



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2024 – 10:52 AM EDT

PDB ID : 1LNL
Title : Structure of deoxygenated hemocyanin from *Rapana thomasiana*
Authors : Perbandt, M.; Guthoehrlein, E.W.; Rypniewski, W.; Idakieva, K.; Stoeva, S.;
Voelter, W.; Genov, N.; Betzel, C.
Deposited on : 2002-05-03
Resolution : 3.30 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

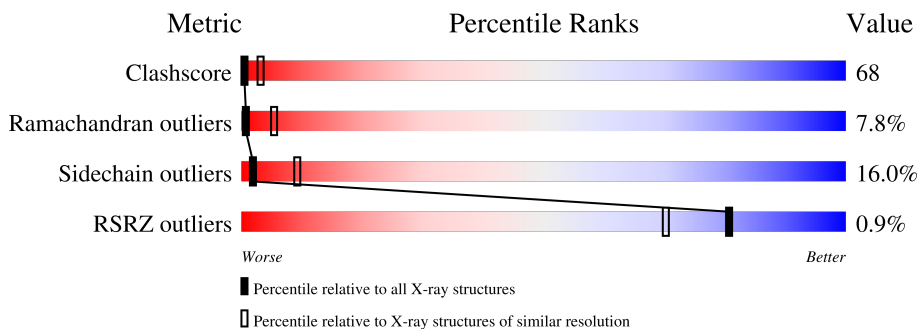
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	180529	1128 (3.32-3.28)
Ramachandran outliers	177936	1125 (3.32-3.28)
Sidechain outliers	177891	1124 (3.32-3.28)
RSRZ outliers	164620	1085 (3.32-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	408	<div> <div></div> <div>20%</div> <div>52%</div> <div>24%</div> <div>5%</div> </div>
1	B	408	<div> <div></div> <div>21%</div> <div>48%</div> <div>26%</div> <div>6%</div> </div>
1	C	408	<div> <div></div> <div>23%</div> <div>47%</div> <div>24%</div> <div>6%</div> </div>

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
3	CU	B	5503	-	-	X	-

2 Entry composition [i](#)

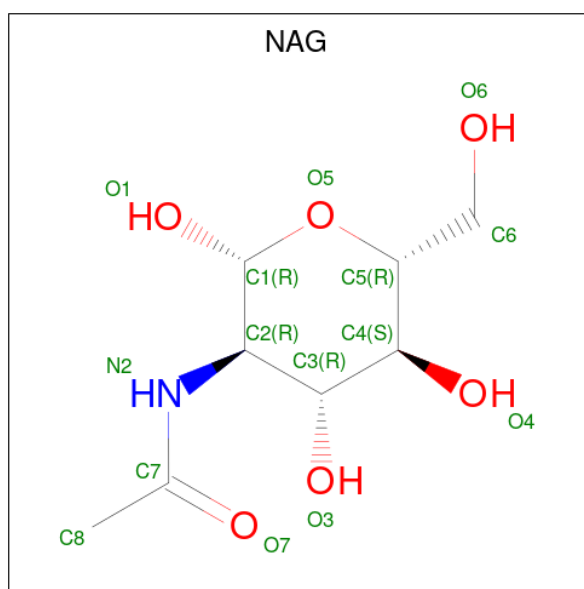
There are 3 unique types of molecules in this entry. The entry contains 9984 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 hemocyanin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	0	0
			3310	2115	558	625	12			
1	B	408	Total	C	N	O	S	0	0	0
			3310	2115	558	625	12			
1	C	408	Total	C	N	O	S	3	0	0
			3310	2115	558	625	12			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	C	1	Total	C	N	O	0	0
			15	8	1	6		
2	C	1	Total	C	N	O	0	0
			15	8	1	6		

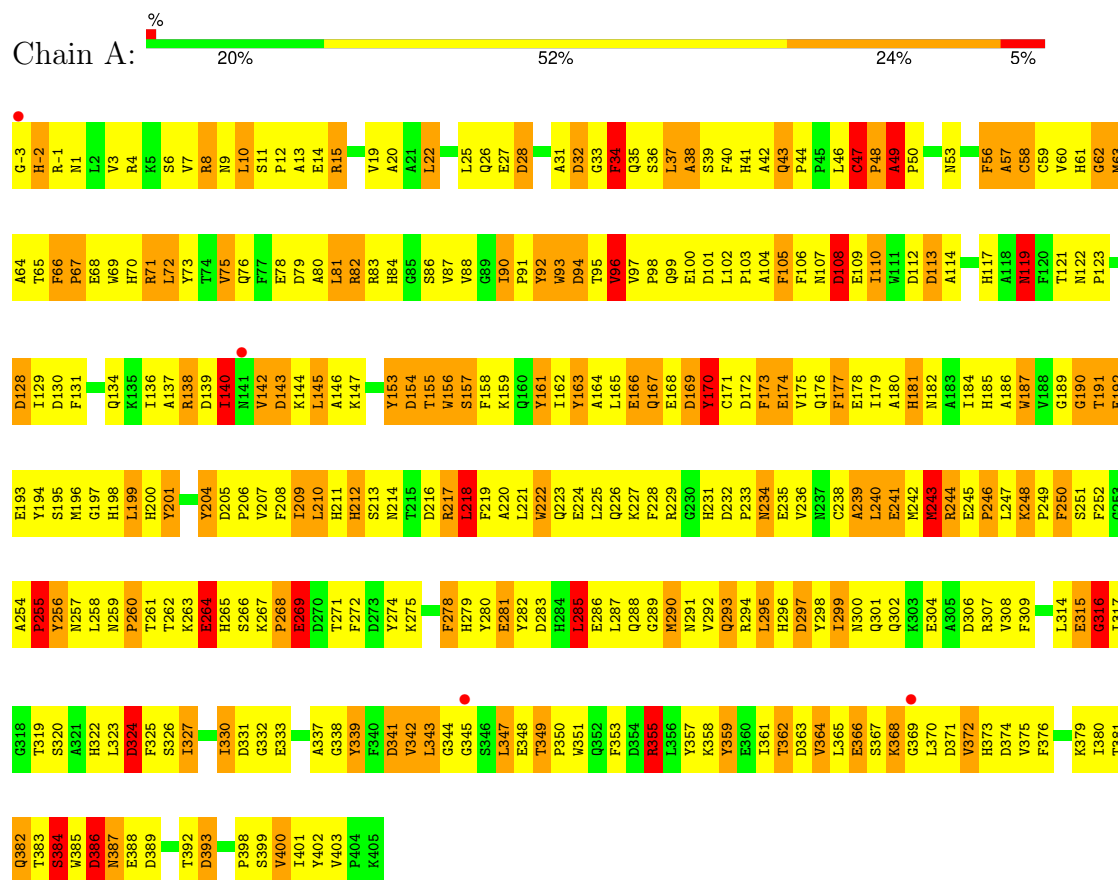
- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Cu 2	0	0
3	B	4	Total 4	Cu 4	0	0
3	C	3	Total 3	Cu 3	0	0

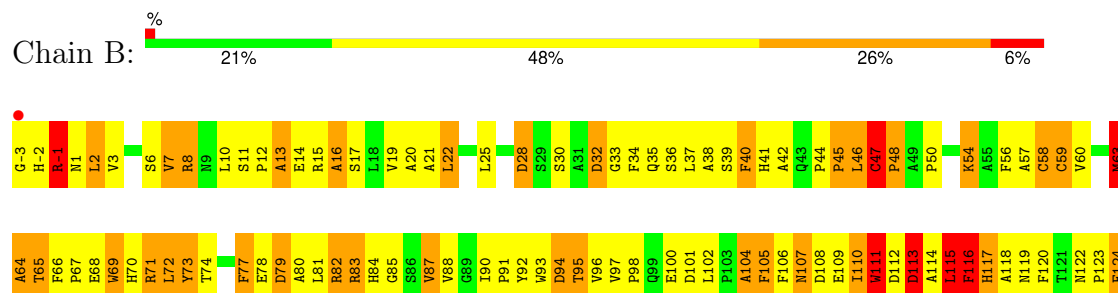
3 Residue-property plots

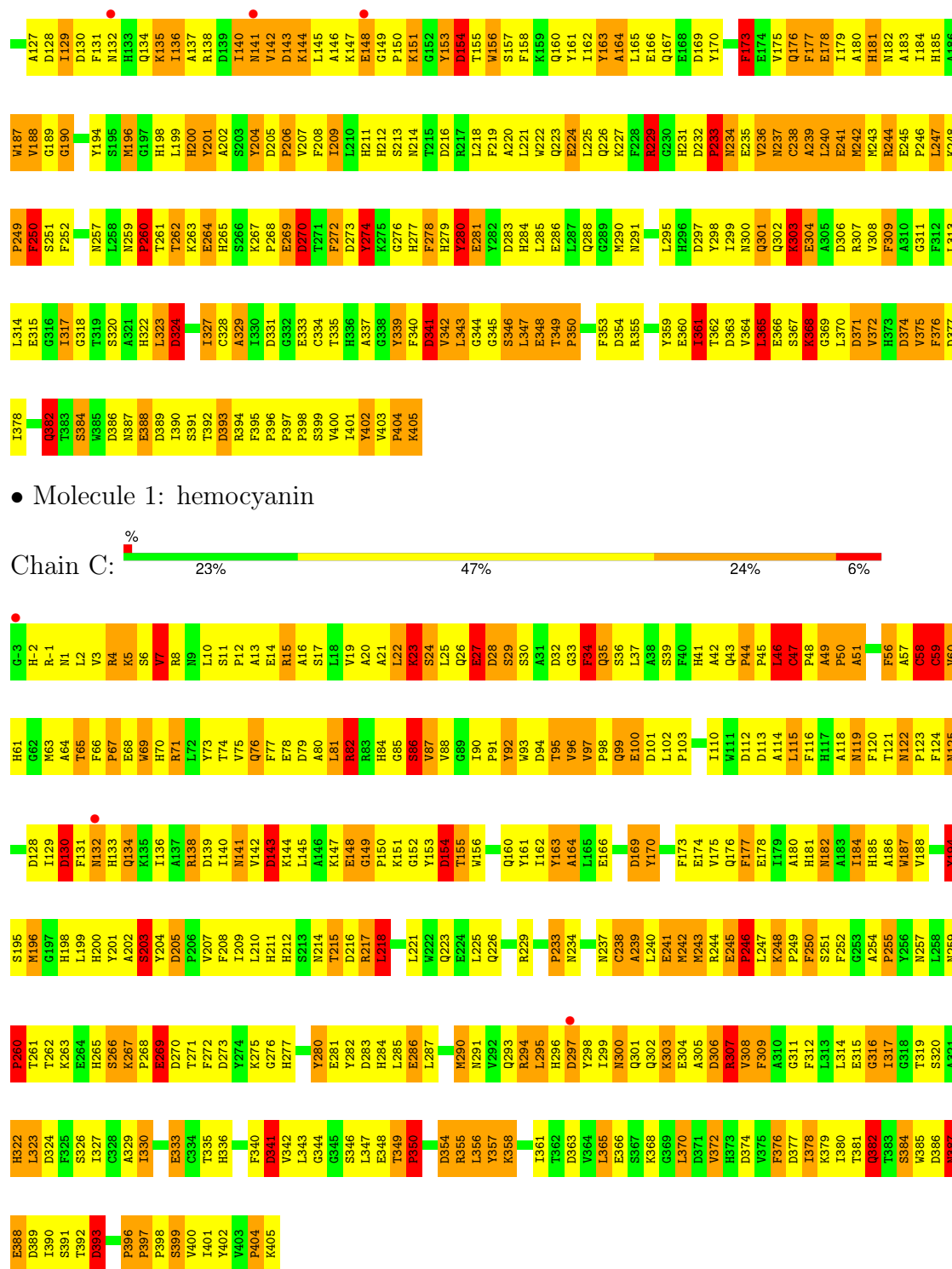
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: hemocyanin



• Molecule 1: hemocyanin





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.49Å 105.49Å 374.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.30 15.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-3.30) 95.8 (15.00-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 3.31Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.248 , 0.288 0.246 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	79.8	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 22.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	9984	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	1.80	53/3415 (1.6%)	1.61	69/4644 (1.5%)
1	B	2.00	91/3415 (2.7%)	1.77	79/4644 (1.7%)
1	C	1.83	64/3415 (1.9%)	1.58	62/4644 (1.3%)
All	All	1.88	208/10245 (2.0%)	1.66	210/13932 (1.5%)

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	C	0	1

All (208) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	333	GLU	CD-OE1	11.16	1.38	1.25
1	B	238	CYS	CB-SG	-10.44	1.64	1.82
1	C	27	GLU	CG-CD	-10.42	1.36	1.51
1	C	69	TRP	CB-CG	-9.38	1.33	1.50
1	B	137	ALA	CA-CB	-9.33	1.32	1.52
1	B	388	GLU	CD-OE2	8.76	1.35	1.25
1	A	264	GLU	CD-OE2	8.75	1.35	1.25
1	B	303	LYS	CD-CE	8.68	1.73	1.51
1	C	366	GLU	CD-OE1	8.40	1.34	1.25
1	B	148	GLU	CD-OE2	8.31	1.34	1.25
1	A	153	TYR	CE1-CZ	8.23	1.49	1.38
1	B	104	ALA	CA-CB	-8.18	1.35	1.52
1	C	388	GLU	CD-OE2	8.17	1.34	1.25
1	A	153	TYR	CG-CD2	7.94	1.49	1.39
1	A	315	GLU	CD-OE2	7.91	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	60	VAL	CB-CG1	-7.87	1.36	1.52
1	C	148	GLU	CD-OE1	7.83	1.34	1.25
1	B	394	ARG	NE-CZ	7.75	1.43	1.33
1	A	163	TYR	CE2-CZ	-7.64	1.28	1.38
1	B	92	TYR	CB-CG	7.63	1.63	1.51
1	B	235	GLU	CG-CD	7.62	1.63	1.51
1	B	16	ALA	CA-CB	-7.60	1.36	1.52
1	A	315	GLU	CD-OE1	7.52	1.33	1.25
1	C	156	TRP	CE3-CZ3	-7.50	1.25	1.38
1	C	164	ALA	CA-CB	-7.43	1.36	1.52
1	B	177	PHE	CG-CD1	-7.41	1.27	1.38
1	C	333	GLU	CD-OE2	7.41	1.33	1.25
1	A	333	GLU	CD-OE1	7.35	1.33	1.25
1	B	201	TYR	CD1-CE1	-7.32	1.28	1.39
1	C	308	VAL	CB-CG2	-7.25	1.37	1.52
1	C	342	VAL	CB-CG2	-7.24	1.37	1.52
1	B	164	ALA	CA-CB	-7.21	1.37	1.52
1	C	194	TYR	CE2-CZ	7.20	1.48	1.38
1	B	60	VAL	CB-CG2	-7.19	1.37	1.52
1	B	403	VAL	CB-CG2	-7.14	1.37	1.52
1	B	156	TRP	CB-CG	7.11	1.63	1.50
1	A	170	TYR	CD2-CE2	-7.11	1.28	1.39
1	B	178	GLU	CD-OE1	-7.10	1.17	1.25
1	A	38	ALA	CA-CB	-7.08	1.37	1.52
1	B	388	GLU	CD-OE1	7.08	1.33	1.25
1	B	73	TYR	CE1-CZ	-7.07	1.29	1.38
1	A	153	TYR	CE2-CZ	7.07	1.47	1.38
1	A	27	GLU	CD-OE1	7.00	1.33	1.25
1	B	342	VAL	CB-CG1	6.97	1.67	1.52
1	C	366	GLU	CD-OE2	6.95	1.33	1.25
1	C	357	TYR	CD1-CE1	-6.91	1.28	1.39
1	B	-3	GLY	N-CA	6.88	1.56	1.46
1	A	355	ARG	CB-CG	-6.84	1.34	1.52
1	B	72	LEU	C-O	-6.77	1.10	1.23
1	C	357	TYR	CD2-CE2	-6.75	1.29	1.39
1	B	187	TRP	CB-CG	-6.71	1.38	1.50
1	B	224	GLU	CD-OE2	6.70	1.33	1.25
1	A	187	TRP	CB-CG	-6.68	1.38	1.50
1	B	372	VAL	CB-CG2	-6.65	1.38	1.52
1	A	142	VAL	CB-CG1	6.61	1.66	1.52
1	C	170	TYR	CG-CD1	-6.61	1.30	1.39
1	C	245	GLU	CD-OE2	6.61	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	177	PHE	CE1-CZ	-6.57	1.24	1.37
1	B	274	TYR	CG-CD1	-6.57	1.30	1.39
1	B	315	GLU	CD-OE1	6.57	1.32	1.25
1	C	242	MET	SD-CE	6.50	2.14	1.77
1	A	204	TYR	CG-CD1	-6.48	1.30	1.39
1	C	76	GLN	CG-CD	-6.46	1.36	1.51
1	C	130	ASP	CB-CG	6.45	1.65	1.51
1	C	47	CYS	CB-SG	-6.45	1.71	1.82
1	A	175	VAL	CA-CB	-6.42	1.41	1.54
1	C	286	GLU	CG-CD	6.40	1.61	1.51
1	B	135	LYS	CD-CE	6.40	1.67	1.51
1	A	66	PHE	C-O	-6.40	1.11	1.23
1	C	239	ALA	CA-CB	-6.37	1.39	1.52
1	C	286	GLU	CD-OE2	6.37	1.32	1.25
1	C	382	GLN	CB-CG	6.36	1.69	1.52
1	B	329	ALA	CA-CB	6.36	1.65	1.52
1	A	222	TRP	CG-CD1	-6.35	1.27	1.36
1	A	281	GLU	CD-OE1	6.33	1.32	1.25
1	C	34	PHE	CD2-CE2	-6.30	1.26	1.39
1	B	73	TYR	CG-CD1	-6.28	1.30	1.39
1	B	20	ALA	CA-CB	6.28	1.65	1.52
1	B	111	TRP	CB-CG	-6.28	1.39	1.50
1	B	64	ALA	CA-CB	-6.27	1.39	1.52
1	B	58	CYS	CA-C	-6.24	1.36	1.52
1	A	269	GLU	CD-OE2	6.18	1.32	1.25
1	C	245	GLU	CD-OE1	6.17	1.32	1.25
1	C	244	ARG	CG-CD	6.16	1.67	1.51
1	C	376	PHE	CB-CG	-6.16	1.40	1.51
1	A	166	GLU	CD-OE2	6.15	1.32	1.25
1	C	269	GLU	CD-OE1	6.13	1.32	1.25
1	B	118	ALA	CA-CB	-6.13	1.39	1.52
1	B	333	GLU	CG-CD	6.12	1.61	1.51
1	C	170	TYR	CB-CG	-6.11	1.42	1.51
1	C	82	ARG	CG-CD	6.07	1.67	1.51
1	B	274	TYR	CE1-CZ	-6.01	1.30	1.38
1	C	56	PHE	CE2-CZ	-6.00	1.25	1.37
1	A	161	TYR	CD2-CE2	-6.00	1.30	1.39
1	B	281	GLU	CD-OE2	5.98	1.32	1.25
1	A	161	TYR	CE1-CZ	-5.95	1.30	1.38
1	B	239	ALA	CA-CB	-5.95	1.40	1.52
1	C	73	TYR	CD2-CE2	-5.94	1.30	1.39
1	B	13	ALA	CA-CB	-5.92	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	242	MET	CG-SD	5.88	1.96	1.81
1	C	69	TRP	CG-CD1	-5.88	1.28	1.36
1	A	27	GLU	CD-OE2	5.87	1.32	1.25
1	B	170	TYR	CE1-CZ	-5.86	1.30	1.38
1	A	62	GLY	C-O	-5.86	1.14	1.23
1	B	353	PHE	CD1-CE1	-5.83	1.27	1.39
1	C	388	GLU	CD-OE1	5.83	1.32	1.25
1	C	378	ILE	CA-CB	-5.82	1.41	1.54
1	B	124	PHE	CE1-CZ	5.79	1.48	1.37
1	A	204	TYR	CD1-CE1	-5.79	1.30	1.39
1	A	245	GLU	CG-CD	5.78	1.60	1.51
1	B	65	THR	CA-C	-5.77	1.38	1.52
1	B	281	GLU	CD-OE1	5.77	1.31	1.25
1	A	342	VAL	CA-CB	-5.77	1.42	1.54
1	B	177	PHE	CE2-CZ	-5.76	1.26	1.37
1	B	280	TYR	CE2-CZ	-5.75	1.31	1.38
1	A	382	GLN	CG-CD	5.74	1.64	1.51
1	C	92	TYR	CD2-CE2	-5.74	1.30	1.39
1	C	267	LYS	CD-CE	5.72	1.65	1.51
1	B	354	ASP	C-O	-5.68	1.12	1.23
1	B	250	PHE	CB-CG	-5.68	1.41	1.51
1	C	86	SER	CB-OG	5.65	1.49	1.42
1	C	358	LYS	CE-NZ	5.65	1.63	1.49
1	C	170	TYR	CG-CD2	-5.62	1.31	1.39
1	B	105	PHE	CE2-CZ	-5.62	1.26	1.37
1	B	235	GLU	CD-OE1	5.62	1.31	1.25
1	C	23	LYS	CE-NZ	-5.61	1.35	1.49
1	B	74	THR	C-O	-5.61	1.12	1.23
1	B	187	TRP	CE3-CZ3	-5.60	1.28	1.38
1	B	272	PHE	CD2-CE2	-5.60	1.28	1.39
1	C	170	TYR	CD2-CE2	-5.58	1.30	1.39
1	B	54	LYS	CD-CE	5.58	1.65	1.51
1	A	400	VAL	CA-CB	-5.57	1.43	1.54
1	C	51	ALA	CA-CB	5.57	1.64	1.52
1	B	224	GLU	CD-OE1	5.56	1.31	1.25
1	A	34	PHE	CE2-CZ	-5.54	1.26	1.37
1	A	250	PHE	CE1-CZ	5.52	1.47	1.37
1	C	203	SER	CB-OG	5.50	1.49	1.42
1	C	163	TYR	CE2-CZ	5.50	1.45	1.38
1	B	160	GLN	N-CA	-5.50	1.35	1.46
1	B	142	VAL	CB-CG1	5.49	1.64	1.52
1	B	353	PHE	CD2-CE2	-5.46	1.28	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	388	GLU	CG-CD	5.46	1.60	1.51
1	B	40	PHE	C-O	-5.46	1.12	1.23
1	C	5	LYS	CD-CE	5.45	1.64	1.51
1	B	22	LEU	CG-CD2	-5.45	1.31	1.51
1	A	20	ALA	CA-CB	5.44	1.63	1.52
1	A	161	TYR	CG-CD2	-5.44	1.32	1.39
1	A	166	GLU	CD-OE1	5.43	1.31	1.25
1	B	339	TYR	CD1-CE1	-5.43	1.31	1.39
1	A	93	TRP	CB-CG	-5.42	1.40	1.50
1	B	382	GLN	CD-NE2	5.40	1.46	1.32
1	B	83	ARG	CZ-NH1	5.37	1.40	1.33
1	B	188	VAL	CB-CG2	5.37	1.64	1.52
1	C	396	PRO	CA-C	-5.37	1.42	1.52
1	A	100	GLU	CG-CD	5.36	1.59	1.51
1	C	125	ASN	CB-CG	5.35	1.63	1.51
1	A	56	PHE	CD2-CE2	-5.35	1.28	1.39
1	A	153	TYR	CG-CD1	5.34	1.46	1.39
1	B	269	GLU	CD-OE1	5.34	1.31	1.25
1	C	317	ILE	CB-CG2	5.33	1.69	1.52
1	A	275	LYS	CD-CE	5.33	1.64	1.51
1	B	147	LYS	CB-CG	5.30	1.66	1.52
1	B	274	TYR	CE2-CZ	-5.30	1.31	1.38
1	A	364	VAL	CA-CB	-5.27	1.43	1.54
1	A	201	TYR	CE2-CZ	-5.26	1.31	1.38
1	B	69	TRP	CG-CD1	-5.26	1.29	1.36
1	A	32	ASP	CB-CG	-5.26	1.40	1.51
1	B	58	CYS	C-O	-5.26	1.13	1.23
1	B	313	LEU	C-O	-5.25	1.13	1.23
1	B	376	PHE	CD1-CE1	-5.25	1.28	1.39
1	C	17	SER	CB-OG	-5.24	1.35	1.42
1	A	75	VAL	CB-CG1	-5.24	1.41	1.52
1	B	309	PHE	CE2-CZ	-5.21	1.27	1.37
1	B	309	PHE	CG-CD1	-5.20	1.30	1.38
1	A	278	PHE	CB-CG	-5.19	1.42	1.51
1	C	182	ASN	C-O	-5.19	1.13	1.23
1	A	63	MET	SD-CE	-5.18	1.48	1.77
1	C	354	ASP	CB-CG	5.17	1.62	1.51
1	B	154	ASP	CB-CG	5.16	1.62	1.51
1	B	201	TYR	CD2-CE2	-5.16	1.31	1.39
1	C	143	ASP	CB-CG	5.16	1.62	1.51
1	C	267	LYS	CE-NZ	5.14	1.61	1.49
1	B	170	TYR	CG-CD1	-5.12	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	278	PHE	CD2-CE2	-5.11	1.29	1.39
1	A	308	VAL	CB-CG1	-5.11	1.42	1.52
1	B	178	GLU	CD-OE2	5.11	1.31	1.25
1	B	376	PHE	CE1-CZ	-5.11	1.27	1.37
1	C	58	CYS	CA-C	-5.11	1.39	1.52
1	C	399	SER	CB-OG	5.10	1.48	1.42
1	A	379	LYS	CB-CG	5.10	1.66	1.52
1	A	192	GLU	CD-OE1	-5.09	1.20	1.25
1	B	83	ARG	CZ-NH2	5.08	1.39	1.33
1	A	388	GLU	CD-OE1	5.08	1.31	1.25
1	C	280	TYR	CE2-CZ	-5.07	1.31	1.38
1	A	308	VAL	CA-CB	-5.07	1.44	1.54
1	C	319	THR	CB-CG2	5.07	1.69	1.52
1	B	236	VAL	CA-CB	-5.07	1.44	1.54
1	B	173	PHE	C-O	-5.06	1.13	1.23
1	B	163	TYR	CD1-CE1	-5.06	1.31	1.39
1	A	49	ALA	CA-CB	5.06	1.63	1.52
1	B	111	TRP	CE3-CZ3	-5.05	1.29	1.38
1	B	92	TYR	CD1-CE1	5.04	1.47	1.39
1	C	147	LYS	CD-CE	5.04	1.63	1.51
1	B	204	TYR	CG-CD1	-5.03	1.32	1.39
1	C	229	ARG	CZ-NH1	5.03	1.39	1.33
1	C	382	GLN	CG-CD	5.03	1.62	1.51
1	A	306	ASP	CB-CG	5.02	1.62	1.51
1	B	69	TRP	CE2-CZ2	-5.00	1.31	1.39

All (210) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	143	ASP	CB-CG-OD2	18.04	134.54	118.30
1	B	47	CYS	CA-CB-SG	-16.17	84.89	114.00
1	B	394	ARG	NE-CZ-NH1	13.36	126.98	120.30
1	A	218	LEU	CB-CG-CD2	-13.07	88.79	111.00
1	B	32	ASP	CB-CG-OD1	12.88	129.89	118.30
1	A	386	ASP	CB-CG-OD2	12.00	129.10	118.30
1	B	79	ASP	CB-CG-OD2	11.38	128.54	118.30
1	C	28	ASP	CB-CG-OD2	11.09	128.28	118.30
1	C	354	ASP	CB-CG-OD2	10.75	127.98	118.30
1	B	244	ARG	NE-CZ-NH1	-10.69	114.96	120.30
1	C	218	LEU	CB-CG-CD2	-10.58	93.02	111.00
1	C	27	GLU	OE1-CD-OE2	10.42	135.80	123.30
1	A	244	ARG	NE-CZ-NH1	-10.39	115.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	47	CYS	CA-CB-SG	-10.31	95.44	114.00
1	B	354	ASP	CB-CG-OD1	10.29	127.56	118.30
1	A	283	ASP	CB-CG-OD2	10.11	127.39	118.30
1	B	-1	ARG	NE-CZ-NH2	-10.08	115.26	120.30
1	B	377	ASP	CB-CG-OD2	10.07	127.36	118.30
1	A	82	ARG	NE-CZ-NH1	-10.02	115.29	120.30
1	A	169	ASP	CB-CG-OD2	9.97	127.28	118.30
1	C	356	LEU	CB-CG-CD1	9.49	127.14	111.00
1	C	363	ASP	CB-CG-OD2	9.48	126.83	118.30
1	A	81	LEU	CB-CG-CD1	-9.03	95.65	111.00
1	C	115	LEU	N-CA-C	-8.95	86.83	111.00
1	B	28	ASP	CB-CG-OD2	8.90	126.31	118.30
1	A	128	ASP	CB-CG-OD2	8.70	126.13	118.30
1	A	94	ASP	CB-CG-OD2	8.66	126.09	118.30
1	A	71	ARG	NE-CZ-NH2	-8.55	116.03	120.30
1	A	72	LEU	CB-CG-CD1	-8.53	96.49	111.00
1	B	238	CYS	CA-CB-SG	-8.51	98.67	114.00
1	A	233	PRO	N-CD-CG	-8.51	90.44	103.20
1	B	371	ASP	CB-CG-OD2	8.41	125.87	118.30
1	B	63	MET	CG-SD-CE	8.25	113.40	100.20
1	C	397	PRO	N-CD-CG	-8.14	90.98	103.20
1	C	217	ARG	NE-CZ-NH1	-8.09	116.26	120.30
1	B	169	ASP	CB-CG-OD2	8.05	125.54	118.30
1	A	285	LEU	CB-CG-CD1	-8.00	97.41	111.00
1	A	393	ASP	CB-CG-OD2	7.97	125.47	118.30
1	B	341	ASP	CB-CG-OD2	7.96	125.46	118.30
1	A	71	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	A	306	ASP	CB-CG-OD2	7.83	125.34	118.30
1	A	244	ARG	NE-CZ-NH2	7.81	124.20	120.30
1	B	324	ASP	CB-CG-OD2	7.76	125.28	118.30
1	A	83	ARG	NE-CZ-NH1	7.73	124.17	120.30
1	A	143	ASP	CB-CG-OD2	7.70	125.23	118.30
1	A	108	ASP	CB-CG-OD2	7.58	125.12	118.30
1	A	48	PRO	N-CD-CG	-7.56	91.85	103.20
1	C	356	LEU	CB-CG-CD2	-7.52	98.21	111.00
1	C	370	LEU	CA-CB-CG	-7.52	98.00	115.30
1	A	217	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	C	358	LYS	CD-CE-NZ	7.45	128.84	111.70
1	B	28	ASP	CB-CG-OD1	-7.45	111.60	118.30
1	C	243	MET	CG-SD-CE	7.25	111.81	100.20
1	A	297	ASP	CB-CG-OD2	7.25	124.82	118.30
1	B	297	ASP	CB-CG-OD2	7.24	124.81	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	306	ASP	CB-CG-OD1	7.19	124.77	118.30
1	A	47	CYS	CA-CB-SG	-7.18	101.07	114.00
1	C	184	ILE	CG1-CB-CG2	-7.16	95.66	111.40
1	C	341	ASP	CB-CG-OD1	7.15	124.74	118.30
1	A	28	ASP	CB-CG-OD2	7.14	124.72	118.30
1	B	154	ASP	CB-CG-OD2	7.14	124.72	118.30
1	A	210	LEU	CA-CB-CG	-7.11	98.95	115.30
1	C	4	ARG	NE-CZ-NH1	-7.09	116.76	120.30
1	B	306	ASP	CB-CG-OD2	7.08	124.67	118.30
1	C	143	ASP	CB-CG-OD2	7.04	124.63	118.30
1	C	143	ASP	CB-CG-OD1	7.02	124.62	118.30
1	A	209	ILE	CG1-CB-CG2	-6.92	96.18	111.40
1	C	229	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	C	377	ASP	CB-CG-OD2	6.89	124.50	118.30
1	C	32	ASP	CB-CG-OD1	6.88	124.50	118.30
1	C	295	LEU	CB-CG-CD2	-6.86	99.33	111.00
1	C	365	LEU	CB-CG-CD2	-6.84	99.37	111.00
1	B	101	ASP	CB-CG-OD2	6.82	124.44	118.30
1	B	46	LEU	CA-CB-CG	6.79	130.93	115.30
1	A	81	LEU	CB-CG-CD2	6.76	122.50	111.00
1	B	350	PRO	N-CD-CG	-6.75	93.08	103.20
1	C	355	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	C	46	LEU	CB-CG-CD1	6.64	122.29	111.00
1	C	143	ASP	OD1-CG-OD2	-6.61	110.74	123.30
1	B	394	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	B	138	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	C	374	ASP	CB-CG-OD1	-6.58	112.38	118.30
1	B	384	SER	CB-CA-C	-6.57	97.63	110.10
1	B	45	PRO	N-CD-CG	-6.54	93.38	103.20
1	A	27	GLU	OE1-CD-OE2	6.54	131.15	123.30
1	B	365	LEU	CA-CB-CG	6.54	130.34	115.30
1	A	47	CYS	N-CA-C	6.52	128.60	111.00
1	A	113	ASP	N-CA-C	6.50	128.56	111.00
1	C	370	LEU	CB-CG-CD2	-6.50	99.95	111.00
1	B	348	GLU	OE1-CD-OE2	-6.49	115.52	123.30
1	C	49	ALA	N-CA-C	-6.49	93.49	111.00
1	C	128	ASP	CB-CG-OD2	6.45	124.11	118.30
1	C	169	ASP	CB-CG-OD1	6.43	124.09	118.30
1	A	82	ARG	NE-CZ-NH2	6.39	123.50	120.30
1	A	359	TYR	CA-CB-CG	6.39	125.55	113.40
1	B	48	PRO	N-CD-CG	-6.39	93.62	103.20
1	C	58	CYS	CB-CA-C	-6.38	97.64	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	44	PRO	N-CD-CG	-6.30	93.75	103.20
1	A	355	ARG	NE-CZ-NH2	6.28	123.44	120.30
1	B	47	CYS	N-CA-C	6.28	127.97	111.00
1	B	377	ASP	CB-CG-OD1	-6.26	112.67	118.30
1	A	243	MET	CG-SD-CE	6.24	110.19	100.20
1	B	361	ILE	CG1-CB-CG2	6.24	125.14	111.40
1	C	205	ASP	CB-CG-OD2	6.24	123.92	118.30
1	B	405	LYS	CA-C-O	-6.22	107.03	120.10
1	A	240	LEU	CB-CG-CD2	-6.21	100.44	111.00
1	B	115	LEU	CA-CB-CG	6.21	129.58	115.30
1	A	324	ASP	CB-CG-OD2	6.20	123.88	118.30
1	B	22	LEU	CB-CG-CD1	6.20	121.54	111.00
1	B	224	GLU	OE1-CD-OE2	6.17	130.71	123.30
1	C	343	LEU	CA-CB-CG	6.16	129.46	115.30
1	C	295	LEU	CB-CG-CD1	6.15	121.45	111.00
1	C	130	ASP	CB-CG-OD2	6.13	123.81	118.30
1	A	67	PRO	N-CD-CG	-6.12	94.02	103.20
1	B	342	VAL	CA-CB-CG1	-6.07	101.79	110.90
1	A	143	ASP	OD1-CG-OD2	-6.06	111.78	123.30
1	B	143	ASP	OD1-CG-OD2	-6.03	111.84	123.30
1	A	308	VAL	CB-CA-C	-6.03	99.94	111.40
1	B	32	ASP	OD1-CG-OD2	-6.01	111.88	123.30
1	A	355	ARG	NE-CZ-NH1	-5.99	117.31	120.30
1	C	27	GLU	CB-CG-CD	-5.98	98.06	114.20
1	A	386	ASP	CB-CG-OD1	-5.97	112.92	118.30
1	C	67	PRO	N-CD-CG	-5.92	94.31	103.20
1	B	129	ILE	CG1-CB-CG2	-5.89	98.44	111.40
1	A	314	LEU	CB-CG-CD2	-5.87	101.02	111.00
1	B	65	THR	N-CA-CB	5.85	121.41	110.30
1	B	91	PRO	N-CD-CG	-5.85	94.43	103.20
1	A	90	ILE	CG1-CB-CG2	-5.84	98.56	111.40
1	A	10	LEU	CA-CB-CG	-5.82	101.92	115.30
1	A	384	SER	CB-CA-C	-5.80	99.08	110.10
1	C	28	ASP	CB-CG-OD1	-5.78	113.10	118.30
1	C	128	ASP	OD1-CG-OD2	-5.77	112.34	123.30
1	A	347	LEU	CA-CB-CG	5.76	128.54	115.30
1	B	229	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	B	349	THR	OG1-CB-CG2	-5.75	96.79	110.00
1	A	349	THR	OG1-CB-CG2	-5.74	96.79	110.00
1	C	393	ASP	CB-CG-OD2	5.73	123.45	118.30
1	A	295	LEU	CA-CB-CG	-5.72	102.15	115.30
1	C	128	ASP	CB-CG-OD1	5.72	123.44	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	73	TYR	CB-CG-CD2	5.71	124.42	121.00
1	A	316	GLY	N-CA-C	5.68	127.31	113.10
1	B	232	ASP	CB-CG-OD2	5.68	123.41	118.30
1	A	306	ASP	OD1-CG-OD2	-5.66	112.55	123.30
1	A	343	LEU	CB-CG-CD1	-5.65	101.39	111.00
1	B	247	LEU	CB-CG-CD1	-5.63	101.42	111.00
1	B	94	ASP	CB-CG-OD1	5.63	123.36	118.30
1	A	295	LEU	CB-CG-CD1	-5.61	101.46	111.00
1	A	46	LEU	CA-CB-CG	5.59	128.15	115.30
1	A	398	PRO	N-CD-CG	-5.57	94.85	103.20
1	B	48	PRO	N-CA-C	-5.56	97.64	112.10
1	A	10	LEU	CB-CG-CD1	-5.55	101.56	111.00
1	B	236	VAL	CA-CB-CG1	-5.54	102.60	110.90
1	B	113	ASP	CB-CG-OD2	5.53	123.28	118.30
1	B	83	ARG	NE-CZ-NH1	-5.51	117.54	120.30
1	C	324	ASP	CB-CG-OD1	5.51	123.26	118.30
1	A	27	GLU	CB-CA-C	-5.50	99.39	110.40
1	C	238	CYS	N-CA-CB	-5.50	100.69	110.60
1	B	393	ASP	CB-CG-OD2	5.48	123.23	118.30
1	B	22	LEU	CB-CG-CD2	-5.47	101.70	111.00
1	B	79	ASP	OD1-CG-OD2	-5.47	112.91	123.30
1	B	128	ASP	CB-CG-OD1	5.46	123.21	118.30
1	B	82	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	C	355	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	C	354	ASP	CB-CG-OD1	-5.42	113.42	118.30
1	B	206	PRO	N-CD-CG	-5.41	95.08	103.20
1	B	394	ARG	CD-NE-CZ	5.40	131.16	123.60
1	B	270	ASP	CB-CG-OD1	5.39	123.15	118.30
1	C	81	LEU	CB-CG-CD1	5.38	120.15	111.00
1	B	50	PRO	N-CD-CG	-5.36	95.16	103.20
1	B	371	ASP	CB-CG-OD1	-5.33	113.50	118.30
1	B	374	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	48	PRO	CA-N-CD	5.30	119.12	111.70
1	A	256	TYR	CB-CG-CD1	-5.29	117.82	121.00
1	C	266	SER	N-CA-CB	-5.29	102.56	110.50
1	C	63	MET	CG-SD-CE	-5.28	91.75	100.20
1	A	255	PRO	N-CD-CG	-5.28	95.28	103.20
1	C	154	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	275	LYS	N-CA-C	-5.27	96.76	111.00
1	B	143	ASP	N-CA-C	-5.27	96.77	111.00
1	A	218	LEU	CB-CG-CD1	-5.26	102.06	111.00
1	A	343	LEU	CB-CG-CD2	-5.26	102.06	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	ASP	CB-CG-OD1	-5.25	113.58	118.30
1	B	240	LEU	CB-CG-CD2	-5.25	102.08	111.00
1	C	7	VAL	CB-CA-C	-5.23	101.47	111.40
1	A	8	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	B	-1	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	317	ILE	CB-CA-C	-5.22	101.17	111.60
1	B	276	GLY	N-CA-C	-5.21	100.06	113.10
1	B	148	GLU	CG-CD-OE1	-5.21	107.88	118.30
1	B	209	ILE	CG1-CB-CG2	-5.20	99.95	111.40
1	B	143	ASP	CB-CG-OD1	-5.20	113.62	118.30
1	B	164	ALA	CB-CA-C	-5.18	102.33	110.10
1	A	143	ASP	CB-CG-OD1	5.17	122.95	118.30
1	B	355	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	C	143	ASP	N-CA-C	-5.14	97.11	111.00
1	B	175	VAL	CA-CB-CG2	-5.14	103.19	110.90
1	A	138	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	C	307	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	B	244	ARG	NH1-CZ-NH2	5.12	125.04	119.40
1	A	140	ILE	CG1-CB-CG2	5.12	122.67	111.40
1	C	215	THR	CA-CB-CG2	-5.08	105.29	112.40
1	B	285	LEU	CB-CG-CD2	-5.08	102.37	111.00
1	A	130	ASP	CB-CG-OD1	5.07	122.86	118.30
1	C	59	CYS	CA-CB-SG	5.07	123.12	114.00
1	C	307	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	C	65	THR	OG1-CB-CG2	-5.06	98.36	110.00
1	B	237	ASN	N-CA-C	-5.05	97.37	111.00
1	C	218	LEU	CB-CG-CD1	5.04	119.58	111.00
1	B	8	ARG	NE-CZ-NH2	5.04	122.82	120.30
1	C	130	ASP	OD1-CG-OD2	-5.02	113.76	123.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	82	ARG	Sidechain

5.2 Too-close contacts

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	3310	0	3075	455	2
1	B	3310	0	3074	400	0
1	C	3310	0	3074	452	0
2	A	15	0	15	3	0
2	C	30	0	30	1	0
3	A	2	0	0	0	0
3	B	4	0	0	0	2
3	C	3	0	0	0	0
All	All	9984	0	9268	1305	2

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 68.

All (1305) 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:290:MET:SD	1:A:290:MET:CE	2.02	1.47
1:B:290:MET:SD	1:B:290:MET:CE	2.05	1.44
1:C:59:CYS:SG	1:C:61:HIS:CE1	2.18	1.36
1:C:242:MET:CE	1:C:242:MET:SD	2.14	1.36
1:C:-2:HIS:CD2	1:C:-1:ARG:HE	1.57	1.22
1:B:200:HIS:CE1	1:B:347:LEU:HB2	1.76	1.20
1:C:71:ARG:HH22	1:C:223:GLN:NE2	1.39	1.20
1:B:372:VAL:HG11	1:B:402:TYR:CD1	1.80	1.16
1:A:316:GLY:O	1:A:317:ILE:HG23	1.44	1.14
1:A:59:CYS:SG	1:A:61:HIS:CE1	2.43	1.11
1:B:226:GLN:NE2	1:B:229:ARG:HH12	1.47	1.11
1:A:59:CYS:SG	1:A:61:HIS:NE2	2.24	1.10
1:A:290:MET:HB2	1:A:294:ARG:HB2	1.20	1.09
1:A:355:ARG:HH11	1:A:355:ARG:HB3	1.19	1.05
1:C:139:ASP:OD1	1:C:141:ASN:HB2	1.56	1.05
1:B:132:ASN:ND2	1:B:134:GLN:HG3	1.73	1.03
1:B:-1:ARG:HH11	1:B:-1:ARG:HG2	1.14	1.03
1:A:69:TRP:HD1	1:A:247:LEU:HD22	1.24	1.02
1:A:69:TRP:CD1	1:A:247:LEU:HD22	1.96	1.01
1:B:328:CYS:HA	1:B:334:CYS:HA	1.41	1.01
1:C:97:VAL:HG12	1:C:98:PRO:HD2	1.40	1.01
1:C:113:ASP:HB3	1:C:118:ALA:HB3	1.40	1.01
1:C:316:GLY:O	1:C:317:ILE:CG1	2.08	1.01
1:A:96:VAL:HG11	1:A:287:LEU:HD11	1.41	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:-2:HIS:CE1	1:B:-1:ARG:NH1	2.30	0.99
1:B:200:HIS:HE1	1:B:347:LEU:HB2	0.84	0.99
1:B:342:VAL:HG12	1:B:343:LEU:H	1.23	0.99
1:B:402:TYR:HE2	1:B:404:PRO:HG3	1.26	0.98
1:C:149:GLY:O	1:C:152:GLY:N	1.96	0.98
1:A:290:MET:HB2	1:A:294:ARG:CB	1.92	0.98
1:A:171:CYS:HB3	1:A:355:ARG:HH21	1.29	0.98
1:B:110:ILE:HD12	1:B:110:ILE:H	1.27	0.98
1:C:7:VAL:HG11	1:C:210:LEU:HD23	1.46	0.98
1:A:365:LEU:O	1:A:370:LEU:HB2	1.63	0.97
1:B:142:VAL:HG13	1:B:144:LYS:HB2	1.42	0.97
1:C:78:GLU:C	1:C:80:ALA:H	1.69	0.96
1:C:316:GLY:O	1:C:317:ILE:HG13	1.63	0.96
1:A:66:PHE:HB3	1:A:67:PRO:HD3	1.45	0.95
1:C:129:ILE:HG13	1:C:136:ILE:HD11	1.46	0.95
1:B:234:ASN:HD21	1:B:273:ASP:CB	1.80	0.95
1:A:182:ASN:HD22	1:A:342:VAL:HA	1.28	0.94
1:C:259:ASN:HD21	1:C:261:THR:N	1.64	0.94
1:B:22:LEU:HD12	1:B:25:LEU:HD23	1.47	0.94
1:B:161:TYR:CD2	1:B:218:LEU:HD13	2.03	0.94
1:C:121:THR:O	1:C:123:PRO:HD3	1.67	0.94
1:A:56:PHE:HD1	1:A:349:THR:HG22	1.32	0.93
1:B:401:ILE:HG22	1:B:402:TYR:N	1.83	0.93
1:B:196:MET:CE	1:B:207:VAL:HG13	1.99	0.93
1:B:372:VAL:HG11	1:B:402:TYR:HD1	1.35	0.92
1:A:39:SER:HB3	1:A:44:PRO:HD2	1.48	0.91
1:C:78:GLU:O	1:C:80:ALA:N	2.03	0.91
1:C:-2:HIS:CD2	1:C:-1:ARG:NE	2.34	0.91
1:C:210:LEU:HD12	1:C:210:LEU:H	1.34	0.91
1:B:145:LEU:HD12	1:B:146:ALA:N	1.84	0.91
1:C:71:ARG:NH2	1:C:223:GLN:HE22	1.67	0.91
1:A:244:ARG:HH11	1:A:244:ARG:HG2	1.36	0.90
1:C:260:PRO:HG2	1:C:261:THR:N	1.86	0.90
1:C:198:HIS:CE1	1:C:200:HIS:HB2	2.05	0.90
1:A:386:ASP:O	1:A:387:ASN:CG	2.10	0.90
1:C:-1:ARG:HB2	1:C:1:ASN:N	1.86	0.90
1:C:136:ILE:HD12	1:C:136:ILE:H	1.35	0.90
1:C:175:VAL:HG23	1:C:176:GLN:H	1.36	0.90
1:C:71:ARG:HH22	1:C:223:GLN:HE22	0.91	0.90
1:C:113:ASP:CB	1:C:118:ALA:HB3	2.02	0.89
1:C:380:ILE:HD11	1:C:392:THR:HB	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:LEU:HD23	1:C:26:GLN:HG3	1.52	0.89
1:B:402:TYR:CE2	1:B:404:PRO:HG3	2.07	0.89
1:A:136:ILE:HD11	1:A:204:TYR:CB	2.02	0.89
1:C:247:LEU:HD22	1:C:268:PRO:HG3	1.52	0.89
1:C:86:SER:O	1:C:88:VAL:N	2.06	0.88
1:B:151:LYS:HE2	1:B:151:LYS:HA	1.56	0.88
1:B:148:GLU:HG2	1:B:155:THR:HB	1.53	0.88
1:A:372:VAL:HG11	1:A:402:TYR:HE1	1.39	0.88
1:A:97:VAL:HG12	1:A:288:GLN:HG3	1.56	0.87
1:B:71:ARG:HD3	1:B:216:ASP:OD2	1.74	0.87
1:A:140:ILE:HG22	1:A:142:VAL:O	1.74	0.87
1:C:265:HIS:CD2	1:C:277:HIS:HB3	2.10	0.87
1:B:132:ASN:ND2	1:B:134:GLN:CG	2.36	0.87
1:C:161:TYR:CD2	1:C:218:LEU:HD22	2.10	0.86
1:A:198:HIS:O	1:A:200:HIS:N	2.08	0.86
1:B:259:ASN:CG	1:B:262:THR:HB	1.94	0.86
1:A:60:VAL:HG11	1:A:65:THR:OG1	1.75	0.86
1:A:-1:ARG:O	1:A:279:HIS:ND1	2.09	0.86
1:B:181:HIS:O	1:B:181:HIS:CG	2.27	0.86
1:B:382:GLN:HB3	1:B:390:ILE:HB	1.58	0.85
1:C:33:GLY:O	1:C:34:PHE:O	1.94	0.85
1:B:132:ASN:HD21	1:B:134:GLN:HG3	1.37	0.84
1:C:4:ARG:HD2	1:C:282:TYR:CE1	2.12	0.84
1:C:81:LEU:HB3	1:C:86:SER:HB3	1.58	0.84
1:C:59:CYS:HG	1:C:61:HIS:CE1	1.90	0.84
1:C:-1:ARG:HB2	1:C:1:ASN:H2	1.41	0.84
1:A:65:THR:HG23	1:A:242:MET:HG3	1.59	0.84
1:A:220:ALA:HA	1:A:223:GLN:HE21	1.41	0.84
1:B:148:GLU:HG2	1:B:155:THR:CB	2.06	0.83
1:B:226:GLN:NE2	1:B:229:ARG:NH1	2.26	0.83
1:A:330:ILE:HD12	1:A:330:ILE:H	1.43	0.83
1:C:346:SER:HB2	1:C:347:LEU:HD22	1.59	0.83
1:A:94:ASP:HA	1:A:214:ASN:ND2	1.94	0.82
1:A:292:VAL:O	1:A:295:LEU:HB2	1.79	0.82
1:A:140:ILE:CG2	1:A:142:VAL:O	2.27	0.82
1:A:47:CYS:HB2	1:A:57:ALA:O	1.79	0.82
1:B:-1:ARG:HG2	1:B:-1:ARG:NH1	1.94	0.82
1:C:238:CYS:O	1:C:239:ALA:HB3	1.79	0.82
1:C:145:LEU:HD23	1:C:145:LEU:H	1.44	0.82
1:A:316:GLY:O	1:A:317:ILE:CG2	2.28	0.82
1:A:153:TYR:HB2	1:A:288:GLN:OE1	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:CYS:O	1:C:59:CYS:HB3	1.78	0.82
1:A:140:ILE:HD12	1:A:140:ILE:H	1.44	0.82
1:B:200:HIS:HE1	1:B:347:LEU:CB	1.81	0.81
1:B:196:MET:HE2	1:B:207:VAL:HG13	1.61	0.81
1:B:236:VAL:HG12	1:B:237:ASN:N	1.95	0.81
1:B:141:ASN:ND2	1:B:142:VAL:H	1.78	0.81
1:C:76:GLN:O	1:C:76:GLN:HG3	1.80	0.81
1:A:15:ARG:O	1:A:19:VAL:HG23	1.80	0.81
1:A:244:ARG:HG2	1:A:244:ARG:NH1	1.94	0.81
1:B:165:LEU:HD23	1:B:222:TRP:HD1	1.44	0.81
1:C:140:ILE:O	1:C:142:VAL:N	2.14	0.81
1:A:56:PHE:CD1	1:A:349:THR:HG22	2.16	0.81
1:B:345:GLY:O	1:B:348:GLU:HG2	1.81	0.80
1:B:11:SER:O	1:B:14:GLU:N	2.13	0.80
1:A:96:VAL:HG11	1:A:287:LEU:CD1	2.12	0.80
1:A:-3:GLY:HA2	1:A:1:ASN:N	1.97	0.80
1:A:207:VAL:HA	1:A:210:LEU:HD12	1.61	0.80
1:B:236:VAL:HG12	1:B:238:CYS:N	1.97	0.80
1:A:290:MET:CB	1:A:294:ARG:HB2	2.09	0.80
1:C:175:VAL:HG23	1:C:176:GLN:N	1.96	0.80
1:C:33:GLY:O	1:C:34:PHE:C	2.17	0.80
1:B:303:LYS:HE2	1:B:405:LYS:HG2	1.63	0.80
1:C:150:PRO:HD2	1:C:154:ASP:HB3	1.61	0.80
1:A:198:HIS:O	1:A:199:LEU:C	2.21	0.80
1:A:98:PRO:HB3	1:A:147:LYS:HA	1.64	0.79
1:C:-2:HIS:O	1:C:-1:ARG:NE	2.15	0.79
1:C:316:GLY:C	1:C:317:ILE:HG13	2.03	0.79
1:C:259:ASN:ND2	1:C:261:THR:N	2.29	0.79
1:B:45:PRO:HG2	1:B:45:PRO:O	1.82	0.79
1:B:327:ILE:HG23	1:B:327:ILE:O	1.81	0.79
1:B:110:ILE:HD12	1:B:110:ILE:N	1.98	0.79
1:C:93:TRP:HE1	1:C:99:GLN:HE22	1.28	0.78
1:B:-2:HIS:CE1	1:B:-1:ARG:HH12	2.01	0.78
1:C:136:ILE:HG21	1:C:205:ASP:HB2	1.64	0.78
1:C:247:LEU:HB2	1:C:266:SER:O	1.82	0.78
1:C:246:PRO:HG3	1:C:267:LYS:HE3	1.64	0.78
1:C:260:PRO:HG2	1:C:261:THR:H	1.46	0.78
1:C:149:GLY:C	1:C:152:GLY:H	1.87	0.78
1:C:234:ASN:OD1	1:C:273:ASP:HB2	1.83	0.78
1:C:245:GLU:O	1:C:246:PRO:O	2.01	0.78
1:A:8:ARG:HE	1:A:103:PRO:HG3	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ILE:HD12	1:A:110:ILE:H	1.48	0.78
1:C:347:LEU:HD22	1:C:347:LEU:N	1.99	0.77
1:C:320:SER:HB3	1:C:344:GLY:H	1.48	0.77
1:A:236:VAL:HG21	1:A:272:PHE:CZ	2.20	0.77
1:B:372:VAL:CG1	1:B:402:TYR:CD1	2.67	0.77
1:C:113:ASP:HB3	1:C:118:ALA:CB	2.14	0.77
1:C:268:PRO:O	1:C:270:ASP:N	2.17	0.77
1:C:402:TYR:CE2	1:C:404:PRO:HG3	2.20	0.77
1:A:1:ASN:HB3	1:A:279:HIS:HB3	1.65	0.77
1:B:342:VAL:HG12	1:B:343:LEU:N	1.98	0.77
1:C:207:VAL:HA	1:C:210:LEU:HD13	1.66	0.77
1:B:262:THR:HG22	1:B:263:LYS:N	1.98	0.77
1:C:401:ILE:HG22	1:C:402:TYR:N	2.00	0.77
1:A:136:ILE:HD11	1:A:204:TYR:C	2.04	0.77
1:C:320:SER:HB3	1:C:344:GLY:N	2.00	0.76
1:B:244:ARG:O	1:B:244:ARG:HG2	1.86	0.76
1:A:108:ASP:HB2	1:A:110:ILE:HD12	1.67	0.76
1:C:150:PRO:HD2	1:C:154:ASP:O	1.85	0.76
1:C:335:THR:HG21	1:C:368:LYS:HE3	1.66	0.76
1:B:41:HIS:O	1:B:59:CYS:HB3	1.84	0.76
1:A:171:CYS:CB	1:A:355:ARG:HH21	1.98	0.76
1:A:264:GLU:HG3	1:A:265:HIS:CE1	2.20	0.76
1:C:39:SER:OG	1:C:44:PRO:HD2	1.86	0.75
1:A:-1:ARG:O	1:A:279:HIS:CG	2.39	0.75
1:B:132:ASN:HD22	1:B:134:GLN:CG	1.98	0.75
1:B:236:VAL:HG12	1:B:238:CYS:H	1.52	0.75
1:C:316:GLY:O	1:C:317:ILE:HG12	1.85	0.75
1:C:354:ASP:O	1:C:355:ARG:HB3	1.84	0.75
1:C:386:ASP:O	1:C:388:GLU:N	2.19	0.75
1:A:68:GLU:HB3	1:A:271:THR:OG1	1.86	0.75
1:A:136:ILE:CG2	1:A:137:ALA:N	2.49	0.75
1:B:39:SER:O	1:B:40:PHE:C	2.18	0.75
1:B:161:TYR:CE2	1:B:218:LEU:HD13	2.21	0.75
1:C:237:ASN:HA	1:C:240:LEU:HD21	1.69	0.75
1:C:174:GLU:OE1	1:C:178:GLU:OE2	2.05	0.75
1:B:257:ASN:HD21	1:B:262:THR:HG22	1.52	0.74
1:A:325:PHE:O	1:A:337:ALA:HB3	1.87	0.74
1:B:166:GLU:OE1	1:B:307:ARG:NH2	2.20	0.74
1:C:71:ARG:NH2	1:C:223:GLN:NE2	2.25	0.74
1:A:69:TRP:HD1	1:A:247:LEU:CD2	1.99	0.74
1:C:259:ASN:ND2	1:C:262:THR:H	1.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:LEU:O	1:A:221:LEU:HB3	1.86	0.74
1:B:32:ASP:HA	1:B:37:LEU:HD21	1.70	0.74
1:A:291:ASN:O	1:A:295:LEU:HD12	1.87	0.74
1:A:380:ILE:HD12	1:A:380:ILE:O	1.88	0.74
1:C:8:ARG:HH12	1:C:103:PRO:HA	1.50	0.74
1:C:112:ASP:C	1:C:114:ALA:H	1.90	0.74
1:B:-1:ARG:HH11	1:B:-1:ARG:CG	1.95	0.74
1:B:249:PRO:O	1:B:250:PHE:C	2.25	0.73
1:C:284:HIS:O	1:C:286:GLU:N	2.21	0.73
1:A:47:CYS:SG	1:A:248:LYS:HG3	2.29	0.73
1:C:7:VAL:O	1:C:10:LEU:HG	1.87	0.73
1:C:205:ASP:OD1	1:C:207:VAL:HG22	1.88	0.73
1:A:384:SER:OG	1:A:386:ASP:N	2.21	0.73
1:C:77:PHE:O	1:C:80:ALA:HB3	1.88	0.73
1:A:355:ARG:HB3	1:A:355:ARG:NH1	2.00	0.73
1:B:317:ILE:N	1:B:317:ILE:HD13	2.04	0.73
1:B:148:GLU:CG	1:B:155:THR:HA	2.19	0.72
1:C:41:HIS:CE1	1:C:61:HIS:HE1	2.06	0.72
1:C:74:THR:OG1	1:C:75:VAL:N	2.20	0.72
1:C:78:GLU:C	1:C:80:ALA:N	2.36	0.72
1:A:57:ALA:O	1:A:58:CYS:HB2	1.88	0.72
1:B:236:VAL:CG1	1:B:237:ASN:N	2.52	0.72
1:B:142:VAL:C	1:B:144:LYS:H	1.90	0.72
1:B:47:CYS:HB2	1:B:56:PHE:O	1.88	0.72
1:C:132:ASN:HB3	1:C:134:GLN:HE22	1.55	0.72
1:B:372:VAL:CG1	1:B:402:TYR:HD1	2.01	0.72
1:C:175:VAL:HG23	1:C:176:GLN:HG2	1.71	0.72
1:C:217:ARG:HA	1:C:282:TYR:CE2	2.24	0.72
1:C:265:HIS:NE2	1:C:277:HIS:HB3	2.04	0.72
1:B:142:VAL:C	1:B:144:LYS:N	2.41	0.72
1:C:198:HIS:O	1:C:199:LEU:C	2.28	0.72
1:A:171:CYS:HB3	1:A:355:ARG:NH2	2.05	0.71
1:B:234:ASN:HD21	1:B:273:ASP:HB3	1.52	0.71
1:C:81:LEU:HB3	1:C:86:SER:CB	2.21	0.71
1:A:91:PRO:HG2	1:A:210:LEU:CD2	2.21	0.71
1:B:257:ASN:ND2	1:B:262:THR:HG22	2.05	0.71
1:A:173:PHE:CE1	1:A:177:PHE:HB2	2.25	0.71
1:B:28:ASP:O	1:B:33:GLY:HA3	1.91	0.71
1:A:31:ALA:HB3	1:A:258:LEU:CD1	2.21	0.71
1:C:22:LEU:HA	1:C:25:LEU:HB3	1.72	0.71
1:B:166:GLU:HB3	1:B:167:GLN:HE21	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:HIS:CE1	1:B:277:HIS:HD2	2.08	0.70
1:B:371:ASP:N	1:B:371:ASP:OD1	2.24	0.70
1:C:401:ILE:HG22	1:C:402:TYR:H	1.55	0.70
1:A:224:GLU:O	1:A:227:LYS:HB3	1.90	0.70
1:B:184:ILE:CD1	1:B:184:ILE:N	2.54	0.70
1:C:68:GLU:HG2	1:C:268:PRO:HB3	1.73	0.70
1:C:202:ALA:O	1:C:203:SER:C	2.29	0.70
1:A:7:VAL:HA	1:A:10:LEU:CD1	2.22	0.70
1:B:142:VAL:HA	1:B:144:LYS:HG2	1.74	0.70
1:C:58:CYS:O	1:C:59:CYS:CB	2.40	0.70
1:C:300:ASN:O	1:C:303:LYS:HG3	1.92	0.70
1:B:148:GLU:HG2	1:B:155:THR:CA	2.22	0.70
1:C:7:VAL:CG1	1:C:210:LEU:HD23	2.20	0.70
1:C:129:ILE:HG13	1:C:136:ILE:CD1	2.21	0.70
1:B:71:ARG:HH22	1:B:223:GLN:HE22	1.39	0.69
1:B:234:ASN:HD21	1:B:273:ASP:HB2	1.56	0.69
1:A:136:ILE:HD13	1:A:205:ASP:CA	2.23	0.69
1:A:136:ILE:HD11	1:A:204:TYR:HB2	1.74	0.69
1:B:198:HIS:HD2	1:B:200:HIS:H	1.38	0.69
1:B:263:LYS:O	1:B:265:HIS:N	2.26	0.69
1:A:136:ILE:CD1	1:A:204:TYR:C	2.61	0.69
1:B:196:MET:HA	1:B:202:ALA:HB2	1.75	0.69
1:B:249:PRO:O	1:B:251:SER:N	2.26	0.69
1:C:200:HIS:CE1	1:C:346:SER:H	2.11	0.69
1:B:238:CYS:SG	1:B:239:ALA:N	2.66	0.68
1:C:322:HIS:HB2	1:C:341:ASP:HB3	1.75	0.68
1:C:4:ARG:CD	1:C:282:TYR:HE1	2.07	0.68
1:C:259:ASN:ND2	1:C:262:THR:N	2.41	0.68
1:A:95:THR:HG21	1:A:184:ILE:HG12	1.75	0.68
1:A:220:ALA:HA	1:A:223:GLN:NE2	2.08	0.68
1:A:319:THR:HA	1:A:344:GLY:O	1.93	0.68
1:A:-3:GLY:O	1:A:-1:ARG:N	2.27	0.68
1:A:161:TYR:O	1:A:165:LEU:HG	1.93	0.68
1:A:372:VAL:HG11	1:A:402:TYR:CE1	2.25	0.68
1:B:150:PRO:O	1:B:151:LYS:HD2	1.93	0.68
1:A:169:ASP:O	1:A:171:CYS:N	2.27	0.68
1:A:184:ILE:O	1:A:185:HIS:C	2.30	0.68
1:B:136:ILE:O	1:B:136:ILE:HD12	1.94	0.68
1:C:11:SER:H	1:C:14:GLU:HB2	1.59	0.68
1:A:323:LEU:HA	1:A:381:THR:O	1.94	0.68
1:B:3:VAL:O	1:B:3:VAL:HG13	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ASN:ND2	1:B:273:ASP:HB2	2.09	0.68
1:B:401:ILE:CG2	1:B:402:TYR:N	2.54	0.67
1:A:91:PRO:HG2	1:A:210:LEU:HD22	1.77	0.67
1:C:150:PRO:CD	1:C:154:ASP:HB3	2.23	0.67
1:A:266:SER:O	1:A:268:PRO:HD3	1.94	0.67
1:B:182:ASN:HD22	1:B:342:VAL:HA	1.59	0.67
1:C:8:ARG:HG2	1:C:8:ARG:HH11	1.58	0.67
1:C:66:PHE:HB3	1:C:67:PRO:HD3	1.77	0.67
1:C:132:ASN:O	1:C:134:GLN:NE2	2.27	0.67
1:C:210:LEU:H	1:C:210:LEU:CD1	2.08	0.67
1:A:286:GLU:HG2	1:A:290:MET:O	1.94	0.67
1:A:299:ILE:O	1:A:302:GLN:N	2.28	0.67
1:A:108:ASP:HB2	1:A:110:ILE:CD1	2.23	0.67
1:C:71:ARG:HD3	1:C:216:ASP:OD1	1.94	0.67
1:B:97:VAL:HG13	1:B:98:PRO:HD2	1.77	0.67
1:B:307:ARG:O	1:B:308:VAL:HG23	1.95	0.67
1:C:330:ILE:H	1:C:330:ILE:CD1	2.07	0.67
1:B:15:ARG:O	1:B:19:VAL:HG23	1.96	0.66
1:C:186:ALA:O	1:C:188:VAL:N	2.27	0.66
1:A:119:ASN:OD1	1:A:119:ASN:O	2.14	0.66
1:A:214:ASN:O	1:A:217:ARG:HB3	1.95	0.66
1:B:226:GLN:HE21	1:B:229:ARG:HH12	1.41	0.66
1:C:131:PHE:CG	1:C:132:ASN:N	2.63	0.66
1:A:136:ILE:HD13	1:A:205:ASP:HA	1.75	0.66
1:A:169:ASP:O	1:A:172:ASP:N	2.19	0.66
1:B:231:HIS:O	1:B:233:PRO:HD3	1.96	0.66
1:A:36:SER:O	1:A:38:ALA:N	2.27	0.66
1:B:320:SER:HA	1:B:344:GLY:H	1.61	0.66
1:A:47:CYS:O	1:A:48:PRO:C	2.31	0.66
1:A:66:PHE:CB	1:A:67:PRO:HD3	2.24	0.66
1:A:330:ILE:H	1:A:330:ILE:CD1	2.03	0.66
1:B:141:ASN:HD21	1:B:187:TRP:HA	1.60	0.66
1:A:110:ILE:HD12	1:A:110:ILE:N	2.11	0.66
1:C:8:ARG:HH12	1:C:103:PRO:CA	2.08	0.66
1:A:98:PRO:HB3	1:A:147:LYS:CA	2.26	0.66
1:B:234:ASN:ND2	1:B:273:ASP:CB	2.57	0.66
1:C:28:ASP:O	1:C:33:GLY:HA3	1.96	0.66
1:C:249:PRO:O	1:C:251:SER:N	2.29	0.66
1:A:325:PHE:CD2	1:A:337:ALA:HB3	2.30	0.66
1:B:196:MET:HE3	1:B:207:VAL:HG13	1.77	0.65
1:A:66:PHE:HB3	1:A:67:PRO:CD	2.23	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:VAL:HG21	1:A:402:TYR:CE1	2.31	0.65
1:B:112:ASP:O	1:B:114:ALA:N	2.29	0.65
1:B:240:LEU:HD12	1:B:240:LEU:H	1.61	0.65
1:B:257:ASN:OD1	1:B:259:ASN:HB3	1.96	0.65
1:C:92:TYR:HB2	1:C:214:ASN:HB2	1.79	0.65
1:B:161:TYR:CE2	1:B:218:LEU:CD1	2.79	0.65
1:A:232:ASP:OD2	1:A:234:ASN:N	2.27	0.65
1:C:136:ILE:HD12	1:C:136:ILE:N	2.08	0.65
1:C:260:PRO:CG	1:C:261:THR:N	2.60	0.65
1:C:22:LEU:HG	1:C:25:LEU:HD23	1.78	0.65
1:C:161:TYR:CD2	1:C:218:LEU:CD2	2.80	0.65
1:A:192:GLU:HB2	1:A:195:SER:OG	1.97	0.65
1:C:59:CYS:SG	1:C:61:HIS:HE1	2.11	0.64
1:A:145:LEU:O	1:A:145:LEU:HD12	1.98	0.64
1:B:104:ALA:O	1:B:107:ASN:N	2.30	0.64
1:B:328:CYS:CA	1:B:334:CYS:HA	2.25	0.64
1:B:141:ASN:HD22	1:B:142:VAL:HG23	1.62	0.64
1:B:225:LEU:O	1:B:229:ARG:HB2	1.98	0.64
1:C:330:ILE:H	1:C:330:ILE:HD12	1.62	0.64
1:A:162:ILE:HD12	1:A:165:LEU:HD12	1.79	0.64
1:C:131:PHE:HE2	1:C:204:TYR:OH	1.80	0.64
1:A:236:VAL:HG12	1:A:238:CYS:H	1.62	0.64
1:B:90:ILE:HG21	1:B:209:ILE:HG22	1.80	0.64
1:A:281:GLU:HG2	1:A:282:TYR:N	2.10	0.64
1:C:122:ASN:HD22	1:C:122:ASN:C	1.99	0.64
1:C:129:ILE:CD1	1:C:136:ILE:HD12	2.28	0.64
1:B:-1:ARG:O	1:B:1:ASN:N	2.31	0.64
1:A:86:SER:OG	1:A:87:VAL:N	2.30	0.63
1:C:145:LEU:H	1:C:145:LEU:CD2	2.11	0.63
1:C:198:HIS:CE1	1:C:200:HIS:CB	2.80	0.63
1:A:205:ASP:OD1	1:A:207:VAL:HG22	1.98	0.63
1:B:155:THR:O	1:B:158:PHE:N	2.31	0.63
1:B:-2:HIS:NE2	1:B:-1:ARG:HG2	2.13	0.63
1:C:11:SER:HB3	1:C:14:GLU:H	1.63	0.63
1:B:-2:HIS:CE1	1:B:-1:ARG:HH11	2.13	0.63
1:B:372:VAL:HG11	1:B:402:TYR:CE1	2.30	0.63
1:A:158:PHE:O	1:A:162:ILE:HG22	1.98	0.63
1:A:292:VAL:HA	1:A:295:LEU:HD12	1.80	0.63
1:C:41:HIS:CE1	1:C:61:HIS:CE1	2.86	0.63
1:C:143:ASP:HA	1:C:145:LEU:HD22	1.81	0.63
1:C:376:PHE:O	1:C:376:PHE:CD1	2.51	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:LEU:CD2	1:C:348:GLU:HB3	2.29	0.63
1:A:316:GLY:HA3	1:A:351:TRP:CZ2	2.33	0.63
1:C:4:ARG:CD	1:C:282:TYR:CE1	2.81	0.63
1:C:4:ARG:HB2	1:C:282:TYR:CD1	2.32	0.63
1:C:93:TRP:HE1	1:C:99:GLN:NE2	1.97	0.63
1:A:36:SER:C	1:A:38:ALA:H	2.02	0.63
1:A:60:VAL:C	1:A:61:HIS:HD2	2.02	0.63
1:B:47:CYS:O	1:B:48:PRO:C	2.36	0.63
1:C:327:ILE:HD11	1:C:361:ILE:CD1	2.29	0.63
1:A:181:HIS:CE1	1:A:185:HIS:CD2	2.86	0.62
1:A:109:GLU:N	1:A:109:GLU:OE2	2.32	0.62
1:B:196:MET:HA	1:B:202:ALA:CB	2.28	0.62
1:A:205:ASP:OD1	1:A:205:ASP:C	2.37	0.62
1:B:145:LEU:HD12	1:B:145:LEU:C	2.18	0.62
1:B:401:ILE:HG22	1:B:402:TYR:H	1.65	0.62
1:A:163:TYR:O	1:A:166:GLU:N	2.33	0.62
1:B:257:ASN:ND2	1:B:262:THR:CG2	2.62	0.62
1:A:291:ASN:O	1:A:295:LEU:CD1	2.47	0.62
1:B:112:ASP:O	1:B:113:ASP:C	2.37	0.62
1:B:184:ILE:HB	1:B:211:HIS:CE1	2.34	0.62
1:B:283:ASP:OD2	1:B:284:HIS:N	2.32	0.62
1:C:249:PRO:O	1:C:250:PHE:C	2.35	0.62
1:A:121:THR:O	1:A:123:PRO:HD3	2.00	0.62
1:B:37:LEU:O	1:B:73:TYR:OH	2.10	0.62
1:C:299:ILE:O	1:C:302:GLN:HB2	1.99	0.62
1:B:54:LYS:HD3	1:B:56:PHE:CZ	2.34	0.62
1:A:228:PHE:HE2	1:A:296:HIS:HD2	1.48	0.61
1:B:148:GLU:HG2	1:B:155:THR:HA	1.82	0.61
1:C:221:LEU:HD21	1:C:295:LEU:CD1	2.30	0.61
1:A:25:LEU:HG	1:A:34:PHE:HB2	1.82	0.61
1:A:322:HIS:O	1:A:382:GLN:HA	2.00	0.61
1:A:324:ASP:N	1:A:324:ASP:OD1	2.33	0.61
1:B:94:ASP:OD2	1:B:95:THR:N	2.33	0.61
1:A:351:TRP:CG	1:A:351:TRP:O	2.52	0.61
1:B:265:HIS:CE1	1:B:277:HIS:CD2	2.88	0.61
1:C:-2:HIS:HB3	1:C:1:ASN:HB2	1.82	0.61
1:B:111:TRP:C	1:B:111:TRP:CD1	2.69	0.61
1:B:47:CYS:HB3	1:B:48:PRO:HD3	1.81	0.61
1:B:184:ILE:N	1:B:184:ILE:HD12	2.14	0.61
1:A:61:HIS:O	1:A:63:MET:HG3	2.01	0.61
1:A:136:ILE:HD11	1:A:204:TYR:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:SER:OG	1:B:347:LEU:HD13	2.00	0.61
1:C:121:THR:O	1:C:123:PRO:CD	2.46	0.61
1:A:32:ASP:O	1:A:37:LEU:HD11	2.01	0.60
1:A:181:HIS:CD2	1:A:212:HIS:NE2	2.69	0.60
1:A:205:ASP:OD1	1:A:206:PRO:N	2.34	0.60
1:B:259:ASN:OD1	1:B:262:THR:HB	2.02	0.60
1:C:5:LYS:HG2	1:C:6:SER:N	2.15	0.60
1:C:8:ARG:CZ	1:C:103:PRO:HG3	2.31	0.60
1:C:60:VAL:HG11	1:C:65:THR:C	2.20	0.60
1:B:324:ASP:HB3	1:B:339:TYR:HB3	1.82	0.60
1:C:129:ILE:H	1:C:129:ILE:HD12	1.64	0.60
1:C:198:HIS:CE1	1:C:200:HIS:H	2.20	0.60
1:A:50:PRO:HD3	1:A:252:PHE:CE2	2.36	0.60
1:A:221:LEU:O	1:A:224:GLU:N	2.35	0.60
1:C:5:LYS:HA	1:C:283:ASP:OD1	2.00	0.60
1:A:104:ALA:O	1:A:106:PHE:N	2.33	0.60
1:A:371:ASP:OD1	1:A:373:HIS:N	2.35	0.60
1:A:32:ASP:OD1	1:A:37:LEU:HD21	2.02	0.60
1:A:179:ILE:HG21	1:A:357:TYR:CZ	2.36	0.60
1:B:342:VAL:CG1	1:B:343:LEU:H	2.06	0.60
1:C:259:ASN:HD21	1:C:262:THR:H	1.50	0.60
1:A:11:SER:OG	1:A:13:ALA:HB3	2.02	0.60
1:A:43:GLN:HG2	1:A:131:PHE:CZ	2.36	0.60
1:A:182:ASN:ND2	1:A:342:VAL:HA	2.09	0.60
1:A:199:LEU:HB3	1:A:345:GLY:N	2.16	0.60
1:C:34:PHE:O	1:C:36:SER:N	2.34	0.60
1:C:248:LYS:HB3	1:C:252:PHE:CE1	2.37	0.60
1:A:169:ASP:O	1:A:170:TYR:C	2.40	0.60
1:B:165:LEU:HD23	1:B:222:TRP:CD1	2.33	0.60
1:B:291:ASN:O	1:B:295:LEU:HG	2.02	0.60
1:A:156:TRP:NE1	1:A:339:TYR:CE2	2.70	0.59
1:A:156:TRP:O	1:A:158:PHE:N	2.35	0.59
1:B:148:GLU:HG3	1:B:155:THR:HA	1.84	0.59
1:C:-2:HIS:CG	1:C:-1:ARG:HE	2.12	0.59
1:C:163:TYR:HD2	1:C:176:GLN:NE2	2.00	0.59
1:A:376:PHE:CD1	1:A:376:PHE:C	2.76	0.59
1:B:201:TYR:O	1:B:202:ALA:C	2.38	0.59
1:B:257:ASN:HD21	1:B:262:THR:CG2	2.15	0.59
1:C:131:PHE:HE2	1:C:204:TYR:HH	1.50	0.59
1:A:7:VAL:HA	1:A:10:LEU:HD11	1.84	0.59
1:A:192:GLU:C	1:A:194:TYR:N	2.54	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:-1:ARG:CB	1:C:1:ASN:N	2.62	0.59
1:A:82:ARG:C	1:A:84:HIS:N	2.54	0.59
1:B:44:PRO:HD3	1:B:131:PHE:CE2	2.37	0.59
1:A:25:LEU:HA	1:A:84:HIS:CE1	2.38	0.59
1:A:82:ARG:C	1:A:84:HIS:H	2.05	0.59
1:A:222:TRP:O	1:A:223:GLN:C	2.41	0.59
1:B:145:LEU:CD1	1:B:146:ALA:N	2.62	0.59
1:B:219:PHE:O	1:B:223:GLN:HG3	2.03	0.59
1:A:1:ASN:CB	1:A:279:HIS:HB3	2.32	0.59
1:B:-2:HIS:NE2	1:B:-1:ARG:CG	2.66	0.59
1:C:347:LEU:HD22	1:C:347:LEU:H	1.66	0.59
1:A:319:THR:HG1	1:A:385:TRP:HE1	1.51	0.59
1:A:400:VAL:HG12	1:A:400:VAL:O	2.02	0.59
1:B:132:ASN:ND2	1:B:132:ASN:O	2.35	0.59
1:B:365:LEU:HD12	1:B:370:LEU:HB3	1.84	0.59
1:B:262:THR:CG2	1:B:263:LYS:N	2.66	0.59
1:A:291:ASN:O	1:A:295:LEU:CG	2.50	0.59
1:B:361:ILE:HG13	1:B:365:LEU:HD23	1.85	0.59
1:C:122:ASN:O	1:C:125:ASN:N	2.36	0.59
1:B:180:ALA:C	1:B:182:ASN:H	2.06	0.58
1:A:286:GLU:OE1	1:A:289:GLY:O	2.20	0.58
1:C:160:GLN:HA	1:C:160:GLN:OE1	2.03	0.58
1:C:217:ARG:NH1	1:C:286:GLU:O	2.36	0.58
1:A:129:ILE:HD11	1:A:136:ILE:HG13	1.85	0.58
1:A:136:ILE:HG23	1:A:137:ALA:H	1.67	0.58
1:A:136:ILE:HG22	1:A:137:ALA:N	2.17	0.58
1:A:192:GLU:O	1:A:194:TYR:N	2.36	0.58
1:B:198:HIS:NE2	1:B:200:HIS:CD2	2.71	0.58
1:C:259:ASN:HD21	1:C:262:THR:N	1.99	0.58
1:A:156:TRP:O	1:A:157:SER:C	2.41	0.58
1:A:242:MET:C	1:A:244:ARG:H	2.07	0.58
1:A:325:PHE:HB3	1:A:380:ILE:HG22	1.83	0.58
1:C:401:ILE:CG2	1:C:402:TYR:N	2.66	0.58
1:A:60:VAL:O	1:A:61:HIS:HD2	1.85	0.58
1:A:162:ILE:HA	1:A:165:LEU:HD12	1.84	0.58
1:A:192:GLU:C	1:A:194:TYR:H	2.07	0.58
1:C:113:ASP:CG	1:C:118:ALA:HB3	2.24	0.58
1:C:247:LEU:O	1:C:250:PHE:HB2	2.04	0.58
1:C:263:LYS:O	1:C:266:SER:OG	2.21	0.58
1:A:380:ILE:HD13	1:A:392:THR:HG21	1.86	0.58
1:B:97:VAL:HG12	1:B:97:VAL:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:LEU:HD12	1:C:210:LEU:N	2.14	0.58
1:B:238:CYS:O	1:B:239:ALA:HB3	2.03	0.58
1:C:136:ILE:HD11	1:C:204:TYR:HB3	1.86	0.58
1:B:222:TRP:O	1:B:223:GLN:C	2.41	0.57
1:C:388:GLU:O	1:C:389:ASP:C	2.41	0.57
1:A:159:LYS:O	1:A:162:ILE:HG22	2.04	0.57
1:B:-1:ARG:HA	1:B:1:ASN:N	2.18	0.57
1:B:166:GLU:CD	1:B:307:ARG:HH22	2.07	0.57
1:A:62:GLY:HA2	1:A:353:PHE:CE2	2.38	0.57
1:A:291:ASN:CG	1:A:292:VAL:H	2.08	0.57
1:B:189:GLY:O	1:B:190:GLY:C	2.42	0.57
1:C:382:GLN:HB3	1:C:390:ILE:HB	1.87	0.57
1:A:72:LEU:HD22	1:A:250:PHE:CD1	2.40	0.57
1:A:184:ILE:HD13	1:A:211:HIS:CE1	2.39	0.57
1:C:44:PRO:O	1:C:44:PRO:HG2	2.04	0.57
1:B:142:VAL:HG12	1:B:145:LEU:N	2.19	0.57
1:A:368:LYS:O	1:A:370:LEU:HG	2.04	0.57
1:B:70:HIS:HD2	1:B:212:HIS:CD2	2.23	0.57
1:C:86:SER:O	1:C:87:VAL:C	2.42	0.57
1:C:401:ILE:CG2	1:C:402:TYR:H	2.17	0.57
1:A:224:GLU:O	1:A:227:LYS:CB	2.52	0.57
1:B:208:PHE:CE1	1:B:212:HIS:CE1	2.93	0.57
1:C:4:ARG:NH1	1:C:282:TYR:OH	2.37	0.57
1:B:127:ALA:H	1:B:136:ILE:HD11	1.69	0.57
1:A:238:CYS:O	1:A:240:LEU:HD12	2.05	0.57
1:A:286:GLU:CD	1:A:289:GLY:C	2.63	0.57
1:A:140:ILE:HG23	1:A:187:TRP:O	2.04	0.56
1:B:299:ILE:O	1:B:302:GLN:N	2.28	0.56
1:B:323:LEU:HB3	1:B:382:GLN:HG3	1.87	0.56
1:C:291:ASN:O	1:C:294:ARG:N	2.38	0.56
1:A:365:LEU:O	1:A:368:LYS:HB3	2.04	0.56
1:B:35:GLN:HE22	1:B:129:ILE:HA	1.68	0.56
1:C:143:ASP:HA	1:C:145:LEU:CD2	2.36	0.56
1:A:200:HIS:NE2	1:A:347:LEU:HB2	2.21	0.56
1:B:140:ILE:O	1:B:143:ASP:N	2.39	0.56
1:B:302:GLN:O	1:B:304:GLU:N	2.33	0.56
1:B:311:GLY:O	1:B:398:PRO:HA	2.06	0.56
1:C:5:LYS:HG2	1:C:6:SER:H	1.69	0.56
1:C:46:LEU:HB2	1:C:50:PRO:HA	1.87	0.56
1:C:198:HIS:ND1	1:C:200:HIS:N	2.53	0.56
1:A:59:CYS:HG	1:A:61:HIS:CE1	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:HIS:C	1:A:213:SER:H	2.09	0.56
1:A:213:SER:O	1:A:217:ARG:HB2	2.05	0.56
1:B:221:LEU:HD11	1:B:295:LEU:HD12	1.88	0.56
1:C:372:VAL:HG21	1:C:402:TYR:CE1	2.40	0.56
1:A:199:LEU:CB	1:A:345:GLY:H	2.18	0.56
1:A:290:MET:CB	1:A:294:ARG:CB	2.78	0.56
1:A:361:ILE:O	1:A:361:ILE:HG13	2.06	0.56
1:B:211:HIS:C	1:B:213:SER:H	2.08	0.56
1:C:114:ALA:HB2	1:C:119:ASN:OD1	2.06	0.56
1:C:259:ASN:ND2	1:C:260:PRO:N	2.54	0.56
1:A:161:TYR:CZ	1:A:180:ALA:HB1	2.41	0.56
1:A:165:LEU:O	1:A:229:ARG:NH2	2.37	0.56
1:A:192:GLU:O	1:A:195:SER:OG	2.24	0.56
1:C:96:VAL:HG12	1:C:96:VAL:O	2.06	0.56
1:C:327:ILE:HD11	1:C:361:ILE:HD12	1.88	0.56
1:A:170:TYR:O	1:A:171:CYS:C	2.44	0.56
1:B:201:TYR:O	1:B:204:TYR:N	2.27	0.56
1:C:70:HIS:HD2	1:C:212:HIS:CD2	2.24	0.56
1:C:223:GLN:O	1:C:226:GLN:HB2	2.06	0.56
1:A:8:ARG:NH2	1:A:101:ASP:O	2.37	0.56
1:A:78:GLU:N	1:A:90:ILE:HD11	2.21	0.56
1:A:244:ARG:NH1	1:A:244:ARG:CG	2.58	0.56
1:B:299:ILE:O	1:B:300:ASN:C	2.43	0.56
1:A:228:PHE:CE1	1:A:293:GLN:HG3	2.41	0.56
1:C:291:ASN:HB3	1:C:294:ARG:HB2	1.86	0.56
1:C:380:ILE:CD1	1:C:392:THR:HB	2.34	0.56
1:B:208:PHE:O	1:B:209:ILE:C	2.43	0.55
1:B:320:SER:OG	1:B:344:GLY:N	2.38	0.55
1:C:34:PHE:O	1:C:37:LEU:N	2.38	0.55
1:A:286:GLU:OE1	1:A:289:GLY:C	2.45	0.55
1:C:145:LEU:HD23	1:C:145:LEU:N	2.15	0.55
1:A:292:VAL:CA	1:A:295:LEU:HD12	2.36	0.55
1:B:234:ASN:OD1	1:B:273:ASP:HB2	2.05	0.55
1:C:267:LYS:H	1:C:267:LYS:HD2	1.72	0.55
1:A:93:TRP:HE1	1:A:99:GLN:NE2	2.05	0.55
1:B:198:HIS:HD2	1:B:200:HIS:N	2.05	0.55
1:A:8:ARG:HH21	1:A:103:PRO:HD3	1.71	0.55
1:A:71:ARG:HH22	1:A:223:GLN:HE22	1.55	0.55
1:B:322:HIS:HA	1:B:341:ASP:HB3	1.88	0.55
1:C:153:TYR:O	1:C:155:THR:HG23	2.06	0.55
1:C:161:TYR:CE2	1:C:218:LEU:HD22	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:PHE:CE2	1:A:296:HIS:HD2	2.23	0.55
1:B:250:PHE:O	1:B:263:LYS:HA	2.07	0.55
1:C:149:GLY:C	1:C:151:LYS:N	2.57	0.55
1:A:69:TRP:HE3	1:A:70:HIS:N	2.05	0.55
1:B:104:ALA:O	1:B:105:PHE:C	2.46	0.55
1:B:141:ASN:ND2	1:B:142:VAL:N	2.53	0.55
1:B:156:TRP:CZ3	1:B:183:ALA:HB2	2.42	0.55
1:B:263:LYS:O	1:B:264:GLU:C	2.44	0.55
1:B:32:ASP:OD2	1:B:37:LEU:HD21	2.06	0.54
1:B:202:ALA:C	1:B:204:TYR:N	2.61	0.54
1:C:78:GLU:O	1:C:81:LEU:N	2.32	0.54
1:A:238:CYS:O	1:A:239:ALA:C	2.41	0.54
1:B:90:ILE:HG21	1:B:209:ILE:CG2	2.37	0.54
1:B:206:PRO:O	1:B:207:VAL:C	2.42	0.54
1:C:205:ASP:OD1	1:C:207:VAL:N	2.37	0.54
1:C:290:MET:SD	1:C:294:ARG:HD2	2.48	0.54
1:B:361:ILE:O	1:B:362:THR:C	2.43	0.54
1:C:217:ARG:HG2	1:C:282:TYR:CD2	2.42	0.54
1:A:4:ARG:N	1:A:281:GLU:O	2.38	0.54
1:B:35:GLN:NE2	1:B:130:ASP:H	2.06	0.54
1:A:341:ASP:OD2	1:A:341:ASP:N	2.39	0.54
1:C:136:ILE:H	1:C:136:ILE:CD1	2.12	0.54
1:C:347:LEU:N	1:C:347:LEU:CD2	2.70	0.54
1:C:378:ILE:HG22	1:C:379:LYS:N	2.22	0.54
1:A:7:VAL:HA	1:A:10:LEU:HD12	1.90	0.54
1:A:34:PHE:O	1:A:35:GLN:C	2.46	0.54
1:A:155:THR:O	1:A:158:PHE:HB3	2.08	0.54
1:B:-2:HIS:CD2	1:B:-1:ARG:HG2	2.43	0.54
1:C:4:ARG:HB2	1:C:282:TYR:HD1	1.72	0.54
1:A:-2:HIS:CE1	1:A:-1:ARG:HG2	2.43	0.54
1:C:85:GLY:O	1:C:87:VAL:N	2.39	0.54
1:B:164:ALA:O	1:B:173:PHE:HD1	1.91	0.54
1:A:22:LEU:HD23	1:A:26:GLN:HG3	1.90	0.54
1:B:402:TYR:C	1:B:402:TYR:CD2	2.81	0.54
1:C:81:LEU:HD12	1:C:90:ILE:CG1	2.37	0.54
1:A:33:GLY:O	1:A:34:PHE:C	2.46	0.54
1:A:60:VAL:C	1:A:61:HIS:CD2	2.81	0.54
1:A:140:ILE:HG22	1:A:142:VAL:C	2.28	0.54
1:B:-1:ARG:NH1	1:B:-1:ARG:CG	2.60	0.53
1:C:42:ALA:HA	1:C:57:ALA:HB1	1.88	0.53
1:C:175:VAL:CG2	1:C:176:GLN:N	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:CYS:O	1:C:239:ALA:CB	2.47	0.53
1:C:293:GLN:O	1:C:297:ASP:HB2	2.07	0.53
1:A:78:GLU:HB2	1:A:90:ILE:CD1	2.38	0.53
1:A:136:ILE:HD13	1:A:205:ASP:N	2.23	0.53
1:A:351:TRP:O	1:A:351:TRP:CD2	2.60	0.53
1:B:-2:HIS:CD2	1:B:-1:ARG:CG	2.91	0.53
1:B:249:PRO:C	1:B:251:SER:N	2.61	0.53
1:C:376:PHE:CD1	1:C:376:PHE:C	2.81	0.53
1:A:236:VAL:CG2	1:A:272:PHE:CZ	2.91	0.53
1:C:267:LYS:HD2	1:C:267:LYS:N	2.22	0.53
1:B:2:LEU:O	1:B:281:GLU:N	2.39	0.53
1:B:164:ALA:HB1	1:B:173:PHE:CD1	2.43	0.53
1:B:259:ASN:OD1	1:B:259:ASN:C	2.47	0.53
1:C:306:ASP:C	1:C:307:ARG:HG3	2.27	0.53
1:C:95:THR:HA	1:C:99:GLN:OE1	2.09	0.53
1:C:198:HIS:HE1	1:C:200:HIS:CG	2.26	0.53
1:C:233:PRO:HG2	1:C:234:ASN:N	2.21	0.53
1:C:386:ASP:O	1:C:387:ASN:C	2.47	0.53
1:A:82:ARG:O	1:A:84:HIS:N	2.42	0.53
1:B:262:THR:HG22	1:B:263:LYS:H	1.73	0.53
1:C:129:ILE:HD11	1:C:136:ILE:N	2.24	0.53
1:A:330:ILE:HD12	1:A:330:ILE:N	2.18	0.53
1:A:383:THR:HG22	1:A:389:ASP:HA	1.91	0.53
1:C:25:LEU:HG	1:C:34:PHE:HB2	1.90	0.53
1:A:9:ASN:ND2	2:A:600:NAG:H5	2.24	0.53
1:A:207:VAL:O	1:A:208:PHE:C	2.46	0.53
1:B:13:ALA:O	1:B:16:ALA:HB3	2.09	0.53
1:B:33:GLY:O	1:B:37:LEU:HG	2.09	0.53
1:B:221:LEU:HD12	1:B:221:LEU:O	2.09	0.53
1:C:4:ARG:NH2	1:C:75:VAL:HG22	2.24	0.53
1:A:322:HIS:HD2	1:A:341:ASP:OD1	1.92	0.52
1:B:66:PHE:CE1	1:B:178:GLU:HG3	2.44	0.52
1:C:-2:HIS:O	1:C:-1:ARG:CD	2.57	0.52
1:C:260:PRO:CG	1:C:261:THR:H	2.20	0.52
1:A:286:GLU:OE2	1:A:290:MET:N	2.42	0.52
1:A:325:PHE:CD2	1:A:337:ALA:CB	2.91	0.52
1:B:113:ASP:O	1:B:114:ALA:C	2.47	0.52
1:C:309:PHE:N	1:C:309:PHE:CD1	2.74	0.52
1:A:43:GLN:HG2	1:A:131:PHE:HZ	1.73	0.52
1:A:57:ALA:O	1:A:58:CYS:CB	2.46	0.52
1:A:338:GLY:HA3	1:A:359:TYR:CE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:LEU:O	1:B:280:TYR:HA	2.08	0.52
1:B:149:GLY:C	1:B:151:LYS:N	2.62	0.52
1:B:164:ALA:HB1	1:B:173:PHE:HD1	1.74	0.52
1:B:180:ALA:C	1:B:182:ASN:N	2.62	0.52
1:C:138:ARG:NH2	1:C:207:VAL:HG13	2.24	0.52
1:A:363:ASP:O	1:A:364:VAL:C	2.47	0.52
1:C:71:ARG:HD2	1:C:280:TYR:OH	2.09	0.52
1:C:268:PRO:O	1:C:271:THR:N	2.43	0.52
1:C:335:THR:CG2	1:C:368:LYS:HE3	2.38	0.52
1:C:174:GLU:O	1:C:175:VAL:C	2.46	0.52
1:A:134:GLN:HG3	1:A:194:TYR:CZ	2.45	0.52
1:A:267:LYS:O	1:A:268:PRO:C	2.47	0.52
1:A:386:ASP:O	1:A:387:ASN:OD1	2.27	0.52
1:C:94:ASP:OD1	1:C:96:VAL:HG23	2.09	0.52
1:C:129:ILE:HD11	1:C:136:ILE:HD12	1.92	0.52
1:A:22:LEU:HA	1:A:25:LEU:HB3	1.91	0.52
1:B:149:GLY:C	1:B:151:LYS:H	2.11	0.52
1:B:163:TYR:HD2	1:B:176:GLN:HG2	1.73	0.52
1:B:259:ASN:OD1	1:B:260:PRO:N	2.42	0.52
1:A:249:PRO:O	1:A:250:PHE:C	2.43	0.52
1:A:299:ILE:O	1:A:300:ASN:C	2.45	0.52
1:C:39:SER:OG	1:C:44:PRO:CD	2.57	0.52
1:C:178:GLU:O	1:C:181:HIS:HB3	2.09	0.52
1:C:259:ASN:ND2	1:C:260:PRO:C	2.63	0.52
1:A:81:LEU:O	1:A:84:HIS:N	2.35	0.52
1:A:104:ALA:O	1:A:105:PHE:C	2.48	0.52
1:B:59:CYS:SG	1:B:199:LEU:HD11	2.50	0.52
1:C:61:HIS:NE2	1:C:70:HIS:HE1	2.06	0.52
1:C:129:ILE:HD12	1:C:134:GLN:O	2.10	0.52
1:A:50:PRO:HG2	1:A:256:TYR:CE2	2.45	0.51
1:A:286:GLU:CG	1:A:290:MET:O	2.57	0.51
1:B:141:ASN:CG	1:B:142:VAL:H	2.14	0.51
1:B:251:SER:O	1:B:252:PHE:C	2.49	0.51
1:C:15:ARG:O	1:C:16:ALA:C	2.46	0.51
1:C:90:ILE:O	1:C:90:ILE:HG22	2.09	0.51
1:A:8:ARG:HH21	1:A:103:PRO:CD	2.22	0.51
1:A:9:ASN:HD22	2:A:600:NAG:C5	2.23	0.51
1:B:-1:ARG:C	1:B:1:ASN:N	2.64	0.51
1:C:163:TYR:CD2	1:C:176:GLN:NE2	2.79	0.51
1:C:306:ASP:N	1:C:405:LYS:O	2.42	0.51
1:A:39:SER:O	1:A:40:PHE:C	2.47	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:THR:HG21	1:A:184:ILE:CG1	2.40	0.51
1:A:95:THR:OG1	1:A:184:ILE:HD11	2.10	0.51
1:A:156:TRP:O	1:A:159:LYS:N	2.43	0.51
1:A:358:LYS:HG2	1:A:401:ILE:HD12	1.91	0.51
1:A:386:ASP:O	1:A:387:ASN:ND2	2.42	0.51
1:B:19:VAL:HG12	1:B:19:VAL:O	2.10	0.51
1:B:36:SER:C	1:B:38:ALA:H	2.14	0.51
1:B:68:GLU:O	1:B:69:TRP:C	2.47	0.51
1:B:208:PHE:O	1:B:211:HIS:N	2.43	0.51
1:C:47:CYS:H	1:C:48:PRO:HD2	1.74	0.51
1:C:82:ARG:HA	1:C:86:SER:H	1.76	0.51
1:C:94:ASP:HA	1:C:214:ASN:ND2	2.25	0.51
1:C:113:ASP:O	1:C:116:PHE:O	2.27	0.51
1:C:268:PRO:O	1:C:269:GLU:C	2.49	0.51
1:B:127:ALA:H	1:B:136:ILE:CG1	2.23	0.51
1:C:249:PRO:HA	1:C:252:PHE:CD1	2.46	0.51
1:A:4:ARG:NE	1:A:280:TYR:CD1	2.79	0.51
1:A:25:LEU:CD1	1:A:34:PHE:H	2.24	0.51
1:A:324:ASP:N	1:A:381:THR:O	2.39	0.51
1:B:181:HIS:CD2	1:B:212:HIS:NE2	2.58	0.51
1:B:366:GLU:OE2	1:B:366:GLU:HA	2.11	0.51
1:A:36:SER:C	1:A:38:ALA:N	2.63	0.51
1:B:-2:HIS:NE2	1:B:-1:ARG:NH1	2.59	0.51
1:C:77:PHE:C	1:C:80:ALA:HB3	2.31	0.51
1:C:102:LEU:CD1	1:C:140:ILE:HD13	2.40	0.51
1:A:1:ASN:HB2	1:A:279:HIS:C	2.30	0.51
1:C:43:GLN:HB3	1:C:131:PHE:CZ	2.46	0.51
1:C:65:THR:HG21	1:C:242:MET:HB3	1.93	0.51
1:C:185:HIS:HA	1:C:196:MET:HE3	1.93	0.51
1:C:259:ASN:HD21	1:C:261:THR:CA	2.24	0.51
1:A:11:SER:O	1:A:14:GLU:N	2.44	0.51
1:A:293:GLN:C	1:A:295:LEU:N	2.64	0.51
1:B:36:SER:C	1:B:38:ALA:N	2.63	0.51
1:C:-1:ARG:CB	1:C:1:ASN:H2	2.20	0.51
1:B:8:ARG:O	1:B:10:LEU:N	2.43	0.50
1:B:211:HIS:C	1:B:213:SER:N	2.65	0.50
1:C:1:ASN:HD22	1:C:281:GLU:HG2	1.76	0.50
1:C:249:PRO:C	1:C:251:SER:N	2.63	0.50
1:A:32:ASP:HA	1:A:37:LEU:HD21	1.93	0.50
1:B:257:ASN:ND2	1:B:259:ASN:O	2.43	0.50
1:B:372:VAL:HG21	1:B:402:TYR:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:SER:HB3	1:B:386:ASP:OD2	2.11	0.50
1:A:226:GLN:HA	1:A:229:ARG:HD2	1.92	0.50
1:B:63:MET:O	1:B:64:ALA:C	2.49	0.50
1:B:240:LEU:HD12	1:B:240:LEU:N	2.26	0.50
1:C:131:PHE:CE1	1:C:132:ASN:OD1	2.64	0.50
1:A:93:TRP:CD1	1:A:93:TRP:C	2.83	0.50
1:C:66:PHE:CB	1:C:67:PRO:HD3	2.41	0.50
1:A:-2:HIS:ND1	1:A:-1:ARG:HG2	2.26	0.50
1:A:66:PHE:CB	1:A:67:PRO:CD	2.84	0.50
1:B:28:ASP:OD1	1:B:28:ASP:C	2.45	0.50
1:B:71:ARG:HH22	1:B:223:GLN:NE2	2.06	0.50
1:B:141:ASN:ND2	1:B:187:TRP:HA	2.26	0.50
1:C:47:CYS:H	1:C:48:PRO:CD	2.25	0.50
1:C:161:TYR:O	1:C:164:ALA:HB3	2.11	0.50
1:C:257:ASN:OD1	1:C:259:ASN:HB3	2.12	0.50
1:A:144:LYS:C	1:A:146:ALA:H	2.13	0.50
1:A:153:TYR:HB2	1:A:288:GLN:CD	2.32	0.50
1:B:198:HIS:CD2	1:B:200:HIS:H	2.25	0.50
1:C:198:HIS:ND1	1:C:198:HIS:C	2.64	0.50
1:A:402:TYR:CD2	1:A:403:VAL:N	2.80	0.50
1:A:339:TYR:O	1:A:339:TYR:CG	2.63	0.50
1:C:187:TRP:N	1:C:187:TRP:CD1	2.77	0.50
1:A:156:TRP:CE3	1:A:157:SER:N	2.79	0.50
1:B:35:GLN:NE2	1:B:129:ILE:HA	2.27	0.50
1:B:78:GLU:HA	1:B:90:ILE:HD11	1.94	0.50
1:B:188:VAL:O	1:B:188:VAL:CG1	2.59	0.50
1:B:318:GLY:HA2	1:B:348:GLU:OE2	2.11	0.50
1:C:161:TYR:O	1:C:162:ILE:C	2.48	0.50
1:C:268:PRO:C	1:C:270:ASP:N	2.65	0.50
1:A:184:ILE:O	1:A:186:ALA:N	2.45	0.49
1:A:12:PRO:O	1:A:13:ALA:C	2.50	0.49
1:A:19:VAL:HG12	1:A:19:VAL:O	2.11	0.49
1:A:87:VAL:C	1:A:88:VAL:HG13	2.31	0.49
1:B:82:ARG:O	1:B:85:GLY:N	2.44	0.49
1:B:119:ASN:O	1:B:120:PHE:CD2	2.65	0.49
1:C:47:CYS:C	1:C:49:ALA:N	2.60	0.49
1:A:-3:GLY:CA	1:A:1:ASN:N	2.72	0.49
1:A:205:ASP:OD1	1:A:207:VAL:N	2.33	0.49
1:A:327:ILE:HD11	1:A:364:VAL:HG12	1.94	0.49
1:B:366:GLU:OE2	1:B:366:GLU:CA	2.59	0.49
1:C:65:THR:CG2	1:C:242:MET:CB	2.91	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:ARG:O	1:C:294:ARG:HD3	2.11	0.49
1:A:372:VAL:HG21	1:A:402:TYR:CD1	2.48	0.49
1:C:113:ASP:OD2	1:C:118:ALA:HB3	2.11	0.49
1:A:174:GLU:C	1:A:176:GLN:N	2.66	0.49
1:A:319:THR:OG1	1:A:385:TRP:NE1	2.40	0.49
1:B:22:LEU:HA	1:B:25:LEU:HB3	1.94	0.49
1:B:184:ILE:CD1	1:B:184:ILE:H	2.23	0.49
1:C:361:ILE:HD12	1:C:365:LEU:HD22	1.95	0.49
1:A:92:TYR:HA	1:A:213:SER:HB3	1.94	0.49
1:A:162:ILE:HG23	1:A:163:TYR:N	2.27	0.49
1:A:319:THR:O	1:A:320:SER:C	2.49	0.49
1:B:111:TRP:CZ2	1:B:113:ASP:HA	2.47	0.49
1:B:150:PRO:O	1:B:151:LYS:CD	2.61	0.49
1:B:185:HIS:CE1	1:B:212:HIS:HE1	2.30	0.49
1:B:202:ALA:C	1:B:204:TYR:H	2.16	0.49
1:C:68:GLU:CB	1:C:268:PRO:HB3	2.43	0.49
1:C:153:TYR:O	1:C:155:THR:N	2.44	0.49
1:A:228:PHE:CZ	1:A:293:GLN:HG3	2.48	0.49
1:B:95:THR:C	1:B:97:VAL:N	2.65	0.49
1:C:68:GLU:H	1:C:68:GLU:CD	2.15	0.49
1:C:129:ILE:CG1	1:C:136:ILE:CD1	2.91	0.49
1:C:130:ASP:O	1:C:131:PHE:C	2.48	0.49
1:C:150:PRO:CG	1:C:154:ASP:HB3	2.43	0.49
1:C:322:HIS:ND1	1:C:322:HIS:C	2.65	0.49
1:B:70:HIS:CD2	1:B:212:HIS:CD2	2.99	0.49
1:B:127:ALA:H	1:B:136:ILE:CD1	2.25	0.49
1:B:234:ASN:CG	1:B:273:ASP:HB2	2.33	0.49
1:C:68:GLU:HB3	1:C:271:THR:HG21	1.94	0.49
1:A:179:ILE:HG21	1:A:357:TYR:OH	2.11	0.49
1:A:182:ASN:ND2	1:A:343:LEU:H	2.11	0.49
1:B:155:THR:O	1:B:156:TRP:C	2.51	0.49
1:C:19:VAL:O	1:C:23:LYS:HB2	2.13	0.49
1:C:161:TYR:O	1:C:164:ALA:N	2.46	0.49
1:C:384:SER:OG	1:C:385:TRP:N	2.45	0.49
1:B:345:GLY:O	1:B:346:SER:C	2.50	0.49
1:C:66:PHE:HZ	1:C:181:HIS:ND1	2.11	0.49
1:A:71:ARG:HH22	1:A:223:GLN:NE2	2.11	0.48
1:A:81:LEU:O	1:A:82:ARG:C	2.50	0.48
1:A:244:ARG:O	1:A:246:PRO:HD3	2.12	0.48
1:B:94:ASP:OD2	1:B:96:VAL:N	2.45	0.48
1:C:225:LEU:HD11	1:C:296:HIS:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:349:THR:O	1:C:350:PRO:O	2.30	0.48
1:A:342:VAL:O	1:A:342:VAL:HG23	2.12	0.48
1:C:59:CYS:O	1:C:61:HIS:N	2.46	0.48
1:A:9:ASN:ND2	2:A:600:NAG:C5	2.76	0.48
1:A:28:ASP:OD1	1:A:28:ASP:C	2.52	0.48
1:A:153:TYR:CD1	1:A:154:ASP:OD1	2.65	0.48
1:A:163:TYR:O	1:A:164:ALA:C	2.50	0.48
1:A:254:ALA:HB1	1:A:255:PRO:HA	1.95	0.48
1:B:320:SER:CA	1:B:344:GLY:H	2.24	0.48
1:C:184:ILE:HB	1:C:211:HIS:CE1	2.48	0.48
1:A:43:GLN:HB3	1:A:200:HIS:HB3	1.95	0.48
1:B:184:ILE:H	1:B:184:ILE:HD13	1.77	0.48
1:C:97:VAL:CG1	1:C:98:PRO:HD2	2.27	0.48
1:C:112:ASP:C	1:C:114:ALA:N	2.63	0.48
1:C:268:PRO:O	1:C:271:THR:HG22	2.14	0.48
1:A:155:THR:OG1	1:A:156:TRP:N	2.46	0.48
1:A:281:GLU:CG	1:A:282:TYR:N	2.76	0.48
1:B:238:CYS:O	1:B:239:ALA:C	2.49	0.48
1:C:122:ASN:O	1:C:123:PRO:C	2.52	0.48
1:C:384:SER:C	1:C:386:ASP:H	2.16	0.48
1:A:345:GLY:O	1:A:348:GLU:HG2	2.14	0.48
1:B:259:ASN:OD1	1:B:261:THR:N	2.46	0.48
1:A:189:GLY:O	1:A:191:THR:N	2.45	0.48
1:B:97:VAL:O	1:B:98:PRO:C	2.49	0.48
1:B:114:ALA:O	1:B:115:LEU:HB2	2.14	0.48
1:B:372:VAL:CB	1:B:402:TYR:HD1	2.27	0.48
1:C:2:LEU:H	1:C:280:TYR:HA	1.79	0.48
1:C:87:VAL:HG12	1:C:88:VAL:HG13	1.95	0.48
1:C:96:VAL:C	1:C:97:VAL:HG22	2.34	0.48
1:C:243:MET:O	1:C:268:PRO:HD2	2.13	0.48
1:A:22:LEU:HD23	1:A:26:GLN:CG	2.42	0.48
1:B:7:VAL:HG12	1:B:93:TRP:HA	1.96	0.48
1:B:112:ASP:O	1:B:114:ALA:CB	2.61	0.48
1:C:4:ARG:HD3	1:C:282:TYR:HE1	1.78	0.48
1:C:6:SER:OG	1:C:8:ARG:HB2	2.14	0.48
1:C:129:ILE:CD1	1:C:136:ILE:CD1	2.92	0.48
1:B:54:LYS:HG3	1:C:387:ASN:ND2	2.29	0.48
1:B:299:ILE:O	1:B:302:GLN:HB2	2.14	0.48
1:C:68:GLU:CG	1:C:268:PRO:HB3	2.41	0.48
1:A:97:VAL:O	1:A:97:VAL:HG23	2.14	0.47
1:A:174:GLU:C	1:A:176:GLN:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ILE:HD12	1:A:184:ILE:H	1.78	0.47
1:A:247:LEU:HD11	1:A:268:PRO:HG3	1.96	0.47
1:A:291:ASN:O	1:A:295:LEU:HG	2.12	0.47
1:A:291:ASN:CG	1:A:292:VAL:N	2.67	0.47
1:B:111:TRP:CD1	1:B:111:TRP:O	2.66	0.47
1:C:202:ALA:O	1:C:204:TYR:N	2.46	0.47
1:A:90:ILE:HG21	1:A:209:ILE:HG22	1.96	0.47
1:C:-2:HIS:C	1:C:-1:ARG:HG2	2.33	0.47
1:C:113:ASP:O	1:C:116:PHE:C	2.53	0.47
1:A:136:ILE:CD1	1:A:205:ASP:N	2.77	0.47
1:A:170:TYR:O	1:A:173:PHE:N	2.46	0.47
1:A:259:ASN:OD1	1:A:259:ASN:C	2.52	0.47
1:B:104:ALA:O	1:B:106:PHE:N	2.48	0.47
1:B:165:LEU:HD23	1:B:165:LEU:HA	1.78	0.47
1:B:350:PRO:O	1:B:350:PRO:HG2	2.15	0.47
1:C:29:SER:O	1:C:29:SER:OG	2.32	0.47
1:C:59:CYS:SG	1:C:61:HIS:NE2	2.81	0.47
1:C:59:CYS:O	1:C:60:VAL:C	2.52	0.47
1:C:239:ALA:C	1:C:241:GLU:H	2.18	0.47
1:A:243:MET:O	1:A:269:GLU:HB2	2.14	0.47
1:A:274:TYR:HB2	1:A:280:TYR:CE2	2.48	0.47
1:A:339:TYR:N	1:A:339:TYR:CD2	2.80	0.47
1:B:42:ALA:CB	1:B:57:ALA:HB1	2.45	0.47
1:B:335:THR:HG21	1:B:368:LYS:HE3	1.95	0.47
1:B:400:VAL:HG12	1:B:400:VAL:O	2.14	0.47
1:C:64:ALA:C	1:C:66:PHE:H	2.17	0.47
1:C:200:HIS:O	1:C:201:TYR:CD2	2.68	0.47
1:C:283:ASP:O	1:C:284:HIS:ND1	2.48	0.47
1:C:312:PHE:HB2	1:C:357:TYR:HB3	1.97	0.47
1:A:50:PRO:HD3	1:A:252:PHE:HE2	1.79	0.47
1:A:199:LEU:HA	1:A:343:LEU:HD21	1.95	0.47
1:B:188:VAL:O	1:B:188:VAL:HG12	2.13	0.47
1:B:369:GLY:O	1:B:370:LEU:HD23	2.14	0.47
1:A:184:ILE:C	1:A:186:ALA:N	2.64	0.47
1:A:298:TYR:O	1:A:299:ILE:C	2.52	0.47
1:A:384:SER:OG	1:A:385:TRP:N	2.45	0.47
1:B:153:TYR:O	1:B:155:THR:HG23	2.15	0.47
1:B:218:LEU:O	1:B:221:LEU:HB3	2.15	0.47
1:A:319:THR:HG23	1:A:320:SER:O	2.15	0.47
1:B:94:ASP:HA	1:B:214:ASN:CG	2.35	0.47
1:B:206:PRO:O	1:B:208:PHE:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:ARG:HG2	1:C:8:ARG:NH1	2.29	0.47
1:C:39:SER:HB3	1:C:46:LEU:HD21	1.96	0.47
1:C:65:THR:CG2	1:C:242:MET:HB3	2.43	0.47
1:C:74:THR:O	1:C:77:PHE:HB2	2.15	0.47
1:C:196:MET:HA	1:C:202:ALA:CB	2.45	0.47
1:A:42:ALA:CB	1:A:200:HIS:HA	2.45	0.47
1:A:281:GLU:HG2	1:A:282:TYR:O	2.15	0.47
1:B:164:ALA:O	1:B:173:PHE:CD1	2.68	0.47
1:B:329:ALA:C	1:B:331:ASP:N	2.67	0.47
1:C:163:TYR:O	1:C:164:ALA:C	2.52	0.47
1:C:186:ALA:C	1:C:188:VAL:H	2.18	0.47
1:C:198:HIS:HE1	1:C:200:HIS:CB	2.27	0.47
1:C:326:SER:OG	1:C:336:HIS:HA	2.15	0.47
1:A:366:GLU:O	1:A:368:LYS:N	2.42	0.47
1:A:207:VAL:O	1:A:210:LEU:N	2.48	0.47
1:A:209:ILE:HD13	1:A:209:ILE:HG21	1.39	0.47
1:A:236:VAL:HG21	1:A:272:PHE:CE2	2.49	0.47
1:B:11:SER:O	1:B:14:GLU:HB2	2.15	0.47
1:B:136:ILE:O	1:B:136:ILE:CD1	2.63	0.47
1:C:131:PHE:CE2	1:C:204:TYR:OH	2.63	0.47
1:A:136:ILE:HD11	1:A:204:TYR:CA	2.43	0.46
1:B:78:GLU:HG3	1:B:90:ILE:HG13	1.97	0.46
1:B:127:ALA:O	1:B:136:ILE:HG13	2.15	0.46
1:B:205:ASP:OD1	1:B:205:ASP:C	2.54	0.46
1:C:327:ILE:HD11	1:C:361:ILE:HD13	1.97	0.46
1:C:397:PRO:HA	1:C:398:PRO:HD3	1.60	0.46
1:B:71:ARG:HD2	1:B:280:TYR:OH	2.15	0.46
1:B:72:LEU:HD12	1:B:247:LEU:HD13	1.97	0.46
1:B:110:ILE:N	1:B:110:ILE:CD1	2.70	0.46
1:B:247:LEU:HD11	1:B:268:PRO:HG3	1.98	0.46
1:B:401:ILE:CG2	1:B:402:TYR:H	2.25	0.46
1:C:47:CYS:O	1:C:48:PRO:C	2.53	0.46
1:C:95:THR:O	1:C:97:VAL:N	2.48	0.46
1:A:6:SER:O	1:A:10:LEU:HG	2.16	0.46
1:A:101:ASP:OD1	1:A:101:ASP:C	2.53	0.46
1:A:368:LYS:HB3	1:A:370:LEU:HD12	1.97	0.46
1:C:347:LEU:H	1:C:347:LEU:CD2	2.26	0.46
1:A:43:GLN:CB	1:A:200:HIS:HB3	2.45	0.46
1:A:225:LEU:O	1:A:228:PHE:N	2.49	0.46
1:B:260:PRO:HG2	1:B:261:THR:N	2.30	0.46
1:B:365:LEU:HD12	1:B:370:LEU:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LEU:HB3	1:A:345:GLY:H	1.78	0.46
1:C:28:ASP:C	1:C:30:SER:H	2.18	0.46
1:C:90:ILE:HG21	1:C:209:ILE:HG22	1.98	0.46
1:C:305:ALA:C	1:C:405:LYS:O	2.53	0.46
1:C:347:LEU:HD13	1:C:347:LEU:HA	1.62	0.46
1:A:22:LEU:HD12	1:A:81:LEU:HD21	1.97	0.46
1:A:214:ASN:OD1	1:A:217:ARG:NE	2.43	0.46
1:B:149:GLY:O	1:B:151:LYS:N	2.49	0.46
1:C:8:ARG:NH2	1:C:103:PRO:HG3	2.30	0.46
1:C:11:SER:O	1:C:14:GLU:N	2.49	0.46
1:C:144:LYS:HD3	1:C:144:LYS:N	2.29	0.46
1:A:92:TYR:CD2	1:A:214:ASN:OD1	2.68	0.46
1:A:198:HIS:HE1	1:A:200:HIS:ND1	2.13	0.46
1:B:324:ASP:OD1	1:B:324:ASP:N	2.49	0.46
1:C:307:ARG:C	1:C:308:VAL:HG23	2.35	0.46
1:A:112:ASP:HA	1:A:119:ASN:HA	1.97	0.46
1:A:217:ARG:HA	1:A:282:TYR:CZ	2.51	0.46
1:C:119:ASN:HD22	2:C:650:NAG:H4	1.81	0.46
1:C:327:ILE:O	1:C:327:ILE:HG22	2.14	0.46
1:A:4:ARG:CZ	1:A:280:TYR:CE1	2.99	0.46
1:A:11:SER:N	1:A:14:GLU:OE2	2.48	0.46
1:B:66:PHE:HB3	1:B:67:PRO:HD3	1.98	0.46
1:A:31:ALA:HB3	1:A:258:LEU:HD11	1.97	0.46
1:A:136:ILE:HG23	1:A:137:ALA:N	2.21	0.46
1:C:163:TYR:O	1:C:166:GLU:N	2.49	0.46
1:C:237:ASN:CA	1:C:240:LEU:HD21	2.40	0.46
1:C:329:ALA:HB3	1:C:333:GLU:HB3	1.98	0.46
1:C:356:LEU:HD23	1:C:356:LEU:HA	1.62	0.46
1:A:195:SER:O	1:A:197:GLY:N	2.49	0.45
1:A:319:THR:CA	1:A:344:GLY:O	2.62	0.45
1:B:6:SER:C	1:B:8:ARG:H	2.18	0.45
1:C:6:SER:C	1:C:8:ARG:N	2.68	0.45
1:C:122:ASN:ND2	1:C:124:PHE:H	2.14	0.45
1:C:194:TYR:HA	1:C:201:TYR:CD1	2.52	0.45
1:C:307:ARG:HB2	1:C:309:PHE:HE1	1.80	0.45
1:A:295:LEU:O	1:A:298:TYR:HB3	2.16	0.45
1:C:47:CYS:N	1:C:48:PRO:CD	2.79	0.45
1:C:102:LEU:O	1:C:103:PRO:C	2.53	0.45
1:C:149:GLY:HA2	1:C:154:ASP:O	2.17	0.45
1:C:242:MET:CE	1:C:242:MET:CG	2.94	0.45
1:A:156:TRP:HE3	1:A:157:SER:N	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:GLN:NE2	1:A:229:ARG:HH11	2.15	0.45
1:B:39:SER:O	1:B:41:HIS:N	2.49	0.45
1:B:148:GLU:CD	1:B:156:TRP:H	2.20	0.45
1:B:181:HIS:CD2	1:B:212:HIS:CD2	3.03	0.45
1:C:112:ASP:HA	1:C:119:ASN:OD1	2.15	0.45
1:C:175:VAL:CG2	1:C:176:GLN:H	2.17	0.45
1:A:241:GLU:H	1:A:241:GLU:HG3	1.42	0.45
1:C:65:THR:HG22	1:C:243:MET:CE	2.47	0.45
1:A:169:ASP:HB3	1:A:172:ASP:HB2	1.99	0.45
1:A:220:ALA:O	1:A:221:LEU:C	2.55	0.45
1:A:242:MET:C	1:A:244:ARG:N	2.70	0.45
1:A:291:ASN:C	1:A:295:LEU:HD12	2.37	0.45
1:B:153:TYR:HB2	1:B:288:GLN:NE2	2.31	0.45
1:B:298:TYR:O	1:B:301:GLN:HB3	2.16	0.45
1:C:41:HIS:NE2	1:C:59:CYS:SG	2.90	0.45
1:C:87:VAL:O	1:C:87:VAL:CG1	2.65	0.45
1:C:131:PHE:CD1	1:C:132:ASN:OD1	2.70	0.45
1:C:150:PRO:HG2	1:C:154:ASP:HB3	1.97	0.45
1:C:323:LEU:C	1:C:323:LEU:HD12	2.37	0.45
1:A:263:LYS:C	1:A:265:HIS:H	2.19	0.45
1:A:386:ASP:C	1:A:387:ASN:CG	2.75	0.45
1:B:107:ASN:O	1:B:108:ASP:C	2.54	0.45
1:B:178:GLU:O	1:B:179:ILE:C	2.54	0.45
1:B:311:GLY:N	1:B:399:SER:O	2.49	0.45
1:C:97:VAL:O	1:C:98:PRO:C	2.54	0.45
1:A:138:ARG:NE	1:A:205:ASP:OD2	2.50	0.45
1:A:195:SER:C	1:A:197:GLY:N	2.69	0.45
1:A:236:VAL:CG2	1:A:272:PHE:CE2	2.99	0.45
1:A:242:MET:O	1:A:244:ARG:N	2.49	0.45
1:A:96:VAL:CG1	1:A:287:LEU:HD11	2.30	0.45
1:A:157:SER:O	1:A:161:TYR:N	2.36	0.45
1:A:286:GLU:OE2	1:A:290:MET:O	2.34	0.45
1:A:323:LEU:HD21	1:A:380:ILE:CG2	2.47	0.45
1:A:362:THR:HG22	1:A:363:ASP:N	2.32	0.45
1:C:184:ILE:O	1:C:185:HIS:C	2.53	0.45
1:A:184:ILE:HD13	1:A:211:HIS:HE1	1.82	0.45
1:A:216:ASP:OD2	1:A:282:TYR:OH	2.32	0.45
1:B:1:ARG:CA	1:B:1:ASN:N	2.80	0.45
1:B:22:LEU:HD11	1:B:34:PHE:CE1	2.52	0.45
1:B:211:HIS:O	1:B:214:ASN:N	2.40	0.45
1:A:34:PHE:O	1:A:37:LEU:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:PRO:CB	1:A:147:LYS:HB2	2.47	0.45
1:A:144:LYS:C	1:A:146:ALA:N	2.71	0.45
1:A:211:HIS:O	1:A:213:SER:N	2.50	0.45
1:A:232:ASP:OD1	1:A:235:GLU:HB2	2.17	0.45
1:A:287:LEU:O	1:A:287:LEU:HG	2.16	0.45
1:A:299:ILE:HD13	1:A:299:ILE:HA	1.82	0.45
1:A:322:HIS:HA	1:A:341:ASP:HB3	1.99	0.45
1:B:148:GLU:HG3	1:B:149:GLY:N	2.32	0.45
1:C:59:CYS:O	1:C:61:HIS:CG	2.70	0.45
1:A:140:ILE:HD12	1:A:140:ILE:N	2.22	0.44
1:A:208:PHE:O	1:A:212:HIS:HB2	2.16	0.44
1:A:228:PHE:CE2	1:A:296:HIS:CD2	3.05	0.44
1:B:268:PRO:O	1:B:269:GLU:C	2.51	0.44
1:B:382:GLN:OE1	1:B:390:ILE:HG21	2.16	0.44
1:A:71:ARG:NE	1:A:216:ASP:OD1	2.32	0.44
1:A:291:ASN:O	1:A:292:VAL:C	2.54	0.44
1:B:72:LEU:HD12	1:B:247:LEU:CD1	2.47	0.44
1:B:140:ILE:HD12	1:B:140:ILE:HG23	1.73	0.44
1:B:241:GLU:H	1:B:241:GLU:HG3	1.38	0.44
1:C:151:LYS:HB2	1:C:154:ASP:HB2	1.99	0.44
1:C:259:ASN:ND2	1:C:259:ASN:C	2.70	0.44
1:B:236:VAL:CG1	1:B:238:CYS:HB3	2.47	0.44
1:B:274:TYR:O	1:B:278:PHE:N	2.43	0.44
1:C:-2:HIS:C	1:C:-1:ARG:CG	2.85	0.44
1:C:22:LEU:O	1:C:26:GLN:N	2.40	0.44
1:C:275:LYS:HG3	1:C:276:GLY:N	2.32	0.44
1:B:65:THR:HG23	1:B:242:MET:HG3	1.99	0.44
1:B:77:PHE:CD1	1:B:209:ILE:HD11	2.52	0.44
1:C:59:CYS:SG	1:C:61:HIS:ND1	2.65	0.44
1:C:61:HIS:CD2	1:C:70:HIS:HE1	2.35	0.44
1:C:145:LEU:CD2	1:C:145:LEU:N	2.76	0.44
1:C:247:LEU:HD12	1:C:247:LEU:HA	1.67	0.44
1:A:143:ASP:O	1:A:146:ALA:HB2	2.17	0.44
1:B:299:ILE:O	1:B:301:GLN:N	2.51	0.44
1:B:309:PHE:CE2	1:B:360:GLU:HB2	2.52	0.44
1:B:323:LEU:HD11	1:B:340:PHE:CZ	2.53	0.44
1:C:4:ARG:HH21	1:C:75:VAL:HG22	1.83	0.44
1:C:42:ALA:O	1:C:45:PRO:HA	2.18	0.44
1:C:69:TRP:HE3	1:C:70:HIS:N	2.15	0.44
1:C:349:THR:O	1:C:350:PRO:C	2.55	0.44
1:A:156:TRP:HE3	1:A:157:SER:H	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:GLU:HA	1:A:226:GLN:HE22	1.83	0.44
1:A:199:LEU:CB	1:A:345:GLY:N	2.78	0.44
1:B:87:VAL:C	1:B:88:VAL:CG1	2.86	0.44
1:C:6:SER:O	1:C:7:VAL:C	2.56	0.44
1:C:27:GLU:H	1:C:27:GLU:HG3	1.55	0.44
1:C:66:PHE:HE2	1:C:70:HIS:CE1	2.36	0.44
1:C:396:PRO:HA	1:C:397:PRO:HD2	1.74	0.44
1:C:404:PRO:C	1:C:405:LYS:O	2.56	0.44
1:A:162:ILE:O	1:A:163:TYR:C	2.56	0.44
1:B:78:GLU:O	1:B:81:LEU:N	2.48	0.44
1:B:365:LEU:HD11	1:B:376:PHE:CE2	2.52	0.44
1:C:136:ILE:HG23	1:C:195:SER:HA	2.00	0.44
1:A:90:ILE:HG21	1:A:90:ILE:HD13	1.77	0.44
1:A:293:GLN:O	1:A:295:LEU:N	2.51	0.44
1:A:370:LEU:HD23	1:A:374:ASP:OD1	2.17	0.44
1:B:163:TYR:O	1:B:164:ALA:C	2.52	0.44
1:B:327:ILE:O	1:B:327:ILE:CG2	2.51	0.44
1:C:71:ARG:HD3	1:C:216:ASP:CG	2.38	0.44
1:C:93:TRP:CD1	1:C:103:PRO:HG2	2.53	0.44
1:A:180:ALA:O	1:A:181:HIS:C	2.56	0.44
1:A:339:TYR:O	1:A:339:TYR:CD2	2.70	0.44
1:B:222:TRP:O	1:B:224:GLU:N	2.50	0.44
1:C:90:ILE:HA	1:C:91:PRO:HD2	1.72	0.44
1:A:181:HIS:ND1	1:A:182:ASN:OD1	2.50	0.43
1:B:238:CYS:N	1:B:240:LEU:HD11	2.33	0.43
1:B:397:PRO:HA	1:B:398:PRO:HD3	1.79	0.43
1:C:211:HIS:O	1:C:215:THR:HG23	2.18	0.43
1:C:312:PHE:N	1:C:356:LEU:HD22	2.33	0.43
1:C:347:LEU:O	1:C:348:GLU:C	2.55	0.43
1:A:257:ASN:OD1	1:A:259:ASN:HB3	2.18	0.43
1:B:94:ASP:HA	1:B:214:ASN:ND2	2.32	0.43
1:B:368:LYS:HE2	1:B:368:LYS:HB2	1.81	0.43
1:B:185:HIS:NE2	1:B:212:HIS:CE1	2.86	0.43
1:C:305:ALA:O	1:C:307:ARG:HG3	2.18	0.43
1:A:-3:GLY:HA2	1:A:1:ASN:H3	1.81	0.43
1:A:104:ALA:O	1:A:107:ASN:N	2.47	0.43
1:A:167:GLN:HG2	1:A:172:ASP:HB3	2.01	0.43
1:B:107:ASN:O	1:B:107:ASN:ND2	2.52	0.43
1:B:202:ALA:O	1:B:204:TYR:N	2.52	0.43
1:B:307:ARG:O	1:B:308:VAL:CG2	2.63	0.43
1:C:41:HIS:CD2	1:C:59:CYS:SG	3.12	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:THR:HG23	1:C:242:MET:CB	2.49	0.43
1:C:95:THR:HG21	1:C:184:ILE:HG12	1.99	0.43
1:A:122:ASN:O	1:A:123:PRO:C	2.54	0.43
1:B:8:ARG:C	1:B:10:LEU:H	2.22	0.43
1:C:42:ALA:CB	1:C:200:HIS:HA	2.48	0.43
1:C:282:TYR:HB2	1:C:285:LEU:HD23	1.99	0.43
1:A:39:SER:C	1:A:41:HIS:N	2.70	0.43
1:A:136:ILE:HG21	1:A:205:ASP:HB2	2.00	0.43
1:A:167:GLN:HE21	1:A:167:GLN:HB2	1.70	0.43
1:A:192:GLU:HB2	1:A:195:SER:HG	1.83	0.43
1:C:65:THR:CG2	1:C:242:MET:HB2	2.49	0.43
1:C:71:ARG:NH2	1:C:272:PHE:O	2.52	0.43
1:C:309:PHE:N	1:C:309:PHE:HD1	2.15	0.43
1:A:61:HIS:HE2	1:A:70:HIS:HE1	1.66	0.43
1:A:301:GLN:HG3	1:A:304:GLU:OE1	2.19	0.43
1:A:371:ASP:O	1:A:372:VAL:C	2.55	0.43
1:C:4:ARG:NH2	1:C:75:VAL:CG2	2.82	0.43
1:C:8:ARG:NH1	1:C:103:PRO:HG3	2.34	0.43
1:C:8:ARG:HH22	1:C:103:PRO:HD3	1.82	0.43
1:C:404:PRO:O	1:C:405:LYS:O	2.37	0.43
1:A:4:ARG:CZ	1:A:280:TYR:CD1	3.01	0.43
1:A:128:ASP:OD1	1:A:128:ASP:N	2.51	0.43
1:B:95:THR:O	1:B:96:VAL:C	2.52	0.43
1:B:127:ALA:N	1:B:136:ILE:HD11	2.33	0.43
1:A:219:PHE:O	1:A:223:GLN:HG3	2.18	0.43
1:A:296:HIS:C	1:A:298:TYR:H	2.20	0.43
1:B:156:TRP:O	1:B:157:SER:C	2.55	0.43
1:B:279:HIS:O	1:B:280:TYR:HB3	2.19	0.43
1:C:237:ASN:C	1:C:240:LEU:HD21	2.39	0.43
1:C:295:LEU:HD23	1:C:295:LEU:HA	1.55	0.43
1:A:198:HIS:C	1:A:200:HIS:N	2.71	0.43
1:A:221:LEU:O	1:A:222:TRP:C	2.58	0.43
1:B:132:ASN:ND2	1:B:134:GLN:CB	2.81	0.43
1:C:176:GLN:O	1:C:177:PHE:C	2.56	0.43
1:A:195:SER:C	1:A:197:GLY:H	2.22	0.42
1:A:343:LEU:C	1:A:343:LEU:HD23	2.40	0.42
1:B:37:LEU:HG	1:B:37:LEU:H	1.65	0.42
1:B:374:ASP:OD2	1:B:375:VAL:N	2.52	0.42
1:B:395:PHE:HA	1:B:396:PRO:HD2	1.84	0.42
1:B:401:ILE:H	1:B:401:ILE:HG13	1.64	0.42
1:C:13:ALA:O	1:C:14:GLU:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:384:SER:C	1:C:386:ASP:N	2.67	0.42
1:A:143:ASP:O	1:A:146:ALA:CB	2.68	0.42
1:B:122:ASN:HA	1:B:123:PRO:HD3	1.78	0.42
1:A:22:LEU:O	1:A:26:GLN:N	2.45	0.42
1:A:263:LYS:C	1:A:265:HIS:N	2.72	0.42
1:C:65:THR:HG23	1:C:242:MET:HB2	2.00	0.42
1:C:132:ASN:C	1:C:134:GLN:HE22	2.23	0.42
1:A:-2:HIS:ND1	1:A:-2:HIS:C	2.72	0.42
1:B:263:LYS:HG2	1:B:264:GLU:N	2.33	0.42
1:C:7:VAL:C	1:C:10:LEU:HG	2.40	0.42
1:A:299:ILE:O	1:A:302:GLN:HB2	2.19	0.42
1:A:315:GLU:O	1:A:316:GLY:C	2.58	0.42
1:A:366:GLU:O	1:A:369:GLY:N	2.50	0.42
1:B:66:PHE:HE2	1:B:70:HIS:CE1	2.38	0.42
1:B:135:LYS:O	1:B:136:ILE:C	2.55	0.42
1:B:177:PHE:C	1:B:177:PHE:CD2	2.92	0.42
1:B:221:LEU:HD11	1:B:295:LEU:CD1	2.49	0.42
1:B:224:GLU:C	1:B:226:GLN:N	2.71	0.42
1:B:252:PHE:HD1	1:B:252:PHE:H	1.66	0.42
1:C:200:HIS:C	1:C:201:TYR:CD2	2.93	0.42
1:C:267:LYS:O	1:C:268:PRO:C	2.56	0.42
1:C:330:ILE:HD12	1:C:330:ILE:N	2.30	0.42
1:A:-3:GLY:CA	1:A:1:ASN:H2	2.32	0.42
1:A:104:ALA:C	1:A:106:PHE:N	2.73	0.42
1:A:293:GLN:C	1:A:295:LEU:H	2.23	0.42
1:B:267:LYS:O	1:B:270:ASP:HB2	2.19	0.42
1:C:20:ALA:O	1:C:21:ALA:C	2.58	0.42
1:C:65:THR:HG21	1:C:242:MET:CB	2.49	0.42
1:C:254:ALA:HB1	1:C:255:PRO:HA	2.00	0.42
1:C:391:SER:HB2	1:C:393:ASP:OD2	2.20	0.42
1:B:150:PRO:O	1:B:151:LYS:CE	2.67	0.42
1:C:275:LYS:HG3	1:C:276:GLY:H	1.85	0.42
1:C:370:LEU:HD23	1:C:370:LEU:HA	1.21	0.42
1:A:10:LEU:HD23	1:A:10:LEU:HA	1.72	0.42
1:A:173:PHE:O	1:A:173:PHE:CD1	2.72	0.42
1:A:249:PRO:O	1:A:251:SER:N	2.53	0.42
1:A:386:ASP:HB2	1:A:387:ASN:H	1.66	0.42
1:B:94:ASP:OD2	1:B:94:ASP:C	2.57	0.42
1:B:132:ASN:OD1	1:B:194:TYR:HE2	2.02	0.42
1:B:220:ALA:O	1:B:221:LEU:C	2.53	0.42
1:B:229:ARG:HH11	1:B:229:ARG:CB	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:GLU:HA	1:B:246:PRO:HD2	1.67	0.42
1:B:303:LYS:CE	1:B:405:LYS:HG2	2.41	0.42
1:A:143:ASP:HA	1:A:145:LEU:HD23	2.01	0.42
1:A:309:PHE:N	1:A:309:PHE:CD1	2.86	0.42
1:B:162:ILE:HD12	1:B:162:ILE:HA	1.93	0.42
1:B:229:ARG:HB2	1:B:229:ARG:HH11	1.84	0.42
1:C:-2:HIS:CB	1:C:1:ASN:HB2	2.48	0.42
1:C:65:THR:HG22	1:C:243:MET:HE1	2.02	0.42
1:C:173:PHE:CE1	1:C:177:PHE:HB2	2.55	0.42
1:C:184:ILE:N	1:C:184:ILE:HD12	2.34	0.42
1:A:66:PHE:CE2	1:A:178:GLU:HG3	2.54	0.42
1:A:106:PHE:HD1	1:A:138:ARG:HH12	1.67	0.42
1:A:210:LEU:HD23	1:A:210:LEU:HA	1.97	0.42
1:B:47:CYS:HB3	1:B:48:PRO:CD	2.45	0.42
1:B:367:SER:O	1:B:368:LYS:HE2	2.20	0.42
1:C:68:GLU:O	1:C:69:TRP:C	2.55	0.42
1:C:99:GLN:O	1:C:100:GLU:C	2.58	0.42
1:C:311:GLY:C	1:C:356:LEU:HD22	2.40	0.42
1:A:53:ASN:HB2	1:B:322:HIS:NE2	2.35	0.41
1:A:92:TYR:CG	1:A:217:ARG:HD3	2.55	0.41
1:A:228:PHE:HE2	1:A:296:HIS:CD2	2.33	0.41
1:B:182:ASN:N	1:B:182:ASN:OD1	2.51	0.41
1:C:122:ASN:HD22	1:C:124:PHE:H	1.68	0.41
1:C:254:ALA:CB	1:C:255:PRO:HA	2.50	0.41
1:A:252:PHE:N	1:A:252:PHE:CD1	2.86	0.41
1:B:78:GLU:C	1:B:80:ALA:N	2.72	0.41
1:B:112:ASP:C	1:B:114:ALA:N	2.74	0.41
1:C:102:LEU:HD11	1:C:140:ILE:HD13	2.02	0.41
1:A:199:LEU:HD22	1:A:348:GLU:HB3	2.02	0.41
1:A:268:PRO:O	1:A:269:GLU:C	2.58	0.41
1:B:17:SER:O	1:B:21:ALA:HB2	2.20	0.41
1:C:96:VAL:HG11	1:C:287:LEU:HD11	2.02	0.41
1:C:131:PHE:N	1:C:131:PHE:CD2	2.87	0.41
1:B:42:ALA:HA	1:B:57:ALA:HB1	2.03	0.41
1:C:-1:ARG:HG2	1:C:1:ASN:H3	1.86	0.41
1:C:132:ASN:C	1:C:134:GLN:NE2	2.73	0.41
1:C:149:GLY:O	1:C:151:LYS:N	2.53	0.41
1:A:94:ASP:HA	1:A:214:ASN:HD21	1.80	0.41
1:A:117:HIS:CD2	1:A:117:HIS:N	2.87	0.41
1:A:205:ASP:CG	1:A:207:VAL:HG22	2.40	0.41
1:B:66:PHE:CE2	1:B:70:HIS:CE1	3.07	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:VAL:HG13	1:B:98:PRO:CD	2.47	0.41
1:B:135:LYS:O	1:B:136:ILE:O	2.39	0.41
1:B:181:HIS:O	1:B:181:HIS:CD2	2.70	0.41
1:C:86:SER:C	1:C:88:VAL:N	2.69	0.41
1:C:241:GLU:H	1:C:241:GLU:HG3	1.55	0.41
1:A:72:LEU:HD22	1:A:250:PHE:CG	2.56	0.41
1:A:136:ILE:CD1	1:A:204:TYR:O	2.69	0.41
1:A:166:GLU:HG3	1:A:299:ILE:HD12	2.01	0.41
1:B:28:ASP:HB2	1:B:84:HIS:CE1	2.56	0.41
1:B:225:LEU:HD12	1:B:225:LEU:HA	1.84	0.41
1:B:280:TYR:C	1:B:281:GLU:OE1	2.58	0.41
1:B:337:ALA:HB1	1:B:361:ILE:HG22	2.02	0.41
1:C:149:GLY:HA3	1:C:152:GLY:O	2.21	0.41
1:A:67:PRO:O	1:A:68:GLU:C	2.55	0.41
1:A:73:TYR:O	1:A:76:GLN:HB3	2.20	0.41
1:A:285:LEU:HD13	1:A:285:LEU:HA	1.68	0.41
1:A:323:LEU:HD21	1:A:380:ILE:HB	2.01	0.41
1:B:-1:ARG:CA	1:B:1:ASN:H3	2.34	0.41
1:B:132:ASN:ND2	1:B:134:GLN:HB2	2.35	0.41
1:B:140:ILE:O	1:B:142:VAL:C	2.59	0.41
1:B:200:HIS:CE1	1:B:347:LEU:H	2.39	0.41
1:B:299:ILE:HG22	1:B:300:ASN:N	2.35	0.41
1:B:314:LEU:H	1:B:314:LEU:HG	1.69	0.41
1:B:388:GLU:O	1:B:389:ASP:C	2.58	0.41
1:C:123:PRO:C	1:C:125:ASN:H	2.24	0.41
1:A:42:ALA:HB1	1:A:200:HIS:HA	2.02	0.41
1:A:325:PHE:O	1:A:337:ALA:CB	2.64	0.41
1:B:166:GLU:HB3	1:B:167:GLN:NE2	2.30	0.41
1:B:205:ASP:OD1	1:B:206:PRO:N	2.53	0.41
1:B:224:GLU:O	1:B:225:LEU:C	2.59	0.41
1:C:346:SER:O	1:C:348:GLU:N	2.54	0.41
1:A:10:LEU:HA	1:A:14:GLU:OE2	2.21	0.41
1:A:87:VAL:HG12	1:A:87:VAL:O	2.21	0.41
1:A:92:TYR:HA	1:A:210:LEU:O	2.21	0.41
1:A:232:ASP:OD2	1:A:232:ASP:C	2.58	0.41
1:A:260:PRO:O	1:A:262:THR:N	2.54	0.41
1:B:34:PHE:O	1:B:35:GLN:C	2.59	0.41
1:B:71:ARG:HD3	1:B:216:ASP:CG	2.41	0.41
1:B:153:TYR:O	1:B:155:THR:N	2.54	0.41
1:B:263:LYS:C	1:B:265:HIS:N	2.74	0.41
1:B:366:GLU:O	1:B:368:LYS:N	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:HIS:CD2	1:C:59:CYS:CB	3.04	0.41
1:C:43:GLN:HA	1:C:44:PRO:C	2.41	0.41
1:C:47:CYS:SG	1:C:248:LYS:HB2	2.60	0.41
1:C:96:VAL:C	1:C:97:VAL:CG2	2.86	0.41
1:C:99:GLN:NE2	1:C:103:PRO:HD3	2.36	0.41
1:C:180:ALA:O	1:C:181:HIS:C	2.59	0.41
1:C:182:ASN:O	1:C:185:HIS:N	2.54	0.41
1:C:323:LEU:HD21	1:C:340:PHE:CZ	2.55	0.41
1:C:346:SER:HB2	1:C:347:LEU:CD2	2.41	0.41
1:A:75:VAL:HG21	1:A:278:PHE:CG	2.56	0.41
1:A:98:PRO:HB2	1:A:147:LYS:HB2	2.03	0.41
1:A:139:ASP:O	1:A:190:GLY:HA3	2.21	0.41
1:A:170:TYR:O	1:A:172:ASP:N	2.54	0.41
1:A:244:ARG:HH11	1:A:244:ARG:CG	2.06	0.41
1:B:32:ASP:O	1:B:37:LEU:HD11	2.21	0.41
1:B:167:GLN:H	1:B:167:GLN:HG2	1.14	0.41
1:C:11:SER:HA	1:C:12:PRO:HD3	1.87	0.41
1:C:169:ASP:O	1:C:170:TYR:C	2.60	0.41
1:C:217:ARG:HG2	1:C:282:TYR:CG	2.55	0.41
1:C:291:ASN:C	1:C:294:ARG:H	2.24	0.41
1:A:47:CYS:C	1:A:49:ALA:N	2.69	0.40
1:B:184:ILE:HG21	1:B:211:HIS:CG	2.56	0.40
1:B:302:GLN:C	1:B:304:GLU:N	2.74	0.40
1:B:320:SER:OG	1:B:343:LEU:HA	2.20	0.40
1:C:139:ASP:O	1:C:140:ILE:C	2.58	0.40
1:C:162:ILE:O	1:C:163:TYR:C	2.58	0.40
1:C:268:PRO:C	1:C:270:ASP:H	2.24	0.40
1:A:380:ILE:HD12	1:A:380:ILE:C	2.41	0.40
1:B:234:ASN:HA	1:B:272:PHE:CB	2.51	0.40
1:B:302:GLN:C	1:B:304:GLU:H	2.19	0.40
1:C:24:SER:HB3	1:C:84:HIS:ND1	2.36	0.40
1:C:48:PRO:HD3	1:C:56:PHE:O	2.21	0.40
1:C:399:SER:C	1:C:400:VAL:HG23	2.42	0.40
1:A:43:GLN:HG3	1:A:44:PRO:N	2.36	0.40
1:A:80:ALA:O	1:A:81:LEU:C	2.57	0.40
1:A:155:THR:O	1:A:159:LYS:HG2	2.22	0.40
1:A:286:GLU:CD	1:A:289:GLY:O	2.59	0.40
1:B:142:VAL:HA	1:B:144:LYS:CG	2.47	0.40
1:B:299:ILE:C	1:B:301:GLN:N	2.69	0.40
1:C:327:ILE:HD13	1:C:365:LEU:HD13	2.03	0.40
1:B:48:PRO:O	1:B:248:LYS:HE2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:ASP:O	1:B:364:VAL:C	2.57	0.40
1:C:86:SER:C	1:C:88:VAL:H	2.24	0.40
1:C:150:PRO:HG2	1:C:154:ASP:CB	2.52	0.40
1:C:298:TYR:O	1:C:302:GLN:HG2	2.21	0.40
1:A:-3:GLY:O	1:A:-2:HIS:C	2.59	0.40
1:A:307:ARG:HB2	1:A:309:PHE:HE1	1.85	0.40
1:B:-2:HIS:NE2	1:B:-1:ARG:HG3	2.35	0.40
1:B:116:PHE:C	1:B:117:HIS:ND1	2.75	0.40
1:C:28:ASP:OD1	1:C:30:SER:HB3	2.21	0.40
1:C:81:LEU:HD12	1:C:90:ILE:HG12	2.04	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-2:HIS:CA	3:B:5503:CU:CU[6_456]	1.67	0.53
1:A:-2:HIS:O	3:B:5503:CU:CU[6_456]	1.69	0.51

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 X-ray entries followed by that with respect to entries of similar resolution.

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	404/408 (99%)	280 (69%)	86 (21%)	38 (9%)	0	3
1	B	404/408 (99%)	311 (77%)	70 (17%)	23 (6%)	1	9
1	C	404/408 (99%)	287 (71%)	83 (20%)	34 (8%)	0	4
All	All	1212/1224 (99%)	878 (72%)	239 (20%)	95 (8%)	1	5

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-2	HIS

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Mol	Chain	Res	Type
1	A	34	PHE
1	A	57	ALA
1	A	58	CYS
1	A	105	PHE
1	A	113	ASP
1	A	114	ALA
1	A	156	TRP
1	A	157	SER
1	A	170	TYR
1	A	199	LEU
1	A	316	GLY
1	A	331	ASP
1	A	362	THR
1	B	113	ASP
1	B	115	LEU
1	B	116	PHE
1	B	124	PHE
1	B	141	ASN
1	B	327	ILE
1	B	404	PRO
1	C	34	PHE
1	C	35	GLN
1	C	59	CYS
1	C	60	VAL
1	C	79	ASP
1	C	87	VAL
1	C	141	ASN
1	C	148	GLU
1	C	187	TRP
1	C	246	PRO
1	C	269	GLU
1	C	316	GLY
1	C	350	PRO
1	C	387	ASN
1	C	404	PRO
1	A	119	ASN
1	A	190	GLY
1	A	368	LYS
1	A	375	VAL
1	A	384	SER
1	A	387	ASN
1	B	47	CYS

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Mol	Chain	Res	Type
1	B	117	HIS
1	B	200	HIS
1	B	234	ASN
1	B	264	GLU
1	B	303	LYS
1	B	368	LYS
1	B	387	ASN
1	C	96	VAL
1	C	100	GLU
1	C	115	LEU
1	C	250	PHE
1	C	260	PRO
1	A	37	LEU
1	A	64	ALA
1	A	193	GLU
1	A	196	MET
1	A	212	HIS
1	A	239	ALA
1	A	269	GLU
1	A	386	ASP
1	B	154	ASP
1	B	250	PHE
1	B	270	ASP
1	C	46	LEU
1	C	51	ALA
1	C	86	SER
1	C	130	ASP
1	C	154	ASP
1	A	350	PRO
1	A	367	SER
1	B	190	GLY
1	B	233	PRO
1	C	132	ASN
1	C	133	HIS
1	C	194	TYR
1	C	304	GLU
1	C	384	SER
1	C	393	ASP
1	A	264	GLU
1	A	297	ASP
1	B	260	PRO
1	C	47	CYS

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Mol	Chain	Res	Type
1	A	177	PHE
1	A	261	THR
1	C	203	SER
1	A	260	PRO
1	A	332	GLY
1	B	7	VAL
1	B	140	ILE
1	C	149	GLY
1	A	49	ALA
1	A	96	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	352/352 (100%)	306 (87%)	46 (13%)	3	14
1	B	352/352 (100%)	289 (82%)	63 (18%)	1	7
1	C	352/352 (100%)	292 (83%)	60 (17%)	1	8
All	All	1056/1056 (100%)	887 (84%)	169 (16%)	2	9

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	15	ARG
1	A	22	LEU
1	A	43	GLN
1	A	47	CYS
1	A	79	ASP
1	A	92	TYR
1	A	96	VAL
1	A	102	LEU
1	A	108	ASP
1	A	110	ILE
1	A	119	ASN

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Mol	Chain	Res	Type
1	A	140	ILE
1	A	145	LEU
1	A	154	ASP
1	A	155	THR
1	A	167	GLN
1	A	173	PHE
1	A	174	GLU
1	A	181	HIS
1	A	191	THR
1	A	201	TYR
1	A	218	LEU
1	A	231	HIS
1	A	234	ASN
1	A	241	GLU
1	A	243	MET
1	A	246	PRO
1	A	248	LYS
1	A	255	PRO
1	A	268	PRO
1	A	285	LEU
1	A	290	MET
1	A	293	GLN
1	A	299	ILE
1	A	324	ASP
1	A	326	SER
1	A	327	ILE
1	A	330	ILE
1	A	339	TYR
1	A	341	ASP
1	A	355	ARG
1	A	366	GLU
1	A	372	VAL
1	A	393	ASP
1	A	399	SER
1	B	-1	ARG
1	B	2	LEU
1	B	12	PRO
1	B	30	SER
1	B	46	LEU
1	B	47	CYS
1	B	58	CYS
1	B	59	CYS

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Mol	Chain	Res	Type
1	B	63	MET
1	B	71	ARG
1	B	77	PHE
1	B	79	ASP
1	B	83	ARG
1	B	87	VAL
1	B	95	THR
1	B	100	GLU
1	B	102	LEU
1	B	107	ASN
1	B	109	GLU
1	B	110	ILE
1	B	111	TRP
1	B	116	PHE
1	B	136	ILE
1	B	144	LYS
1	B	151	LYS
1	B	153	TYR
1	B	154	ASP
1	B	173	PHE
1	B	176	GLN
1	B	181	HIS
1	B	196	MET
1	B	227	LYS
1	B	229	ARG
1	B	233	PRO
1	B	241	GLU
1	B	243	MET
1	B	249	PRO
1	B	260	PRO
1	B	262	THR
1	B	274	TYR
1	B	280	TYR
1	B	286	GLU
1	B	301	GLN
1	B	303	LYS
1	B	304	GLU
1	B	323	LEU
1	B	324	ASP
1	B	341	ASP
1	B	343	LEU
1	B	346	SER

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Mol	Chain	Res	Type
1	B	347	LEU
1	B	349	THR
1	B	359	TYR
1	B	361	ILE
1	B	365	LEU
1	B	368	LYS
1	B	375	VAL
1	B	378	ILE
1	B	382	GLN
1	B	391	SER
1	B	392	THR
1	B	393	ASP
1	B	402	TYR
1	C	3	VAL
1	C	7	VAL
1	C	15	ARG
1	C	22	LEU
1	C	23	LYS
1	C	24	SER
1	C	27	GLU
1	C	29	SER
1	C	35	GLN
1	C	46	LEU
1	C	47	CYS
1	C	50	PRO
1	C	58	CYS
1	C	71	ARG
1	C	82	ARG
1	C	95	THR
1	C	97	VAL
1	C	99	GLN
1	C	101	ASP
1	C	110	ILE
1	C	119	ASN
1	C	120	PHE
1	C	122	ASN
1	C	130	ASP
1	C	134	GLN
1	C	138	ARG
1	C	143	ASP
1	C	154	ASP
1	C	155	THR

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Mol	Chain	Res	Type
1	C	196	MET
1	C	203	SER
1	C	208	PHE
1	C	218	LEU
1	C	233	PRO
1	C	241	GLU
1	C	246	PRO
1	C	248	LYS
1	C	255	PRO
1	C	260	PRO
1	C	290	MET
1	C	294	ARG
1	C	297	ASP
1	C	300	ASN
1	C	301	GLN
1	C	303	LYS
1	C	307	ARG
1	C	309	PHE
1	C	314	LEU
1	C	315	GLU
1	C	322	HIS
1	C	323	LEU
1	C	330	ILE
1	C	341	ASP
1	C	349	THR
1	C	350	PRO
1	C	358	LYS
1	C	372	VAL
1	C	381	THR
1	C	382	GLN
1	C	387	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	76	GLN
1	A	84	HIS
1	A	99	GLN
1	A	117	HIS
1	A	119	ASN
1	A	122	ASN

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Mol	Chain	Res	Type
1	A	167	GLN
1	A	182	ASN
1	A	198	HIS
1	A	211	HIS
1	A	223	GLN
1	A	226	GLN
1	A	291	ASN
1	A	296	HIS
1	A	322	HIS
1	B	-2	HIS
1	B	1	ASN
1	B	35	GLN
1	B	107	ASN
1	B	119	ASN
1	B	132	ASN
1	B	141	ASN
1	B	167	GLN
1	B	176	GLN
1	B	200	HIS
1	B	211	HIS
1	B	223	GLN
1	B	226	GLN
1	B	234	ASN
1	B	265	HIS
1	B	277	HIS
1	B	301	GLN
1	B	302	GLN
1	B	387	ASN
1	C	-2	HIS
1	C	99	GLN
1	C	117	HIS
1	C	119	ASN
1	C	122	ASN
1	C	125	ASN
1	C	132	ASN
1	C	134	GLN
1	C	167	GLN
1	C	176	GLN
1	C	223	GLN
1	C	226	GLN
1	C	237	ASN
1	C	259	ASN

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Mol	Chain	Res	Type
1	C	265	HIS
1	C	293	GLN
1	C	336	HIS
1	C	387	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 9 are monoatomic - leaving 3 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	$\# Z > 2$
2	NAG	C	650	-	15,15,15	1.89	4 (26%)	21,21,21	1.82	6 (28%)
2	NAG	A	600	-	15,15,15	1.71	3 (20%)	21,21,21	1.96	6 (28%)
2	NAG	C	651	-	15,15,15	1.80	4 (26%)	21,21,21	4.28	11 (52%)

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
2	NAG	C	650	-	-	2/6/26/26	0/1/1/1
2	NAG	A	600	-	-	3/6/26/26	0/1/1/1
2	NAG	C	651	-	-	4/6/26/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	650	NAG	O7-C7	4.74	1.33	1.23
2	A	600	NAG	C3-C2	3.62	1.59	1.53
2	C	650	NAG	C8-C7	3.14	1.57	1.50
2	C	651	NAG	C8-C7	2.92	1.56	1.50
2	C	651	NAG	O1-C1	2.74	1.48	1.39
2	A	600	NAG	C1-C2	2.48	1.55	1.52
2	C	650	NAG	C1-C2	2.42	1.55	1.52
2	C	650	NAG	O1-C1	2.38	1.47	1.39
2	C	651	NAG	C6-C5	2.28	1.59	1.51
2	C	651	NAG	C4-C5	2.25	1.57	1.53
2	A	600	NAG	C8-C7	2.25	1.55	1.50

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	651	NAG	C1-C2-C3	-13.28	92.43	110.54
2	C	651	NAG	O1-C1-C2	8.11	126.06	109.22
2	C	651	NAG	C1-O5-C5	-7.08	99.96	113.65
2	C	651	NAG	O5-C5-C6	4.81	118.36	106.44
2	A	600	NAG	C1-C2-N2	-4.63	105.37	110.73
2	A	600	NAG	C1-C2-C3	3.89	115.85	110.54
2	C	650	NAG	C1-C2-C3	3.58	115.42	110.54
2	C	650	NAG	O1-C1-C2	3.32	116.11	109.22
2	C	650	NAG	C2-N2-C7	-3.20	115.62	123.11
2	C	651	NAG	O1-C1-O5	3.19	119.89	110.41
2	C	650	NAG	O3-C3-C4	-3.17	102.89	110.38
2	A	600	NAG	O3-C3-C2	3.14	115.83	109.58
2	C	651	NAG	O5-C1-C2	-3.11	106.39	109.52
2	C	651	NAG	C2-N2-C7	2.96	130.03	123.11
2	C	651	NAG	C3-C4-C5	2.78	115.27	110.23
2	C	651	NAG	C1-C2-N2	2.71	113.86	110.73
2	A	600	NAG	O5-C5-C6	2.69	113.12	106.44
2	C	650	NAG	O3-C3-C2	2.58	114.73	109.58
2	C	651	NAG	C8-C7-N2	2.36	120.02	116.12
2	A	600	NAG	C2-N2-C7	-2.29	117.73	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	650	NAG	O5-C1-C2	-2.25	107.26	109.52
2	C	651	NAG	O3-C3-C2	2.11	113.79	109.58
2	A	600	NAG	C8-C7-N2	2.05	119.51	116.12

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	NAG	C8-C7-N2-C2
2	A	600	NAG	O7-C7-N2-C2
2	C	650	NAG	C8-C7-N2-C2
2	C	650	NAG	O7-C7-N2-C2
2	C	651	NAG	C8-C7-N2-C2
2	C	651	NAG	O7-C7-N2-C2
2	C	651	NAG	C4-C5-C6-O6
2	A	600	NAG	O5-C5-C6-O6
2	C	651	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	650	NAG	1	0
2	A	600	NAG	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	C	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	-1:ARG	C	1:ASN	N	5.08
1	C	-1:ARG	C	1:ASN	N	3.99
1	B	-1:ARG	C	1:ASN	N	2.64

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	408/408 (100%)	-0.16	4 (0%) 79 68	43, 43, 43, 78	0
1	B	408/408 (100%)	-0.24	4 (0%) 79 68	43, 43, 43, 78	0
1	C	408/408 (100%)	-0.06	3 (0%) 84 75	31, 43, 43, 78	1 (0%)
All	All	1224/1224 (100%)	-0.15	11 (0%) 81 70	31, 43, 43, 78	1 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	-3	GLY	7.3
1	B	141	ASN	4.6
1	B	132	ASN	3.1
1	C	132	ASN	3.0
1	B	148	GLU	2.8
1	C	297	ASP	2.3
1	A	141	ASN	2.3
1	A	-3	GLY	2.3
1	A	369	GLY	2.3
1	A	345	GLY	2.2
1	B	-3	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	C	651	15/15	0.57	0.23	77,77,77,77	0
2	NAG	A	600	15/15	0.63	0.30	77,77,77,77	0
2	NAG	C	650	15/15	0.72	0.14	77,77,77,77	0
3	CU	A	5001	1/1	0.97	0.07	77,77,77,77	0
3	CU	B	5503	1/1	0.97	0.07	77,77,77,77	0
3	CU	B	5506	1/1	0.97	0.07	77,77,77,77	0
3	CU	A	5012	1/1	0.98	0.04	77,77,77,77	0
3	CU	C	5509	1/1	0.98	0.05	77,77,77,77	0
3	CU	B	5004	1/1	0.99	0.08	77,77,77,77	0
3	CU	C	5007	1/1	0.99	0.03	77,77,77,77	0
3	CU	C	5018	1/1	0.99	0.04	77,77,77,77	0
3	CU	B	5015	1/1	0.99	0.06	77,77,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.