1:D:2:TRP:CD1	2.67	0.76
1:B:196:LEU:HB2	1:B:199:ALA:HB3	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:THR:HG23	1:B:524:VAL:HG22	1.67	0.76
1:C:4:ILE:HG21	1:D:87:PRO:HG2	1.68	0.76
1:D:362:GLN:O	1:D:364:ILE:HG23	1.85	0.76
1:B:501:GLN:O	1:B:501:GLN:HG2	1.84	0.76
1:C:88:VAL:C	1:D:38:ILE:HG13	2.05	0.76
1:C:196:LEU:HB2	1:C:199:ALA:HB3	1.67	0.76
1:D:156:GLU:HG3	1:D:160:PRO:HB3	1.66	0.76
1:D:366:LYS:CG	1:D:367:LEU:N	2.48	0.76
1:D:432:ASP:CG	1:D:464:ILE:HG22	2.05	0.76
1:A:440:PRO:HB3	1:A:457:LEU:HD21	1.67	0.76
1:A:523:THR:CG2	1:A:524:VAL:N	2.46	0.76
1:B:82:SER:CB	1:C:27:ASN:HB3	2.15	0.76
1:B:223:PRO:HD2	1:B:226:TYR:OH	1.85	0.76
1:D:371:ILE:HD12	1:D:410:MET:HB3	1.68	0.76
1:A:91:PRO:CA	1:B:1:ASP:O	2.34	0.76
1:C:501:GLN:HG2	1:C:501:GLN:O	1.84	0.76
1:D:196:LEU:HB2	1:D:199:ALA:HB3	1.67	0.76
1:D:448:CYS:SG	1:D:537:ILE:HG22	2.26	0.76
1:B:301:THR:HG21	2:B:805:NAG:C8	2.12	0.75
1:A:371:ILE:HD12	1:A:410:MET:HB3	1.68	0.75
1:B:84:ASN:HD22	1:D:91:PRO:HB2	1.49	0.75
1:C:301:THR:HG21	2:C:805:NAG:C8	2.13	0.75
1:C:371:ILE:HD12	1:C:410:MET:HB3	1.68	0.75
1:A:188:THR:HG23	1:A:208:ILE:CG1	2.16	0.75
1:B:88:VAL:HG13	1:C:27:ASN:OD1	1.87	0.75
1:B:272:THR:HG22	1:B:273:THR:H	1.51	0.75
1:B:364:ILE:HG13	1:B:364:ILE:O	1.87	0.75
1:C:366:LYS:CG	1:C:367:LEU:N	2.48	0.75
1:C:272:THR:HG22	1:C:273:THR:H	1.50	0.75
1:D:501:GLN:O	1:D:501:GLN:HG2	1.84	0.75
1:B:448:CYS:SG	1:B:537:ILE:HG22	2.27	0.75
1:A:362:GLN:O	1:A:364:ILE:HG23	1.85	0.75
1:A:396:ARG:NH2	1:A:464:ILE:HB	2.02	0.75
1:B:31:PHE:CE2	1:C:29:ASP:CB	2.68	0.75
1:B:194:THR:HB	1:B:198:GLY:HA2	1.67	0.75
1:B:482:THR:CG2	1:B:499:THR:CG2	2.62	0.75
1:C:448:CYS:SG	1:C:537:ILE:HG22	2.27	0.75
1:D:290:PHE:CD2	1:D:293:ARG:N	2.55	0.75
1:B:396:ARG:NH2	1:B:464:ILE:HB	2.02	0.75
1:C:440:PRO:HB3	1:C:457:LEU:HD21	1.67	0.75
1:D:449:ASP:HB3	1:D:532:CYS:N	2.02	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:PHE:HD2	1:C:293:ARG:H	1.28	0.75
1:A:5:PRO:HD2	1:B:90:GLU:OE2	1.87	0.75
1:A:448:CYS:SG	1:A:537:ILE:HG22	2.27	0.74
1:A:449:ASP:HB3	1:A:532:CYS:N	2.02	0.74
1:B:371:ILE:HD12	1:B:410:MET:HB3	1.68	0.74
1:A:523:THR:HG23	1:A:524:VAL:HG22	1.67	0.74
1:C:396:ARG:NH2	1:C:464:ILE:HB	2.02	0.74
1:D:523:THR:HG23	1:D:524:VAL:HG22	1.67	0.74
1:A:241:ARG:HE	1:A:281:ILE:HD12	1.51	0.74
1:A:272:THR:HG22	1:A:273:THR:H	1.50	0.74
1:C:2:TRP:N	1:D:89:GLU:HA	2.01	0.74
1:C:188:THR:HG23	1:C:208:ILE:CG1	2.16	0.74
1:A:3:VAL:HG23	1:B:91:PRO:CB	2.17	0.74
1:B:368:SER:HG	1:B:370:PHE:HE1	1.36	0.74
1:C:241:ARG:HE	1:C:281:ILE:HD12	1.51	0.74
1:D:188:THR:HG23	1:D:208:ILE:CG1	2.16	0.74
1:D:450:GLN:HG3	1:D:533:GLU:OE2	1.88	0.74
1:A:79:HIS:HA	1:B:1:ASP:H2	1.53	0.74
1:B:84:ASN:O	1:C:24:ILE:HB	1.87	0.74
1:B:84:ASN:HD21	1:D:91:PRO:HB2	1.53	0.74
1:B:396:ARG:HH21	1:B:464:ILE:CG2	1.99	0.74
1:B:449:ASP:HB3	1:B:532:CYS:N	2.02	0.74
1:B:450:GLN:HG3	1:B:533:GLU:OE2	1.88	0.74
1:C:90:GLU:C	1:D:79:HIS:H	1.78	0.74
1:A:364:ILE:O	1:A:364:ILE:HG13	1.87	0.74
1:C:80:ALA:HB3	1:D:39:THR:OG1	1.88	0.74
1:C:88:VAL:HG22	1:D:76:LEU:CD2	1.96	0.74
1:C:482:THR:CG2	1:C:499:THR:CG2	2.62	0.74
1:D:451:ASN:O	1:D:534:GLY:HA2	1.88	0.74
1:A:79:HIS:HA	1:B:1:ASP:N	2.03	0.74
1:A:298:LEU:N	1:A:298:LEU:HD23	2.03	0.74
1:C:87:PRO:C	1:D:76:LEU:CD2	2.53	0.74
1:C:290:PHE:HZ	1:C:296:TYR:HH	1.35	0.74
1:D:523:THR:CG2	1:D:524:VAL:N	2.46	0.74
1:A:450:GLN:HG3	1:A:533:GLU:OE2	1.88	0.74
1:C:31:PHE:CB	1:D:75:VAL:HG22	2.13	0.74
1:C:523:THR:HG23	1:C:524:VAL:HG22	1.67	0.74
1:A:90:GLU:C	1:B:3:VAL:CG2	2.57	0.73
1:B:188:THR:HG23	1:B:208:ILE:CG1	2.16	0.73
1:B:290:PHE:HZ	1:B:296:TYR:HH	1.33	0.73
1:B:320:THR:CG2	2:B:807:NAG:HN2	2.01	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:GLU:OE2	1:D:37:SER:CA	2.30	0.73
1:C:450:GLN:HG3	1:C:533:GLU:OE2	1.88	0.73
1:A:223:PRO:HB2	1:A:226:TYR:CE2	2.23	0.73
1:B:31:PHE:HA	1:C:30:ARG:HA	1.67	0.73
1:C:1:ASP:H1	1:D:28:LYS:HB2	1.53	0.73
1:C:26:SER:OG	1:D:77:SER:CB	2.36	0.73
1:C:449:ASP:HB3	1:C:532:CYS:N	2.02	0.73
1:D:320:THR:CG2	2:D:807:NAG:HN2	2.02	0.73
1:A:320:THR:CG2	2:A:807:NAG:N2	2.52	0.73
1:A:482:THR:CG2	1:A:499:THR:CG2	2.62	0.73
1:B:31:PHE:CE2	1:C:29:ASP:HB3	2.14	0.73
1:B:451:ASN:O	1:B:534:GLY:HA2	1.88	0.73
1:C:4:ILE:HG22	1:D:87:PRO:CG	2.16	0.73
1:C:88:VAL:HG12	1:D:94:ILE:CB	2.18	0.73
1:C:223:PRO:HB2	1:C:226:TYR:CE2	2.23	0.73
1:C:364:ILE:O	1:C:364:ILE:HG13	1.87	0.73
1:A:451:ASN:O	1:A:534:GLY:HA2	1.88	0.73
1:B:241:ARG:HE	1:B:281:ILE:HD12	1.51	0.73
1:C:79:HIS:CG	1:D:44:ASP:OD1	2.41	0.73
1:D:223:PRO:HB2	1:D:226:TYR:CE2	2.23	0.73
1:D:364:ILE:O	1:D:364:ILE:HG13	1.87	0.73
1:A:276:GLU:HG3	1:A:277:SER:H	1.54	0.73
1:B:298:LEU:N	1:B:298:LEU:HD23	2.03	0.73
1:C:1:ASP:H1	1:D:28:LYS:HD3	1.47	0.73
1:C:84:ASN:O	1:D:47:PRO:HG2	1.88	0.73
1:C:91:PRO:C	1:D:37:SER:OG	2.26	0.73
1:D:333:VAL:CB	1:D:334:PRO:HD3	2.18	0.73
1:C:451:ASN:O	1:C:534:GLY:HA2	1.88	0.73
1:D:373:ASN:ND2	1:D:374:ASP:H	1.87	0.73
1:A:333:VAL:CB	1:A:334:PRO:HD3	2.18	0.73
1:B:276:GLU:HG3	1:B:277:SER:H	1.54	0.73
1:C:290:PHE:HE2	1:C:293:ARG:HB2	1.52	0.73
1:B:223:PRO:HB2	1:B:226:TYR:CE2	2.23	0.73
1:B:273:THR:O	2:B:803:NAG:H82	1.89	0.73
1:B:290:PHE:HE2	1:B:293:ARG:HB2	1.52	0.73
1:B:320:THR:CG2	2:B:807:NAG:N2	2.52	0.73
1:B:373:ASN:ND2	1:B:374:ASP:H	1.87	0.73
1:D:298:LEU:N	1:D:298:LEU:HD23	2.03	0.73
1:D:301:THR:HG21	2:D:805:NAG:C8	2.12	0.73
1:A:342:SER:HA	1:A:431:LEU:HB2	1.71	0.73
1:B:364:ILE:O	1:B:364:ILE:CG1	2.37	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:364:ILE:O	1:D:364:ILE:CG1	2.37	0.73
1:D:396:ARG:HH21	1:D:464:ILE:CG2	1.98	0.73
1:A:373:ASN:ND2	1:A:374:ASP:H	1.87	0.72
1:C:273:THR:O	2:C:803:NAG:H82	1.89	0.72
1:C:511:VAL:HG23	1:C:523:THR:O	1.89	0.72
1:A:90:GLU:CB	1:B:3:VAL:O	2.34	0.72
1:A:273:THR:O	2:A:803:NAG:H82	1.89	0.72
1:A:320:THR:CG2	2:A:807:NAG:HN2	2.01	0.72
1:B:32:ASN:HA	1:C:29:ASP:OD2	1.87	0.72
1:B:33:LYS:HB3	1:B:83:GLU:HG2	1.71	0.72
1:C:1:ASP:N	1:D:88:VAL:CB	2.52	0.72
1:C:298:LEU:HD23	1:C:298:LEU:N	2.03	0.72
1:D:33:LYS:HB3	1:D:83:GLU:HG2	1.71	0.72
1:D:290:PHE:HE2	1:D:293:ARG:HB2	1.52	0.72
1:D:320:THR:CG2	2:D:807:NAG:N2	2.52	0.72
1:C:320:THR:CG2	2:C:807:NAG:N2	2.52	0.72
1:D:482:THR:CG2	1:D:499:THR:CG2	2.62	0.72
1:A:99:ILE:CG2	1:D:30:ARG:NH1	2.50	0.72
1:A:511:VAL:HG23	1:A:523:THR:O	1.89	0.72
1:C:373:ASN:ND2	1:C:374:ASP:H	1.87	0.72
1:D:273:THR:O	2:D:803:NAG:H82	1.89	0.72
1:D:511:VAL:HG23	1:D:523:THR:O	1.89	0.72
1:A:364:ILE:O	1:A:364:ILE:CG1	2.37	0.72
1:B:511:VAL:HG23	1:B:523:THR:O	1.89	0.72
1:C:333:VAL:CB	1:C:334:PRO:HD3	2.18	0.72
1:C:32:ASN:H	1:D:75:VAL:HG21	0.57	0.72
1:C:276:GLU:HG3	1:C:277:SER:H	1.54	0.72
1:A:394:LEU:HD12	1:A:394:LEU:N	2.05	0.72
1:B:333:VAL:CB	1:B:334:PRO:HD3	2.18	0.72
1:C:366:LYS:HG3	1:C:367:LEU:N	2.04	0.72
1:B:32:ASN:C	1:C:25:LYS:HE2	2.06	0.72
1:C:82:SER:HB2	1:D:75:VAL:H	1.52	0.72
1:D:276:GLU:HG3	1:D:277:SER:H	1.54	0.72
1:A:474:SER:CB	1:A:512:LEU:HG	2.14	0.71
1:B:88:VAL:C	1:D:1:ASP:HB2	2.09	0.71
1:D:396:ARG:NH2	1:D:464:ILE:HB	2.02	0.71
1:A:4:ILE:C	1:B:91:PRO:HB2	2.10	0.71
1:B:394:LEU:N	1:B:394:LEU:HD12	2.05	0.71
1:D:342:SER:HA	1:D:431:LEU:HB2	1.71	0.71
1:C:90:GLU:HB3	1:D:79:HIS:N	2.05	0.71
1:C:227:THR:O	2:C:812:NAG:O5	2.09	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:SER:HA	1:C:431:LEU:HB2	1.71	0.71
1:C:364:ILE:O	1:C:364:ILE:CG1	2.37	0.71
1:B:316:THR:O	2:B:806:NAG:H82	1.91	0.71
1:C:229:LEU:HD23	1:C:322:THR:HB	1.73	0.71
1:C:394:LEU:HD12	1:C:394:LEU:N	2.05	0.71
1:D:229:LEU:HD23	1:D:322:THR:HB	1.73	0.71
1:D:414:ASP:HB3	1:D:420:GLY:HA3	1.73	0.71
1:A:276:GLU:CG	1:A:277:SER:H	2.03	0.71
1:C:434:ASN:OD1	1:C:467:ASN:HB3	1.91	0.71
1:D:438:PRO:HB3	1:D:471:TYR:CE2	2.26	0.71
1:B:434:ASN:OD1	1:B:467:ASN:HB3	1.91	0.71
1:C:90:GLU:HB3	1:D:79:HIS:CA	2.20	0.71
1:A:289:ASP:O	1:A:289:ASP:CG	2.29	0.71
1:A:335:ALA:HB1	3:A:811:NDG:H6	1.55	0.71
1:A:403:ASN:CB	2:A:902:NAG:N2	2.54	0.71
1:B:187:TYR:HA	2:B:801:NAG:C7	2.21	0.71
1:B:30:ARG:O	1:C:30:ARG:CA	2.39	0.71
1:B:290:PHE:CD2	1:B:293:ARG:N	2.55	0.71
1:C:81:VAL:CG1	1:D:40:GLY:N	2.49	0.71
1:C:187:TYR:HA	2:C:801:NAG:C7	2.21	0.71
1:D:337:SER:CA	1:D:427:ILE:HG23	2.19	0.71
1:A:91:PRO:CA	1:B:3:VAL:HG22	2.21	0.71
1:C:93:GLU:OE2	1:D:85:GLY:CA	2.30	0.71
1:D:276:GLU:CG	1:D:277:SER:H	2.03	0.71
1:A:187:TYR:HA	2:A:801:NAG:C7	2.21	0.70
1:A:414:ASP:HB3	1:A:420:GLY:HA3	1.73	0.70
1:B:483:TRP:CZ2	1:B:507:TYR:HE1	2.09	0.70
1:C:26:SER:OG	1:D:77:SER:HB2	1.90	0.70
1:C:33:LYS:HB3	1:C:83:GLU:HG2	1.71	0.70
1:C:320:THR:CG2	2:C:807:NAG:HN2	2.02	0.70
1:D:394:LEU:HD12	1:D:394:LEU:N	2.05	0.70
1:A:290:PHE:HE2	1:A:293:ARG:HB2	1.52	0.70
1:A:290:PHE:CD2	1:A:293:ARG:N	2.54	0.70
1:B:33:LYS:H	1:C:25:LYS:HE2	0.84	0.70
1:B:227:THR:O	2:B:812:NAG:O5	2.09	0.70
1:B:229:LEU:HD23	1:B:322:THR:HB	1.73	0.70
1:B:342:SER:HA	1:B:431:LEU:HB2	1.71	0.70
1:C:85:GLY:N	1:D:74:TYR:CE2	2.59	0.70
1:D:187:TYR:HA	2:D:801:NAG:C7	2.21	0.70
1:B:414:ASP:HB3	1:B:420:GLY:HA3	1.73	0.70
1:D:434:ASN:OD1	1:D:467:ASN:HB3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LYS:HB3	1:A:83:GLU:HG2	1.71	0.70
1:B:405:THR:OG1	1:B:406:TYR:N	2.22	0.70
1:D:227:THR:O	2:D:812:NAG:O5	2.09	0.70
1:D:316:THR:O	2:D:806:NAG:H82	1.91	0.70
1:A:1:ASP:HB3	1:B:92:MET:HB3	1.72	0.70
1:C:289:ASP:O	1:C:289:ASP:CG	2.29	0.70
1:A:3:VAL:CG2	1:B:78:SER:H	2.01	0.70
1:A:316:THR:O	2:A:806:NAG:H82	1.91	0.70
1:C:276:GLU:CG	1:C:277:SER:H	2.03	0.70
1:D:403:ASN:CB	2:D:902:NAG:N2	2.54	0.70
1:A:523:THR:HG23	1:A:524:VAL:HG23	1.73	0.70
1:C:31:PHE:CD1	1:D:95:THR:CG2	2.75	0.70
1:C:80:ALA:HB3	1:D:77:SER:CB	2.21	0.70
1:A:434:ASN:OD1	1:A:467:ASN:HB3	1.91	0.70
1:A:485:ALA:C	1:A:486:GLU:HG2	2.12	0.70
1:A:229:LEU:HD23	1:A:322:THR:HB	1.73	0.70
1:A:405:THR:OG1	1:A:406:TYR:N	2.22	0.70
1:B:83:GLU:N	1:C:25:LYS:CD	2.43	0.70
1:B:523:THR:HG23	1:B:524:VAL:HG23	1.74	0.70
1:C:4:ILE:CG2	1:D:87:PRO:CB	2.68	0.69
1:C:396:ARG:HE	1:C:432:ASP:HB2	1.57	0.69
1:C:414:ASP:HB3	1:C:420:GLY:HA3	1.73	0.69
1:D:474:SER:HB2	1:D:512:LEU:CG	2.15	0.69
1:A:227:THR:O	2:A:812:NAG:O5	2.09	0.69
1:A:438:PRO:HB3	1:A:471:TYR:CE2	2.26	0.69
1:C:1:ASP:H3	1:D:88:VAL:CG1	2.03	0.69
1:C:290:PHE:CD2	1:C:293:ARG:N	2.55	0.69
1:C:316:THR:O	2:C:806:NAG:H82	1.91	0.69
1:C:337:SER:CA	1:C:427:ILE:HG23	2.20	0.69
1:C:403:ASN:CB	2:C:902:NAG:N2	2.54	0.69
1:D:405:THR:OG1	1:D:406:TYR:N	2.22	0.69
1:D:485:ALA:C	1:D:486:GLU:HG2	2.11	0.69
1:A:483:TRP:CZ2	1:A:507:TYR:HE1	2.09	0.69
1:C:1:ASP:C	1:D:28:LYS:NZ	2.44	0.69
1:B:276:GLU:CG	1:B:277:SER:H	2.03	0.69
1:B:438:PRO:HB3	1:B:471:TYR:CE2	2.26	0.69
1:D:1:ASP:CG	1:D:2:TRP:H	1.96	0.69
1:B:485:ALA:C	1:B:486:GLU:HG2	2.11	0.69
1:C:35:TYR:CD2	1:D:45:ASN:CG	2.65	0.69
1:C:82:SER:HB3	1:D:75:VAL:O	1.92	0.69
1:C:186:GLU:OE1	2:C:801:NAG:H62	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ILE:HG13	1:A:59:TRP:O	1.93	0.69
1:B:83:GLU:HG2	1:C:25:LYS:CD	2.20	0.69
1:C:483:TRP:CZ2	1:C:507:TYR:HE1	2.09	0.69
1:D:53:ILE:HG13	1:D:59:TRP:O	1.93	0.69
1:D:186:GLU:OE1	2:D:801:NAG:H62	1.93	0.69
1:A:10:SER:N	1:D:30:ARG:HG3	2.08	0.69
1:A:242:LEU:HD12	1:A:280:GLY:O	1.93	0.69
1:B:27:ASN:C	1:B:27:ASN:ND2	2.46	0.69
1:B:403:ASN:CB	2:B:902:NAG:N2	2.54	0.69
1:B:474:SER:CB	1:B:512:LEU:HG	2.14	0.69
1:C:79:HIS:HB3	1:D:39:THR:CG2	2.20	0.69
1:C:90:GLU:HG2	1:D:36:TYR:CB	2.08	0.69
1:C:289:ASP:O	1:C:290:PHE:CB	2.25	0.69
1:D:289:ASP:O	1:D:289:ASP:CG	2.29	0.69
1:B:83:GLU:O	1:C:25:LYS:N	2.17	0.69
1:B:242:LEU:HD12	1:B:280:GLY:O	1.93	0.69
1:C:83:GLU:CB	1:D:41:GLN:NE2	2.56	0.69
1:C:523:THR:HG23	1:C:524:VAL:HG23	1.74	0.69
1:A:27:ASN:C	1:A:27:ASN:ND2	2.46	0.69
1:A:366:LYS:HG3	1:A:367:LEU:N	2.04	0.69
1:C:405:THR:OG1	1:C:406:TYR:N	2.22	0.69
1:C:485:ALA:C	1:C:486:GLU:HG2	2.11	0.69
1:D:523:THR:HG23	1:D:524:VAL:HG23	1.74	0.69
1:A:1:ASP:H3	1:B:94:ILE:HD11	0.87	0.68
1:A:1:ASP:HA	1:B:24:ILE:CD1	2.22	0.68
1:A:186:GLU:OE1	2:A:801:NAG:H62	1.93	0.68
1:A:282:LEU:HD23	1:A:283:THR:N	2.08	0.68
1:B:282:LEU:HD23	1:B:283:THR:N	2.08	0.68
1:B:81:VAL:HB	1:D:90:GLU:HG2	1.74	0.68
1:C:31:PHE:HB3	1:D:95:THR:HG23	1.72	0.68
1:C:242:LEU:HD12	1:C:280:GLY:O	1.93	0.68
1:C:474:SER:HB2	1:C:512:LEU:CG	2.15	0.68
1:A:290:PHE:HZ	1:A:296:TYR:OH	1.76	0.68
1:A:320:THR:HG21	2:A:807:NAG:H2	1.76	0.68
1:B:289:ASP:O	1:B:289:ASP:CG	2.29	0.68
1:C:272:THR:HG22	1:C:273:THR:N	2.09	0.68
1:C:290:PHE:HZ	1:C:296:TYR:OH	1.77	0.68
1:D:272:THR:HG22	1:D:273:THR:N	2.09	0.68
1:D:396:ARG:HD3	1:D:431:LEU:O	1.94	0.68
1:A:396:ARG:HD3	1:A:431:LEU:O	1.93	0.68
1:B:282:LEU:HD23	1:B:283:THR:H	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:THR:HG21	2:B:807:NAG:H2	1.76	0.68
1:C:87:PRO:N	1:D:43:ALA:CB	2.35	0.68
1:C:282:LEU:HD23	1:C:283:THR:N	2.08	0.68
1:D:242:LEU:HD12	1:D:280:GLY:O	1.93	0.68
1:C:87:PRO:HD3	1:D:43:ALA:N	2.08	0.68
1:C:195:ASP:HB2	1:C:201:LEU:N	2.08	0.68
1:C:282:LEU:HD23	1:C:283:THR:H	1.58	0.68
1:A:482:THR:HG21	1:A:500:GLN:H	1.59	0.68
1:B:396:ARG:HD3	1:B:431:LEU:O	1.94	0.68
1:C:84:ASN:HA	1:D:71:TYR:CG	2.28	0.68
1:B:53:ILE:HG13	1:B:59:TRP:O	1.93	0.68
1:B:155:PRO:HB2	2:B:801:NAG:C8	2.24	0.68
1:B:333:VAL:HB	1:B:334:PRO:CD	2.24	0.68
1:B:337:SER:CA	1:B:427:ILE:HG23	2.20	0.68
1:C:89:GLU:CA	1:D:38:ILE:HG13	2.24	0.68
1:C:517:GLN:C	1:C:519:ASN:N	2.46	0.68
1:A:368:SER:HG	1:A:370:PHE:HE1	1.42	0.68
1:A:371:ILE:CG2	1:A:372:GLY:N	2.57	0.68
1:B:88:VAL:C	1:D:1:ASP:CB	2.62	0.68
1:B:347:ARG:CD	1:B:392:GLY:H	2.07	0.68
1:C:4:ILE:HG23	1:D:87:PRO:CG	2.17	0.68
1:C:53:ILE:HG13	1:C:59:TRP:O	1.93	0.68
1:D:396:ARG:HE	1:D:432:ASP:HB2	1.57	0.68
1:B:87:PRO:HG2	1:C:2:TRP:CB	2.21	0.68
1:B:221:PHE:CE1	1:B:315:SER:O	2.45	0.68
1:B:396:ARG:HE	1:B:432:ASP:CB	2.07	0.68
1:C:396:ARG:HD3	1:C:431:LEU:O	1.94	0.68
1:B:371:ILE:CG2	1:B:372:GLY:N	2.57	0.68
1:C:1:ASP:CA	1:D:89:GLU:CG	2.57	0.68
1:C:93:GLU:HB3	1:D:81:VAL:HG11	1.73	0.68
1:C:137:ASP:OD2	1:C:139:ILE:HG22	1.94	0.68
1:C:155:PRO:HB2	2:C:801:NAG:C8	2.24	0.68
1:C:371:ILE:CG2	1:C:372:GLY:N	2.57	0.68
1:C:440:PRO:HA	1:C:458:THR:O	1.94	0.68
1:D:347:ARG:CD	1:D:392:GLY:H	2.07	0.68
1:A:1:ASP:CG	1:A:2:TRP:H	1.96	0.67
1:A:272:THR:HG22	1:A:273:THR:N	2.09	0.67
1:A:282:LEU:HD23	1:A:283:THR:H	1.58	0.67
1:B:1:ASP:CG	1:B:2:TRP:H	1.96	0.67
1:B:186:GLU:OE1	2:B:801:NAG:H62	1.93	0.67
1:B:289:ASP:O	1:B:290:PHE:CB	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:ASP:O	1:C:222:ASP:CG	2.32	0.67
1:D:282:LEU:HD23	1:D:283:THR:H	1.58	0.67
1:D:333:VAL:HB	1:D:334:PRO:CD	2.24	0.67
1:D:440:PRO:HA	1:D:458:THR:O	1.94	0.67
1:A:347:ARG:CD	1:A:392:GLY:H	2.07	0.67
1:B:32:ASN:HB2	1:C:27:ASN:HA	1.74	0.67
1:B:84:ASN:OD1	1:C:27:ASN:N	2.25	0.67
1:C:333:VAL:HB	1:C:334:PRO:CD	2.24	0.67
1:D:195:ASP:HB2	1:D:201:LEU:N	2.08	0.67
1:D:222:ASP:O	1:D:222:ASP:CG	2.32	0.67
1:D:396:ARG:HE	1:D:432:ASP:CB	2.07	0.67
1:D:423:THR:HB	2:D:810:NAG:C8	2.24	0.67
1:B:137:ASP:OD2	1:B:139:ILE:HG22	1.94	0.67
1:D:137:ASP:OD2	1:D:139:ILE:HG22	1.94	0.67
1:A:155:PRO:HB2	2:A:801:NAG:C8	2.24	0.67
1:C:91:PRO:C	1:D:79:HIS:CD2	2.66	0.67
1:C:347:ARG:CD	1:C:392:GLY:H	2.07	0.67
1:C:474:SER:CB	1:C:512:LEU:HG	2.14	0.67
1:A:24:ILE:C	1:D:2:TRP:CZ2	2.48	0.67
1:B:272:THR:HG22	1:B:273:THR:N	2.09	0.67
1:B:440:PRO:HA	1:B:458:THR:O	1.94	0.67
1:B:482:THR:HG21	1:B:500:GLN:H	1.59	0.67
1:C:90:GLU:HG2	1:D:36:TYR:HB3	1.75	0.67
1:D:27:ASN:C	1:D:27:ASN:ND2	2.46	0.67
1:D:282:LEU:HD23	1:D:283:THR:N	2.08	0.67
1:D:474:SER:CB	1:D:512:LEU:HG	2.14	0.67
1:D:483:TRP:CZ2	1:D:507:TYR:HE1	2.09	0.67
1:D:524:VAL:HG21	2:D:904:NAG:H81	1.77	0.67
1:B:290:PHE:HZ	1:B:296:TYR:OH	1.76	0.67
1:C:482:THR:HG21	1:C:500:GLN:H	1.58	0.67
1:D:396:ARG:NH2	1:D:464:ILE:CB	2.58	0.67
1:B:474:SER:HB2	1:B:512:LEU:CG	2.15	0.67
1:B:524:VAL:HG21	2:B:904:NAG:H81	1.76	0.67
1:D:187:TYR:HA	2:D:801:NAG:C8	2.25	0.67
1:A:90:GLU:N	1:B:2:TRP:CE3	2.60	0.67
1:A:396:ARG:HE	1:A:432:ASP:CB	2.07	0.67
1:B:396:ARG:HE	1:B:432:ASP:HB2	1.57	0.67
1:B:401:VAL:HG13	1:B:405:THR:O	1.95	0.67
1:C:224:LYS:HE3	1:C:316:THR:O	1.95	0.67
1:C:396:ARG:HE	1:C:432:ASP:CB	2.07	0.67
1:C:401:VAL:HG13	1:C:405:THR:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:SER:N	1:D:30:ARG:CG	2.58	0.67
1:A:137:ASP:OD2	1:A:139:ILE:HG22	1.94	0.67
1:A:423:THR:HB	2:A:810:NAG:C8	2.24	0.67
1:C:187:TYR:HA	2:C:801:NAG:C8	2.25	0.67
1:C:221:PHE:CE1	1:C:315:SER:O	2.45	0.67
1:B:195:ASP:HB2	1:B:201:LEU:N	2.08	0.67
1:B:222:ASP:O	1:B:222:ASP:CG	2.32	0.67
2:C:902:NAG:O7	2:C:902:NAG:H3	1.95	0.67
1:D:347:ARG:CG	1:D:392:GLY:H	2.08	0.67
1:D:373:ASN:ND2	1:D:374:ASP:N	2.43	0.67
1:D:446:THR:CG2	1:D:537:ILE:O	2.43	0.67
1:A:396:ARG:NH2	1:A:464:ILE:CB	2.58	0.66
1:B:446:THR:CG2	1:B:537:ILE:O	2.43	0.66
1:C:32:ASN:CG	1:C:33:LYS:H	1.98	0.66
1:D:401:VAL:HG13	1:D:405:THR:O	1.95	0.66
2:D:902:NAG:H3	2:D:902:NAG:O7	1.95	0.66
1:C:82:SER:CB	1:D:75:VAL:N	2.49	0.66
1:C:423:THR:HB	2:C:810:NAG:C8	2.24	0.66
1:D:32:ASN:CG	1:D:33:LYS:H	1.99	0.66
1:B:187:TYR:HA	2:B:801:NAG:C8	2.25	0.66
1:C:27:ASN:ND2	1:D:93:GLU:CA	2.58	0.66
1:C:232:GLU:HG3	1:C:290:PHE:H	1.61	0.66
1:C:524:VAL:HG21	2:C:904:NAG:H81	1.77	0.66
1:D:320:THR:HG21	2:D:807:NAG:H2	1.76	0.66
1:A:187:TYR:HA	2:A:801:NAG:C8	2.25	0.66
1:A:482:THR:OG1	1:A:500:GLN:CG	2.44	0.66
1:A:347:ARG:HD2	1:A:392:GLY:H	1.60	0.66
1:A:440:PRO:HA	1:A:458:THR:O	1.94	0.66
1:C:86:SER:CB	1:D:76:LEU:HD11	2.26	0.66
1:C:396:ARG:NH2	1:C:464:ILE:CB	2.58	0.66
1:D:232:GLU:HG2	1:D:289:ASP:HA	1.77	0.66
1:D:290:PHE:HZ	1:D:296:TYR:OH	1.77	0.66
1:D:371:ILE:CG2	1:D:372:GLY:N	2.57	0.66
1:D:403:ASN:HB2	2:D:902:NAG:N2	2.10	0.66
1:D:440:PRO:HD2	1:D:522:LEU:CD1	2.26	0.66
1:A:36:TYR:CE2	1:D:2:TRP:HH2	2.13	0.66
1:A:347:ARG:CG	1:A:392:GLY:H	2.08	0.66
1:B:347:ARG:HD2	1:B:392:GLY:H	1.60	0.66
1:B:396:ARG:NH2	1:B:464:ILE:CB	2.58	0.66
1:B:403:ASN:HB2	2:B:902:NAG:N2	2.10	0.66
1:B:423:THR:HB	2:B:810:NAG:C8	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:THR:OG1	1:B:500:GLN:CG	2.44	0.66
1:C:440:PRO:HD2	1:C:522:LEU:CD1	2.26	0.66
1:A:224:LYS:HE3	1:A:316:THR:O	1.95	0.66
1:A:524:VAL:HG21	2:A:904:NAG:H81	1.77	0.66
1:C:90:GLU:OE1	1:D:53:ILE:HG21	1.95	0.66
1:C:373:ASN:ND2	1:C:374:ASP:N	2.43	0.66
1:C:438:PRO:HB3	1:C:471:TYR:CE2	2.26	0.66
1:D:347:ARG:HD2	1:D:392:GLY:H	1.60	0.66
1:D:464:ILE:O	1:D:467:ASN:HB2	1.96	0.66
1:A:8:LYS:HB2	1:D:30:ARG:HE	1.61	0.66
1:A:195:ASP:HB2	1:A:201:LEU:N	2.08	0.66
1:A:373:ASN:ND2	1:A:374:ASP:N	2.43	0.66
1:C:232:GLU:HG2	1:C:289:ASP:HA	1.77	0.66
1:A:32:ASN:CG	1:A:33:LYS:H	1.99	0.66
1:A:396:ARG:HE	1:A:432:ASP:HB2	1.57	0.66
1:A:401:VAL:HG13	1:A:405:THR:O	1.95	0.66
1:A:440:PRO:HD2	1:A:522:LEU:CD1	2.26	0.66
1:B:440:PRO:HD3	1:B:522:LEU:HD12	1.78	0.66
2:B:805:NAG:C6	2:B:806:NAG:C7	2.74	0.66
1:B:232:GLU:HG3	1:B:290:PHE:H	1.61	0.66
1:B:347:ARG:CG	1:B:392:GLY:H	2.08	0.66
1:B:464:ILE:O	1:B:467:ASN:HB2	1.95	0.66
1:C:347:ARG:CG	1:C:392:GLY:H	2.08	0.66
1:C:482:THR:OG1	1:C:500:GLN:CG	2.44	0.66
1:D:366:LYS:HG3	1:D:367:LEU:HG	1.77	0.66
1:A:222:ASP:O	1:A:222:ASP:CG	2.32	0.65
1:A:337:SER:CA	1:A:427:ILE:HG23	2.20	0.65
1:A:403:ASN:HB2	2:A:902:NAG:N2	2.10	0.65
1:B:265:GLU:HB3	1:B:268:PHE:CE2	2.31	0.65
2:C:805:NAG:C6	2:C:806:NAG:C7	2.74	0.65
1:D:482:THR:HG21	1:D:500:GLN:H	1.59	0.65
1:B:224:LYS:HE3	1:B:316:THR:O	1.95	0.65
1:B:373:ASN:ND2	1:B:374:ASP:N	2.43	0.65
1:B:524:VAL:HG23	2:B:904:NAG:H81	1.78	0.65
1:C:88:VAL:HG12	1:D:94:ILE:N	2.10	0.65
1:C:320:THR:HG21	2:C:807:NAG:H2	1.76	0.65
1:A:10:SER:HB2	1:D:30:ARG:CG	2.26	0.65
1:A:232:GLU:HG2	1:A:289:ASP:HA	1.77	0.65
1:A:446:THR:CG2	1:A:537:ILE:O	2.44	0.65
1:A:464:ILE:O	1:A:467:ASN:HB2	1.96	0.65
1:C:1:ASP:H1	1:D:28:LYS:CD	2.03	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:LYS:HG3	1:C:367:LEU:HG	1.77	0.65
1:D:32:ASN:ND2	1:D:83:GLU:N	2.45	0.65
1:D:155:PRO:HB2	2:D:801:NAG:C8	2.24	0.65
1:D:482:THR:OG1	1:D:500:GLN:CG	2.44	0.65
2:A:902:NAG:H3	2:A:902:NAG:O7	1.95	0.65
1:B:30:ARG:HH11	1:C:30:ARG:HG2	1.60	0.65
1:C:347:ARG:HD2	1:C:392:GLY:H	1.60	0.65
1:D:488:ASP:HB2	1:D:493:SER:OG	1.97	0.65
1:A:90:GLU:HG3	1:B:3:VAL:CG2	2.14	0.65
1:A:333:VAL:HB	1:A:334:PRO:CD	2.24	0.65
1:B:440:PRO:HD2	1:B:522:LEU:CD1	2.26	0.65
1:A:32:ASN:ND2	1:A:83:GLU:N	2.44	0.65
1:B:84:ASN:OD1	1:C:26:SER:HA	1.71	0.65
1:B:232:GLU:HG2	1:B:289:ASP:HA	1.77	0.65
1:B:406:TYR:CE1	2:B:808:NAG:H83	2.32	0.65
1:C:464:ILE:O	1:C:467:ASN:HB2	1.96	0.65
1:C:488:ASP:HB2	1:C:493:SER:OG	1.97	0.65
1:C:524:VAL:HG23	2:C:904:NAG:H81	1.78	0.65
2:C:809:NAG:C6	2:C:810:NAG:H62	2.26	0.65
2:A:805:NAG:C6	2:A:806:NAG:C7	2.74	0.65
2:B:809:NAG:C6	2:B:810:NAG:H62	2.26	0.65
2:B:904:NAG:O7	2:B:904:NAG:C3	2.45	0.65
1:C:79:HIS:CG	1:D:39:THR:HG22	2.32	0.65
1:C:346:SER:OG	1:C:349:GLU:HG3	1.97	0.65
1:D:224:LYS:HE3	1:D:316:THR:O	1.95	0.65
1:A:89:GLU:OE1	1:B:2:TRP:CB	2.26	0.65
1:A:212:THR:HG22	1:A:213:ASP:H	1.62	0.65
1:B:31:PHE:CZ	1:C:34:VAL:HG21	2.32	0.65
1:C:403:ASN:HB2	2:C:902:NAG:N2	2.10	0.65
1:C:446:THR:CG2	1:C:537:ILE:O	2.44	0.65
1:A:2:TRP:CE2	1:B:79:HIS:O	2.43	0.65
1:A:327:ASN:HA	1:A:360:ASP:OD2	1.97	0.65
1:A:364:ILE:O	1:A:364:ILE:HD12	1.97	0.65
1:B:346:SER:OG	1:B:349:GLU:HG3	1.97	0.65
1:B:488:ASP:HB2	1:B:493:SER:OG	1.97	0.65
1:B:517:GLN:C	1:B:519:ASN:N	2.47	0.65
1:C:88:VAL:HG23	1:D:39:THR:O	1.97	0.65
1:A:2:TRP:CE2	1:B:80:ALA:HB1	2.16	0.65
1:A:440:PRO:HD3	1:A:522:LEU:HD12	1.78	0.65
1:B:366:LYS:HG3	1:B:367:LEU:HG	1.77	0.65
1:B:482:THR:HG21	1:B:499:THR:CA	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:VAL:CG1	1:D:43:ALA:CA	2.70	0.65
1:C:440:PRO:HD3	1:C:522:LEU:HD12	1.78	0.65
2:D:809:NAG:C6	2:D:810:NAG:H62	2.26	0.65
1:B:212:THR:HG22	1:B:213:ASP:H	1.62	0.64
1:B:327:ASN:HA	1:B:360:ASP:OD2	1.97	0.64
1:B:364:ILE:O	1:B:364:ILE:HD12	1.97	0.64
1:C:32:ASN:ND2	1:C:83:GLU:N	2.45	0.64
1:A:366:LYS:HG3	1:A:367:LEU:HG	1.77	0.64
1:C:31:PHE:HD2	1:D:75:VAL:HG23	1.62	0.64
1:A:482:THR:HG21	1:A:499:THR:CA	2.27	0.64
1:B:341:VAL:HG21	1:B:345:LEU:HD12	1.79	0.64
2:C:904:NAG:O7	2:C:904:NAG:C3	2.45	0.64
1:A:469:TYR:CD2	1:A:470:PRO:CD	2.81	0.64
1:D:212:THR:HG22	1:D:213:ASP:H	1.62	0.64
1:D:232:GLU:HG3	1:D:290:PHE:H	1.61	0.64
1:D:265:GLU:HB3	1:D:268:PHE:CE2	2.31	0.64
1:D:482:THR:HG21	1:D:499:THR:CA	2.27	0.64
1:A:346:SER:OG	1:A:349:GLU:HG3	1.97	0.64
1:A:482:THR:HG22	1:A:499:THR:N	2.13	0.64
2:B:902:NAG:H3	2:B:902:NAG:O7	1.95	0.64
1:C:364:ILE:O	1:C:364:ILE:HD12	1.97	0.64
1:D:406:TYR:CE1	2:D:808:NAG:H83	2.32	0.64
1:D:524:VAL:HG23	2:D:904:NAG:H81	1.78	0.64
1:A:154:ASP:O	2:A:801:NAG:H82	1.98	0.64
1:A:347:ARG:HG3	1:A:392:GLY:H	1.62	0.64
1:A:406:TYR:CE1	2:A:808:NAG:H83	2.32	0.64
2:A:809:NAG:C6	2:A:810:NAG:H62	2.26	0.64
1:C:504:LYS:NZ	1:C:531:SER:OG	2.31	0.64
1:D:341:VAL:HG21	1:D:345:LEU:HD12	1.79	0.64
1:D:346:SER:OG	1:D:349:GLU:HG3	1.97	0.64
1:D:409:ILE:HG12	1:D:425:THR:HG23	1.80	0.64
1:C:90:GLU:OE2	1:D:37:SER:HA	1.98	0.64
1:C:409:ILE:HG12	1:C:425:THR:HG23	1.80	0.64
1:A:343:GLU:HB3	1:A:433:VAL:CG2	2.28	0.64
1:A:524:VAL:HG23	2:A:904:NAG:H81	1.78	0.64
1:C:81:VAL:HG21	1:D:45:ASN:HB2	0.64	0.64
1:C:347:ARG:HG3	1:C:392:GLY:H	1.62	0.64
1:A:364:ILE:O	1:A:364:ILE:CD1	2.46	0.64
1:A:419:VAL:HG13	2:A:809:NAG:O7	1.98	0.64
1:B:409:ILE:HG12	1:B:425:THR:HG23	1.80	0.64
1:C:341:VAL:HG21	1:C:345:LEU:HD12	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:347:ARG:HG3	1:D:392:GLY:H	1.62	0.64
1:D:375:PRO:HB3	1:D:400:TYR:CD2	2.33	0.64
1:A:474:SER:HB2	1:A:512:LEU:CG	2.15	0.64
1:C:327:ASN:HA	1:C:360:ASP:OD2	1.97	0.64
1:C:364:ILE:O	1:C:364:ILE:CD1	2.46	0.64
1:C:486:GLU:O	1:C:494:MET:CA	2.46	0.64
2:D:904:NAG:O7	2:D:904:NAG:C3	2.45	0.64
1:A:488:ASP:HB2	1:A:493:SER:OG	1.97	0.63
1:C:406:TYR:CE1	2:C:808:NAG:H83	2.32	0.63
1:D:327:ASN:HA	1:D:360:ASP:OD2	1.97	0.63
1:A:22:VAL:HG22	1:A:23:GLN:N	2.14	0.63
1:A:341:VAL:HG21	1:A:345:LEU:HD12	1.79	0.63
1:A:486:GLU:O	1:A:494:MET:CA	2.46	0.63
1:A:504:LYS:NZ	1:A:531:SER:OG	2.31	0.63
1:B:419:VAL:HG13	2:B:809:NAG:O7	1.98	0.63
1:C:343:GLU:HB3	1:C:433:VAL:CG2	2.28	0.63
1:D:221:PHE:CE1	1:D:315:SER:O	2.45	0.63
1:D:440:PRO:HD3	1:D:522:LEU:HD12	1.78	0.63
1:B:343:GLU:HB3	1:B:433:VAL:CG2	2.28	0.63
1:B:375:PRO:HB3	1:B:400:TYR:CD2	2.33	0.63
1:C:142:LEU:HB3	1:C:196:LEU:HA	1.81	0.63
1:A:10:SER:HA	1:D:30:ARG:HD2	1.81	0.63
1:B:87:PRO:HD2	1:D:90:GLU:O	1.97	0.63
1:B:142:LEU:HB3	1:B:196:LEU:HA	1.81	0.63
1:B:469:TYR:CD2	1:B:470:PRO:CD	2.81	0.63
1:C:84:ASN:HB3	1:D:73:LYS:O	1.98	0.63
1:C:154:ASP:O	1:C:155:PRO:C	2.36	0.63
1:C:265:GLU:HB3	1:C:268:PHE:CE2	2.31	0.63
1:C:375:PRO:HB3	1:C:400:TYR:CD2	2.33	0.63
1:C:419:VAL:HG13	2:C:809:NAG:O7	1.98	0.63
1:D:504:LYS:NZ	1:D:531:SER:OG	2.31	0.63
1:A:221:PHE:CE1	1:A:315:SER:O	2.45	0.63
1:B:371:ILE:HG22	1:B:372:GLY:N	2.14	0.63
1:C:371:ILE:HG22	1:C:372:GLY:N	2.14	0.63
1:A:154:ASP:CA	2:A:801:NAG:H82	2.29	0.63
1:A:232:GLU:HG3	1:A:290:PHE:H	1.61	0.63
1:A:486:GLU:O	1:A:495:LEU:N	2.31	0.63
1:B:127:VAL:HG22	1:B:128:MET:N	2.14	0.63
1:B:504:LYS:NZ	1:B:531:SER:OG	2.31	0.63
1:C:1:ASP:N	1:D:88:VAL:HB	2.11	0.63
1:C:446:THR:CG2	1:C:539:CYS:SG	2.86	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:LEU:HB3	1:D:196:LEU:HA	1.81	0.63
1:D:364:ILE:O	1:D:364:ILE:CD1	2.46	0.63
1:A:517:GLN:C	1:A:519:ASN:N	2.47	0.63
1:C:90:GLU:CD	1:D:36:TYR:HB3	2.18	0.63
1:C:469:TYR:CD2	1:C:470:PRO:CD	2.81	0.63
1:C:482:THR:HG21	1:C:499:THR:CA	2.27	0.63
1:D:154:ASP:O	1:D:155:PRO:C	2.36	0.63
1:D:469:TYR:CE1	1:D:470:PRO:HD2	2.34	0.63
1:D:486:GLU:O	1:D:494:MET:CA	2.46	0.63
1:B:347:ARG:HG3	1:B:392:GLY:H	1.62	0.63
1:C:403:ASN:CB	2:C:902:NAG:C7	2.76	0.63
1:D:22:VAL:HG22	1:D:23:GLN:N	2.14	0.63
1:D:364:ILE:O	1:D:364:ILE:HD12	1.97	0.63
1:D:419:VAL:HG13	2:D:809:NAG:O7	1.98	0.63
1:B:364:ILE:O	1:B:364:ILE:CD1	2.46	0.63
1:C:22:VAL:HG22	1:C:23:GLN:N	2.14	0.63
1:C:127:VAL:HG22	1:C:128:MET:N	2.14	0.63
1:C:154:ASP:CA	2:C:801:NAG:H82	2.29	0.63
1:C:212:THR:HG22	1:C:213:ASP:H	1.62	0.63
1:D:371:ILE:HG22	1:D:372:GLY:N	2.14	0.63
1:A:3:VAL:CG2	1:B:78:SER:N	2.60	0.62
1:A:142:LEU:HB3	1:A:196:LEU:HA	1.81	0.62
1:A:409:ILE:HG12	1:A:425:THR:HG23	1.80	0.62
1:B:22:VAL:HG22	1:B:23:GLN:N	2.14	0.62
1:B:154:ASP:O	1:B:155:PRO:C	2.36	0.62
1:C:81:VAL:CG1	1:D:43:ALA:CB	2.26	0.62
1:D:411:LEU:HD22	1:D:421:THR:HG23	1.81	0.62
1:A:127:VAL:HG22	1:A:128:MET:N	2.14	0.62
1:A:375:PRO:HB3	1:A:400:TYR:CD2	2.33	0.62
1:C:374:ASP:O	1:C:375:PRO:O	2.17	0.62
1:C:449:ASP:H	1:C:532:CYS:CB	2.12	0.62
1:B:154:ASP:O	2:B:801:NAG:H82	1.98	0.62
1:C:90:GLU:OE2	1:D:36:TYR:O	2.15	0.62
1:C:227:THR:CG2	2:C:807:NAG:C7	2.76	0.62
1:C:411:LEU:HD22	1:C:421:THR:HG23	1.81	0.62
1:D:343:GLU:HB3	1:D:433:VAL:CG2	2.27	0.62
1:D:508:SER:HB3	1:D:526:ASN:OD1	2.00	0.62
1:B:374:ASP:O	1:B:375:PRO:O	2.17	0.62
1:C:524:VAL:HG23	2:C:904:NAG:C8	2.29	0.62
1:D:127:VAL:HG22	1:D:128:MET:N	2.14	0.62
1:D:524:VAL:HG23	2:D:904:NAG:C8	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ARG:HD3	1:A:100:ASP:HA	1.82	0.62
1:A:89:GLU:O	1:B:1:ASP:O	2.18	0.62
1:B:154:ASP:CA	2:B:801:NAG:H82	2.29	0.62
1:C:87:PRO:O	1:D:38:ILE:HD11	2.00	0.62
1:C:524:VAL:CG2	2:C:904:NAG:C8	2.78	0.62
1:A:227:THR:CG2	2:A:807:NAG:C7	2.76	0.62
1:A:403:ASN:CB	2:A:902:NAG:C7	2.76	0.62
1:B:88:VAL:O	1:D:1:ASP:OD2	2.17	0.62
1:B:524:VAL:CG2	2:B:904:NAG:C8	2.78	0.62
1:C:154:ASP:O	2:C:801:NAG:H82	1.98	0.62
1:C:469:TYR:CE1	1:C:470:PRO:HD2	2.34	0.62
1:D:371:ILE:CG2	1:D:372:GLY:H	2.13	0.62
1:D:518:ASN:O	1:D:520:PRO:CD	2.46	0.62
2:D:805:NAG:C6	2:D:806:NAG:C7	2.74	0.62
1:A:1:ASP:H2	1:B:94:ILE:CD1	1.98	0.62
1:A:147:SER:OG	1:A:167:ARG:HG3	1.99	0.62
1:B:33:LYS:H	1:C:25:LYS:NZ	1.97	0.62
1:B:83:GLU:HG2	1:C:25:LYS:HD2	1.79	0.62
1:B:366:LYS:HG3	1:B:367:LEU:N	2.04	0.62
1:B:508:SER:HB3	1:B:526:ASN:OD1	1.99	0.62
1:C:508:SER:HB3	1:C:526:ASN:OD1	2.00	0.62
1:C:518:ASN:O	1:C:520:PRO:CD	2.46	0.62
1:A:212:THR:HG22	1:A:213:ASP:N	2.15	0.62
1:A:371:ILE:HG22	1:A:372:GLY:N	2.14	0.62
1:A:449:ASP:H	1:A:532:CYS:CB	2.12	0.62
1:A:524:VAL:HG23	2:A:904:NAG:C8	2.29	0.62
1:B:486:GLU:O	1:B:495:LEU:N	2.31	0.62
1:C:482:THR:HG22	1:C:499:THR:N	2.13	0.62
1:B:371:ILE:CG2	1:B:372:GLY:H	2.13	0.62
1:B:411:LEU:HD22	1:B:421:THR:HG23	1.81	0.62
1:B:518:ASN:O	1:B:520:PRO:CD	2.46	0.62
1:B:469:TYR:CE1	1:B:470:PRO:HD2	2.34	0.62
1:C:212:THR:HG22	1:C:213:ASP:N	2.15	0.62
1:D:154:ASP:CA	2:D:801:NAG:H82	2.29	0.62
1:A:91:PRO:CD	1:B:3:VAL:HG22	2.28	0.61
1:B:446:THR:CG2	1:B:539:CYS:SG	2.86	0.61
1:C:68:ARG:HD3	1:C:100:ASP:HA	1.82	0.61
1:C:486:GLU:O	1:C:495:LEU:N	2.31	0.61
1:D:68:ARG:HD3	1:D:100:ASP:HA	1.82	0.61
1:D:235:ILE:HG12	1:D:287:GLY:HA2	1.82	0.61
1:D:415:ASP:OD1	1:D:416:GLY:N	2.26	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:SER:HB3	1:A:526:ASN:OD1	2.00	0.61
1:A:524:VAL:CG2	2:A:904:NAG:C8	2.78	0.61
1:B:486:GLU:O	1:B:494:MET:CA	2.46	0.61
1:C:1:ASP:H1	1:D:28:LYS:CB	2.13	0.61
1:C:81:VAL:HG11	1:D:43:ALA:C	2.21	0.61
1:D:403:ASN:O	1:D:405:THR:N	2.33	0.61
1:A:374:ASP:O	1:A:375:PRO:O	2.17	0.61
1:C:181:ARG:NE	1:C:213:ASP:OD1	2.34	0.61
1:B:212:THR:HG22	1:B:213:ASP:N	2.15	0.61
1:C:27:ASN:HD21	1:D:93:GLU:H	1.45	0.61
1:C:85:GLY:HA3	1:D:47:PRO:HB2	1.82	0.61
1:D:374:ASP:O	1:D:375:PRO:O	2.17	0.61
1:A:2:TRP:CD1	1:B:80:ALA:HB2	2.35	0.61
1:A:154:ASP:O	1:A:155:PRO:C	2.36	0.61
1:A:411:LEU:HD22	1:A:421:THR:HG23	1.81	0.61
1:C:379:LEU:HD23	1:C:379:LEU:H	1.66	0.61
1:D:403:ASN:CB	2:D:902:NAG:C7	2.76	0.61
1:D:154:ASP:O	2:D:801:NAG:H82	1.98	0.61
1:D:524:VAL:CG2	2:D:904:NAG:C8	2.78	0.61
1:A:91:PRO:N	1:B:1:ASP:O	2.33	0.61
1:B:181:ARG:NE	1:B:213:ASP:OD1	2.34	0.61
1:B:403:ASN:O	1:B:405:THR:N	2.33	0.61
1:C:403:ASN:O	1:C:405:THR:N	2.33	0.61
1:D:469:TYR:CD2	1:D:470:PRO:CD	2.80	0.61
1:D:475:LEU:O	1:D:479:SER:HB3	2.01	0.61
1:A:9:VAL:N	1:D:30:ARG:HD3	2.15	0.61
1:A:403:ASN:O	1:A:405:THR:N	2.33	0.61
1:A:415:ASP:OD1	1:A:416:GLY:N	2.27	0.61
1:B:524:VAL:HG23	2:B:904:NAG:C8	2.29	0.61
1:C:31:PHE:O	1:D:73:LYS:CD	2.47	0.61
1:D:212:THR:HG22	1:D:213:ASP:N	2.15	0.61
1:A:181:ARG:NE	1:A:213:ASP:OD1	2.34	0.61
1:A:379:LEU:HD23	1:A:379:LEU:H	1.66	0.61
1:A:469:TYR:CE1	1:A:470:PRO:HD2	2.34	0.61
1:B:475:LEU:O	1:B:479:SER:HB3	2.01	0.61
1:C:368:SER:HG	1:C:370:PHE:HE1	1.48	0.61
1:D:181:ARG:NE	1:D:213:ASP:OD1	2.34	0.61
1:D:379:LEU:HD23	1:D:379:LEU:H	1.66	0.61
1:A:475:LEU:O	1:A:479:SER:HB3	2.01	0.61
1:D:449:ASP:H	1:D:532:CYS:CB	2.12	0.61
1:A:232:GLU:CG	1:A:290:PHE:N	2.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:ARG:HD3	1:B:100:ASP:HA	1.82	0.60
1:C:371:ILE:CG2	1:C:372:GLY:H	2.13	0.60
1:C:88:VAL:CA	1:D:38:ILE:HD11	2.31	0.60
1:C:189:LEU:N	1:C:189:LEU:HD23	2.16	0.60
1:D:189:LEU:N	1:D:189:LEU:HD23	2.16	0.60
1:A:9:VAL:C	1:D:30:ARG:HD2	2.16	0.60
1:B:379:LEU:HD23	1:B:379:LEU:H	1.66	0.60
1:B:450:GLN:HB2	1:B:533:GLU:CA	2.26	0.60
1:C:232:GLU:CG	1:C:290:PHE:N	2.64	0.60
1:C:81:VAL:H	1:D:45:ASN:HD22	1.48	0.60
1:C:90:GLU:CG	1:D:36:TYR:HB3	2.32	0.60
1:D:523:THR:CG2	1:D:524:VAL:H	1.94	0.60
1:B:189:LEU:N	1:B:189:LEU:HD23	2.17	0.60
1:D:403:ASN:CB	2:D:902:NAG:H83	2.21	0.60
1:C:336:VAL:HB	1:C:426:LEU:HD23	1.84	0.60
1:C:514:SER:HA	1:C:517:GLN:O	2.02	0.60
1:A:189:LEU:HD23	1:A:189:LEU:N	2.16	0.60
1:A:265:GLU:HB3	1:A:268:PHE:CE2	2.31	0.60
1:A:371:ILE:CG2	1:A:372:GLY:H	2.13	0.60
1:B:336:VAL:HB	1:B:426:LEU:HD23	1.84	0.60
1:D:227:THR:CG2	2:D:807:NAG:C7	2.76	0.60
1:A:2:TRP:CZ2	1:B:36:TYR:CD2	2.75	0.60
1:C:146:LEU:HA	1:C:194:THR:O	2.02	0.60
1:C:475:LEU:O	1:C:479:SER:HB3	2.01	0.60
1:D:446:THR:CG2	1:D:539:CYS:SG	2.86	0.60
1:B:227:THR:CG2	2:B:807:NAG:C7	2.76	0.60
1:B:396:ARG:NH2	1:B:464:ILE:HG21	2.17	0.60
1:C:32:ASN:CB	1:D:75:VAL:HG23	2.31	0.60
1:C:508:SER:HA	1:C:526:ASN:HA	1.84	0.60
1:C:116:SER:HA	1:C:210:GLN:O	2.02	0.60
1:B:88:VAL:O	1:D:1:ASP:CG	2.40	0.59
1:C:450:GLN:HB2	1:C:533:GLU:CA	2.26	0.59
1:B:508:SER:HA	1:B:526:ASN:HA	1.84	0.59
1:C:81:VAL:HG13	1:D:44:ASP:H	1.63	0.59
1:D:367:LEU:CB	1:D:413:THR:O	2.51	0.59
1:B:514:SER:HA	1:B:517:GLN:O	2.02	0.59
1:C:1:ASP:C	1:D:28:LYS:HZ3	1.97	0.59
1:D:116:SER:HA	1:D:210:GLN:O	2.02	0.59
1:D:232:GLU:CG	1:D:290:PHE:N	2.64	0.59
1:D:514:SER:HA	1:D:517:GLN:O	2.02	0.59
1:A:446:THR:CG2	1:A:539:CYS:SG	2.86	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:SER:HA	1:B:210:GLN:O	2.02	0.59
1:D:49:GLY:O	1:D:63:THR:HG21	2.02	0.59
1:D:146:LEU:HA	1:D:194:THR:O	2.02	0.59
1:D:239:VAL:HG13	1:D:240:GLN:H	1.67	0.59
1:B:239:VAL:HG13	1:B:240:GLN:H	1.67	0.59
1:B:268:PHE:HA	1:B:285:ALA:HB3	1.84	0.59
1:C:31:PHE:CB	1:D:95:THR:HG21	2.10	0.59
1:D:396:ARG:NH2	1:D:464:ILE:HG21	2.17	0.59
1:A:239:VAL:HG13	1:A:240:GLN:H	1.67	0.59
1:B:449:ASP:H	1:B:532:CYS:CB	2.12	0.59
1:C:443:ARG:HG3	1:C:443:ARG:HH11	1.67	0.59
1:D:336:VAL:HB	1:D:426:LEU:HD23	1.84	0.59
2:A:904:NAG:O7	2:A:904:NAG:C3	2.45	0.59
1:B:49:GLY:O	1:B:63:THR:HG21	2.02	0.59
1:B:286:LYS:O	1:B:287:GLY:O	2.21	0.59
1:C:235:ILE:HG12	1:C:287:GLY:HA2	1.82	0.59
1:C:239:VAL:HG13	1:C:240:GLN:H	1.67	0.59
1:A:49:GLY:O	1:A:63:THR:HG21	2.02	0.59
1:A:116:SER:HA	1:A:210:GLN:O	2.02	0.59
1:A:450:GLN:HB2	1:A:533:GLU:CA	2.26	0.59
1:A:514:SER:HA	1:A:517:GLN:O	2.02	0.59
1:A:518:ASN:O	1:A:520:PRO:CD	2.46	0.59
1:B:155:PRO:C	1:B:157:GLU:N	2.56	0.59
1:C:268:PHE:HA	1:C:285:ALA:HB3	1.84	0.59
1:C:286:LYS:O	1:C:287:GLY:O	2.21	0.59
1:A:90:GLU:CB	1:B:3:VAL:HG23	2.33	0.59
1:A:367:LEU:CB	1:A:413:THR:O	2.51	0.59
1:A:396:ARG:NH2	1:A:464:ILE:HG21	2.17	0.59
1:B:38:ILE:HG22	1:B:53:ILE:HG22	1.85	0.59
1:B:146:LEU:HA	1:B:194:THR:O	2.02	0.59
1:B:367:LEU:CB	1:B:413:THR:O	2.51	0.59
1:B:482:THR:HG22	1:B:499:THR:N	2.13	0.59
1:C:28:LYS:HB3	1:D:76:LEU:O	2.03	0.59
1:C:335:ALA:HB1	3:C:811:NDG:C6	2.33	0.59
1:D:363:GLN:O	1:D:364:ILE:HG22	2.03	0.59
1:D:486:GLU:O	1:D:495:LEU:N	2.31	0.59
1:D:508:SER:HA	1:D:526:ASN:HA	1.84	0.59
1:A:38:ILE:HG22	1:A:53:ILE:HG22	1.85	0.59
1:A:195:ASP:CB	1:A:200:GLY:HA3	2.33	0.59
1:C:49:GLY:O	1:C:63:THR:HG21	2.02	0.59
1:D:289:ASP:O	1:D:290:PHE:CB	2.25	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ILE:CG2	1:B:91:PRO:O	2.33	0.58
1:B:88:VAL:O	1:D:1:ASP:HB3	2.01	0.58
1:B:473:VAL:HA	1:B:513:LEU:HD23	1.85	0.58
1:C:443:ARG:HA	1:C:525:VAL:HG13	1.85	0.58
1:A:146:LEU:HA	1:A:194:THR:O	2.02	0.58
1:A:299:GLN:C	1:A:300:ILE:HD12	2.24	0.58
1:C:367:LEU:CB	1:C:413:THR:O	2.51	0.58
1:D:38:ILE:HG22	1:D:53:ILE:HG22	1.85	0.58
1:A:286:LYS:O	1:A:287:GLY:O	2.21	0.58
1:B:232:GLU:HG2	1:B:289:ASP:CA	2.33	0.58
1:B:335:ALA:HB1	3:B:811:NDG:C6	2.33	0.58
1:B:403:ASN:CB	2:B:902:NAG:C7	2.76	0.58
1:C:86:SER:N	1:D:74:TYR:HD2	1.94	0.58
1:C:88:VAL:CG2	1:D:76:LEU:HD23	2.25	0.58
1:C:155:PRO:C	1:C:157:GLU:N	2.56	0.58
1:D:443:ARG:HA	1:D:525:VAL:HG13	1.85	0.58
1:A:91:PRO:HA	1:B:1:ASP:C	2.23	0.58
1:A:443:ARG:HH11	1:A:443:ARG:HG3	1.67	0.58
1:B:537:ILE:HG12	1:B:538:LYS:N	2.19	0.58
1:C:309:SER:O	1:C:310:VAL:HG23	2.03	0.58
1:D:232:GLU:HG2	1:D:289:ASP:CA	2.33	0.58
1:D:286:LYS:O	1:D:287:GLY:O	2.21	0.58
1:D:366:LYS:HG3	1:D:367:LEU:N	2.04	0.58
1:B:522:LEU:CD2	1:B:523:THR:HB	2.26	0.58
1:C:28:LYS:HD3	1:D:76:LEU:O	2.02	0.58
1:C:406:TYR:HB3	1:C:428:LEU:CD2	2.33	0.58
1:A:336:VAL:HB	1:A:426:LEU:HD23	1.84	0.58
1:C:31:PHE:HA	1:D:73:LYS:HZ1	1.69	0.58
1:C:226:TYR:CE2	1:C:242:LEU:HD23	2.39	0.58
1:C:447:MET:HB2	1:C:529:VAL:HG22	1.84	0.58
1:D:221:PHE:HA	1:D:244:VAL:HG12	1.85	0.58
1:D:226:TYR:CE2	1:D:242:LEU:HD23	2.39	0.58
1:A:1:ASP:CA	1:B:24:ILE:HD13	2.33	0.58
1:B:42:GLY:HA2	1:B:47:PRO:O	2.04	0.58
1:B:232:GLU:CG	1:B:290:PHE:N	2.64	0.58
1:B:235:ILE:HG12	1:B:287:GLY:HA2	1.82	0.58
1:D:406:TYR:HB3	1:D:428:LEU:CD2	2.33	0.58
1:D:443:ARG:HH11	1:D:443:ARG:HG3	1.67	0.58
1:D:522:LEU:CD2	1:D:523:THR:HB	2.26	0.58
1:D:537:ILE:HG12	1:D:538:LYS:N	2.19	0.58
1:A:363:GLN:O	1:A:364:ILE:HG22	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:VAL:HA	1:A:513:LEU:HD23	1.85	0.58
1:C:42:GLY:HA2	1:C:47:PRO:O	2.04	0.58
1:C:232:GLU:HG2	1:C:289:ASP:CA	2.33	0.58
1:C:396:ARG:NH2	1:C:464:ILE:HG21	2.17	0.58
1:D:473:VAL:HA	1:D:513:LEU:HD23	1.85	0.58
1:A:232:GLU:HG2	1:A:289:ASP:CA	2.33	0.58
1:A:537:ILE:HG12	1:A:538:LYS:N	2.19	0.58
1:B:406:TYR:HB3	1:B:428:LEU:CD2	2.33	0.58
1:B:443:ARG:HH11	1:B:443:ARG:HG3	1.67	0.58
1:C:27:ASN:ND2	1:C:27:ASN:C	2.46	0.58
1:C:79:HIS:ND1	1:D:39:THR:HG22	2.19	0.58
1:D:296:TYR:HB2	1:D:321:VAL:HB	1.86	0.58
1:A:89:GLU:CD	1:B:2:TRP:CD1	2.51	0.58
1:A:154:ASP:CB	1:A:155:PRO:CD	2.82	0.58
1:A:221:PHE:HA	1:A:244:VAL:HG12	1.85	0.58
1:A:309:SER:O	1:A:310:VAL:HG23	2.03	0.58
1:A:406:TYR:HB3	1:A:428:LEU:CD2	2.33	0.58
1:A:508:SER:HA	1:A:526:ASN:HA	1.84	0.58
1:B:415:ASP:OD1	1:B:416:GLY:N	2.27	0.58
1:B:443:ARG:HA	1:B:525:VAL:HG13	1.85	0.58
1:C:38:ILE:HG22	1:C:53:ILE:HG22	1.85	0.58
1:C:299:GLN:C	1:C:300:ILE:HD12	2.24	0.58
1:C:332:PHE:CD2	1:C:424:GLY:HA3	2.39	0.58
1:D:42:GLY:HA2	1:D:47:PRO:O	2.04	0.58
1:A:42:GLY:HA2	1:A:47:PRO:O	2.04	0.57
1:A:406:TYR:HB3	1:A:428:LEU:HD21	1.86	0.57
1:B:87:PRO:CG	1:C:2:TRP:HB2	2.29	0.57
1:B:309:SER:O	1:B:310:VAL:HG23	2.03	0.57
1:C:90:GLU:CG	1:D:79:HIS:O	2.51	0.57
1:A:268:PHE:HA	1:A:285:ALA:HB3	1.84	0.57
1:A:447:MET:HB2	1:A:529:VAL:HG22	1.84	0.57
1:B:299:GLN:C	1:B:300:ILE:HD12	2.24	0.57
1:B:332:PHE:CD2	1:B:424:GLY:HA3	2.39	0.57
1:B:406:TYR:HB3	1:B:428:LEU:HD21	1.87	0.57
1:C:84:ASN:O	1:D:74:TYR:CE2	2.57	0.57
1:C:88:VAL:CG1	1:D:94:ILE:O	2.52	0.57
1:C:240:GLN:HG3	1:C:241:ARG:N	2.19	0.57
1:D:240:GLN:HG3	1:D:241:ARG:N	2.19	0.57
1:D:268:PHE:HA	1:D:285:ALA:HB3	1.84	0.57
1:A:332:PHE:CD2	1:A:424:GLY:HA3	2.39	0.57
1:B:154:ASP:CB	1:B:155:PRO:CD	2.82	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:PHE:HA	1:B:244:VAL:HG12	1.85	0.57
1:B:226:TYR:CE2	1:B:242:LEU:HD23	2.39	0.57
1:B:523:THR:CG2	1:B:524:VAL:H	1.94	0.57
1:C:296:TYR:HB2	1:C:321:VAL:HB	1.86	0.57
1:C:473:VAL:HA	1:C:513:LEU:HD23	1.85	0.57
1:D:299:GLN:C	1:D:300:ILE:HD12	2.24	0.57
1:D:447:MET:HB2	1:D:529:VAL:HG22	1.84	0.57
1:B:155:PRO:N	2:B:801:NAG:H82	2.20	0.57
1:B:447:MET:HB2	1:B:529:VAL:HG22	1.84	0.57
1:C:87:PRO:C	1:D:38:ILE:HD11	2.24	0.57
1:C:154:ASP:CB	2:C:801:NAG:HN2	2.16	0.57
1:D:154:ASP:CB	1:D:155:PRO:CD	2.82	0.57
1:D:330:PRO:HD3	1:D:414:ASP:HB2	1.86	0.57
1:A:336:VAL:HG12	1:A:338:ARG:HB2	1.87	0.57
1:B:28:LYS:NZ	1:D:2:TRP:O	2.33	0.57
1:C:79:HIS:HB3	1:D:44:ASP:CG	2.25	0.57
1:C:83:GLU:CB	1:D:41:GLN:HE22	2.16	0.57
1:A:2:TRP:CZ2	1:B:79:HIS:O	2.38	0.57
1:B:68:ARG:HG3	1:B:69:GLU:N	2.19	0.57
1:B:330:PRO:HD3	1:B:414:ASP:HB2	1.86	0.57
1:C:87:PRO:CD	1:D:43:ALA:N	2.65	0.57
1:C:363:GLN:O	1:C:364:ILE:HG22	2.03	0.57
1:D:32:ASN:HD22	1:D:83:GLU:H	1.51	0.57
1:D:195:ASP:CB	1:D:200:GLY:HA3	2.33	0.57
1:D:482:THR:HG22	1:D:499:THR:N	2.13	0.57
1:A:10:SER:CA	1:D:30:ARG:HD2	2.35	0.57
1:A:235:ILE:HG12	1:A:287:GLY:HA2	1.82	0.57
1:B:195:ASP:CB	1:B:200:GLY:HA3	2.33	0.57
1:B:363:GLN:O	1:B:364:ILE:HG22	2.03	0.57
1:B:393:ASN:C	1:B:394:LEU:HD12	2.25	0.57
1:D:332:PHE:CD2	1:D:424:GLY:HA3	2.39	0.57
1:D:406:TYR:HB3	1:D:428:LEU:HD21	1.87	0.57
1:A:330:PRO:HD3	1:A:414:ASP:HB2	1.86	0.57
1:C:195:ASP:CB	1:C:200:GLY:HA3	2.33	0.57
1:C:505:GLY:HA2	1:C:529:VAL:H	1.69	0.57
1:D:154:ASP:CB	2:D:801:NAG:HN2	2.16	0.57
1:A:108:PHE:CE1	1:A:203:VAL:HG23	2.40	0.57
1:A:296:TYR:HB2	1:A:321:VAL:HB	1.86	0.57
1:A:335:ALA:HB1	3:A:811:NDG:C6	2.33	0.57
1:A:369:TYR:HD1	1:A:383:LYS:O	1.88	0.57
1:B:189:LEU:HD21	1:B:209:ILE:HD12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:ASP:N	1:B:243:SER:O	2.38	0.57
1:B:240:GLN:HG3	1:B:241:ARG:N	2.19	0.57
1:B:259:TYR:O	1:B:260:LYS:HB3	2.05	0.57
1:B:336:VAL:HG12	1:B:338:ARG:HB2	1.87	0.57
1:C:89:GLU:N	1:D:38:ILE:CG1	2.58	0.57
1:D:369:TYR:HD1	1:D:383:LYS:O	1.88	0.57
1:C:26:SER:CB	1:D:77:SER:HB2	2.34	0.57
1:C:154:ASP:CB	1:C:155:PRO:CD	2.82	0.57
1:C:221:PHE:HA	1:C:244:VAL:HG12	1.85	0.57
1:C:537:ILE:HG12	1:C:538:LYS:N	2.19	0.57
1:A:240:GLN:HG3	1:A:241:ARG:N	2.19	0.56
1:B:118:ARG:HA	1:B:212:THR:HB	1.87	0.56
1:D:335:ALA:HB1	3:D:811:NDG:C6	2.33	0.56
1:A:118:ARG:HA	1:A:212:THR:HB	1.87	0.56
1:A:393:ASN:C	1:A:394:LEU:HD12	2.25	0.56
1:A:443:ARG:HA	1:A:525:VAL:HG13	1.85	0.56
1:B:85:GLY:O	1:D:90:GLU:HA	2.05	0.56
1:B:378:TRP:O	1:B:391:ASN:HB2	2.06	0.56
1:D:68:ARG:HG3	1:D:69:GLU:N	2.19	0.56
1:A:68:ARG:HG3	1:A:69:GLU:N	2.19	0.56
1:A:226:TYR:CE2	1:A:242:LEU:HD23	2.39	0.56
1:A:505:GLY:HA2	1:A:529:VAL:H	1.69	0.56
1:B:369:TYR:HD1	1:B:383:LYS:O	1.88	0.56
1:C:27:ASN:HD21	1:D:93:GLU:HB3	1.60	0.56
1:C:82:SER:OG	1:D:74:TYR:HB3	2.05	0.56
1:C:155:PRO:N	2:C:801:NAG:H82	2.20	0.56
1:C:369:TYR:HD1	1:C:383:LYS:O	1.88	0.56
1:D:189:LEU:HD21	1:D:209:ILE:HD12	1.87	0.56
1:D:309:SER:O	1:D:310:VAL:HG23	2.03	0.56
1:B:154:ASP:CB	2:B:801:NAG:HN2	2.16	0.56
1:B:296:TYR:HB2	1:B:321:VAL:HB	1.86	0.56
1:C:32:ASN:CG	1:C:33:LYS:N	2.59	0.56
1:C:68:ARG:HG3	1:C:69:GLU:N	2.19	0.56
1:C:85:GLY:HA2	1:D:41:GLN:C	2.13	0.56
1:C:335:ALA:HB1	3:C:811:NDG:H6	1.66	0.56
1:C:336:VAL:HG12	1:C:338:ARG:HB2	1.87	0.56
1:C:393:ASN:C	1:C:394:LEU:HD12	2.25	0.56
1:D:378:TRP:O	1:D:391:ASN:HB2	2.06	0.56
1:D:517:GLN:C	1:D:519:ASN:N	2.47	0.56
1:A:5:PRO:N	1:B:91:PRO:HB2	2.21	0.56
1:A:259:TYR:O	1:A:260:LYS:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:GLU:CG	1:C:25:LYS:HD3	2.25	0.56
1:B:394:LEU:N	1:B:394:LEU:CD1	2.69	0.56
1:C:432:ASP:CG	1:C:464:ILE:CG2	2.74	0.56
1:D:222:ASP:N	1:D:243:SER:O	2.38	0.56
1:A:155:PRO:C	1:A:157:GLU:N	2.56	0.56
1:A:189:LEU:HD21	1:A:209:ILE:HD12	1.87	0.56
1:A:222:ASP:N	1:A:243:SER:O	2.38	0.56
1:B:30:ARG:NH1	1:C:30:ARG:HB3	2.21	0.56
1:C:108:PHE:CE1	1:C:203:VAL:HG23	2.40	0.56
1:C:378:TRP:O	1:C:391:ASN:HB2	2.06	0.56
1:C:415:ASP:OD1	1:C:416:GLY:N	2.26	0.56
1:D:155:PRO:N	2:D:801:NAG:H82	2.20	0.56
1:A:403:ASN:CB	2:A:902:NAG:H83	2.21	0.56
1:B:108:PHE:CE1	1:B:203:VAL:HG23	2.40	0.56
1:C:189:LEU:HD21	1:C:209:ILE:HD12	1.87	0.56
1:D:32:ASN:CG	1:D:33:LYS:N	2.59	0.56
1:A:4:ILE:CA	1:B:91:PRO:CD	2.69	0.56
1:C:162:LEU:O	1:C:174:LEU:HD12	2.06	0.56
1:C:365:GLN:O	1:C:365:GLN:CG	2.54	0.56
1:D:108:PHE:CE1	1:D:203:VAL:HG23	2.40	0.56
1:D:162:LEU:O	1:D:174:LEU:HD12	2.06	0.56
1:D:393:ASN:C	1:D:394:LEU:HD12	2.25	0.56
1:D:450:GLN:HB2	1:D:533:GLU:CA	2.26	0.56
1:B:505:GLY:HA2	1:B:529:VAL:H	1.69	0.56
1:C:118:ARG:HA	1:C:212:THR:HB	1.87	0.56
1:C:406:TYR:HB3	1:C:428:LEU:HD21	1.86	0.56
1:D:432:ASP:CG	1:D:464:ILE:CG2	2.74	0.56
1:C:31:PHE:O	1:D:73:LYS:CE	2.54	0.56
1:C:88:VAL:HG13	1:D:94:ILE:O	2.05	0.56
1:C:222:ASP:N	1:C:243:SER:O	2.38	0.56
1:C:482:THR:HG21	1:C:499:THR:C	2.27	0.56
1:D:336:VAL:HG12	1:D:338:ARG:HB2	1.87	0.56
1:A:2:TRP:CH2	1:B:35:TYR:O	2.58	0.55
1:A:394:LEU:N	1:A:394:LEU:CD1	2.69	0.55
1:D:339:VAL:HG21	1:D:351:ILE:CG2	2.36	0.55
1:B:162:LEU:O	1:B:174:LEU:HD12	2.06	0.55
1:C:35:TYR:HB3	1:D:45:ASN:ND2	2.22	0.55
1:C:330:PRO:HD3	1:C:414:ASP:HB2	1.86	0.55
1:D:259:TYR:O	1:D:260:LYS:HB3	2.05	0.55
1:B:318:THR:CG2	2:B:806:NAG:H5	2.34	0.55
1:C:1:ASP:N	1:D:89:GLU:OE2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:GLU:C	1:D:38:ILE:HG13	2.26	0.55
1:C:352:ILE:HG13	1:C:388:VAL:CB	2.33	0.55
1:C:403:ASN:CB	2:C:902:NAG:H83	2.21	0.55
1:D:155:PRO:HG2	2:D:801:NAG:O7	2.07	0.55
1:D:505:GLY:HA2	1:D:529:VAL:H	1.70	0.55
1:A:333:VAL:CG2	1:A:334:PRO:HD3	2.36	0.55
1:A:482:THR:HG21	1:A:499:THR:C	2.27	0.55
1:B:339:VAL:HG21	1:B:351:ILE:CG2	2.37	0.55
1:C:79:HIS:HB3	1:D:39:THR:CB	2.36	0.55
1:C:259:TYR:O	1:C:260:LYS:HB3	2.05	0.55
1:C:339:VAL:HG21	1:C:351:ILE:CG2	2.37	0.55
1:D:118:ARG:HA	1:D:212:THR:HB	1.87	0.55
1:D:268:PHE:CD2	1:D:268:PHE:N	2.75	0.55
1:D:394:LEU:N	1:D:394:LEU:CD1	2.69	0.55
1:A:365:GLN:O	1:A:365:GLN:CG	2.54	0.55
1:B:30:ARG:NH1	1:C:30:ARG:CG	2.69	0.55
1:C:278:ASN:HD22	1:C:278:ASN:N	2.05	0.55
1:D:28:LYS:HB3	1:D:88:VAL:HG11	1.89	0.55
1:A:154:ASP:CG	1:A:155:PRO:CD	2.75	0.55
1:A:162:LEU:O	1:A:174:LEU:HD12	2.06	0.55
1:A:318:THR:CG2	2:A:806:NAG:H5	2.34	0.55
1:C:79:HIS:N	1:D:39:THR:HG21	2.10	0.55
1:C:459:ILE:HG21	1:C:471:TYR:CE2	2.42	0.55
1:D:155:PRO:C	1:D:157:GLU:N	2.56	0.55
1:D:419:VAL:CG1	1:D:420:GLY:N	2.70	0.55
1:A:32:ASN:CG	1:A:33:LYS:N	2.59	0.55
1:B:330:PRO:HB3	1:B:358:ASP:HB2	1.89	0.55
1:C:333:VAL:CG2	1:C:334:PRO:HD3	2.36	0.55
1:C:394:LEU:N	1:C:394:LEU:CD1	2.69	0.55
1:C:439:VAL:HG13	1:C:522:LEU:HD11	1.88	0.55
1:A:419:VAL:CG1	1:A:420:GLY:N	2.70	0.55
1:B:28:LYS:HE3	1:D:4:ILE:N	2.13	0.55
1:B:226:TYR:O	1:B:227:THR:CG2	2.55	0.55
1:B:419:VAL:CG1	1:B:420:GLY:N	2.70	0.55
1:B:482:THR:HG21	1:B:499:THR:C	2.27	0.55
1:C:81:VAL:HG21	1:D:45:ASN:N	2.20	0.55
1:C:86:SER:O	1:D:41:GLN:O	2.25	0.55
1:D:154:ASP:CG	1:D:155:PRO:CD	2.75	0.55
1:A:155:PRO:N	2:A:801:NAG:H82	2.20	0.55
1:A:226:TYR:O	1:A:227:THR:CG2	2.55	0.55
1:B:83:GLU:CB	1:C:25:LYS:CG	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:VAL:CG2	1:B:334:PRO:HD3	2.36	0.55
1:B:432:ASP:CG	1:B:464:ILE:CG2	2.74	0.55
1:C:82:SER:OG	1:D:74:TYR:CD2	2.60	0.55
1:C:83:GLU:CA	1:D:41:GLN:HE22	2.06	0.55
1:C:155:PRO:HG2	2:C:801:NAG:O7	2.07	0.55
1:D:278:ASN:HD22	1:D:278:ASN:N	2.05	0.55
1:D:459:ILE:HG21	1:D:471:TYR:CE2	2.42	0.55
1:D:466:PRO:O	1:D:468:THR:N	2.40	0.55
1:A:10:SER:N	1:D:30:ARG:HD2	2.20	0.55
1:A:363:GLN:C	1:A:364:ILE:CG2	2.76	0.55
1:A:378:TRP:O	1:A:391:ASN:HB2	2.06	0.55
1:A:438:PRO:HB2	1:A:513:LEU:HD12	1.89	0.55
1:A:459:ILE:HG21	1:A:471:TYR:CE2	2.42	0.55
1:B:154:ASP:CG	1:B:155:PRO:CD	2.75	0.55
1:B:155:PRO:HG2	2:B:801:NAG:O7	2.07	0.55
1:C:31:PHE:CB	1:D:75:VAL:CG2	2.80	0.55
1:D:333:VAL:CG2	1:D:334:PRO:HD3	2.36	0.55
1:D:482:THR:HG21	1:D:499:THR:C	2.27	0.55
1:A:75:VAL:O	1:A:76:LEU:HD23	2.07	0.54
1:B:28:LYS:HB3	1:B:88:VAL:HG11	1.89	0.54
1:B:32:ASN:C	1:C:25:LYS:CE	2.68	0.54
1:B:466:PRO:O	1:B:468:THR:N	2.40	0.54
1:C:31:PHE:CD2	1:D:74:TYR:O	2.60	0.54
1:D:363:GLN:C	1:D:364:ILE:CG2	2.75	0.54
1:D:439:VAL:HG13	1:D:522:LEU:HD11	1.88	0.54
1:A:339:VAL:HG21	1:A:351:ILE:CG2	2.37	0.54
1:C:226:TYR:HB2	1:C:319:VAL:HG22	1.89	0.54
1:D:272:THR:CG2	1:D:273:THR:H	2.19	0.54
1:A:90:GLU:HB2	1:B:3:VAL:O	2.06	0.54
1:A:330:PRO:HB3	1:A:358:ASP:HB2	1.89	0.54
1:A:432:ASP:CG	1:A:464:ILE:CG2	2.74	0.54
1:A:466:PRO:O	1:A:468:THR:N	2.40	0.54
1:A:490:LYS:O	1:A:490:LYS:HG2	2.08	0.54
1:B:169:THR:OG1	1:B:171:VAL:HG23	2.07	0.54
1:C:32:ASN:HD22	1:C:83:GLU:H	1.51	0.54
1:C:169:THR:OG1	1:C:171:VAL:HG23	2.08	0.54
1:D:226:TYR:O	1:D:227:THR:CG2	2.55	0.54
1:D:330:PRO:HB3	1:D:358:ASP:HB2	1.89	0.54
1:B:439:VAL:HG13	1:B:522:LEU:HD11	1.88	0.54
1:B:450:GLN:CB	1:B:532:CYS:O	2.56	0.54
1:C:154:ASP:CG	1:C:155:PRO:CD	2.75	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:LEU:C	1:C:367:LEU:HD12	2.28	0.54
1:C:419:VAL:CG1	1:C:420:GLY:N	2.70	0.54
1:B:226:TYR:HB2	1:B:319:VAL:HG22	1.89	0.54
1:C:28:LYS:HB3	1:C:88:VAL:HG11	1.89	0.54
1:D:117:VAL:O	1:D:211:ILE:HA	2.07	0.54
1:A:10:SER:CB	1:D:30:ARG:HG3	2.36	0.54
1:A:268:PHE:CD2	1:A:268:PHE:N	2.75	0.54
1:A:332:PHE:HD2	1:A:424:GLY:HA3	1.73	0.54
1:A:439:VAL:HG13	1:A:522:LEU:HD11	1.88	0.54
1:C:87:PRO:CG	1:D:43:ALA:HB2	1.86	0.54
1:C:88:VAL:CG2	1:D:75:VAL:O	2.43	0.54
1:C:268:PHE:CD2	1:C:268:PHE:N	2.75	0.54
1:C:466:PRO:O	1:C:468:THR:N	2.40	0.54
1:D:367:LEU:C	1:D:367:LEU:HD12	2.28	0.54
1:D:490:LYS:O	1:D:490:LYS:HG2	2.08	0.54
1:B:217:ASN:N	1:B:217:ASN:ND2	2.56	0.54
1:B:367:LEU:C	1:B:367:LEU:HD12	2.28	0.54
1:C:1:ASP:N	1:D:28:LYS:CB	2.71	0.54
1:D:169:THR:OG1	1:D:171:VAL:HG23	2.07	0.54
1:A:28:LYS:HB3	1:A:88:VAL:HG11	1.89	0.54
1:A:155:PRO:HG2	2:A:801:NAG:O7	2.07	0.54
1:B:459:ILE:HG21	1:B:471:TYR:CE2	2.42	0.54
1:C:26:SER:HG	1:D:77:SER:CB	2.19	0.54
1:C:93:GLU:HB3	1:D:81:VAL:CG1	2.37	0.54
1:C:117:VAL:O	1:C:211:ILE:HA	2.07	0.54
1:C:226:TYR:O	1:C:227:THR:CG2	2.55	0.54
1:C:330:PRO:HB3	1:C:358:ASP:HB2	1.89	0.54
1:D:217:ASN:N	1:D:217:ASN:ND2	2.56	0.54
1:D:332:PHE:HD2	1:D:424:GLY:HA3	1.73	0.54
1:A:272:THR:CG2	1:A:273:THR:H	2.18	0.54
1:A:367:LEU:HD12	1:A:367:LEU:C	2.28	0.54
1:B:363:GLN:C	1:B:364:ILE:CG2	2.76	0.54
1:B:403:ASN:CB	2:B:902:NAG:H83	2.21	0.54
1:D:241:ARG:NE	1:D:281:ILE:HD12	2.22	0.54
1:D:438:PRO:HB2	1:D:513:LEU:HD12	1.89	0.54
1:B:252:THR:HG23	1:B:253:PRO:HD2	1.90	0.54
1:B:490:LYS:O	1:B:490:LYS:HG2	2.08	0.54
1:C:90:GLU:H	1:D:79:HIS:N	1.91	0.54
1:C:217:ASN:N	1:C:217:ASN:ND2	2.56	0.54
1:C:252:THR:HG23	1:C:253:PRO:HD2	1.90	0.54
1:C:363:GLN:C	1:C:364:ILE:CG2	2.75	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:443:ARG:HG3	1:D:443:ARG:NH1	2.24	0.54
1:A:32:ASN:HD22	1:A:83:GLU:H	1.51	0.53
1:A:217:ASN:N	1:A:217:ASN:ND2	2.56	0.53
1:B:75:VAL:O	1:B:76:LEU:HD23	2.08	0.53
1:B:81:VAL:CB	1:D:90:GLU:HG2	2.37	0.53
1:B:86:SER:N	1:D:91:PRO:CD	2.70	0.53
1:B:117:VAL:O	1:B:211:ILE:HA	2.07	0.53
1:B:249:MET:O	1:B:252:THR:HB	2.08	0.53
1:B:272:THR:CG2	1:B:273:THR:H	2.19	0.53
1:A:249:MET:O	1:A:252:THR:HB	2.09	0.53
1:A:373:ASN:HB3	1:A:409:ILE:H	1.74	0.53
1:B:403:ASN:C	1:B:405:THR:H	2.12	0.53
1:B:438:PRO:HB2	1:B:513:LEU:HD12	1.89	0.53
1:B:458:THR:HG22	1:B:493:SER:HB3	1.91	0.53
1:C:85:GLY:N	1:D:74:TYR:CD2	2.77	0.53
1:A:117:VAL:O	1:A:211:ILE:HA	2.07	0.53
1:A:443:ARG:HG3	1:A:443:ARG:NH1	2.23	0.53
1:C:75:VAL:O	1:C:76:LEU:HD23	2.08	0.53
1:C:79:HIS:CB	1:D:39:THR:CB	2.80	0.53
1:C:438:PRO:HB2	1:C:513:LEU:HD12	1.89	0.53
1:C:522:LEU:CD2	1:C:523:THR:HB	2.26	0.53
1:D:105:ARG:HG3	1:D:106:PRO:HD2	1.91	0.53
1:D:373:ASN:HB3	1:D:409:ILE:H	1.73	0.53
1:D:450:GLN:CB	1:D:532:CYS:O	2.56	0.53
1:A:22:VAL:HG22	1:A:23:GLN:H	1.73	0.53
1:A:458:THR:HG22	1:A:493:SER:HB3	1.91	0.53
1:C:88:VAL:C	1:D:38:ILE:CG1	2.76	0.53
1:C:154:ASP:C	2:C:801:NAG:C8	2.62	0.53
1:C:443:ARG:HG3	1:C:443:ARG:NH1	2.23	0.53
1:C:450:GLN:CB	1:C:532:CYS:O	2.56	0.53
1:D:458:THR:HG22	1:D:493:SER:HB3	1.91	0.53
1:B:332:PHE:HD2	1:B:424:GLY:HA3	1.73	0.53
1:B:373:ASN:HB3	1:B:409:ILE:H	1.74	0.53
1:C:83:GLU:C	1:D:41:GLN:NE2	2.61	0.53
1:C:490:LYS:HG2	1:C:490:LYS:O	2.08	0.53
1:C:533:GLU:HA	1:C:533:GLU:OE2	2.09	0.53
1:D:22:VAL:HG22	1:D:23:GLN:H	1.73	0.53
1:D:367:LEU:HD13	1:D:412:VAL:HG23	1.91	0.53
1:A:320:THR:CG2	2:A:807:NAG:C2	2.77	0.53
1:C:105:ARG:HG3	1:C:106:PRO:HD2	1.91	0.53
1:C:272:THR:CG2	1:C:273:THR:H	2.18	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:GLU:CG	1:C:277:SER:N	2.71	0.53
1:D:75:VAL:O	1:D:76:LEU:HD23	2.08	0.53
1:A:169:THR:OG1	1:A:171:VAL:HG23	2.07	0.53
1:C:312:LEU:O	3:C:804:NDG:C8	2.57	0.53
1:C:369:TYR:O	1:C:383:LYS:HG2	2.09	0.53
1:D:242:LEU:O	1:D:279:GLN:HB3	2.09	0.53
1:D:249:MET:O	1:D:252:THR:HB	2.08	0.53
1:B:379:LEU:H	1:B:379:LEU:CD2	2.22	0.53
1:C:318:THR:CG2	2:C:806:NAG:H5	2.34	0.53
1:C:332:PHE:HD2	1:C:424:GLY:HA3	1.73	0.53
1:A:154:ASP:CB	2:A:801:NAG:HN2	2.16	0.53
1:A:242:LEU:O	1:A:279:GLN:HB3	2.09	0.53
1:A:312:LEU:O	3:A:804:NDG:C8	2.57	0.53
1:A:347:ARG:HG3	1:A:391:ASN:HA	1.91	0.53
1:A:403:ASN:C	1:A:405:THR:H	2.12	0.53
1:B:276:GLU:CG	1:B:277:SER:N	2.71	0.53
1:B:369:TYR:O	1:B:383:LYS:HG2	2.09	0.53
1:A:4:ILE:CB	1:B:90:GLU:C	2.76	0.53
1:A:252:THR:HG23	1:A:253:PRO:HD2	1.90	0.53
1:A:278:ASN:HD22	1:A:278:ASN:N	2.05	0.53
1:C:249:MET:O	1:C:252:THR:HB	2.08	0.53
1:D:403:ASN:C	1:D:405:THR:H	2.12	0.53
1:A:289:ASP:O	1:A:290:PHE:CB	2.25	0.52
1:B:347:ARG:HG3	1:B:391:ASN:HA	1.91	0.52
1:C:1:ASP:O	1:D:28:LYS:CD	2.57	0.52
1:D:31:PHE:CD2	1:D:32:ASN:HB2	2.44	0.52
1:D:227:THR:CG2	2:D:807:NAG:H83	2.32	0.52
1:A:226:TYR:HB2	1:A:319:VAL:HG22	1.89	0.52
1:A:369:TYR:O	1:A:383:LYS:HG2	2.09	0.52
1:A:2:TRP:CZ2	1:B:36:TYR:HA	2.43	0.52
1:A:4:ILE:CA	1:B:91:PRO:CB	2.81	0.52
1:A:24:ILE:HA	1:D:2:TRP:CB	2.33	0.52
1:A:24:ILE:CG2	1:D:2:TRP:HE1	2.18	0.52
1:A:31:PHE:CD2	1:A:32:ASN:HB2	2.45	0.52
1:A:352:ILE:HG13	1:A:388:VAL:CB	2.33	0.52
1:A:450:GLN:CB	1:A:532:CYS:O	2.56	0.52
1:A:512:LEU:HD11	1:A:519:ASN:HD21	1.75	0.52
1:B:31:PHE:CD2	1:B:32:ASN:HB2	2.44	0.52
1:C:81:VAL:CG1	1:D:43:ALA:H	2.22	0.52
1:D:312:LEU:O	3:D:804:NDG:C8	2.57	0.52
1:D:496:LEU:HD21	1:D:509:ILE:CD1	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:512:LEU:HD11	1:D:519:ASN:HD21	1.74	0.52
1:D:533:GLU:HA	1:D:533:GLU:OE2	2.09	0.52
1:A:2:TRP:HH2	1:B:35:TYR:O	1.92	0.52
1:B:443:ARG:HG3	1:B:443:ARG:NH1	2.23	0.52
1:C:31:PHE:CD2	1:C:32:ASN:HB2	2.45	0.52
1:C:91:PRO:N	1:D:79:HIS:HD2	2.03	0.52
1:C:268:PHE:C	1:C:285:ALA:HB3	2.30	0.52
1:C:379:LEU:H	1:C:379:LEU:CD2	2.22	0.52
1:D:272:THR:CG2	2:D:803:NAG:HN2	2.23	0.52
1:A:367:LEU:HD13	1:A:412:VAL:HG23	1.91	0.52
1:B:22:VAL:HG22	1:B:23:GLN:H	1.73	0.52
1:B:312:LEU:O	3:B:804:NDG:C8	2.57	0.52
1:B:496:LEU:HD21	1:B:509:ILE:CD1	2.38	0.52
1:C:403:ASN:C	1:C:405:THR:H	2.12	0.52
1:D:226:TYR:HB2	1:D:319:VAL:HG22	1.89	0.52
1:B:30:ARG:NH1	1:C:30:ARG:HG2	2.25	0.52
1:B:512:LEU:HD11	1:B:519:ASN:HD21	1.75	0.52
1:C:28:LYS:CB	1:D:76:LEU:O	2.57	0.52
1:C:194:THR:HG22	1:C:195:ASP:N	2.25	0.52
1:C:512:LEU:HD11	1:C:519:ASN:HD21	1.74	0.52
1:D:318:THR:CG2	2:D:806:NAG:H5	2.34	0.52
1:D:396:ARG:NH2	1:D:464:ILE:HG22	2.12	0.52
1:A:268:PHE:C	1:A:285:ALA:HB3	2.30	0.52
1:A:338:ARG:HB3	1:A:339:VAL:HG22	1.92	0.52
1:A:371:ILE:HG23	1:A:372:GLY:H	1.73	0.52
1:A:402:LYS:C	1:A:403:ASN:O	2.46	0.52
1:C:1:ASP:CA	1:D:89:GLU:OE1	2.39	0.52
1:C:93:GLU:CA	1:D:81:VAL:HG11	2.38	0.52
1:C:242:LEU:O	1:C:279:GLN:HB3	2.09	0.52
1:C:336:VAL:O	1:C:426:LEU:HD22	2.10	0.52
1:C:338:ARG:HB3	1:C:339:VAL:HG22	1.92	0.52
1:C:367:LEU:HD13	1:C:412:VAL:HG23	1.91	0.52
1:C:371:ILE:HG23	1:C:372:GLY:H	1.73	0.52
1:C:458:THR:HG22	1:C:493:SER:HB3	1.90	0.52
1:D:338:ARG:HB3	1:D:339:VAL:HG22	1.92	0.52
1:A:496:LEU:HD21	1:A:509:ILE:CD1	2.38	0.52
1:A:505:GLY:O	1:A:506:ASP:OD1	2.28	0.52
1:B:272:THR:CG2	2:B:803:NAG:HN2	2.23	0.52
1:B:371:ILE:HG23	1:B:372:GLY:H	1.73	0.52
1:B:426:LEU:O	1:B:426:LEU:HD13	2.10	0.52
1:C:27:ASN:HD21	1:D:93:GLU:N	2.04	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:ARG:HG3	1:C:391:ASN:HA	1.91	0.52
1:C:373:ASN:HB3	1:C:409:ILE:H	1.73	0.52
1:C:450:GLN:CB	1:C:533:GLU:HA	2.29	0.52
1:D:365:GLN:O	1:D:365:GLN:CG	2.54	0.52
1:A:105:ARG:HG3	1:A:106:PRO:HD2	1.91	0.52
1:A:138:ASN:HD22	1:A:138:ASN:C	2.13	0.52
1:B:89:GLU:N	1:D:1:ASP:CB	2.46	0.52
1:B:194:THR:HG22	1:B:195:ASP:N	2.25	0.52
1:D:138:ASN:C	1:D:138:ASN:HD22	2.13	0.52
1:D:155:PRO:CD	2:D:801:NAG:H82	2.40	0.52
1:D:482:THR:CG2	1:D:499:THR:CA	2.87	0.52
1:B:105:ARG:HG3	1:B:106:PRO:HD2	1.91	0.52
1:B:221:PHE:HB3	1:B:223:PRO:O	2.10	0.52
1:B:367:LEU:HD13	1:B:412:VAL:HG23	1.91	0.52
1:D:221:PHE:HB3	1:D:223:PRO:O	2.10	0.52
1:D:252:THR:HG23	1:D:253:PRO:HD2	1.90	0.52
1:D:347:ARG:HD2	1:D:392:GLY:N	2.25	0.52
1:D:371:ILE:HG23	1:D:372:GLY:H	1.73	0.52
1:D:482:THR:HG22	1:D:482:THR:O	2.09	0.52
1:D:505:GLY:O	1:D:506:ASP:OD1	2.28	0.52
1:A:272:THR:CG2	2:A:803:NAG:HN2	2.23	0.51
1:A:482:THR:CG2	1:A:499:THR:CA	2.87	0.51
1:B:533:GLU:HA	1:B:533:GLU:OE2	2.09	0.51
1:C:30:ARG:NH2	1:D:6:PRO:HG3	2.25	0.51
1:D:234:GLU:HB2	1:D:235:ILE:HG22	1.93	0.51
1:D:369:TYR:O	1:D:383:LYS:HG2	2.09	0.51
1:A:3:VAL:HG21	1:B:77:SER:OG	2.10	0.51
1:A:221:PHE:HB3	1:A:223:PRO:O	2.10	0.51
1:A:514:SER:HB3	1:A:517:GLN:O	2.10	0.51
1:A:533:GLU:HA	1:A:533:GLU:OE2	2.09	0.51
1:B:142:LEU:O	1:B:196:LEU:HD23	2.11	0.51
1:B:242:LEU:O	1:B:279:GLN:HB3	2.09	0.51
1:B:266:GLY:N	1:B:268:PHE:CE2	2.76	0.51
1:B:268:PHE:C	1:B:285:ALA:HB3	2.30	0.51
1:C:22:VAL:HG22	1:C:23:GLN:H	1.73	0.51
1:C:272:THR:CG2	2:C:803:NAG:HN2	2.23	0.51
1:C:482:THR:CG2	1:C:499:THR:CA	2.87	0.51
1:C:514:SER:HB3	1:C:517:GLN:O	2.11	0.51
1:A:234:GLU:HB2	1:A:235:ILE:HG22	1.93	0.51
1:B:81:VAL:CG1	1:D:90:GLU:HG2	2.40	0.51
1:B:155:PRO:CD	2:B:801:NAG:H82	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:VAL:CB	1:B:334:PRO:CD	2.88	0.51
1:C:33:LYS:HB3	1:C:83:GLU:CG	2.40	0.51
1:C:88:VAL:HG22	1:D:75:VAL:O	2.03	0.51
1:C:426:LEU:O	1:C:426:LEU:HD13	2.10	0.51
1:D:333:VAL:CB	1:D:334:PRO:CD	2.88	0.51
1:D:347:ARG:HG3	1:D:391:ASN:HA	1.91	0.51
1:D:426:LEU:O	1:D:426:LEU:HD13	2.09	0.51
1:D:514:SER:HB3	1:D:517:GLN:O	2.10	0.51
1:A:90:GLU:CB	1:B:3:VAL:CA	2.60	0.51
1:A:396:ARG:CZ	1:A:432:ASP:HB2	2.41	0.51
1:A:426:LEU:O	1:A:426:LEU:HD13	2.09	0.51
1:B:138:ASN:C	1:B:138:ASN:HD22	2.13	0.51
1:B:514:SER:HB3	1:B:517:GLN:O	2.10	0.51
1:C:88:VAL:CG1	1:D:94:ILE:N	2.73	0.51
1:C:155:PRO:CD	2:C:801:NAG:H82	2.40	0.51
1:C:347:ARG:HD2	1:C:392:GLY:N	2.25	0.51
1:D:33:LYS:HB3	1:D:83:GLU:CG	2.40	0.51
1:D:336:VAL:O	1:D:426:LEU:HD22	2.10	0.51
1:B:471:TYR:N	1:B:471:TYR:CD1	2.79	0.51
1:C:82:SER:HB2	1:D:74:TYR:HA	1.92	0.51
1:C:142:LEU:O	1:C:196:LEU:HD23	2.11	0.51
1:C:151:LEU:HD12	1:C:190:THR:O	2.11	0.51
1:D:151:LEU:HD12	1:D:190:THR:O	2.11	0.51
1:A:276:GLU:CG	1:A:277:SER:N	2.71	0.51
1:A:297:VAL:CG2	2:A:807:NAG:H62	2.41	0.51
1:A:458:THR:HA	1:A:493:SER:HA	1.93	0.51
1:B:297:VAL:CG2	2:B:807:NAG:H62	2.41	0.51
1:B:336:VAL:O	1:B:426:LEU:HD22	2.10	0.51
1:C:82:SER:OG	1:D:74:TYR:HD2	1.93	0.51
1:C:90:GLU:H	1:D:78:SER:CB	1.92	0.51
1:C:90:GLU:H	1:D:78:SER:HB2	1.74	0.51
1:C:138:ASN:HD22	1:C:138:ASN:C	2.13	0.51
1:A:333:VAL:CB	1:A:334:PRO:CD	2.88	0.51
1:A:428:LEU:O	1:A:428:LEU:HD23	2.11	0.51
1:B:482:THR:CG2	1:B:499:THR:CA	2.87	0.51
1:B:505:GLY:O	1:B:506:ASP:OD1	2.28	0.51
1:C:266:GLY:N	1:C:268:PHE:CE2	2.76	0.51
1:C:505:GLY:O	1:C:506:ASP:OD1	2.28	0.51
1:A:4:ILE:HA	1:B:90:GLU:CA	2.37	0.51
1:A:151:LEU:HD12	1:A:190:THR:O	2.11	0.51
1:A:450:GLN:CG	1:A:533:GLU:OE2	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:THR:HA	1:B:493:SER:HA	1.93	0.51
1:C:31:PHE:CE2	1:D:73:LYS:C	2.36	0.51
1:C:333:VAL:CB	1:C:334:PRO:CD	2.88	0.51
1:D:268:PHE:C	1:D:285:ALA:HB3	2.30	0.51
1:A:194:THR:HG22	1:A:195:ASP:N	2.25	0.51
1:B:76:LEU:O	1:B:94:ILE:N	2.44	0.51
1:B:352:ILE:HG13	1:B:388:VAL:CB	2.33	0.51
1:B:428:LEU:HD23	1:B:428:LEU:O	2.11	0.51
1:C:25:LYS:NZ	1:C:29:ASP:OD2	2.40	0.51
1:C:31:PHE:CD1	1:D:95:THR:HG21	2.44	0.51
1:C:234:GLU:HB2	1:C:235:ILE:HG22	1.93	0.51
1:C:368:SER:OG	1:C:370:PHE:HE1	1.94	0.51
2:C:809:NAG:H61	2:C:810:NAG:C6	2.39	0.51
1:D:396:ARG:CZ	1:D:432:ASP:HB2	2.41	0.51
2:D:809:NAG:H61	2:D:810:NAG:C6	2.39	0.51
1:A:336:VAL:O	1:A:426:LEU:HD22	2.10	0.51
1:A:458:THR:HG22	1:A:493:SER:CB	2.41	0.51
1:A:471:TYR:CD1	1:A:471:TYR:N	2.79	0.51
1:B:151:LEU:HD12	1:B:190:THR:O	2.11	0.51
1:B:338:ARG:HB3	1:B:339:VAL:HG22	1.92	0.51
1:C:88:VAL:HG12	1:D:94:ILE:CA	2.40	0.51
1:C:241:ARG:NE	1:C:281:ILE:HD12	2.22	0.51
1:D:76:LEU:O	1:D:94:ILE:N	2.44	0.51
1:D:276:GLU:HG3	1:D:277:SER:N	2.25	0.51
1:D:352:ILE:HG13	1:D:388:VAL:CB	2.33	0.51
1:A:513:LEU:C	1:A:514:SER:HG	2.14	0.50
1:B:32:ASN:HB2	1:C:26:SER:O	2.11	0.50
1:C:31:PHE:CA	1:D:73:LYS:NZ	2.72	0.50
1:C:155:PRO:HG2	2:C:801:NAG:C7	2.42	0.50
1:C:458:THR:HA	1:C:493:SER:HA	1.93	0.50
1:D:80:ALA:O	1:D:88:VAL:HG23	2.11	0.50
1:D:194:THR:HG22	1:D:195:ASP:N	2.25	0.50
1:D:458:THR:HA	1:D:493:SER:HA	1.93	0.50
1:B:432:ASP:CB	1:B:464:ILE:CG2	2.90	0.50
1:B:450:GLN:CG	1:B:533:GLU:OE2	2.58	0.50
1:C:221:PHE:HB3	1:C:223:PRO:O	2.10	0.50
1:C:428:LEU:O	1:C:428:LEU:HD23	2.11	0.50
1:D:217:ASN:N	1:D:217:ASN:HD22	2.09	0.50
1:D:458:THR:HG22	1:D:493:SER:CB	2.42	0.50
1:A:80:ALA:O	1:A:88:VAL:HG23	2.11	0.50
1:A:155:PRO:CD	2:A:801:NAG:H82	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ARG:NE	1:A:281:ILE:HD12	2.22	0.50
1:A:290:PHE:CE2	1:A:293:ARG:CB	2.92	0.50
1:A:419:VAL:HG22	2:A:809:NAG:H81	1.93	0.50
1:C:28:LYS:CD	1:C:88:VAL:HG12	2.38	0.50
1:C:261:ILE:HD11	1:C:264:ASN:HD22	1.77	0.50
1:C:352:ILE:CG1	1:C:388:VAL:HB	2.33	0.50
1:C:450:GLN:CG	1:C:533:GLU:OE2	2.58	0.50
1:D:142:LEU:O	1:D:196:LEU:HD23	2.11	0.50
1:D:297:VAL:CG2	2:D:807:NAG:H62	2.41	0.50
1:A:2:TRP:CD2	1:B:80:ALA:HB3	2.30	0.50
1:A:142:LEU:O	1:A:196:LEU:HD23	2.11	0.50
1:B:227:THR:CG2	2:B:807:NAG:H83	2.32	0.50
1:B:268:PHE:CD2	1:B:268:PHE:N	2.75	0.50
1:B:419:VAL:HG22	2:B:809:NAG:H81	1.93	0.50
1:C:90:GLU:CD	1:D:37:SER:C	2.66	0.50
1:C:297:VAL:CG2	2:C:807:NAG:H62	2.41	0.50
1:C:382:ASN:OD1	1:C:385:ASN:N	2.45	0.50
1:C:396:ARG:CZ	1:C:432:ASP:HB2	2.41	0.50
1:D:382:ASN:OD1	1:D:385:ASN:N	2.45	0.50
1:D:432:ASP:CB	1:D:464:ILE:CG2	2.89	0.50
1:A:11:GLU:OE2	1:A:69:GLU:OE1	2.30	0.50
1:A:76:LEU:O	1:A:94:ILE:N	2.44	0.50
1:B:217:ASN:N	1:B:217:ASN:HD22	2.09	0.50
1:B:327:ASN:OD1	1:B:360:ASP:OD1	2.30	0.50
1:B:458:THR:HG22	1:B:493:SER:CB	2.42	0.50
1:C:290:PHE:CE2	1:C:293:ARG:CB	2.92	0.50
1:C:458:THR:HG22	1:C:493:SER:CB	2.42	0.50
1:D:428:LEU:O	1:D:428:LEU:HD23	2.11	0.50
1:D:471:TYR:CD1	1:D:471:TYR:N	2.79	0.50
1:A:382:ASN:OD1	1:A:385:ASN:N	2.44	0.50
1:B:155:PRO:HG2	2:B:801:NAG:C7	2.42	0.50
1:B:216:ASP:HB2	1:B:217:ASN:ND2	2.27	0.50
1:B:373:ASN:ND2	1:B:374:ASP:OD1	2.45	0.50
1:C:216:ASP:HB2	1:C:217:ASN:ND2	2.27	0.50
1:C:471:TYR:N	1:C:471:TYR:CD1	2.79	0.50
1:C:482:THR:HG22	1:C:482:THR:O	2.09	0.50
1:D:11:GLU:OE2	1:D:69:GLU:OE1	2.30	0.50
1:D:261:ILE:HD11	1:D:264:ASN:HD22	1.77	0.50
1:D:363:GLN:C	1:D:364:ILE:HG23	2.32	0.50
1:D:450:GLN:CB	1:D:533:GLU:HA	2.29	0.50
1:A:1:ASP:HB3	1:B:92:MET:CB	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:THR:HG22	1:A:110:GLN:HG3	1.94	0.50
1:A:155:PRO:HG2	2:A:801:NAG:C7	2.42	0.50
1:A:423:THR:HB	2:A:810:NAG:H83	1.93	0.50
1:B:80:ALA:O	1:B:88:VAL:HG23	2.11	0.50
1:B:363:GLN:C	1:B:364:ILE:HG23	2.32	0.50
1:B:423:THR:HB	2:B:810:NAG:H83	1.93	0.50
1:B:482:THR:HG22	1:B:482:THR:O	2.09	0.50
2:B:809:NAG:H61	2:B:810:NAG:C6	2.39	0.50
1:C:87:PRO:C	1:D:38:ILE:CD1	2.80	0.50
1:C:88:VAL:HG21	1:D:75:VAL:O	2.07	0.50
1:C:496:LEU:HD21	1:C:509:ILE:CD1	2.38	0.50
1:D:155:PRO:HG2	2:D:801:NAG:C7	2.42	0.50
1:D:320:THR:CG2	2:D:807:NAG:C2	2.77	0.50
1:A:347:ARG:HD2	1:A:392:GLY:N	2.25	0.50
1:A:352:ILE:CG1	1:A:388:VAL:HB	2.34	0.50
1:B:290:PHE:CE2	1:B:293:ARG:CB	2.93	0.50
1:B:449:ASP:CB	1:B:532:CYS:H	2.22	0.50
2:B:812:NAG:O7	2:B:812:NAG:C1	2.60	0.50
1:C:87:PRO:N	1:D:43:ALA:CA	2.69	0.50
1:C:402:LYS:C	1:C:403:ASN:O	2.46	0.50
2:C:812:NAG:O7	2:C:812:NAG:C1	2.60	0.50
2:D:807:NAG:O7	2:D:807:NAG:H3	2.11	0.50
1:A:327:ASN:OD1	1:A:360:ASP:OD1	2.30	0.50
1:B:366:LYS:HG2	1:B:367:LEU:H	1.74	0.50
1:B:367:LEU:HB2	1:B:413:THR:O	2.12	0.50
1:C:217:ASN:N	1:C:217:ASN:HD22	2.09	0.50
1:C:432:ASP:CB	1:C:464:ILE:CG2	2.90	0.50
1:D:352:ILE:CG1	1:D:388:VAL:HB	2.33	0.50
1:D:373:ASN:ND2	1:D:374:ASP:OD1	2.45	0.50
1:A:1:ASP:CA	1:B:24:ILE:HG21	2.32	0.49
1:B:11:GLU:OE2	1:B:69:GLU:OE1	2.30	0.49
1:B:347:ARG:HD2	1:B:392:GLY:N	2.25	0.49
1:B:449:ASP:CB	1:B:532:CYS:N	2.74	0.49
1:B:457:LEU:HD23	1:B:494:MET:SD	2.52	0.49
1:C:11:GLU:OE2	1:C:69:GLU:OE1	2.30	0.49
1:C:81:VAL:HB	1:D:43:ALA:H	1.76	0.49
1:C:327:ASN:OD1	1:C:360:ASP:OD1	2.30	0.49
1:C:335:ALA:CB	3:C:811:NDG:C6	2.90	0.49
1:D:367:LEU:HB2	1:D:413:THR:O	2.12	0.49
1:D:457:LEU:HD23	1:D:494:MET:SD	2.52	0.49
1:B:352:ILE:CG1	1:B:388:VAL:HB	2.34	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:ASP:O	2:C:801:NAG:C8	2.60	0.49
1:C:373:ASN:ND2	1:C:374:ASP:OD1	2.45	0.49
1:D:154:ASP:O	2:D:801:NAG:C8	2.60	0.49
1:A:10:SER:CA	1:D:30:ARG:CD	2.89	0.49
1:B:33:LYS:HB3	1:B:83:GLU:CG	2.40	0.49
2:B:807:NAG:H3	2:B:807:NAG:O7	2.11	0.49
1:D:273:THR:H	2:D:803:NAG:HN2	1.60	0.49
1:D:335:ALA:CB	3:D:811:NDG:C6	2.90	0.49
1:D:419:VAL:HG22	2:D:809:NAG:H81	1.93	0.49
1:B:68:ARG:HD3	1:B:100:ASP:CA	2.43	0.49
1:B:234:GLU:HB2	1:B:235:ILE:HG22	1.92	0.49
1:B:396:ARG:CZ	1:B:432:ASP:HB2	2.41	0.49
1:C:68:ARG:HD3	1:C:100:ASP:CA	2.43	0.49
1:C:86:SER:N	1:D:74:TYR:CD2	2.73	0.49
1:C:151:LEU:HD12	1:C:151:LEU:H	1.77	0.49
1:C:336:VAL:CG1	1:C:338:ARG:HB2	2.43	0.49
1:C:367:LEU:HB2	1:C:413:THR:O	2.12	0.49
1:D:397:GLU:OE1	1:D:397:GLU:N	2.45	0.49
1:D:402:LYS:C	1:D:403:ASN:O	2.46	0.49
1:D:451:ASN:O	1:D:534:GLY:CA	2.60	0.49
1:A:252:THR:CG2	1:A:253:PRO:HD2	2.43	0.49
1:B:192:GLN:HA	1:B:203:VAL:O	2.13	0.49
1:B:226:TYR:C	1:B:227:THR:HG23	2.33	0.49
1:C:109:THR:HG22	1:C:110:GLN:HG3	1.94	0.49
1:C:423:THR:HB	2:C:810:NAG:H83	1.94	0.49
1:D:68:ARG:HD3	1:D:100:ASP:CA	2.43	0.49
1:D:252:THR:CG2	1:D:253:PRO:HD2	2.43	0.49
1:A:87:PRO:O	1:B:2:TRP:CH2	2.66	0.49
1:A:217:ASN:N	1:A:217:ASN:HD22	2.09	0.49
1:A:272:THR:CG2	1:A:273:THR:N	2.76	0.49
1:B:109:THR:HG22	1:B:110:GLN:CG	2.42	0.49
1:B:224:LYS:HE3	2:B:806:NAG:H82	1.95	0.49
1:B:365:GLN:HA	1:B:416:GLY:HA3	1.95	0.49
1:B:382:ASN:OD1	1:B:385:ASN:N	2.45	0.49
1:D:224:LYS:HE3	2:D:806:NAG:H82	1.95	0.49
1:D:226:TYR:C	1:D:227:THR:HG23	2.33	0.49
1:D:276:GLU:CG	1:D:277:SER:N	2.71	0.49
1:D:336:VAL:CG1	1:D:338:ARG:HB2	2.43	0.49
1:D:423:THR:HB	2:D:810:NAG:H83	1.94	0.49
1:A:226:TYR:C	1:A:227:THR:HG23	2.33	0.49
1:A:373:ASN:ND2	1:A:374:ASP:OD1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:ASP:CB	1:A:464:ILE:CG2	2.89	0.49
1:A:457:LEU:HD23	1:A:494:MET:SD	2.52	0.49
1:B:151:LEU:HD12	1:B:151:LEU:H	1.77	0.49
1:B:261:ILE:HD11	1:B:264:ASN:HD22	1.77	0.49
1:B:276:GLU:HG3	1:B:277:SER:N	2.25	0.49
1:C:109:THR:HG22	1:C:110:GLN:CG	2.42	0.49
1:C:226:TYR:C	1:C:227:THR:HG23	2.33	0.49
1:D:310:VAL:HG12	1:D:312:LEU:HG	1.95	0.49
1:A:89:GLU:OE1	1:B:2:TRP:CG	2.62	0.49
1:A:186:GLU:OE1	2:A:801:NAG:C6	2.59	0.49
1:B:154:ASP:CG	1:B:155:PRO:HD2	2.33	0.49
1:B:365:GLN:O	1:B:365:GLN:CG	2.54	0.49
1:C:31:PHE:CD2	1:D:75:VAL:HG23	2.44	0.49
1:C:252:THR:CG2	1:C:253:PRO:HD2	2.43	0.49
1:C:281:ILE:HG23	1:C:281:ILE:O	2.13	0.49
1:C:512:LEU:HD11	1:C:519:ASN:ND2	2.28	0.49
1:D:216:ASP:HB2	1:D:217:ASN:ND2	2.27	0.49
1:A:216:ASP:HB2	1:A:217:ASN:ND2	2.27	0.49
1:A:367:LEU:HD13	1:A:412:VAL:CG2	2.43	0.49
1:B:28:LYS:CD	1:B:88:VAL:HG12	2.38	0.49
1:B:109:THR:HG22	1:B:110:GLN:HG3	1.94	0.49
1:B:335:ALA:CB	3:B:811:NDG:C6	2.90	0.49
1:B:336:VAL:CG1	1:B:338:ARG:HB2	2.43	0.49
1:B:451:ASN:O	1:B:534:GLY:CA	2.60	0.49
1:C:282:LEU:CD2	1:C:283:THR:N	2.76	0.49
1:C:397:GLU:OE1	1:C:397:GLU:N	2.45	0.49
2:D:809:NAG:H62	2:D:810:NAG:O6	2.13	0.49
1:A:224:LYS:HE3	2:A:806:NAG:H82	1.95	0.49
1:A:261:ILE:HD11	1:A:264:ASN:HD22	1.77	0.49
1:A:365:GLN:HA	1:A:416:GLY:HA3	1.95	0.49
1:A:432:ASP:CB	1:A:464:ILE:HG21	2.43	0.49
1:B:87:PRO:HG2	1:C:2:TRP:CD1	2.47	0.49
1:B:154:ASP:O	2:B:801:NAG:C8	2.60	0.49
1:B:273:THR:H	2:B:803:NAG:HN2	1.60	0.49
1:C:310:VAL:HG12	1:C:312:LEU:HG	1.95	0.49
1:C:363:GLN:C	1:C:364:ILE:HG23	2.32	0.49
1:C:419:VAL:HG22	2:C:809:NAG:H81	1.93	0.49
1:C:449:ASP:CB	1:C:532:CYS:H	2.22	0.49
1:D:151:LEU:HD12	1:D:151:LEU:H	1.78	0.49
1:D:186:GLU:OE1	2:D:801:NAG:C6	2.59	0.49
1:D:250:PRO:O	1:D:255:TRP:CE3	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:449:ASP:CB	1:D:532:CYS:H	2.22	0.49
1:A:273:THR:H	2:A:803:NAG:HN2	1.60	0.48
1:B:67:ASP:OD2	1:B:69:GLU:HB2	2.13	0.48
1:B:84:ASN:O	1:C:24:ILE:CB	2.57	0.48
1:B:250:PRO:O	1:B:255:TRP:CE3	2.66	0.48
1:B:278:ASN:HD22	1:B:278:ASN:N	2.05	0.48
1:C:67:ASP:OD2	1:C:69:GLU:HB2	2.13	0.48
1:C:151:LEU:O	1:C:152:LYS:HB2	2.13	0.48
1:C:154:ASP:CG	1:C:155:PRO:HD2	2.33	0.48
1:C:457:LEU:HD23	1:C:494:MET:SD	2.52	0.48
1:D:109:THR:HG22	1:D:110:GLN:HG3	1.94	0.48
1:D:432:ASP:CB	1:D:464:ILE:HG21	2.43	0.48
1:A:28:LYS:CD	1:A:88:VAL:HG12	2.38	0.48
1:A:151:LEU:HD12	1:A:151:LEU:H	1.78	0.48
1:A:310:VAL:HG12	1:A:312:LEU:HG	1.95	0.48
1:A:335:ALA:CB	3:A:811:NDG:C6	2.90	0.48
1:A:522:LEU:CD2	1:A:523:THR:HB	2.26	0.48
2:A:807:NAG:O7	2:A:807:NAG:H3	2.11	0.48
1:B:32:ASN:ND2	1:B:83:GLU:N	2.44	0.48
1:B:150:ILE:HD11	1:B:165:ILE:HB	1.96	0.48
1:B:241:ARG:NE	1:B:281:ILE:HD12	2.22	0.48
1:C:80:ALA:O	1:C:88:VAL:HG23	2.11	0.48
1:C:432:ASP:CB	1:C:464:ILE:HG21	2.43	0.48
1:D:224:LYS:CE	2:D:806:NAG:C8	2.91	0.48
1:D:513:LEU:C	1:D:514:SER:HG	2.16	0.48
1:A:266:GLY:N	1:A:268:PHE:CE2	2.76	0.48
1:B:27:ASN:C	1:B:29:ASP:H	2.15	0.48
1:B:186:GLU:OE1	2:B:801:NAG:C6	2.59	0.48
1:C:192:GLN:HA	1:C:203:VAL:O	2.13	0.48
1:C:250:PRO:O	1:C:255:TRP:CE3	2.66	0.48
1:C:367:LEU:HD13	1:C:412:VAL:CG2	2.43	0.48
1:D:151:LEU:O	1:D:152:LYS:HB2	2.13	0.48
1:D:327:ASN:OD1	1:D:360:ASP:OD1	2.30	0.48
1:D:367:LEU:HD13	1:D:412:VAL:CG2	2.43	0.48
1:D:368:SER:OG	1:D:370:PHE:HE1	1.94	0.48
1:A:8:LYS:CB	1:D:30:ARG:HH21	2.26	0.48
1:A:192:GLN:HA	1:A:203:VAL:O	2.13	0.48
1:A:512:LEU:HD11	1:A:519:ASN:ND2	2.28	0.48
1:B:119:GLU:OE2	1:B:216:ASP:OD1	2.32	0.48
1:B:272:THR:CG2	1:B:273:THR:N	2.76	0.48
1:B:512:LEU:HD11	1:B:519:ASN:ND2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:809:NAG:C6	2:B:810:NAG:C6	2.92	0.48
1:C:32:ASN:HB3	1:D:75:VAL:HG23	1.94	0.48
2:C:807:NAG:H3	2:C:807:NAG:O7	2.11	0.48
1:A:27:ASN:C	1:A:29:ASP:H	2.15	0.48
1:A:41:GLN:HA	1:A:45:ASN:HB2	1.95	0.48
1:A:109:THR:HG22	1:A:110:GLN:CG	2.42	0.48
1:A:154:ASP:CG	1:A:155:PRO:HD2	2.33	0.48
1:A:281:ILE:HG23	1:A:281:ILE:O	2.13	0.48
2:A:809:NAG:H62	2:A:810:NAG:O6	2.13	0.48
1:B:151:LEU:O	1:B:152:LYS:HB2	2.13	0.48
2:B:809:NAG:H62	2:B:810:NAG:O6	2.13	0.48
1:C:81:VAL:CG1	1:D:43:ALA:C	2.80	0.48
1:C:119:GLU:OE2	1:C:216:ASP:OD1	2.32	0.48
2:C:809:NAG:C6	2:C:810:NAG:C6	2.92	0.48
1:D:117:VAL:O	1:D:212:THR:N	2.46	0.48
1:D:154:ASP:CG	1:D:155:PRO:HD2	2.33	0.48
1:D:448:CYS:SG	1:D:537:ILE:CG2	3.01	0.48
1:A:282:LEU:CD2	1:A:283:THR:N	2.76	0.48
1:A:483:TRP:CZ2	1:A:507:TYR:CE1	2.87	0.48
1:B:261:ILE:CD1	1:B:264:ASN:ND2	2.77	0.48
1:B:432:ASP:CB	1:B:464:ILE:HG21	2.43	0.48
1:D:192:GLN:HA	1:D:203:VAL:O	2.13	0.48
1:A:10:SER:H	1:D:30:ARG:HG3	1.75	0.48
1:A:155:PRO:O	1:A:157:GLU:N	2.43	0.48
1:A:336:VAL:CG1	1:A:338:ARG:HB2	2.43	0.48
1:A:363:GLN:C	1:A:364:ILE:HG23	2.32	0.48
1:A:397:GLU:OE1	1:A:397:GLU:N	2.44	0.48
1:B:31:PHE:CG	1:C:30:ARG:N	2.57	0.48
1:B:241:ARG:HE	1:B:281:ILE:CD1	2.24	0.48
1:C:261:ILE:CD1	1:C:264:ASN:ND2	2.77	0.48
1:A:5:PRO:N	1:B:91:PRO:CB	2.75	0.48
1:A:154:ASP:O	2:A:801:NAG:C8	2.60	0.48
1:A:367:LEU:HB2	1:A:413:THR:O	2.12	0.48
1:A:449:ASP:CB	1:A:532:CYS:H	2.22	0.48
1:B:252:THR:CG2	1:B:253:PRO:HD2	2.43	0.48
1:B:281:ILE:HG23	1:B:281:ILE:O	2.13	0.48
1:B:397:GLU:N	1:B:397:GLU:OE1	2.45	0.48
1:C:224:LYS:HE3	2:C:806:NAG:H82	1.95	0.48
1:C:225:THR:HA	1:C:318:THR:O	2.14	0.48
1:A:225:THR:HA	1:A:318:THR:O	2.14	0.48
1:B:224:LYS:CE	2:B:806:NAG:C8	2.91	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:THR:HA	1:B:318:THR:O	2.14	0.48
1:B:282:LEU:CD2	1:B:283:THR:N	2.76	0.48
1:B:367:LEU:HD13	1:B:412:VAL:CG2	2.43	0.48
1:B:448:CYS:SG	1:B:537:ILE:CG2	3.01	0.48
1:B:537:ILE:CG1	1:B:538:LYS:N	2.77	0.48
1:C:273:THR:H	2:C:803:NAG:HN2	1.60	0.48
1:C:418:SER:O	1:C:419:VAL:HG23	2.14	0.48
1:D:41:GLN:HA	1:D:45:ASN:HB2	1.95	0.48
1:D:119:GLU:OE2	1:D:216:ASP:OD1	2.32	0.48
2:D:812:NAG:O7	2:D:812:NAG:C1	2.60	0.48
1:C:41:GLN:HA	1:C:45:ASN:HB2	1.96	0.48
2:C:809:NAG:H62	2:C:810:NAG:O6	2.13	0.48
1:D:27:ASN:C	1:D:29:ASP:H	2.15	0.48
1:D:150:ILE:HD11	1:D:165:ILE:HB	1.96	0.48
1:D:241:ARG:HE	1:D:281:ILE:CD1	2.24	0.48
1:D:281:ILE:O	1:D:281:ILE:HG23	2.13	0.48
1:D:512:LEU:HD11	1:D:519:ASN:ND2	2.28	0.48
2:A:809:NAG:C6	2:A:810:NAG:C6	2.92	0.47
1:C:227:THR:CG2	2:C:807:NAG:H83	2.32	0.47
1:D:225:THR:HA	1:D:318:THR:O	2.14	0.47
1:D:450:GLN:CG	1:D:533:GLU:OE2	2.58	0.47
1:A:67:ASP:OD2	1:A:69:GLU:HB2	2.13	0.47
1:A:151:LEU:O	1:A:152:LYS:HB2	2.13	0.47
1:A:224:LYS:CE	2:A:806:NAG:C8	2.91	0.47
1:A:268:PHE:CA	1:A:285:ALA:HB3	2.45	0.47
1:A:368:SER:OG	1:A:370:PHE:HE1	1.94	0.47
1:A:482:THR:HG22	1:A:482:THR:O	2.09	0.47
1:B:41:GLN:HA	1:B:45:ASN:HB2	1.95	0.47
1:C:76:LEU:O	1:C:94:ILE:N	2.44	0.47
1:C:150:ILE:HD11	1:C:165:ILE:HB	1.96	0.47
1:D:261:ILE:CD1	1:D:264:ASN:ND2	2.77	0.47
1:D:282:LEU:CD2	1:D:283:THR:N	2.76	0.47
1:D:300:ILE:HD12	1:D:300:ILE:N	2.29	0.47
1:D:365:GLN:HA	1:D:416:GLY:HA3	1.95	0.47
1:D:537:ILE:CG1	1:D:538:LYS:N	2.77	0.47
1:A:33:LYS:HB3	1:A:83:GLU:CG	2.40	0.47
1:A:150:ILE:HD11	1:A:165:ILE:HB	1.96	0.47
1:A:418:SER:O	1:A:419:VAL:HG23	2.14	0.47
1:B:246:ASP:C	1:B:247:LEU:HD12	2.35	0.47
1:C:155:PRO:O	1:C:157:GLU:N	2.43	0.47
1:C:301:THR:CG2	1:C:316:THR:HG23	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:ASN:CG	1:C:374:ASP:H	2.18	0.47
1:D:109:THR:HG22	1:D:110:GLN:CG	2.42	0.47
1:D:514:SER:CA	1:D:517:GLN:O	2.62	0.47
1:A:119:GLU:OE2	1:A:216:ASP:OD1	2.32	0.47
1:B:27:ASN:ND2	1:B:28:LYS:N	2.50	0.47
1:B:28:LYS:HG3	1:D:3:VAL:HG21	1.87	0.47
1:B:268:PHE:CA	1:B:285:ALA:HB3	2.45	0.47
1:C:32:ASN:CA	1:D:75:VAL:CG2	2.88	0.47
1:C:50:VAL:HB	1:C:51:PHE:CD1	2.50	0.47
1:C:226:TYR:O	1:C:227:THR:HG23	2.15	0.47
1:C:320:THR:CB	2:C:807:NAG:N2	2.78	0.47
1:C:365:GLN:HA	1:C:416:GLY:HA3	1.95	0.47
1:D:8:LYS:CD	1:D:8:LYS:N	2.51	0.47
1:D:67:ASP:OD2	1:D:69:GLU:HB2	2.13	0.47
1:A:250:PRO:O	1:A:255:TRP:CE3	2.67	0.47
1:A:450:GLN:CB	1:A:533:GLU:HA	2.29	0.47
1:A:514:SER:CA	1:A:517:GLN:O	2.62	0.47
1:A:537:ILE:CG1	1:A:538:LYS:N	2.77	0.47
1:B:300:ILE:HD12	1:B:300:ILE:N	2.30	0.47
1:C:92:MET:HG3	1:D:79:HIS:ND1	2.29	0.47
1:C:224:LYS:CE	2:C:806:NAG:C8	2.91	0.47
1:C:449:ASP:CB	1:C:532:CYS:N	2.74	0.47
1:D:246:ASP:C	1:D:247:LEU:HD12	2.35	0.47
1:D:320:THR:CB	2:D:807:NAG:N2	2.78	0.47
1:A:50:VAL:HB	1:A:51:PHE:CD1	2.50	0.47
1:A:261:ILE:CD1	1:A:264:ASN:ND2	2.77	0.47
1:B:33:LYS:N	1:C:25:LYS:NZ	2.61	0.47
1:B:226:TYR:O	1:B:227:THR:HG23	2.14	0.47
1:B:310:VAL:HG12	1:B:312:LEU:HG	1.95	0.47
1:B:418:SER:O	1:B:419:VAL:HG23	2.14	0.47
1:C:36:TYR:O	1:C:55:TRP:HA	2.15	0.47
1:C:246:ASP:C	1:C:247:LEU:HD12	2.35	0.47
1:D:373:ASN:CG	1:D:374:ASP:H	2.18	0.47
1:A:68:ARG:HD3	1:A:100:ASP:CA	2.43	0.47
2:A:812:NAG:O7	2:A:812:NAG:C1	2.60	0.47
1:B:402:LYS:C	1:B:403:ASN:O	2.46	0.47
1:C:186:GLU:OE1	2:C:801:NAG:C6	2.59	0.47
1:C:440:PRO:HB3	1:C:457:LEU:CD2	2.43	0.47
2:D:809:NAG:C6	2:D:810:NAG:C6	2.92	0.47
1:A:90:GLU:CB	1:B:3:VAL:CG2	2.93	0.47
1:A:246:ASP:C	1:A:247:LEU:HD12	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:THR:CB	2:A:807:NAG:N2	2.78	0.47
1:B:50:VAL:HB	1:B:51:PHE:CD1	2.50	0.47
1:C:23:GLN:HB2	1:C:59:TRP:CE3	2.50	0.47
1:C:300:ILE:HD12	1:C:300:ILE:N	2.30	0.47
1:C:537:ILE:CG1	1:C:538:LYS:N	2.77	0.47
1:D:23:GLN:HB2	1:D:59:TRP:CE3	2.50	0.47
1:A:226:TYR:O	1:A:227:THR:HG23	2.15	0.47
1:A:301:THR:CG2	1:A:316:THR:HG23	2.45	0.47
1:B:271:ILE:O	1:B:271:ILE:HG23	2.15	0.47
1:B:373:ASN:CG	1:B:374:ASP:H	2.18	0.47
1:B:539:CYS:HB3	1:B:540:GLN:H	1.46	0.47
1:C:81:VAL:HG12	1:D:43:ALA:HB3	0.53	0.47
1:C:81:VAL:CG1	1:D:43:ALA:N	2.77	0.47
1:D:50:VAL:HB	1:D:51:PHE:CD1	2.50	0.47
1:A:8:LYS:HB3	1:D:30:ARG:HH21	1.79	0.47
1:A:23:GLN:HB2	1:A:59:TRP:CE3	2.50	0.47
1:A:108:PHE:HE1	1:A:203:VAL:HG23	1.80	0.47
1:B:88:VAL:CG1	1:C:27:ASN:OD1	2.60	0.47
1:B:320:THR:CB	2:B:807:NAG:N2	2.78	0.47
1:C:82:SER:OG	1:D:41:GLN:O	2.12	0.47
1:C:272:THR:CG2	1:C:273:THR:N	2.76	0.47
1:C:514:SER:CA	1:C:517:GLN:O	2.62	0.47
1:D:226:TYR:O	1:D:227:THR:HG23	2.15	0.47
1:D:418:SER:O	1:D:419:VAL:HG23	2.14	0.47
1:A:4:ILE:C	1:B:91:PRO:CB	2.82	0.46
1:A:89:GLU:O	1:B:1:ASP:C	2.54	0.46
1:A:270:ASN:OD1	1:A:271:ILE:N	2.49	0.46
1:A:300:ILE:HD12	1:A:300:ILE:N	2.30	0.46
1:A:373:ASN:CG	1:A:374:ASP:H	2.18	0.46
1:D:268:PHE:CA	1:D:285:ALA:HB3	2.45	0.46
1:D:301:THR:CG2	1:D:316:THR:HG23	2.45	0.46
1:D:482:THR:HG22	1:D:499:THR:H	1.70	0.46
1:B:155:PRO:O	1:B:157:GLU:N	2.43	0.46
1:B:310:VAL:HG12	1:B:311:PRO:O	2.15	0.46
1:B:408:VAL:O	1:B:426:LEU:N	2.48	0.46
1:C:3:VAL:HB	1:C:4:ILE:H	1.51	0.46
1:C:88:VAL:N	1:D:38:ILE:HG12	2.30	0.46
1:C:310:VAL:HG12	1:C:311:PRO:O	2.15	0.46
1:D:36:TYR:O	1:D:55:TRP:HA	2.15	0.46
1:D:272:THR:HG23	2:D:803:NAG:HN2	1.81	0.46
1:D:363:GLN:O	1:D:364:ILE:CG2	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:THR:CG2	2:A:807:NAG:H83	2.32	0.46
1:A:271:ILE:HG23	1:A:271:ILE:O	2.15	0.46
1:A:449:ASP:N	1:A:532:CYS:HB3	2.19	0.46
1:B:23:GLN:HB2	1:B:59:TRP:CE3	2.50	0.46
1:B:31:PHE:CD2	1:C:29:ASP:OD2	2.69	0.46
1:B:301:THR:CG2	1:B:316:THR:HG23	2.45	0.46
1:D:194:THR:CG2	1:D:195:ASP:N	2.79	0.46
1:A:194:THR:CG2	1:A:195:ASP:N	2.79	0.46
1:A:262:ARG:HG3	1:A:299:GLN:HB2	1.98	0.46
1:A:511:VAL:N	1:A:523:THR:O	2.46	0.46
1:B:368:SER:OG	1:B:370:PHE:HE1	1.94	0.46
1:A:87:PRO:O	1:B:2:TRP:HZ2	1.83	0.46
1:A:227:THR:N	2:A:812:NAG:H2	2.31	0.46
1:A:506:ASP:OD1	1:A:506:ASP:N	2.49	0.46
1:B:36:TYR:O	1:B:55:TRP:HA	2.15	0.46
1:C:54:GLU:HB2	1:C:57:THR:OG1	2.16	0.46
1:C:81:VAL:H	1:D:45:ASN:ND2	2.10	0.46
1:C:108:PHE:HE1	1:C:203:VAL:HG23	1.80	0.46
1:C:262:ARG:HG3	1:C:299:GLN:HB2	1.97	0.46
1:C:539:CYS:HB3	1:C:540:GLN:H	1.45	0.46
1:D:54:GLU:HB2	1:D:57:THR:OG1	2.16	0.46
1:D:155:PRO:O	1:D:157:GLU:N	2.43	0.46
1:D:506:ASP:OD1	1:D:506:ASP:N	2.49	0.46
1:A:36:TYR:O	1:A:55:TRP:HA	2.15	0.46
1:A:310:VAL:HG12	1:A:311:PRO:O	2.15	0.46
1:A:440:PRO:HB3	1:A:457:LEU:CD2	2.43	0.46
2:A:809:NAG:H61	2:A:810:NAG:C6	2.39	0.46
1:C:459:ILE:HD12	1:C:459:ILE:N	2.31	0.46
1:D:310:VAL:HG12	1:D:311:PRO:O	2.15	0.46
1:D:459:ILE:N	1:D:459:ILE:HD12	2.31	0.46
1:A:8:LYS:HE2	1:D:28:LYS:HG3	1.94	0.46
1:A:54:GLU:HB2	1:A:57:THR:OG1	2.16	0.46
1:A:79:HIS:CA	1:B:1:ASP:N	2.70	0.46
1:A:374:ASP:N	1:A:374:ASP:OD1	2.49	0.46
1:B:117:VAL:O	1:B:212:THR:N	2.46	0.46
1:B:155:PRO:CB	2:B:801:NAG:C8	2.94	0.46
1:B:194:THR:CG2	1:B:195:ASP:N	2.79	0.46
1:B:272:THR:HG23	2:B:803:NAG:HN2	1.80	0.46
1:B:459:ILE:HD12	1:B:459:ILE:N	2.31	0.46
1:C:3:VAL:HB	1:D:87:PRO:HB2	1.97	0.46
1:C:272:THR:HG23	2:C:803:NAG:HN2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:THR:HG21	2:C:809:NAG:H61	1.98	0.46
1:D:187:TYR:HE1	1:D:211:ILE:HD11	1.81	0.46
1:D:374:ASP:N	1:D:374:ASP:OD1	2.49	0.46
1:B:109:THR:CB	1:B:131:SER:HB2	2.46	0.46
1:B:461:ASP:HB3	1:B:468:THR:CG2	2.46	0.46
1:B:514:SER:CA	1:B:517:GLN:O	2.62	0.46
1:C:31:PHE:C	1:D:73:LYS:CE	2.83	0.46
1:C:100:ASP:OD1	1:C:101:GLN:N	2.49	0.46
1:C:194:THR:CG2	1:C:195:ASP:N	2.79	0.46
1:C:374:ASP:N	1:C:374:ASP:OD1	2.49	0.46
1:C:415:ASP:CG	1:C:416:GLY:H	2.16	0.46
1:C:448:CYS:SG	1:C:537:ILE:CG2	3.01	0.46
1:D:100:ASP:OD1	1:D:101:GLN:N	2.49	0.46
1:D:339:VAL:HG11	1:D:351:ILE:HG23	1.98	0.46
1:A:363:GLN:O	1:A:364:ILE:CG2	2.63	0.46
1:B:450:GLN:CB	1:B:533:GLU:HA	2.29	0.46
1:B:506:ASP:OD1	1:B:506:ASP:N	2.49	0.46
1:C:90:GLU:N	1:D:78:SER:C	2.30	0.46
1:C:227:THR:N	2:C:812:NAG:H2	2.31	0.46
1:C:241:ARG:HE	1:C:281:ILE:CD1	2.24	0.46
1:C:286:LYS:C	1:C:287:GLY:O	2.55	0.46
1:C:408:VAL:O	1:C:426:LEU:N	2.49	0.46
1:D:270:ASN:OD1	1:D:271:ILE:N	2.49	0.46
1:A:286:LYS:C	1:A:287:GLY:O	2.55	0.46
1:A:374:ASP:C	1:A:375:PRO:O	2.54	0.46
1:A:380:THR:CG2	1:A:381:VAL:N	2.79	0.46
1:A:449:ASP:CB	1:A:532:CYS:N	2.74	0.46
1:B:100:ASP:OD1	1:B:101:GLN:N	2.49	0.46
1:B:227:THR:N	2:B:812:NAG:H2	2.31	0.46
1:B:363:GLN:O	1:B:364:ILE:CG2	2.63	0.46
1:B:380:THR:CG2	1:B:381:VAL:N	2.79	0.46
1:C:1:ASP:CA	1:D:28:LYS:CD	2.88	0.46
1:C:276:GLU:HG3	1:C:277:SER:N	2.25	0.46
2:C:805:NAG:C5	2:C:806:NAG:H83	2.46	0.46
1:D:109:THR:CB	1:D:131:SER:HB2	2.46	0.46
1:D:290:PHE:CE2	1:D:293:ARG:CB	2.92	0.46
1:D:524:VAL:HG21	2:D:904:NAG:C8	2.44	0.46
1:A:8:LYS:CD	1:A:8:LYS:N	2.51	0.45
1:B:30:ARG:NH1	1:C:30:ARG:CB	2.78	0.45
1:B:262:ARG:HG3	1:B:299:GLN:HB2	1.98	0.45
1:B:374:ASP:N	1:B:374:ASP:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:VAL:CG2	1:B:487:LEU:HD21	2.47	0.45
1:C:32:ASN:CA	1:D:75:VAL:HG23	2.44	0.45
1:C:109:THR:CB	1:C:131:SER:HB2	2.46	0.45
1:C:227:THR:HG22	1:C:320:THR:HB	1.98	0.45
1:C:271:ILE:HG23	1:C:271:ILE:O	2.15	0.45
1:C:451:ASN:O	1:C:534:GLY:CA	2.60	0.45
1:D:227:THR:HG22	1:D:320:THR:HB	1.99	0.45
1:D:415:ASP:CG	1:D:416:GLY:H	2.16	0.45
1:D:461:ASP:HB3	1:D:468:THR:CG2	2.46	0.45
2:D:805:NAG:C5	2:D:806:NAG:H83	2.46	0.45
1:A:117:VAL:O	1:A:212:THR:N	2.46	0.45
1:A:155:PRO:CB	2:A:801:NAG:C8	2.94	0.45
1:A:241:ARG:HE	1:A:281:ILE:CD1	2.24	0.45
1:A:276:GLU:HG3	1:A:277:SER:N	2.25	0.45
1:A:298:LEU:N	1:A:298:LEU:CD2	2.75	0.45
1:A:312:LEU:O	3:A:804:NDG:H8C1	2.17	0.45
1:A:408:VAL:O	1:A:426:LEU:N	2.48	0.45
1:A:459:ILE:N	1:A:459:ILE:HD12	2.31	0.45
1:A:519:ASN:CG	1:A:519:ASN:O	2.55	0.45
1:B:227:THR:HG22	1:B:320:THR:HB	1.98	0.45
1:B:381:VAL:HA	1:B:387:ILE:O	2.17	0.45
1:B:468:THR:C	1:B:469:TYR:O	2.54	0.45
1:C:1:ASP:O	1:D:28:LYS:HD3	2.16	0.45
1:C:28:LYS:CG	1:D:93:GLU:HG2	2.11	0.45
1:C:268:PHE:CA	1:C:285:ALA:HB3	2.45	0.45
1:C:371:ILE:HD12	1:C:371:ILE:HA	1.65	0.45
1:C:450:GLN:CB	1:C:533:GLU:OE2	2.64	0.45
1:C:514:SER:HG	1:C:519:ASN:HA	1.81	0.45
1:D:108:PHE:HE1	1:D:203:VAL:HG23	1.80	0.45
1:D:271:ILE:HG23	1:D:271:ILE:O	2.15	0.45
1:D:408:VAL:O	1:D:426:LEU:N	2.49	0.45
1:A:421:THR:HG21	2:A:809:NAG:H61	1.98	0.45
1:B:85:GLY:N	1:C:25:LYS:O	2.47	0.45
1:B:261:ILE:HD11	1:B:264:ASN:ND2	2.32	0.45
1:C:506:ASP:OD1	1:C:506:ASP:N	2.49	0.45
1:D:152:LYS:O	1:D:189:LEU:HA	2.17	0.45
1:D:473:VAL:CG2	1:D:487:LEU:HD21	2.47	0.45
1:A:381:VAL:HA	1:A:387:ILE:O	2.17	0.45
1:B:8:LYS:CD	1:B:8:LYS:N	2.51	0.45
1:B:187:TYR:HE1	1:B:211:ILE:HD11	1.81	0.45
1:B:270:ASN:OD1	1:B:271:ILE:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:LYS:C	1:B:287:GLY:O	2.55	0.45
1:B:450:GLN:CB	1:B:533:GLU:OE2	2.64	0.45
1:C:1:ASP:C	1:D:28:LYS:HD3	2.37	0.45
1:C:187:TYR:HE1	1:C:211:ILE:HD11	1.81	0.45
1:D:381:VAL:HA	1:D:387:ILE:O	2.17	0.45
1:D:440:PRO:HB3	1:D:457:LEU:CD2	2.43	0.45
1:A:187:TYR:HE1	1:A:211:ILE:HD11	1.81	0.45
1:A:336:VAL:HG11	1:A:338:ARG:HD2	1.99	0.45
1:A:380:THR:HG22	1:A:381:VAL:N	2.32	0.45
1:B:152:LYS:O	1:B:189:LEU:HA	2.17	0.45
1:B:421:THR:HG21	2:B:809:NAG:H61	1.98	0.45
1:B:519:ASN:O	1:B:519:ASN:CG	2.55	0.45
1:B:524:VAL:HG21	2:B:904:NAG:C8	2.44	0.45
1:C:93:GLU:CB	1:D:81:VAL:CG1	2.79	0.45
1:C:363:GLN:O	1:C:364:ILE:CG2	2.63	0.45
1:D:266:GLY:N	1:D:268:PHE:CE2	2.76	0.45
1:D:421:THR:HG21	2:D:809:NAG:H61	1.98	0.45
1:A:100:ASP:OD1	1:A:101:GLN:N	2.49	0.45
1:A:261:ILE:HD11	1:A:264:ASN:ND2	2.32	0.45
1:A:339:VAL:HG11	1:A:351:ILE:HG23	1.98	0.45
1:A:367:LEU:H	1:A:367:LEU:HG	1.41	0.45
1:A:451:ASN:O	1:A:534:GLY:CA	2.60	0.45
1:A:461:ASP:HB3	1:A:468:THR:CG2	2.46	0.45
1:A:481:LEU:HD12	1:A:481:LEU:HA	1.50	0.45
2:A:805:NAG:C5	2:A:806:NAG:H83	2.46	0.45
1:B:371:ILE:HD12	1:B:371:ILE:HA	1.65	0.45
1:B:469:TYR:CD2	1:B:470:PRO:N	2.85	0.45
1:C:339:VAL:HG11	1:C:351:ILE:HG23	1.98	0.45
1:C:381:VAL:HA	1:C:387:ILE:O	2.17	0.45
1:C:449:ASP:N	1:C:532:CYS:HB3	2.19	0.45
1:C:461:ASP:HB3	1:C:468:THR:CG2	2.46	0.45
1:D:449:ASP:CB	1:D:532:CYS:N	2.74	0.45
1:A:426:LEU:HD13	1:A:426:LEU:C	2.37	0.45
1:B:187:TYR:CE1	1:B:211:ILE:HD11	2.52	0.45
1:B:482:THR:O	1:B:483:TRP:CD2	2.70	0.45
2:B:805:NAG:H62	2:B:806:NAG:N2	2.31	0.45
1:C:298:LEU:N	1:C:298:LEU:CD2	2.75	0.45
1:C:371:ILE:HD13	1:C:381:VAL:HG11	1.95	0.45
1:D:336:VAL:HG11	1:D:338:ARG:HD2	1.99	0.45
1:D:450:GLN:CB	1:D:533:GLU:OE2	2.64	0.45
1:A:272:THR:HG23	2:A:803:NAG:HN2	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:CYS:SG	1:A:537:ILE:CG2	3.01	0.45
1:A:482:THR:O	1:A:483:TRP:CD2	2.70	0.45
1:B:54:GLU:HB2	1:B:57:THR:OG1	2.16	0.45
1:B:128:MET:HB3	1:B:129:ALA:H	1.62	0.45
1:B:134:ASP:HB2	1:B:146:LEU:HD11	1.99	0.45
1:B:162:LEU:HB2	1:B:163:PHE:CE1	2.52	0.45
1:B:312:LEU:O	3:B:804:NDG:H8C1	2.17	0.45
1:C:117:VAL:O	1:C:212:THR:N	2.46	0.45
1:C:187:TYR:CE1	1:C:211:ILE:HD11	2.52	0.45
1:C:336:VAL:HG11	1:C:338:ARG:HD2	1.99	0.45
1:C:426:LEU:HD13	1:C:426:LEU:C	2.37	0.45
1:D:109:THR:HB	1:D:131:SER:HB2	1.99	0.45
1:D:162:LEU:HB2	1:D:163:PHE:CE1	2.52	0.45
1:A:1:ASP:OD1	1:B:24:ILE:HB	2.17	0.45
1:A:232:GLU:HA	1:A:288:LEU:HD12	1.99	0.45
1:A:450:GLN:CB	1:A:533:GLU:OE2	2.64	0.45
1:A:469:TYR:CE2	1:A:470:PRO:HB2	2.52	0.45
1:B:380:THR:HG22	1:B:381:VAL:N	2.32	0.45
1:C:78:SER:O	1:D:39:THR:HG21	2.17	0.45
1:D:262:ARG:HG3	1:D:299:GLN:HB2	1.97	0.45
1:D:482:THR:O	1:D:483:TRP:CD2	2.70	0.45
1:A:162:LEU:HB2	1:A:163:PHE:CE1	2.52	0.45
1:A:473:VAL:CG2	1:A:487:LEU:HD21	2.47	0.45
1:A:485:ALA:O	1:A:486:GLU:OE1	2.35	0.45
1:B:108:PHE:HE1	1:B:203:VAL:HG23	1.80	0.45
1:C:31:PHE:O	1:D:73:LYS:NZ	2.47	0.45
1:C:134:ASP:HB2	1:C:146:LEU:HD11	1.99	0.45
1:C:270:ASN:OD1	1:C:271:ILE:N	2.49	0.45
1:C:380:THR:HG22	1:C:381:VAL:N	2.32	0.45
1:D:187:TYR:CE1	1:D:211:ILE:HD11	2.52	0.45
1:D:286:LYS:C	1:D:287:GLY:O	2.55	0.45
1:D:469:TYR:CD2	1:D:470:PRO:N	2.85	0.45
1:D:485:ALA:O	1:D:486:GLU:OE1	2.35	0.45
1:A:36:TYR:CE2	1:D:2:TRP:CH2	3.00	0.44
1:A:109:THR:CB	1:A:131:SER:HB2	2.46	0.44
1:B:441:SER:CB	1:B:442:PRO:HD3	2.47	0.44
1:C:3:VAL:CB	1:D:87:PRO:HB2	2.47	0.44
1:C:79:HIS:HB3	1:D:39:THR:HB	1.96	0.44
1:C:109:THR:HB	1:C:131:SER:HB2	1.99	0.44
1:D:227:THR:N	2:D:812:NAG:H2	2.31	0.44
1:B:30:ARG:CZ	1:C:30:ARG:HB3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:PHE:CE1	1:D:75:VAL:HG12	2.38	0.44
1:B:426:LEU:HD13	1:B:426:LEU:C	2.37	0.44
1:C:83:GLU:N	1:D:41:GLN:CD	2.66	0.44
1:C:482:THR:O	1:C:483:TRP:CD2	2.70	0.44
1:A:109:THR:HB	1:A:131:SER:HB2	1.99	0.44
1:A:134:ASP:HB2	1:A:146:LEU:HD11	1.99	0.44
1:A:415:ASP:CG	1:A:416:GLY:H	2.16	0.44
1:B:339:VAL:HG11	1:B:351:ILE:HG23	1.98	0.44
1:C:469:TYR:CE2	1:C:470:PRO:HB2	2.52	0.44
1:C:473:VAL:CG2	1:C:487:LEU:HD21	2.47	0.44
1:D:312:LEU:O	3:D:804:NDG:H8C1	2.17	0.44
1:A:67:ASP:OD1	1:A:69:GLU:HB2	2.18	0.44
1:A:469:TYR:CD2	1:A:470:PRO:N	2.85	0.44
1:B:336:VAL:HG11	1:B:338:ARG:HD2	1.99	0.44
1:B:439:VAL:HA	1:B:440:PRO:HD3	1.81	0.44
1:C:461:ASP:HB3	1:C:468:THR:HG22	2.00	0.44
1:C:468:THR:C	1:C:469:TYR:O	2.54	0.44
1:D:519:ASN:CG	1:D:519:ASN:O	2.55	0.44
1:A:86:SER:HA	1:A:87:PRO:HD3	1.83	0.44
1:A:152:LYS:O	1:A:189:LEU:HA	2.17	0.44
1:A:224:LYS:HE3	2:A:806:NAG:C8	2.48	0.44
1:B:224:LYS:HE3	2:B:806:NAG:C8	2.48	0.44
1:B:442:PRO:HD2	1:B:457:LEU:HD12	2.00	0.44
2:B:805:NAG:C5	2:B:806:NAG:H83	2.46	0.44
1:C:84:ASN:C	1:D:74:TYR:HE2	2.07	0.44
1:C:261:ILE:HD11	1:C:264:ASN:ND2	2.32	0.44
1:D:28:LYS:CD	1:D:88:VAL:HG12	2.38	0.44
1:D:374:ASP:C	1:D:375:PRO:O	2.54	0.44
1:D:511:VAL:N	1:D:523:THR:O	2.46	0.44
1:A:22:VAL:CG2	1:A:23:GLN:N	2.81	0.44
1:A:252:THR:HA	1:A:253:PRO:HD3	1.81	0.44
1:A:441:SER:CB	1:A:442:PRO:HD3	2.47	0.44
1:B:31:PHE:O	1:C:29:ASP:C	2.56	0.44
1:B:485:ALA:O	1:B:486:GLU:OE1	2.35	0.44
1:C:85:GLY:CA	1:D:47:PRO:HD2	2.48	0.44
1:D:67:ASP:OD1	1:D:69:GLU:HB2	2.18	0.44
1:D:224:LYS:HE3	2:D:806:NAG:C8	2.48	0.44
1:D:232:GLU:HA	1:D:288:LEU:HD12	1.99	0.44
1:D:380:THR:CG2	1:D:381:VAL:N	2.79	0.44
1:B:194:THR:HG23	1:B:201:LEU:O	2.18	0.44
1:B:290:PHE:CD2	1:B:293:ARG:O	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:THR:CG2	2:B:807:NAG:C2	2.76	0.44
1:C:22:VAL:CG2	1:C:23:GLN:N	2.81	0.44
1:C:67:ASP:OD1	1:C:69:GLU:HB2	2.18	0.44
1:C:152:LYS:O	1:C:189:LEU:HA	2.17	0.44
1:C:220:ILE:O	1:C:220:ILE:HG22	2.18	0.44
1:D:290:PHE:CD2	1:D:293:ARG:O	2.71	0.44
1:D:421:THR:CG2	1:D:422:GLY:N	2.81	0.44
1:A:227:THR:HG22	1:A:320:THR:HB	1.98	0.44
1:A:442:PRO:HD2	1:A:457:LEU:HD12	2.00	0.44
1:A:524:VAL:HG21	2:A:904:NAG:C8	2.44	0.44
1:C:88:VAL:HA	1:D:38:ILE:HD11	1.99	0.44
1:C:380:THR:CG2	1:C:381:VAL:N	2.79	0.44
1:D:155:PRO:CB	2:D:801:NAG:C8	2.94	0.44
1:D:261:ILE:HD11	1:D:264:ASN:ND2	2.32	0.44
1:D:435:ASP:HB2	1:D:436:ASN:H	1.58	0.44
1:A:3:VAL:HG21	1:B:77:SER:HA	2.00	0.44
1:A:92:MET:HB2	1:B:1:ASP:CB	2.48	0.44
1:A:290:PHE:CD2	1:A:293:ARG:O	2.71	0.44
1:A:540:GLN:O	1:A:540:GLN:NE2	2.47	0.44
1:B:22:VAL:CG2	1:B:23:GLN:N	2.81	0.44
1:B:368:SER:CB	1:B:370:PHE:HE1	2.31	0.44
1:B:469:TYR:CE2	1:B:470:PRO:HB2	2.52	0.44
1:C:32:ASN:HD22	1:C:83:GLU:N	2.13	0.44
1:C:151:LEU:HD12	1:C:151:LEU:N	2.33	0.44
1:C:162:LEU:HB2	1:C:163:PHE:CE1	2.52	0.44
1:A:419:VAL:HG13	1:A:420:GLY:N	2.33	0.43
1:B:3:VAL:HB	1:B:4:ILE:H	1.51	0.43
1:B:109:THR:HB	1:B:131:SER:HB2	1.99	0.43
1:B:151:LEU:HD12	1:B:151:LEU:N	2.33	0.43
1:B:421:THR:CG2	1:B:422:GLY:N	2.81	0.43
1:B:522:LEU:HA	1:B:522:LEU:HD23	1.36	0.43
1:C:374:ASP:C	1:C:375:PRO:O	2.54	0.43
1:C:469:TYR:CD2	1:C:470:PRO:N	2.85	0.43
1:C:485:ALA:O	1:C:486:GLU:OE1	2.35	0.43
1:D:468:THR:C	1:D:469:TYR:O	2.54	0.43
1:D:469:TYR:CE2	1:D:470:PRO:HB2	2.52	0.43
1:A:8:LYS:CB	1:D:30:ARG:HE	2.30	0.43
1:A:92:MET:CG	1:B:3:VAL:HG12	2.47	0.43
1:A:421:THR:CG2	1:A:422:GLY:N	2.81	0.43
1:A:468:THR:C	1:A:469:TYR:O	2.54	0.43
1:B:374:ASP:C	1:B:375:PRO:O	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:VAL:HG13	1:B:420:GLY:N	2.33	0.43
1:C:312:LEU:O	3:C:804:NDG:H8C1	2.17	0.43
1:D:220:ILE:O	1:D:220:ILE:HG22	2.18	0.43
2:D:805:NAG:H62	2:D:806:NAG:N2	2.31	0.43
1:A:299:GLN:CG	1:A:318:THR:HG23	2.42	0.43
1:A:335:ALA:HB3	3:A:811:NDG:O6	2.15	0.43
1:B:232:GLU:HA	1:B:288:LEU:HD12	2.00	0.43
1:B:450:GLN:HG3	1:B:532:CYS:O	2.10	0.43
1:C:89:GLU:HB3	1:D:78:SER:O	2.01	0.43
1:C:232:GLU:HA	1:C:288:LEU:HD12	1.99	0.43
1:C:511:VAL:N	1:C:523:THR:O	2.46	0.43
1:D:426:LEU:HD13	1:D:426:LEU:C	2.37	0.43
1:D:441:SER:CB	1:D:442:PRO:HD3	2.47	0.43
1:A:194:THR:HG23	1:A:201:LEU:O	2.18	0.43
1:A:247:LEU:HD12	1:A:247:LEU:N	2.33	0.43
1:B:252:THR:HA	1:B:253:PRO:HD3	1.81	0.43
1:B:297:VAL:HG21	2:B:807:NAG:H62	2.01	0.43
1:C:92:MET:CE	1:D:91:PRO:CG	2.97	0.43
1:C:128:MET:HB3	1:C:129:ALA:H	1.62	0.43
1:C:290:PHE:CD2	1:C:293:ARG:O	2.71	0.43
1:C:441:SER:CB	1:C:442:PRO:HD3	2.47	0.43
1:D:128:MET:HB3	1:D:129:ALA:H	1.62	0.43
1:A:187:TYR:CE1	1:A:211:ILE:HD11	2.52	0.43
1:A:368:SER:CB	1:A:370:PHE:HE1	2.31	0.43
1:C:224:LYS:HE3	2:C:806:NAG:C8	2.48	0.43
1:C:442:PRO:HD2	1:C:457:LEU:HD12	2.00	0.43
1:C:518:ASN:C	1:C:520:PRO:CD	2.87	0.43
1:D:247:LEU:HD12	1:D:247:LEU:N	2.33	0.43
1:D:380:THR:HG22	1:D:381:VAL:N	2.32	0.43
1:D:419:VAL:HG13	1:D:420:GLY:N	2.33	0.43
1:D:461:ASP:HB3	1:D:468:THR:HG22	2.00	0.43
1:A:4:ILE:HB	1:B:90:GLU:HB3	1.48	0.43
1:B:354:LEU:HD12	1:B:386:GLY:O	2.18	0.43
1:C:31:PHE:C	1:D:75:VAL:CG2	2.79	0.43
1:C:421:THR:CG2	1:C:422:GLY:N	2.81	0.43
1:D:3:VAL:HB	1:D:4:ILE:H	1.51	0.43
1:D:194:THR:HG23	1:D:201:LEU:O	2.18	0.43
1:D:249:MET:HA	1:D:250:PRO:HD3	1.85	0.43
1:D:335:ALA:HB3	3:D:811:NDG:O6	2.15	0.43
1:D:368:SER:CB	1:D:370:PHE:HE1	2.31	0.43
1:D:442:PRO:HD2	1:D:457:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:ASN:HA	1:C:29:ASP:CG	2.36	0.43
1:B:83:GLU:HB3	1:C:25:LYS:HB2	1.45	0.43
1:B:333:VAL:HG23	1:B:334:PRO:HD3	2.01	0.43
1:B:540:GLN:O	1:B:540:GLN:NE2	2.47	0.43
1:C:155:PRO:CB	2:C:801:NAG:C8	2.94	0.43
1:D:134:ASP:HB2	1:D:146:LEU:HD11	1.99	0.43
1:D:450:GLN:HG3	1:D:532:CYS:O	2.10	0.43
1:A:1:ASP:CA	1:B:24:ILE:CD1	2.95	0.43
1:A:9:VAL:O	1:D:30:ARG:CD	2.62	0.43
1:A:32:ASN:HD22	1:A:83:GLU:N	2.13	0.43
1:A:79:HIS:CA	1:B:1:ASP:H1	2.30	0.43
1:A:195:ASP:HB3	1:A:196:LEU:HG	2.01	0.43
1:C:154:ASP:HB3	2:C:801:NAG:C7	2.48	0.43
1:C:194:THR:HG23	1:C:201:LEU:O	2.18	0.43
1:C:344:ASP:CG	1:C:344:ASP:O	2.57	0.43
1:D:22:VAL:CG2	1:D:23:GLN:N	2.81	0.43
1:D:32:ASN:HD22	1:D:83:GLU:N	2.13	0.43
1:D:175:ILE:CG2	1:D:176:GLY:N	2.82	0.43
1:A:297:VAL:HG21	2:A:807:NAG:H62	2.01	0.43
1:A:333:VAL:HG23	1:A:334:PRO:HD3	2.01	0.43
1:A:354:LEU:HD12	1:A:386:GLY:O	2.18	0.43
1:B:67:ASP:OD1	1:B:69:GLU:HB2	2.18	0.43
1:B:247:LEU:HD12	1:B:247:LEU:N	2.33	0.43
1:C:40:GLY:O	1:C:45:ASN:HB2	2.19	0.43
1:C:354:LEU:HD12	1:C:386:GLY:O	2.18	0.43
1:C:368:SER:CB	1:C:370:PHE:HE1	2.31	0.43
1:D:367:LEU:H	1:D:367:LEU:HG	1.41	0.43
1:D:371:ILE:HG13	1:D:410:MET:SD	2.59	0.43
1:A:24:ILE:O	1:D:2:TRP:CH2	2.58	0.43
1:A:518:ASN:C	1:A:520:PRO:CD	2.87	0.43
1:B:371:ILE:HG13	1:B:410:MET:SD	2.59	0.43
1:C:519:ASN:CG	1:C:519:ASN:O	2.55	0.43
1:D:138:ASN:C	1:D:138:ASN:ND2	2.73	0.43
1:D:344:ASP:O	1:D:344:ASP:CG	2.57	0.43
1:D:354:LEU:HD12	1:D:386:GLY:O	2.18	0.43
1:A:188:THR:H	2:A:801:NAG:H83	1.84	0.42
1:A:344:ASP:O	1:A:344:ASP:CG	2.57	0.42
1:A:409:ILE:HD13	3:A:811:NDG:H8C3	2.01	0.42
1:B:220:ILE:O	1:B:220:ILE:HG22	2.18	0.42
2:B:810:NAG:O7	2:B:810:NAG:C1	2.67	0.42
1:C:333:VAL:HG23	1:C:334:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:524:VAL:HG21	2:C:904:NAG:C8	2.44	0.42
1:D:298:LEU:N	1:D:298:LEU:CD2	2.75	0.42
1:D:339:VAL:HG21	1:D:351:ILE:HG22	2.01	0.42
1:A:90:GLU:O	1:A:91:PRO:O	2.37	0.42
1:A:230:VAL:O	1:A:323:VAL:HA	2.20	0.42
1:A:461:ASP:HB3	1:A:468:THR:HG22	2.00	0.42
1:B:435:ASP:HB2	1:B:436:ASN:H	1.58	0.42
1:B:461:ASP:HB3	1:B:468:THR:HG22	2.00	0.42
1:C:261:ILE:H	1:C:261:ILE:HD13	1.85	0.42
1:C:490:LYS:O	1:C:490:LYS:CG	2.67	0.42
1:D:518:ASN:C	1:D:520:PRO:CD	2.87	0.42
1:A:371:ILE:HG13	1:A:410:MET:SD	2.59	0.42
1:B:175:ILE:CG2	1:B:176:GLY:N	2.82	0.42
1:C:4:ILE:HA	1:C:5:PRO:HD3	1.72	0.42
1:C:450:GLN:HG3	1:C:532:CYS:O	2.10	0.42
1:A:92:MET:HG2	1:B:3:VAL:HG12	2.01	0.42
1:A:151:LEU:HD12	1:A:151:LEU:N	2.33	0.42
1:A:347:ARG:HD2	1:A:392:GLY:CA	2.50	0.42
1:B:40:GLY:O	1:B:45:ASN:HB2	2.19	0.42
1:B:409:ILE:HD13	3:B:811:NDG:H8C3	2.01	0.42
1:C:5:PRO:HA	1:C:6:PRO:HD3	1.85	0.42
1:C:88:VAL:O	1:D:94:ILE:CD1	2.50	0.42
1:C:247:LEU:HD12	1:C:247:LEU:N	2.33	0.42
1:C:371:ILE:HA	1:C:410:MET:HB3	2.02	0.42
1:C:515:ASP:OD1	1:C:516:ALA:N	2.53	0.42
1:D:333:VAL:HG23	1:D:334:PRO:HD3	2.01	0.42
1:D:409:ILE:HD13	3:D:811:NDG:H8C3	2.01	0.42
1:A:5:PRO:HA	1:A:6:PRO:HD3	1.85	0.42
1:A:175:ILE:CG2	1:A:176:GLY:N	2.82	0.42
1:A:239:VAL:HG11	1:A:282:LEU:HD22	2.02	0.42
1:A:250:PRO:HA	1:A:255:TRP:CG	2.55	0.42
1:C:88:VAL:N	1:D:38:ILE:CG1	2.82	0.42
1:C:339:VAL:HG21	1:C:351:ILE:HG22	2.01	0.42
1:D:347:ARG:HD2	1:D:392:GLY:CA	2.49	0.42
1:D:448:CYS:C	1:D:452:PRO:HG3	2.40	0.42
1:D:482:THR:HG23	1:D:499:THR:HG23	1.88	0.42
1:A:138:ASN:C	1:A:138:ASN:ND2	2.73	0.42
1:A:220:ILE:O	1:A:220:ILE:HG22	2.18	0.42
2:A:805:NAG:H62	2:A:806:NAG:N2	2.31	0.42
1:B:339:VAL:HG21	1:B:351:ILE:HG22	2.01	0.42
1:B:469:TYR:CE2	1:B:470:PRO:HD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:GLU:CD	1:D:92:MET:H	2.22	0.42
1:C:252:THR:HA	1:C:253:PRO:HD3	1.81	0.42
1:D:195:ASP:HB3	1:D:196:LEU:HG	2.01	0.42
1:D:261:ILE:HD13	1:D:261:ILE:H	1.85	0.42
1:D:264:ASN:HB3	1:D:267:GLY:HA2	2.01	0.42
1:D:469:TYR:CE2	1:D:470:PRO:HD2	2.54	0.42
1:A:505:GLY:H	1:A:529:VAL:HB	1.85	0.42
1:B:502:LEU:HA	1:B:502:LEU:HD23	1.82	0.42
1:B:518:ASN:C	1:B:520:PRO:CD	2.87	0.42
1:C:67:ASP:CG	1:C:69:GLU:HB2	2.40	0.42
1:C:83:GLU:CA	1:D:41:GLN:OE1	2.59	0.42
1:C:175:ILE:CG2	1:C:176:GLY:N	2.82	0.42
1:C:367:LEU:H	1:C:367:LEU:HG	1.41	0.42
1:D:7:ILE:O	1:D:96:ILE:HG23	2.20	0.42
1:D:188:THR:H	2:D:801:NAG:H83	1.84	0.42
1:D:250:PRO:HA	1:D:255:TRP:CG	2.54	0.42
1:D:297:VAL:HG21	2:D:807:NAG:H62	2.01	0.42
1:A:108:PHE:HA	1:A:132:ALA:CB	2.50	0.42
1:A:264:ASN:HB3	1:A:267:GLY:HA2	2.01	0.42
1:B:84:ASN:O	1:C:24:ILE:CA	2.68	0.42
1:B:87:PRO:HG2	1:D:90:GLU:H	1.82	0.42
1:B:87:PRO:CG	1:C:2:TRP:CB	2.94	0.42
1:B:108:PHE:HA	1:B:132:ALA:CB	2.50	0.42
1:B:188:THR:H	2:B:801:NAG:H83	1.84	0.42
1:B:230:VAL:O	1:B:323:VAL:HA	2.20	0.42
1:B:298:LEU:N	1:B:298:LEU:CD2	2.75	0.42
1:B:344:ASP:CG	1:B:344:ASP:O	2.57	0.42
1:C:239:VAL:HG11	1:C:282:LEU:HD22	2.02	0.42
1:C:371:ILE:HG13	1:C:410:MET:SD	2.59	0.42
1:D:67:ASP:CG	1:D:69:GLU:HB2	2.40	0.42
1:D:151:LEU:HD12	1:D:151:LEU:N	2.33	0.42
1:D:483:TRP:CZ2	1:D:507:TYR:CE1	2.87	0.42
1:B:67:ASP:CG	1:B:69:GLU:HB2	2.40	0.42
1:B:87:PRO:CG	1:C:2:TRP:CD1	3.03	0.42
1:C:7:ILE:O	1:C:96:ILE:HG23	2.20	0.42
1:C:138:ASN:C	1:C:138:ASN:ND2	2.73	0.42
1:C:188:THR:H	2:C:801:NAG:H83	1.84	0.42
1:C:347:ARG:HD2	1:C:392:GLY:CA	2.50	0.42
1:C:409:ILE:HD13	3:C:811:NDG:H8C3	2.01	0.42
1:D:231:PRO:O	1:D:288:LEU:HD12	2.20	0.42
1:B:31:PHE:CE2	1:C:27:ASN:N	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:ASP:HB3	1:B:196:LEU:HG	2.01	0.42
1:B:264:ASN:HB3	1:B:267:GLY:HA2	2.01	0.42
1:B:335:ALA:HB3	3:B:811:NDG:O6	2.15	0.42
1:B:347:ARG:HD2	1:B:392:GLY:CA	2.50	0.42
1:B:515:ASP:OD1	1:B:516:ALA:N	2.52	0.42
1:C:8:LYS:CD	1:C:8:LYS:N	2.51	0.42
1:C:23:GLN:HB2	1:C:59:TRP:CD2	2.55	0.42
1:C:90:GLU:HG2	1:D:36:TYR:HA	1.43	0.42
1:C:237:PHE:N	1:C:284:THR:OG1	2.42	0.42
1:C:366:LYS:HG2	1:C:367:LEU:H	1.74	0.42
1:C:419:VAL:HG13	1:C:420:GLY:N	2.33	0.42
1:D:490:LYS:O	1:D:490:LYS:CG	2.67	0.42
1:A:5:PRO:HG3	1:B:91:PRO:HG2	1.22	0.41
1:A:23:GLN:HB2	1:A:59:TRP:CD2	2.55	0.41
1:A:212:THR:CG2	1:A:213:ASP:H	2.32	0.41
1:B:7:ILE:O	1:B:96:ILE:HG23	2.20	0.41
1:B:81:VAL:HG12	1:D:90:GLU:HG2	2.02	0.41
1:C:250:PRO:HA	1:C:255:TRP:CG	2.54	0.41
1:D:522:LEU:HB3	1:D:523:THR:H	1.57	0.41
2:D:810:NAG:O7	2:D:810:NAG:C1	2.67	0.41
1:A:127:VAL:HG22	1:A:128:MET:HG3	2.03	0.41
1:A:230:VAL:HG23	1:A:323:VAL:HA	2.03	0.41
1:A:502:LEU:HD22	1:A:503:LYS:H	1.85	0.41
1:B:23:GLN:HB2	1:B:59:TRP:CD2	2.55	0.41
1:B:250:PRO:HA	1:B:255:TRP:CG	2.54	0.41
1:B:367:LEU:H	1:B:367:LEU:HG	1.41	0.41
1:D:4:ILE:HA	1:D:5:PRO:HD3	1.72	0.41
1:D:272:THR:CG2	1:D:273:THR:N	2.76	0.41
1:A:4:ILE:HB	1:B:90:GLU:C	2.39	0.41
1:A:7:ILE:O	1:A:96:ILE:HG23	2.20	0.41
1:A:515:ASP:OD1	1:A:516:ALA:N	2.52	0.41
1:B:212:THR:CG2	1:B:213:ASP:H	2.32	0.41
1:B:231:PRO:O	1:B:288:LEU:HD12	2.20	0.41
1:B:511:VAL:N	1:B:523:THR:O	2.46	0.41
1:C:231:PRO:O	1:C:235:ILE:HD13	2.21	0.41
1:C:264:ASN:HB3	1:C:267:GLY:HA2	2.01	0.41
1:C:297:VAL:HG21	2:C:807:NAG:H62	2.01	0.41
1:C:347:ARG:HG3	1:C:392:GLY:N	2.33	0.41
1:C:423:THR:CG2	2:C:810:NAG:N2	2.84	0.41
1:C:502:LEU:HD22	1:C:503:LYS:H	1.85	0.41
1:D:230:VAL:O	1:D:323:VAL:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:474:SER:N	1:D:512:LEU:O	2.53	0.41
1:A:339:VAL:HG21	1:A:351:ILE:HG22	2.01	0.41
1:A:469:TYR:CE2	1:A:470:PRO:HD2	2.54	0.41
2:A:810:NAG:O7	2:A:810:NAG:C1	2.67	0.41
1:B:23:GLN:HA	1:B:58:GLY:O	2.21	0.41
1:B:347:ARG:HG3	1:B:392:GLY:N	2.33	0.41
1:B:371:ILE:HA	1:B:410:MET:HB3	2.02	0.41
1:C:1:ASP:HB2	1:D:89:GLU:HG2	1.11	0.41
1:C:231:PRO:O	1:C:288:LEU:HD12	2.20	0.41
1:C:522:LEU:HA	1:C:522:LEU:HD23	1.36	0.41
1:D:108:PHE:HA	1:D:132:ALA:CB	2.50	0.41
1:A:23:GLN:HA	1:A:58:GLY:O	2.21	0.41
1:A:40:GLY:O	1:A:45:ASN:HB2	2.19	0.41
1:A:154:ASP:HB3	2:A:801:NAG:C7	2.48	0.41
1:B:127:VAL:HG22	1:B:128:MET:HG3	2.03	0.41
1:B:231:PRO:O	1:B:235:ILE:HD13	2.21	0.41
1:C:32:ASN:ND2	1:C:83:GLU:CB	2.62	0.41
1:C:108:PHE:HA	1:C:132:ALA:CB	2.50	0.41
1:D:23:GLN:HB2	1:D:59:TRP:CD2	2.55	0.41
1:D:108:PHE:HA	1:D:132:ALA:HB2	2.03	0.41
1:D:111:ASP:O	1:D:112:VAL:HG13	2.21	0.41
1:D:231:PRO:O	1:D:235:ILE:HD13	2.21	0.41
1:D:347:ARG:HG3	1:D:392:GLY:N	2.33	0.41
1:D:371:ILE:HA	1:D:410:MET:HB3	2.02	0.41
1:D:515:ASP:OD1	1:D:516:ALA:N	2.52	0.41
1:A:4:ILE:HD12	1:B:90:GLU:HB3	1.53	0.41
1:A:67:ASP:CG	1:A:69:GLU:HB2	2.40	0.41
1:A:68:ARG:HD3	1:A:100:ASP:CB	2.51	0.41
1:A:423:THR:CG2	2:A:810:NAG:N2	2.84	0.41
1:B:19:LYS:HB3	1:B:62:VAL:HG12	2.03	0.41
1:B:108:PHE:CZ	1:B:191:VAL:HG23	2.56	0.41
1:B:111:ASP:O	1:B:112:VAL:HG13	2.21	0.41
1:B:118:ARG:CA	1:B:212:THR:HB	2.51	0.41
1:B:474:SER:N	1:B:512:LEU:O	2.53	0.41
1:C:111:ASP:O	1:C:112:VAL:HG13	2.21	0.41
1:C:195:ASP:HB3	1:C:196:LEU:HG	2.01	0.41
1:D:68:ARG:HD3	1:D:100:ASP:CB	2.51	0.41
1:D:118:ARG:CA	1:D:212:THR:HB	2.51	0.41
1:A:62:VAL:O	1:A:62:VAL:HG13	2.21	0.41
1:C:68:ARG:HD3	1:C:100:ASP:CB	2.51	0.41
1:C:88:VAL:N	1:D:38:ILE:HD11	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:PHE:HA	1:C:132:ALA:HB2	2.03	0.41
1:C:108:PHE:CZ	1:C:191:VAL:HG23	2.56	0.41
1:C:474:SER:N	1:C:512:LEU:O	2.54	0.41
1:D:297:VAL:HG22	2:D:807:NAG:H62	2.03	0.41
1:A:36:TYR:CZ	1:D:2:TRP:HH2	2.39	0.41
1:A:111:ASP:O	1:A:112:VAL:HG13	2.21	0.41
1:A:448:CYS:C	1:A:452:PRO:HG3	2.40	0.41
1:B:432:ASP:CG	1:B:433:VAL:N	2.74	0.41
1:B:490:LYS:O	1:B:490:LYS:CG	2.67	0.41
1:B:505:GLY:H	1:B:529:VAL:HB	1.85	0.41
1:C:212:THR:CG2	1:C:213:ASP:H	2.32	0.41
1:C:274:ASP:HA	1:C:275:PRO:HD3	1.93	0.41
1:C:540:GLN:O	1:C:540:GLN:NE2	2.47	0.41
1:A:371:ILE:HA	1:A:410:MET:HB3	2.02	0.41
1:A:432:ASP:CG	1:A:433:VAL:N	2.74	0.41
1:A:474:SER:N	1:A:512:LEU:O	2.54	0.41
1:B:108:PHE:HA	1:B:132:ALA:HB2	2.03	0.41
1:B:261:ILE:HD13	1:B:261:ILE:H	1.85	0.41
1:B:316:THR:OG1	2:B:806:NAG:H83	2.21	0.41
1:B:409:ILE:HD13	3:B:811:NDG:C8	2.51	0.41
1:B:440:PRO:HB3	1:B:457:LEU:CD2	2.43	0.41
1:C:33:LYS:NZ	1:C:56:GLU:OE1	2.42	0.41
1:C:42:GLY:CA	1:C:47:PRO:O	2.69	0.41
1:C:62:VAL:O	1:C:62:VAL:HG13	2.21	0.41
1:C:118:ARG:CA	1:C:212:THR:HB	2.51	0.41
1:C:230:VAL:O	1:C:323:VAL:HA	2.20	0.41
1:C:239:VAL:HG13	1:C:240:GLN:N	2.33	0.41
1:C:297:VAL:HG22	2:C:807:NAG:H62	2.03	0.41
1:C:432:ASP:CG	1:C:433:VAL:N	2.74	0.41
1:D:119:GLU:CG	1:D:214:ALA:HB3	2.51	0.41
1:D:127:VAL:HG22	1:D:128:MET:HG3	2.03	0.41
1:D:239:VAL:HG11	1:D:282:LEU:HD22	2.02	0.41
1:D:432:ASP:CG	1:D:433:VAL:N	2.74	0.41
1:D:449:ASP:HB2	1:D:531:SER:HA	2.03	0.41
1:A:193:ALA:O	1:A:202:SER:HA	2.21	0.41
1:B:249:MET:O	1:B:252:THR:CB	2.69	0.41
1:C:84:ASN:C	1:D:74:TYR:CZ	2.90	0.41
1:C:252:THR:O	1:C:255:TRP:N	2.54	0.41
1:D:62:VAL:O	1:D:62:VAL:HG13	2.21	0.41
1:A:33:LYS:NZ	1:A:56:GLU:OE1	2.42	0.40
1:A:231:PRO:O	1:A:288:LEU:HD12	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:VAL:HG13	1:A:240:GLN:N	2.33	0.40
1:A:319:VAL:CG1	1:A:320:THR:N	2.84	0.40
1:A:490:LYS:O	1:A:490:LYS:CG	2.67	0.40
1:B:119:GLU:CG	1:B:214:ALA:HB3	2.51	0.40
1:B:230:VAL:HG23	1:B:323:VAL:HA	2.03	0.40
1:B:400:TYR:O	1:B:401:VAL:C	2.59	0.40
1:C:119:GLU:CG	1:C:214:ALA:HB3	2.51	0.40
1:C:193:ALA:O	1:C:202:SER:HA	2.21	0.40
1:C:320:THR:CG2	2:C:807:NAG:C2	2.76	0.40
2:C:810:NAG:O7	2:C:810:NAG:C1	2.67	0.40
1:D:138:ASN:HD22	1:D:138:ASN:N	2.19	0.40
1:D:259:TYR:O	1:D:260:LYS:CB	2.69	0.40
1:D:502:LEU:HD22	1:D:503:LYS:H	1.85	0.40
1:D:505:GLY:H	1:D:529:VAL:HB	1.85	0.40
1:D:522:LEU:HA	1:D:522:LEU:HD23	1.36	0.40
1:A:19:LYS:HB3	1:A:62:VAL:HG12	2.03	0.40
1:A:108:PHE:CZ	1:A:191:VAL:HG23	2.56	0.40
1:A:119:GLU:CG	1:A:214:ALA:HB3	2.51	0.40
1:A:316:THR:OG1	2:A:806:NAG:H83	2.21	0.40
1:B:19:LYS:HB3	1:B:62:VAL:CG1	2.52	0.40
1:C:400:TYR:O	1:C:401:VAL:C	2.59	0.40
1:D:108:PHE:CZ	1:D:191:VAL:HG23	2.56	0.40
1:D:252:THR:HA	1:D:253:PRO:HD3	1.81	0.40
1:D:316:THR:OG1	2:D:806:NAG:H83	2.21	0.40
1:A:272:THR:O	1:A:281:ILE:HG22	2.22	0.40
1:C:79:HIS:CB	1:D:39:THR:HB	2.35	0.40
1:C:230:VAL:HG23	1:C:323:VAL:HA	2.03	0.40
1:C:249:MET:O	1:C:252:THR:CB	2.69	0.40
1:C:249:MET:HA	1:C:250:PRO:HD3	1.85	0.40
1:C:290:PHE:CG	1:C:292:LEU:HB2	2.56	0.40
1:C:505:GLY:H	1:C:529:VAL:HB	1.85	0.40
1:D:23:GLN:HA	1:D:58:GLY:O	2.21	0.40
1:D:154:ASP:HB3	2:D:801:NAG:C7	2.48	0.40
1:D:249:MET:O	1:D:252:THR:CB	2.69	0.40
1:D:299:GLN:CG	1:D:318:THR:HG23	2.42	0.40
1:A:261:ILE:HD13	1:A:261:ILE:H	1.85	0.40
1:A:297:VAL:HG22	2:A:807:NAG:H62	2.03	0.40
1:B:68:ARG:HD3	1:B:100:ASP:CB	2.51	0.40
1:B:274:ASP:HA	1:B:275:PRO:HD3	1.93	0.40
1:B:449:ASP:N	1:B:532:CYS:HB3	2.19	0.40
1:C:34:VAL:CG1	1:C:80:ALA:HB1	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:GLU:HB3	1:D:79:HIS:H	1.59	0.40
1:C:329:ALA:HA	1:C:330:PRO:HD3	1.87	0.40
1:C:385:ASN:O	1:C:385:ASN:ND2	2.55	0.40
1:C:396:ARG:HH21	1:C:432:ASP:CG	2.25	0.40
1:C:469:TYR:CE2	1:C:470:PRO:HD2	2.54	0.40
1:D:19:LYS:HB3	1:D:62:VAL:HG12	2.03	0.40
1:D:34:VAL:CG1	1:D:80:ALA:HB1	2.52	0.40
1:D:193:ALA:O	1:D:202:SER:HA	2.21	0.40
1:D:230:VAL:HG23	1:D:323:VAL:HA	2.03	0.40
1:D:345:LEU:HD22	1:D:349:GLU:HB2	2.03	0.40
1:D:385:ASN:ND2	1:D:385:ASN:O	2.55	0.40
1:D:409:ILE:HD13	3:D:811:NDG:C8	2.51	0.40
1:A:231:PRO:O	1:A:235:ILE:HD13	2.21	0.40
1:A:249:MET:O	1:A:252:THR:CB	2.69	0.40
1:A:396:ARG:HH21	1:A:432:ASP:CG	2.25	0.40
1:A:482:THR:HG22	1:A:499:THR:H	1.70	0.40
1:B:373:ASN:CG	1:B:374:ASP:N	2.75	0.40
1:B:378:TRP:HB2	1:B:379:LEU:H	1.64	0.40
1:B:385:ASN:ND2	1:B:385:ASN:O	2.55	0.40
1:C:87:PRO:O	1:D:38:ILE:CD1	2.68	0.40
1:C:259:TYR:O	1:C:260:LYS:CB	2.69	0.40
1:C:445:PHE:CD2	1:C:445:PHE:N	2.89	0.40
1:D:19:LYS:HB3	1:D:62:VAL:CG1	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	538/880 (61%)	402 (75%)	91 (17%)	45 (8%)	0	9
1	B	538/880 (61%)	401 (74%)	93 (17%)	44 (8%)	1	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	538/880 (61%)	401 (74%)	92 (17%)	45 (8%)	0	9
1	D	538/880 (61%)	401 (74%)	92 (17%)	45 (8%)	0	9
All	All	2152/3520 (61%)	1605 (75%)	368 (17%)	179 (8%)	1	9

All (179) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	PRO
1	A	155	PRO
1	A	235	ILE
1	A	347	ARG
1	A	363	GLN
1	A	364	ILE
1	A	374	ASP
1	A	404	ASN
1	A	467	ASN
1	A	476	SER
1	A	502	LEU
1	A	517	GLN
1	A	518	ASN
1	A	519	ASN
1	B	91	PRO
1	B	155	PRO
1	B	235	ILE
1	B	347	ARG
1	B	363	GLN
1	B	364	ILE
1	B	374	ASP
1	B	404	ASN
1	B	467	ASN
1	B	476	SER
1	B	502	LEU
1	B	517	GLN
1	B	518	ASN
1	B	519	ASN
1	C	91	PRO
1	C	155	PRO
1	C	235	ILE
1	C	347	ARG
1	C	363	GLN
1	C	364	ILE

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Mol	Chain	Res	Type
1	C	374	ASP
1	C	404	ASN
1	C	467	ASN
1	C	476	SER
1	C	502	LEU
1	C	517	GLN
1	C	518	ASN
1	C	519	ASN
1	D	91	PRO
1	D	155	PRO
1	D	235	ILE
1	D	347	ARG
1	D	363	GLN
1	D	364	ILE
1	D	374	ASP
1	D	404	ASN
1	D	467	ASN
1	D	476	SER
1	D	502	LEU
1	D	517	GLN
1	D	518	ASN
1	D	519	ASN
1	A	3	VAL
1	A	156	GLU
1	A	260	LYS
1	A	287	GLY
1	A	470	PRO
1	A	503	LYS
1	B	3	VAL
1	B	156	GLU
1	B	260	LYS
1	B	287	GLY
1	B	470	PRO
1	B	503	LYS
1	C	3	VAL
1	C	156	GLU
1	C	260	LYS
1	C	287	GLY
1	C	470	PRO
1	C	503	LYS
1	D	3	VAL
1	D	156	GLU

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Mol	Chain	Res	Type
1	D	260	LYS
1	D	287	GLY
1	D	470	PRO
1	D	503	LYS
1	A	55	TRP
1	A	212	THR
1	A	250	PRO
1	A	333	VAL
1	A	360	ASP
1	A	372	GLY
1	A	377	ARG
1	A	506	ASP
1	B	55	TRP
1	B	212	THR
1	B	250	PRO
1	B	333	VAL
1	B	360	ASP
1	B	372	GLY
1	B	377	ARG
1	B	506	ASP
1	C	55	TRP
1	C	212	THR
1	C	250	PRO
1	C	333	VAL
1	C	360	ASP
1	C	372	GLY
1	C	377	ARG
1	C	506	ASP
1	D	55	TRP
1	D	212	THR
1	D	250	PRO
1	D	333	VAL
1	D	360	ASP
1	D	372	GLY
1	D	377	ARG
1	D	506	ASP
1	A	152	LYS
1	A	223	PRO
1	A	359	PRO
1	A	375	PRO
1	B	152	LYS
1	B	223	PRO

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Mol	Chain	Res	Type
1	B	359	PRO
1	B	375	PRO
1	C	152	LYS
1	C	223	PRO
1	C	359	PRO
1	C	375	PRO
1	D	152	LYS
1	D	223	PRO
1	D	359	PRO
1	D	375	PRO
1	A	160	PRO
1	A	265	GLU
1	A	278	ASN
1	A	289	ASP
1	A	482	THR
1	B	160	PRO
1	B	265	GLU
1	B	278	ASN
1	B	289	ASP
1	B	482	THR
1	C	160	PRO
1	C	265	GLU
1	C	278	ASN
1	C	289	ASP
1	C	482	THR
1	D	160	PRO
1	D	265	GLU
1	D	278	ASN
1	D	289	ASP
1	D	482	THR
1	A	498	PRO
1	A	523	THR
1	B	498	PRO
1	B	523	THR
1	C	498	PRO
1	C	523	THR
1	D	498	PRO
1	D	523	THR
1	A	154	ASP
1	A	307	PRO
1	B	154	ASP
1	B	307	PRO

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Mol	Chain	Res	Type
1	C	154	ASP
1	C	307	PRO
1	D	154	ASP
1	D	307	PRO
1	A	222	ASP
1	B	222	ASP
1	C	222	ASP
1	D	222	ASP
1	A	200	GLY
1	B	200	GLY
1	C	200	GLY
1	D	200	GLY
1	A	47	PRO
1	A	158	PRO
1	B	47	PRO
1	C	47	PRO
1	C	158	PRO
1	D	47	PRO
1	D	158	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	480/779 (62%)	381 (79%)	99 (21%)	1	6
1	B	480/779 (62%)	381 (79%)	99 (21%)	1	6
1	C	480/779 (62%)	381 (79%)	99 (21%)	1	6
1	D	480/779 (62%)	381 (79%)	99 (21%)	1	6
All	All	1920/3116 (62%)	1524 (79%)	396 (21%)	3	6

All (396) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	18	PRO

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Mol	Chain	Res	Type
1	A	19	LYS
1	A	27	ASN
1	A	52	ARG
1	A	61	LEU
1	A	66	LEU
1	A	68	ARG
1	A	88	VAL
1	A	91	PRO
1	A	92	MET
1	A	117	VAL
1	A	138	ASN
1	A	146	LEU
1	A	151	LEU
1	A	155	PRO
1	A	156	GLU
1	A	161	ASN
1	A	163	PHE
1	A	189	LEU
1	A	195	ASP
1	A	202	SER
1	A	216	ASP
1	A	217	ASN
1	A	223	PRO
1	A	226	TYR
1	A	231	PRO
1	A	233	ASN
1	A	234	GLU
1	A	235	ILE
1	A	237	PHE
1	A	250	PRO
1	A	253	PRO
1	A	261	ILE
1	A	264	ASN
1	A	268	PHE
1	A	273	THR
1	A	277	SER
1	A	278	ASN
1	A	282	LEU
1	A	284	THR
1	A	288	LEU
1	A	298	LEU
1	A	309	SER

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Mol	Chain	Res	Type
1	A	310	VAL
1	A	315	SER
1	A	316	THR
1	A	318	THR
1	A	333	VAL
1	A	336	VAL
1	A	339	VAL
1	A	345	LEU
1	A	353	SER
1	A	354	LEU
1	A	360	ASP
1	A	363	GLN
1	A	364	ILE
1	A	365	GLN
1	A	371	ILE
1	A	373	ASN
1	A	375	PRO
1	A	379	LEU
1	A	382	ASN
1	A	384	ASP
1	A	385	ASN
1	A	393	ASN
1	A	394	LEU
1	A	395	ASP
1	A	398	SER
1	A	399	GLU
1	A	404	ASN
1	A	405	THR
1	A	407	THR
1	A	410	MET
1	A	423	THR
1	A	425	THR
1	A	427	ILE
1	A	428	LEU
1	A	433	VAL
1	A	436	ASN
1	A	447	MET
1	A	448	CYS
1	A	461	ASP
1	A	464	ILE
1	A	465	PRO
1	A	466	PRO

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Mol	Chain	Res	Type
1	A	470	PRO
1	A	477	HIS
1	A	492	THR
1	A	509	ILE
1	A	512	LEU
1	A	517	GLN
1	A	518	ASN
1	A	519	ASN
1	A	520	PRO
1	A	522	LEU
1	A	523	THR
1	A	532	CYS
1	A	540	GLN
1	B	8	LYS
1	B	18	PRO
1	B	19	LYS
1	B	27	ASN
1	B	52	ARG
1	B	61	LEU
1	B	66	LEU
1	B	68	ARG
1	B	88	VAL
1	B	91	PRO
1	B	92	MET
1	B	117	VAL
1	B	138	ASN
1	B	146	LEU
1	B	151	LEU
1	B	155	PRO
1	B	156	GLU
1	B	161	ASN
1	B	163	PHE
1	B	189	LEU
1	B	195	ASP
1	B	202	SER
1	B	216	ASP
1	B	217	ASN
1	B	223	PRO
1	B	226	TYR
1	B	231	PRO
1	B	233	ASN
1	B	234	GLU

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Mol	Chain	Res	Type
1	B	235	ILE
1	B	237	PHE
1	B	250	PRO
1	B	253	PRO
1	B	261	ILE
1	B	264	ASN
1	B	268	PHE
1	B	273	THR
1	B	277	SER
1	B	278	ASN
1	B	282	LEU
1	B	284	THR
1	B	288	LEU
1	B	298	LEU
1	B	309	SER
1	B	310	VAL
1	B	315	SER
1	B	316	THR
1	B	318	THR
1	B	333	VAL
1	B	336	VAL
1	B	339	VAL
1	B	345	LEU
1	B	353	SER
1	B	354	LEU
1	B	360	ASP
1	B	363	GLN
1	B	364	ILE
1	B	365	GLN
1	B	371	ILE
1	B	373	ASN
1	B	375	PRO
1	B	379	LEU
1	B	382	ASN
1	B	384	ASP
1	B	385	ASN
1	B	393	ASN
1	B	394	LEU
1	B	395	ASP
1	B	398	SER
1	B	399	GLU
1	B	404	ASN

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Mol	Chain	Res	Type
1	B	405	THR
1	B	407	THR
1	B	410	MET
1	B	423	THR
1	B	425	THR
1	B	427	ILE
1	B	428	LEU
1	B	433	VAL
1	B	436	ASN
1	B	447	MET
1	B	448	CYS
1	B	461	ASP
1	B	464	ILE
1	B	465	PRO
1	B	466	PRO
1	B	470	PRO
1	B	477	HIS
1	B	492	THR
1	B	509	ILE
1	B	512	LEU
1	B	517	GLN
1	B	518	ASN
1	B	519	ASN
1	B	520	PRO
1	B	522	LEU
1	B	523	THR
1	B	532	CYS
1	B	540	GLN
1	C	8	LYS
1	C	18	PRO
1	C	19	LYS
1	C	27	ASN
1	C	52	ARG
1	C	61	LEU
1	C	66	LEU
1	C	68	ARG
1	C	88	VAL
1	C	91	PRO
1	C	92	MET
1	C	117	VAL
1	C	138	ASN
1	C	146	LEU

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Mol	Chain	Res	Type
1	C	151	LEU
1	C	155	PRO
1	C	156	GLU
1	C	161	ASN
1	C	163	PHE
1	C	189	LEU
1	C	195	ASP
1	C	202	SER
1	C	216	ASP
1	C	217	ASN
1	C	223	PRO
1	C	226	TYR
1	C	231	PRO
1	C	233	ASN
1	C	234	GLU
1	C	235	ILE
1	C	237	PHE
1	C	250	PRO
1	C	253	PRO
1	C	261	ILE
1	C	264	ASN
1	C	268	PHE
1	C	273	THR
1	C	277	SER
1	C	278	ASN
1	C	282	LEU
1	C	284	THR
1	C	288	LEU
1	C	298	LEU
1	C	309	SER
1	C	310	VAL
1	C	315	SER
1	C	316	THR
1	C	318	THR
1	C	333	VAL
1	C	336	VAL
1	C	339	VAL
1	C	345	LEU
1	C	353	SER
1	C	354	LEU
1	C	360	ASP
1	C	363	GLN

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Mol	Chain	Res	Type
1	C	364	ILE
1	C	365	GLN
1	C	371	ILE
1	C	373	ASN
1	C	375	PRO
1	C	379	LEU
1	C	382	ASN
1	C	384	ASP
1	C	385	ASN
1	C	393	ASN
1	C	394	LEU
1	C	395	ASP
1	C	398	SER
1	C	399	GLU
1	C	404	ASN
1	C	405	THR
1	C	407	THR
1	C	410	MET
1	C	423	THR
1	C	425	THR
1	C	427	ILE
1	C	428	LEU
1	C	433	VAL
1	C	436	ASN
1	C	447	MET
1	C	448	CYS
1	C	461	ASP
1	C	464	ILE
1	C	465	PRO
1	C	466	PRO
1	C	470	PRO
1	C	477	HIS
1	C	492	THR
1	C	509	ILE
1	C	512	LEU
1	C	517	GLN
1	C	518	ASN
1	C	519	ASN
1	C	520	PRO
1	C	522	LEU
1	C	523	THR
1	C	532	CYS

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Mol	Chain	Res	Type
1	C	540	GLN
1	D	8	LYS
1	D	18	PRO
1	D	19	LYS
1	D	27	ASN
1	D	52	ARG
1	D	61	LEU
1	D	66	LEU
1	D	68	ARG
1	D	88	VAL
1	D	91	PRO
1	D	92	MET
1	D	117	VAL
1	D	138	ASN
1	D	146	LEU
1	D	151	LEU
1	D	155	PRO
1	D	156	GLU
1	D	161	ASN
1	D	163	PHE
1	D	189	LEU
1	D	195	ASP
1	D	202	SER
1	D	216	ASP
1	D	217	ASN
1	D	223	PRO
1	D	226	TYR
1	D	231	PRO
1	D	233	ASN
1	D	234	GLU
1	D	235	ILE
1	D	237	PHE
1	D	250	PRO
1	D	253	PRO
1	D	261	ILE
1	D	264	ASN
1	D	268	PHE
1	D	273	THR
1	D	277	SER
1	D	278	ASN
1	D	282	LEU
1	D	284	THR

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Mol	Chain	Res	Type
1	D	288	LEU
1	D	298	LEU
1	D	309	SER
1	D	310	VAL
1	D	315	SER
1	D	316	THR
1	D	318	THR
1	D	333	VAL
1	D	336	VAL
1	D	339	VAL
1	D	345	LEU
1	D	353	SER
1	D	354	LEU
1	D	360	ASP
1	D	363	GLN
1	D	364	ILE
1	D	365	GLN
1	D	371	ILE
1	D	373	ASN
1	D	375	PRO
1	D	379	LEU
1	D	382	ASN
1	D	384	ASP
1	D	385	ASN
1	D	393	ASN
1	D	394	LEU
1	D	395	ASP
1	D	398	SER
1	D	399	GLU
1	D	404	ASN
1	D	405	THR
1	D	407	THR
1	D	410	MET
1	D	423	THR
1	D	425	THR
1	D	427	ILE
1	D	428	LEU
1	D	433	VAL
1	D	436	ASN
1	D	447	MET
1	D	448	CYS
1	D	461	ASP

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Mol	Chain	Res	Type
1	D	464	ILE
1	D	465	PRO
1	D	466	PRO
1	D	470	PRO
1	D	477	HIS
1	D	492	THR
1	D	509	ILE
1	D	512	LEU
1	D	517	GLN
1	D	518	ASN
1	D	519	ASN
1	D	520	PRO
1	D	522	LEU
1	D	523	THR
1	D	532	CYS
1	D	540	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	27	ASN
1	A	32	ASN
1	A	45	ASN
1	A	104	ASN
1	A	110	GLN
1	A	122	GLN
1	A	138	ASN
1	A	217	ASN
1	A	233	ASN
1	A	240	GLN
1	A	264	ASN
1	A	278	ASN
1	A	299	GLN
1	A	373	ASN
1	A	385	ASN
1	A	391	ASN
1	A	393	ASN
1	A	404	ASN
1	A	455	GLN
1	A	467	ASN
1	A	517	GLN

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Mol	Chain	Res	Type
1	A	519	ASN
1	B	12	ASN
1	B	27	ASN
1	B	45	ASN
1	B	104	ASN
1	B	110	GLN
1	B	122	GLN
1	B	138	ASN
1	B	217	ASN
1	B	233	ASN
1	B	240	GLN
1	B	264	ASN
1	B	278	ASN
1	B	299	GLN
1	B	373	ASN
1	B	385	ASN
1	B	391	ASN
1	B	393	ASN
1	B	404	ASN
1	B	455	GLN
1	B	467	ASN
1	B	517	GLN
1	B	519	ASN
1	C	12	ASN
1	C	27	ASN
1	C	32	ASN
1	C	45	ASN
1	C	104	ASN
1	C	110	GLN
1	C	122	GLN
1	C	138	ASN
1	C	217	ASN
1	C	233	ASN
1	C	240	GLN
1	C	264	ASN
1	C	278	ASN
1	C	299	GLN
1	C	373	ASN
1	C	385	ASN
1	C	391	ASN
1	C	393	ASN
1	C	404	ASN

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Mol	Chain	Res	Type
1	C	455	GLN
1	C	467	ASN
1	C	517	GLN
1	C	519	ASN
1	D	12	ASN
1	D	27	ASN
1	D	32	ASN
1	D	79	HIS
1	D	104	ASN
1	D	110	GLN
1	D	122	GLN
1	D	138	ASN
1	D	217	ASN
1	D	233	ASN
1	D	240	GLN
1	D	264	ASN
1	D	278	ASN
1	D	299	GLN
1	D	373	ASN
1	D	385	ASN
1	D	391	ASN
1	D	393	ASN
1	D	404	ASN
1	D	455	GLN
1	D	467	ASN
1	D	517	GLN
1	D	519	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 108 ligands modelled in this entry, 48 are monoatomic - leaving 60 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NDG	D	811	1	14,14,15	0.87	0	17,19,21	1.96	1 (5%)
2	NAG	C	801	1	14,14,15	0.70	0	17,19,21	0.98	1 (5%)
2	NAG	A	903	1	14,14,15	0.55	0	17,19,21	0.79	0
2	NAG	C	808	1	14,14,15	0.67	0	17,19,21	0.70	0
3	NDG	B	811	1	14,14,15	0.86	0	17,19,21	1.96	1 (5%)
2	NAG	D	812	1	14,14,15	0.83	1 (7%)	17,19,21	0.75	1 (5%)
2	NAG	A	807	1	14,14,15	0.64	0	17,19,21	1.19	2 (11%)
2	NAG	A	802	1	14,14,15	0.78	1 (7%)	17,19,21	0.85	0
2	NAG	B	809	1	14,14,15	0.76	0	17,19,21	0.94	0
2	NAG	D	805	1	14,14,15	0.71	0	17,19,21	1.05	1 (5%)
2	NAG	C	902	1	14,14,15	1.13	1 (7%)	17,19,21	1.09	2 (11%)
2	NAG	D	904	1	14,14,15	0.78	1 (7%)	17,19,21	0.70	1 (5%)
2	NAG	C	802	1	14,14,15	0.78	1 (7%)	17,19,21	0.85	0
2	NAG	B	904	1	14,14,15	0.77	1 (7%)	17,19,21	0.69	0
2	NAG	B	903	1	14,14,15	0.56	0	17,19,21	0.79	0
2	NAG	C	806	1	14,14,15	0.57	0	17,19,21	1.39	3 (17%)
2	NAG	D	902	1	14,14,15	1.13	1 (7%)	17,19,21	1.09	1 (5%)
2	NAG	C	903	1	14,14,15	0.55	0	17,19,21	0.78	0
2	NAG	D	806	1	14,14,15	0.55	0	17,19,21	1.38	3 (17%)
2	NAG	D	903	1	14,14,15	0.54	0	17,19,21	0.79	0
3	NDG	A	811	1	14,14,15	0.87	0	17,19,21	1.96	1 (5%)
2	NAG	B	802	1	14,14,15	0.78	1 (7%)	17,19,21	0.85	0
2	NAG	C	807	1	14,14,15	0.64	0	17,19,21	1.19	2 (11%)
2	NAG	A	801	1	14,14,15	0.71	0	17,19,21	0.99	1 (5%)
2	NAG	B	807	1	14,14,15	0.65	0	17,19,21	1.20	2 (11%)
2	NAG	C	803	1	14,14,15	1.00	1 (7%)	17,19,21	1.17	2 (11%)
2	NAG	C	904	1	14,14,15	0.77	1 (7%)	17,19,21	0.70	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	D	803	1	14,14,15	1.00	1 (7%)	17,19,21	1.16	2 (11%)
2	NAG	B	808	1	14,14,15	0.66	0	17,19,21	0.70	0
3	NDG	A	804	1	14,14,15	0.65	0	17,19,21	0.78	0
3	NDG	B	804	1	14,14,15	0.64	0	17,19,21	0.78	0
3	NDG	C	811	1	14,14,15	0.87	0	17,19,21	1.96	1 (5%)
2	NAG	B	803	1	14,14,15	1.00	1 (7%)	17,19,21	1.17	2 (11%)
2	NAG	A	803	1	14,14,15	1.00	1 (7%)	17,19,21	1.16	2 (11%)
2	NAG	C	809	1	14,14,15	0.77	1 (7%)	17,19,21	0.94	0
2	NAG	C	812	1	14,14,15	0.83	1 (7%)	17,19,21	0.76	1 (5%)
3	NDG	D	804	1	14,14,15	0.64	0	17,19,21	0.78	0
2	NAG	D	809	1	14,14,15	0.77	1 (7%)	17,19,21	0.94	0
2	NAG	B	805	1	14,14,15	0.72	0	17,19,21	1.05	1 (5%)
2	NAG	A	810	1	14,14,15	0.67	0	17,19,21	1.33	4 (23%)
2	NAG	D	801	1	14,14,15	0.70	0	17,19,21	0.98	1 (5%)
2	NAG	B	812	1	14,14,15	0.83	1 (7%)	17,19,21	0.76	1 (5%)
2	NAG	C	810	1	14,14,15	0.66	0	17,19,21	1.33	4 (23%)
2	NAG	B	801	1	14,14,15	0.70	0	17,19,21	0.98	1 (5%)
2	NAG	B	902	1	14,14,15	1.12	1 (7%)	17,19,21	1.09	2 (11%)
2	NAG	A	806	1	14,14,15	0.55	0	17,19,21	1.39	3 (17%)
2	NAG	B	810	1	14,14,15	0.67	0	17,19,21	1.33	4 (23%)
2	NAG	A	812	1	14,14,15	0.84	1 (7%)	17,19,21	0.76	1 (5%)
2	NAG	D	810	1	14,14,15	0.67	0	17,19,21	1.33	4 (23%)
2	NAG	D	807	1	14,14,15	0.65	0	17,19,21	1.19	2 (11%)
2	NAG	A	808	1	14,14,15	0.67	0	17,19,21	0.70	0
2	NAG	A	904	1	14,14,15	0.77	1 (7%)	17,19,21	0.70	1 (5%)
3	NDG	C	804	1	14,14,15	0.64	0	17,19,21	0.78	0
2	NAG	A	809	1	14,14,15	0.77	1 (7%)	17,19,21	0.94	0
2	NAG	D	802	1	14,14,15	0.78	1 (7%)	17,19,21	0.85	0
2	NAG	A	805	1	14,14,15	0.72	0	17,19,21	1.06	1 (5%)
2	NAG	B	806	1	14,14,15	0.56	0	17,19,21	1.39	3 (17%)
2	NAG	D	808	1	14,14,15	0.66	0	17,19,21	0.70	0
2	NAG	A	902	1	14,14,15	1.15	1 (7%)	17,19,21	1.08	2 (11%)
2	NAG	C	805	1	14,14,15	0.72	0	17,19,21	1.05	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDG	D	811	1	-	2/6/23/26	0/1/1/1
2	NAG	C	801	1	-	4/6/23/26	0/1/1/1
2	NAG	A	903	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	C	808	1	-	3/6/23/26	0/1/1/1
3	NDG	B	811	1	-	2/6/23/26	0/1/1/1
2	NAG	D	812	1	-	4/6/23/26	0/1/1/1
2	NAG	D	805	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	A	802	1	-	2/6/23/26	0/1/1/1
2	NAG	A	807	1	-	5/6/23/26	0/1/1/1
2	NAG	B	809	1	-	2/6/23/26	0/1/1/1
2	NAG	C	902	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	D	904	1	-	3/6/23/26	0/1/1/1
2	NAG	C	806	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	D	902	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	B	903	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	B	904	1	-	3/6/23/26	0/1/1/1
2	NAG	C	802	1	-	2/6/23/26	0/1/1/1
2	NAG	C	903	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	D	806	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	D	903	1	1/1/5/7	2/6/23/26	0/1/1/1
3	NDG	A	811	1	-	2/6/23/26	0/1/1/1
2	NAG	B	802	1	-	2/6/23/26	0/1/1/1
2	NAG	C	807	1	-	5/6/23/26	0/1/1/1
2	NAG	A	801	1	-	4/6/23/26	0/1/1/1
2	NAG	B	807	1	-	5/6/23/26	0/1/1/1
2	NAG	C	803	1	-	2/6/23/26	0/1/1/1
2	NAG	C	904	1	-	3/6/23/26	0/1/1/1
2	NAG	D	803	1	-	2/6/23/26	0/1/1/1
2	NAG	B	808	1	-	3/6/23/26	0/1/1/1
3	NDG	A	804	1	-	0/6/23/26	0/1/1/1
3	NDG	B	804	1	-	0/6/23/26	0/1/1/1
3	NDG	C	811	1	-	2/6/23/26	0/1/1/1
2	NAG	B	803	1	-	2/6/23/26	0/1/1/1
2	NAG	A	803	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	809	1	-	2/6/23/26	0/1/1/1
2	NAG	C	812	1	-	4/6/23/26	0/1/1/1
3	NDG	D	804	1	-	0/6/23/26	0/1/1/1
2	NAG	D	809	1	-	2/6/23/26	0/1/1/1
2	NAG	B	805	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	A	810	1	-	3/6/23/26	0/1/1/1
2	NAG	D	801	1	-	4/6/23/26	0/1/1/1
2	NAG	B	812	1	-	4/6/23/26	0/1/1/1
2	NAG	C	810	1	-	3/6/23/26	0/1/1/1
2	NAG	B	801	1	-	4/6/23/26	0/1/1/1
2	NAG	B	902	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	B	810	1	-	3/6/23/26	0/1/1/1
2	NAG	A	805	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	A	812	1	-	4/6/23/26	0/1/1/1
2	NAG	D	810	1	-	3/6/23/26	0/1/1/1
2	NAG	D	807	1	-	5/6/23/26	0/1/1/1
2	NAG	A	808	1	-	3/6/23/26	0/1/1/1
2	NAG	A	904	1	-	3/6/23/26	0/1/1/1
3	NDG	C	804	1	-	0/6/23/26	0/1/1/1
2	NAG	A	809	1	-	2/6/23/26	0/1/1/1
2	NAG	D	802	1	-	2/6/23/26	0/1/1/1
2	NAG	A	806	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	B	806	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	D	808	1	-	3/6/23/26	0/1/1/1
2	NAG	A	902	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	C	805	1	1/1/5/7	2/6/23/26	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	902	NAG	C1-C2	3.42	1.57	1.52
2	C	902	NAG	C1-C2	3.37	1.56	1.52
2	B	902	NAG	C1-C2	3.34	1.56	1.52
2	D	902	NAG	C1-C2	3.33	1.56	1.52
2	C	803	NAG	O5-C5	2.65	1.48	1.43
2	D	803	NAG	O5-C5	2.64	1.48	1.43
2	B	803	NAG	O5-C5	2.62	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	803	NAG	O5-C5	2.62	1.48	1.43
2	D	904	NAG	C1-C2	-2.45	1.49	1.52
2	C	904	NAG	C1-C2	-2.42	1.49	1.52
2	A	904	NAG	C1-C2	-2.41	1.49	1.52
2	B	904	NAG	C1-C2	-2.39	1.49	1.52
2	A	812	NAG	C1-C2	-2.35	1.49	1.52
2	C	812	NAG	C1-C2	-2.31	1.49	1.52
2	D	812	NAG	C1-C2	-2.29	1.49	1.52
2	B	812	NAG	C1-C2	-2.27	1.49	1.52
2	A	802	NAG	C1-C2	2.13	1.55	1.52
2	D	802	NAG	C1-C2	2.11	1.55	1.52
2	B	802	NAG	C1-C2	2.10	1.55	1.52
2	D	809	NAG	C1-C2	-2.07	1.49	1.52
2	C	802	NAG	C1-C2	2.06	1.55	1.52
2	C	809	NAG	C1-C2	-2.06	1.49	1.52
2	A	809	NAG	C1-C2	-2.04	1.49	1.52

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	811	NDG	C2-N2-C7	-7.43	112.94	122.90
3	A	811	NDG	C2-N2-C7	-7.42	112.95	122.90
3	B	811	NDG	C2-N2-C7	-7.42	112.95	122.90
3	C	811	NDG	C2-N2-C7	-7.41	112.97	122.90
2	B	806	NAG	C2-N2-C7	-3.65	118.01	122.90
2	C	806	NAG	C2-N2-C7	-3.62	118.04	122.90
2	A	806	NAG	C2-N2-C7	-3.59	118.08	122.90
2	D	806	NAG	C2-N2-C7	-3.58	118.10	122.90
2	C	805	NAG	C2-N2-C7	-3.18	118.64	122.90
2	A	805	NAG	C2-N2-C7	-3.17	118.65	122.90
2	B	805	NAG	C2-N2-C7	-3.16	118.67	122.90
2	D	805	NAG	C2-N2-C7	-3.14	118.69	122.90
2	B	807	NAG	C2-N2-C7	-3.09	118.77	122.90
2	D	807	NAG	C2-N2-C7	-3.07	118.79	122.90
2	A	807	NAG	C2-N2-C7	-3.06	118.80	122.90
2	C	807	NAG	C2-N2-C7	-3.04	118.82	122.90
2	C	803	NAG	C2-N2-C7	-3.01	118.87	122.90
2	B	803	NAG	C2-N2-C7	-3.00	118.88	122.90
2	D	803	NAG	C2-N2-C7	-3.00	118.88	122.90
2	A	803	NAG	C2-N2-C7	-2.98	118.91	122.90
2	C	810	NAG	C1-C2-N2	2.53	114.42	110.43
2	A	810	NAG	C1-C2-N2	2.52	114.41	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	810	NAG	C1-C2-N2	2.52	114.40	110.43
2	D	810	NAG	C1-C2-N2	2.50	114.37	110.43
2	B	810	NAG	C4-C3-C2	-2.47	107.40	111.02
2	C	803	NAG	C1-O5-C5	2.46	115.49	112.19
2	B	803	NAG	C1-O5-C5	2.46	115.49	112.19
2	A	806	NAG	C4-C3-C2	-2.46	107.41	111.02
2	C	810	NAG	C4-C3-C2	-2.46	107.41	111.02
2	A	803	NAG	C1-O5-C5	2.46	115.48	112.19
2	A	810	NAG	C4-C3-C2	-2.45	107.42	111.02
2	D	810	NAG	C4-C3-C2	-2.45	107.42	111.02
2	B	806	NAG	C4-C3-C2	-2.45	107.42	111.02
2	D	806	NAG	C4-C3-C2	-2.44	107.44	111.02
2	C	806	NAG	C4-C3-C2	-2.43	107.46	111.02
2	D	803	NAG	C1-O5-C5	2.42	115.43	112.19
2	D	810	NAG	O5-C1-C2	-2.39	107.60	111.29
2	A	810	NAG	O5-C1-C2	-2.37	107.63	111.29
2	B	810	NAG	O5-C1-C2	-2.36	107.64	111.29
2	C	810	NAG	O5-C1-C2	-2.35	107.65	111.29
2	B	810	NAG	C1-O5-C5	-2.26	109.16	112.19
2	C	810	NAG	C1-O5-C5	-2.25	109.18	112.19
2	D	810	NAG	C1-O5-C5	-2.23	109.20	112.19
2	A	810	NAG	C1-O5-C5	-2.22	109.21	112.19
2	C	812	NAG	C2-N2-C7	-2.18	119.98	122.90
2	A	812	NAG	C2-N2-C7	-2.18	119.98	122.90
2	C	902	NAG	O5-C1-C2	2.17	114.66	111.29
2	B	812	NAG	C2-N2-C7	-2.16	120.00	122.90
2	A	801	NAG	C1-C2-N2	-2.16	107.03	110.43
2	D	801	NAG	C1-C2-N2	-2.15	107.05	110.43
2	B	902	NAG	O5-C1-C2	2.14	114.61	111.29
2	C	801	NAG	C1-C2-N2	-2.14	107.07	110.43
2	D	902	NAG	O5-C1-C2	2.14	114.59	111.29
2	B	801	NAG	C1-C2-N2	-2.13	107.08	110.43
2	A	902	NAG	O5-C1-C2	2.13	114.58	111.29
2	D	812	NAG	C2-N2-C7	-2.12	120.06	122.90
2	A	807	NAG	O5-C1-C2	-2.08	108.07	111.29
2	C	807	NAG	O5-C1-C2	-2.06	108.11	111.29
2	B	807	NAG	O5-C1-C2	-2.05	108.12	111.29
2	B	902	NAG	C1-O5-C5	2.05	114.93	112.19
2	A	806	NAG	O5-C1-C2	-2.04	108.13	111.29
2	A	904	NAG	C2-N2-C7	-2.04	120.17	122.90
2	D	807	NAG	O5-C1-C2	-2.04	108.14	111.29
2	C	904	NAG	C2-N2-C7	-2.04	120.17	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	904	NAG	C2-N2-C7	-2.03	120.17	122.90
2	B	806	NAG	O5-C1-C2	-2.02	108.17	111.29
2	C	902	NAG	C1-O5-C5	2.02	114.89	112.19
2	D	806	NAG	O5-C1-C2	-2.02	108.17	111.29
2	C	806	NAG	O5-C1-C2	-2.01	108.19	111.29
2	A	902	NAG	C1-O5-C5	2.01	114.88	112.19

All (16) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	805	NAG	C1
2	A	806	NAG	C1
2	A	902	NAG	C1
2	A	903	NAG	C1
2	B	805	NAG	C1
2	B	806	NAG	C1
2	B	902	NAG	C1
2	B	903	NAG	C1
2	C	805	NAG	C1
2	C	806	NAG	C1
2	C	902	NAG	C1
2	C	903	NAG	C1
2	D	805	NAG	C1
2	D	806	NAG	C1
2	D	902	NAG	C1
2	D	903	NAG	C1

All (152) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	807	NAG	C3-C2-N2-C7
2	A	808	NAG	C1-C2-N2-C7
2	A	810	NAG	C1-C2-N2-C7
2	A	812	NAG	C1-C2-N2-C7
2	A	902	NAG	C3-C2-N2-C7
2	A	904	NAG	C3-C2-N2-C7
2	B	807	NAG	C3-C2-N2-C7
2	B	808	NAG	C1-C2-N2-C7
2	B	810	NAG	C1-C2-N2-C7
2	B	812	NAG	C1-C2-N2-C7
2	B	902	NAG	C3-C2-N2-C7
2	B	904	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
2	C	807	NAG	C3-C2-N2-C7
2	C	808	NAG	C1-C2-N2-C7
2	C	810	NAG	C1-C2-N2-C7
2	C	812	NAG	C1-C2-N2-C7
2	C	902	NAG	C3-C2-N2-C7
2	C	904	NAG	C3-C2-N2-C7
2	D	807	NAG	C3-C2-N2-C7
2	D	808	NAG	C1-C2-N2-C7
2	D	810	NAG	C1-C2-N2-C7
2	D	812	NAG	C1-C2-N2-C7
2	D	902	NAG	C3-C2-N2-C7
2	D	904	NAG	C3-C2-N2-C7
3	A	811	NDG	C4-C5-C6-O6
3	B	811	NDG	C4-C5-C6-O6
3	C	811	NDG	C4-C5-C6-O6
3	D	811	NDG	C4-C5-C6-O6
2	A	802	NAG	C4-C5-C6-O6
2	A	807	NAG	C4-C5-C6-O6
2	B	802	NAG	C4-C5-C6-O6
2	B	807	NAG	C4-C5-C6-O6
2	C	802	NAG	C4-C5-C6-O6
2	C	807	NAG	C4-C5-C6-O6
2	D	807	NAG	C4-C5-C6-O6
3	A	811	NDG	O5-C5-C6-O6
3	B	811	NDG	O5-C5-C6-O6
3	C	811	NDG	O5-C5-C6-O6
3	D	811	NDG	O5-C5-C6-O6
2	D	802	NAG	C4-C5-C6-O6
2	A	809	NAG	O5-C5-C6-O6
2	B	809	NAG	O5-C5-C6-O6
2	C	809	NAG	O5-C5-C6-O6
2	D	809	NAG	O5-C5-C6-O6
2	A	809	NAG	C4-C5-C6-O6
2	B	809	NAG	C4-C5-C6-O6
2	C	809	NAG	C4-C5-C6-O6
2	D	809	NAG	C4-C5-C6-O6
2	A	807	NAG	O5-C5-C6-O6
2	B	807	NAG	O5-C5-C6-O6
2	C	807	NAG	O5-C5-C6-O6
2	D	807	NAG	O5-C5-C6-O6
2	A	807	NAG	C8-C7-N2-C2
2	B	807	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	C	807	NAG	C8-C7-N2-C2
2	D	807	NAG	C8-C7-N2-C2
2	A	805	NAG	O5-C5-C6-O6
2	B	805	NAG	O5-C5-C6-O6
2	C	805	NAG	O5-C5-C6-O6
2	D	805	NAG	O5-C5-C6-O6
2	A	802	NAG	O5-C5-C6-O6
2	B	802	NAG	O5-C5-C6-O6
2	C	802	NAG	O5-C5-C6-O6
2	D	802	NAG	O5-C5-C6-O6
2	B	904	NAG	C4-C5-C6-O6
2	A	904	NAG	C4-C5-C6-O6
2	C	904	NAG	C4-C5-C6-O6
2	D	904	NAG	C4-C5-C6-O6
2	A	805	NAG	C4-C5-C6-O6
2	C	805	NAG	C4-C5-C6-O6
2	D	805	NAG	C4-C5-C6-O6
2	B	805	NAG	C4-C5-C6-O6
2	A	810	NAG	C4-C5-C6-O6
2	B	810	NAG	C4-C5-C6-O6
2	C	810	NAG	C4-C5-C6-O6
2	D	810	NAG	C4-C5-C6-O6
2	A	812	NAG	O5-C5-C6-O6
2	B	812	NAG	O5-C5-C6-O6
2	C	812	NAG	O5-C5-C6-O6
2	D	812	NAG	O5-C5-C6-O6
2	A	807	NAG	O7-C7-N2-C2
2	B	807	NAG	O7-C7-N2-C2
2	C	807	NAG	O7-C7-N2-C2
2	D	807	NAG	O7-C7-N2-C2
2	A	803	NAG	C4-C5-C6-O6
2	B	803	NAG	C4-C5-C6-O6
2	C	803	NAG	C4-C5-C6-O6
2	D	803	NAG	C4-C5-C6-O6
2	A	810	NAG	O5-C5-C6-O6
2	B	810	NAG	O5-C5-C6-O6
2	C	810	NAG	O5-C5-C6-O6
2	D	810	NAG	O5-C5-C6-O6
2	B	904	NAG	O5-C5-C6-O6
2	C	904	NAG	O5-C5-C6-O6
2	A	904	NAG	O5-C5-C6-O6
2	D	904	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	B	801	NAG	C4-C5-C6-O6
2	D	801	NAG	C4-C5-C6-O6
2	A	801	NAG	C4-C5-C6-O6
2	C	801	NAG	C4-C5-C6-O6
2	A	803	NAG	O5-C5-C6-O6
2	B	803	NAG	O5-C5-C6-O6
2	C	803	NAG	O5-C5-C6-O6
2	D	803	NAG	O5-C5-C6-O6
2	D	903	NAG	C4-C5-C6-O6
2	C	903	NAG	C4-C5-C6-O6
2	A	903	NAG	C4-C5-C6-O6
2	B	903	NAG	C4-C5-C6-O6
2	A	808	NAG	C4-C5-C6-O6
2	C	808	NAG	C4-C5-C6-O6
2	A	806	NAG	C4-C5-C6-O6
2	B	808	NAG	C4-C5-C6-O6
2	D	806	NAG	C4-C5-C6-O6
2	D	808	NAG	C4-C5-C6-O6
2	B	806	NAG	C4-C5-C6-O6
2	A	801	NAG	C3-C2-N2-C7
2	A	903	NAG	C3-C2-N2-C7
2	B	801	NAG	C3-C2-N2-C7
2	B	903	NAG	C3-C2-N2-C7
2	C	801	NAG	C3-C2-N2-C7
2	C	903	NAG	C3-C2-N2-C7
2	D	801	NAG	C3-C2-N2-C7
2	D	903	NAG	C3-C2-N2-C7
2	C	806	NAG	C4-C5-C6-O6
2	B	801	NAG	O5-C5-C6-O6
2	D	801	NAG	O5-C5-C6-O6
2	A	801	NAG	O5-C5-C6-O6
2	C	801	NAG	O5-C5-C6-O6
2	A	801	NAG	C1-C2-N2-C7
2	A	902	NAG	C1-C2-N2-C7
2	B	801	NAG	C1-C2-N2-C7
2	B	902	NAG	C1-C2-N2-C7
2	C	801	NAG	C1-C2-N2-C7
2	C	902	NAG	C1-C2-N2-C7
2	D	801	NAG	C1-C2-N2-C7
2	D	902	NAG	C1-C2-N2-C7
2	D	806	NAG	O5-C5-C6-O6
2	A	806	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	C	806	NAG	O5-C5-C6-O6
2	B	806	NAG	O5-C5-C6-O6
2	A	808	NAG	C3-C2-N2-C7
2	A	812	NAG	C3-C2-N2-C7
2	B	808	NAG	C3-C2-N2-C7
2	B	812	NAG	C3-C2-N2-C7
2	C	808	NAG	C3-C2-N2-C7
2	C	812	NAG	C3-C2-N2-C7
2	D	808	NAG	C3-C2-N2-C7
2	D	812	NAG	C3-C2-N2-C7
2	B	812	NAG	C4-C5-C6-O6
2	C	812	NAG	C4-C5-C6-O6
2	D	812	NAG	C4-C5-C6-O6
2	A	812	NAG	C4-C5-C6-O6

There are no ring outliers.

52 monomers are involved in 403 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	811	NDG	7	0
2	C	801	NAG	22	0
2	C	808	NAG	2	0
3	B	811	NDG	8	0
2	D	812	NAG	3	0
2	A	807	NAG	17	0
2	B	809	NAG	8	0
2	D	805	NAG	7	0
2	C	902	NAG	8	0
2	D	904	NAG	8	0
2	B	904	NAG	8	0
2	C	806	NAG	10	0
2	D	902	NAG	8	0
2	D	806	NAG	12	0
3	A	811	NDG	7	0
2	C	807	NAG	17	0
2	A	801	NAG	21	0
2	B	807	NAG	16	0
2	C	803	NAG	4	0
2	C	904	NAG	8	0
2	D	803	NAG	4	0
2	B	808	NAG	2	0
3	A	804	NDG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	804	NDG	2	0
3	C	811	NDG	6	0
2	B	803	NAG	4	0
2	A	803	NAG	4	0
2	C	809	NAG	8	0
2	C	812	NAG	3	0
3	D	804	NDG	2	0
2	D	809	NAG	8	0
2	B	805	NAG	7	0
2	A	810	NAG	13	0
2	D	801	NAG	21	0
2	B	812	NAG	3	0
2	C	810	NAG	13	0
2	B	801	NAG	20	0
2	B	902	NAG	8	0
2	A	806	NAG	12	0
2	B	810	NAG	12	0
2	A	812	NAG	3	0
2	D	810	NAG	12	0
2	D	807	NAG	17	0
2	A	808	NAG	2	0
2	A	904	NAG	8	0
3	C	804	NDG	2	0
2	A	809	NAG	8	0
2	A	805	NAG	7	0
2	B	806	NAG	12	0
2	D	808	NAG	2	0
2	A	902	NAG	8	0
2	C	805	NAG	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Tomogram visualisation

This section contains visualisations of the EMDB entry EMD-1052. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Tomogram analysis

This section contains the results of statistical analysis of the tomogram.

7.1 Map-value distribution

This section was not generated.

8 Map-model fit

This section was not generated.