



## Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 01:54 pm BST

PDB ID : 7QDG  
EMDB ID : EMD-13916  
Title : SARS-CoV-2 S protein S:A222V + S:D614G mutant 1-up  
Authors : Ginex, T.; Marco-Marin, C.; Wieczor, M.; Mata, C.P.; Krieger, J.; Lopez-Redondo, M.L.; Frances-Gomez, C.; Ruiz-Rodriguez, P.; Melero, R.; Sanchez-Sorzano, C.O.; Martinez, M.; Gougéard, N.; Forcada-Nadal, A.; Zamora-Caballero, S.; Gozalbo-Rovira, R.; Sanz-Frasquet, C.; Bravo, J.; Rubio, V.; Marina, A.; Geller, R.; Comas, I.; Gil, C.; Coscolla, M.; Orozco, M.; LLacer, J.L.; Carazo, J.M.  
Deposited on : 2021-11-27  
Resolution : 3.40 Å(reported)  
Based on initial model : 7BNN

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

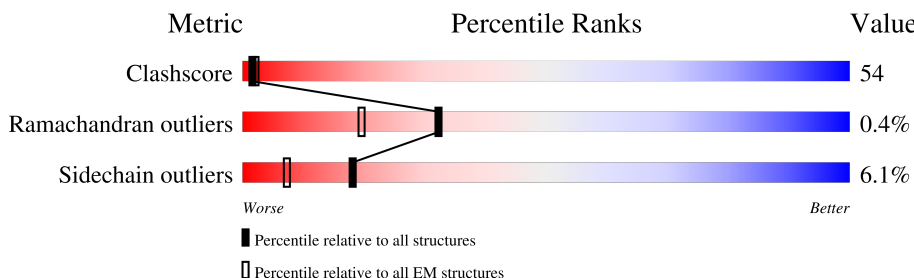
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

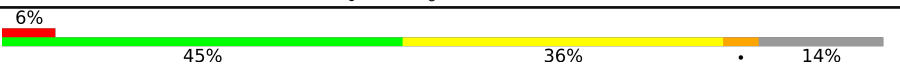


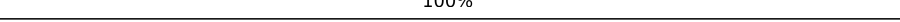
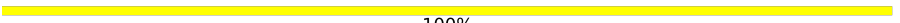

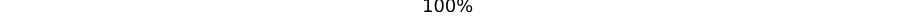
The reported resolution of this entry is 3.40 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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 EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1250	
1	B	1250	
1	C	1250	
2	E	2	
2	G	2	
2	I	2	
2	J	2	

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Validation Pipeline (wwPDB-VP) : 2.39

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Mol	Chain	Length	Quality of chain
2	K	2	<div><div></div>100%</div>
2	L	2	<div><div></div>50%<div></div>50%</div>
2	M	2	<div><div></div>50%<div></div>50%</div>
2	N	2	<div><div></div>100%<div></div>50%<div></div>50%</div>
2	O	2	<div><div></div>50%<div></div>100%</div>
2	P	2	<div><div></div>50%<div></div>50%</div>
3	Q	2	<div><div></div>50%<div></div>50%</div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25570 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein,Fibritin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1070	Total	C	N	O	S	0	0
			8356	5334	1392	1592	38		
1	B	1049	Total	C	N	O	S	0	0
			8191	5230	1365	1560	36		
1	C	1074	Total	C	N	O	S	0	0
			8365	5342	1393	1592	38		

There are 99 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	VAL	ALA	conflict	UNP P0DTC2
A	614	GLY	ASP	conflict	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	685	ALA	ARG	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1214	LEU	-	linker	UNP P0DTC2
A	1215	VAL	-	linker	UNP P0DTC2
A	1216	PRO	-	linker	UNP P0DTC2
A	1217	ARG	-	linker	UNP P0DTC2
A	1218	GLY	-	linker	UNP P0DTC2
A	1219	SER	-	linker	UNP P0DTC2
A	1249	HIS	-	expression tag	UNP P10104
A	1250	HIS	-	expression tag	UNP P10104
A	1251	HIS	-	expression tag	UNP P10104
A	1252	HIS	-	expression tag	UNP P10104
A	1253	HIS	-	expression tag	UNP P10104
A	1254	HIS	-	expression tag	UNP P10104
A	1255	HIS	-	expression tag	UNP P10104
A	1256	HIS	-	expression tag	UNP P10104
A	1257	HIS	-	expression tag	UNP P10104
A	1258	GLU	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1259	GLN	-	expression tag	UNP P10104
A	1260	LYS	-	expression tag	UNP P10104
A	1261	LEU	-	expression tag	UNP P10104
A	1262	ILE	-	expression tag	UNP P10104
A	1263	SER	-	expression tag	UNP P10104
A	1264	GLU	-	expression tag	UNP P10104
A	1265	GLU	-	expression tag	UNP P10104
A	1266	ASP	-	expression tag	UNP P10104
A	1267	LEU	-	expression tag	UNP P10104
B	222	VAL	ALA	conflict	UNP P0DTC2
B	614	GLY	ASP	conflict	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	685	ALA	ARG	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1214	LEU	-	linker	UNP P0DTC2
B	1215	VAL	-	linker	UNP P0DTC2
B	1216	PRO	-	linker	UNP P0DTC2
B	1217	ARG	-	linker	UNP P0DTC2
B	1218	GLY	-	linker	UNP P0DTC2
B	1219	SER	-	linker	UNP P0DTC2
B	1249	HIS	-	expression tag	UNP P10104
B	1250	HIS	-	expression tag	UNP P10104
B	1251	HIS	-	expression tag	UNP P10104
B	1252	HIS	-	expression tag	UNP P10104
B	1253	HIS	-	expression tag	UNP P10104
B	1254	HIS	-	expression tag	UNP P10104
B	1255	HIS	-	expression tag	UNP P10104
B	1256	HIS	-	expression tag	UNP P10104
B	1257	HIS	-	expression tag	UNP P10104
B	1258	GLU	-	expression tag	UNP P10104
B	1259	GLN	-	expression tag	UNP P10104
B	1260	LYS	-	expression tag	UNP P10104
B	1261	LEU	-	expression tag	UNP P10104
B	1262	ILE	-	expression tag	UNP P10104
B	1263	SER	-	expression tag	UNP P10104
B	1264	GLU	-	expression tag	UNP P10104
B	1265	GLU	-	expression tag	UNP P10104
B	1266	ASP	-	expression tag	UNP P10104
B	1267	LEU	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
C	222	VAL	ALA	conflict	UNP P0DTC2
C	614	GLY	ASP	conflict	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	685	ALA	ARG	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1214	LEU	-	linker	UNP P0DTC2
C	1215	VAL	-	linker	UNP P0DTC2
C	1216	PRO	-	linker	UNP P0DTC2
C	1217	ARG	-	linker	UNP P0DTC2
C	1218	GLY	-	linker	UNP P0DTC2
C	1219	SER	-	linker	UNP P0DTC2
C	1249	HIS	-	expression tag	UNP P10104
C	1250	HIS	-	expression tag	UNP P10104
C	1251	HIS	-	expression tag	UNP P10104
C	1252	HIS	-	expression tag	UNP P10104
C	1253	HIS	-	expression tag	UNP P10104
C	1254	HIS	-	expression tag	UNP P10104
C	1255	HIS	-	expression tag	UNP P10104
C	1256	HIS	-	expression tag	UNP P10104
C	1257	HIS	-	expression tag	UNP P10104
C	1258	GLU	-	expression tag	UNP P10104
C	1259	GLN	-	expression tag	UNP P10104
C	1260	LYS	-	expression tag	UNP P10104
C	1261	LEU	-	expression tag	UNP P10104
C	1262	ILE	-	expression tag	UNP P10104
C	1263	SER	-	expression tag	UNP P10104
C	1264	GLU	-	expression tag	UNP P10104
C	1265	GLU	-	expression tag	UNP P10104
C	1266	ASP	-	expression tag	UNP P10104
C	1267	LEU	-	expression tag	UNP P10104

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	O	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	P	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	Q	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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

### 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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Spike glycoprotein,Fibritin







W152	M153	E154	S155	E156	F157	M164	M165	C166	T167	F168	W171	F175	L176	M177	D178	L179	E180	G181	K182	Q183	G184	N185	F186	K187	F192	F193	F194	K195	N196	I197	Y200	P201	K202	I203	Y204	I210	M211	L212	V213	L216	P217	Q218	G219	F220	S221	V222	L223	E224	P225	L226	V227	D228	
P85	F86	N87	D88	G89	V90	Y91	F92	Y95	F96	X97	S98	N99	I100	I101	R102	G103	W104	I105	F106	G107	T108	T109	L110	K113	T114	Q115	S116	L117	L118	I119	V120	A123	V126	V127	I128	K129	F133	H134	F135	C136	N137	D138	L141	G142	V143	Y144	Y145	H146	K147	N148	N149	K150	S151
C15	V16	M17	L18	T19	T20	R21	T22	Q23	L24	P25	P26	A27	S31	F32	T33	G34	R35	V36	X37	Y38	V42	F43	R44	S45	S46	V47	L48	T51	F55	L56	P57	F58	F59	W64	F65	H66	A67	I68	H69	V70	SER	GLY	THR	ASN	GLY	T76	K77	F79	D80	N81	P82	V83	F84



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%

MAG1  
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  50%  50%

MAG1  
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%

MAG1  
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%

MAG1  
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  50%  50%

MAG1  
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  50%  50%

MAG1  
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	145681	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	32.4	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.176	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.048	Depositor
Map size (Å)	420.0, 420.0, 420.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.54	2/8552 (0.0%)	0.71	7/11644 (0.1%)
1	B	0.55	5/8379 (0.1%)	0.67	6/11404 (0.1%)
1	C	0.63	9/8561 (0.1%)	0.71	9/11658 (0.1%)
All	All	0.57	16/25492 (0.1%)	0.70	22/34706 (0.1%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1146	ASP	C-O	-21.21	0.83	1.23
1	B	1146	ASP	C-O	-13.83	0.97	1.23
1	B	815	ARG	CZ-NH1	-8.44	1.22	1.33
1	C	70	VAL	C-O	-7.37	1.09	1.23
1	C	1043	CYS	CB-SG	-6.82	1.70	1.82
1	B	70	VAL	C-O	-6.60	1.10	1.23
1	C	392	PHE	CE2-CZ	-6.42	1.25	1.37
1	A	1032	CYS	CB-SG	5.88	1.92	1.82
1	A	940	SER	C-O	-5.79	1.12	1.23
1	C	676	THR	C-O	-5.50	1.12	1.23
1	C	522	ALA	CA-CB	-5.36	1.41	1.52
1	C	423	TYR	CD1-CE1	-5.32	1.31	1.39
1	B	1042	PHE	CG-CD2	-5.22	1.30	1.38
1	C	129	LYS	N-CA	-5.21	1.35	1.46
1	B	1126	CYS	CB-SG	-5.14	1.73	1.81
1	C	361	CYS	CB-SG	-5.00	1.73	1.81

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	825	LYS	CD-CE-NZ	-9.60	89.62	111.70
1	A	1032	CYS	CA-CB-SG	-8.76	98.24	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1043	CYS	CA-CB-SG	-7.71	100.12	114.00
1	B	815	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	B	291	CYS	CA-CB-SG	6.78	126.20	114.00
1	B	1146	ASP	CA-C-O	-6.61	106.21	120.10
1	A	1146	ASP	CA-C-O	-6.41	106.64	120.10
1	B	34	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	C	34	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	B	1032	CYS	CA-CB-SG	6.29	125.31	114.00
1	C	165	ASN	CB-CA-C	6.21	122.81	110.40
1	A	361	CYS	CA-CB-SG	-6.06	103.09	114.00
1	B	118	LEU	CB-CG-CD2	5.92	121.07	111.00
1	C	70	VAL	CA-C-O	-5.85	107.81	120.10
1	A	1014	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	118	LEU	CB-CG-CD2	5.61	120.53	111.00
1	C	128	ILE	CB-CA-C	-5.47	100.66	111.60
1	C	522	ALA	CB-CA-C	-5.33	102.10	110.10
1	C	522	ALA	N-CA-CB	-5.24	102.76	110.10
1	C	646	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	301	CYS	CA-CB-SG	-5.13	104.76	114.00
1	A	662	CYS	CA-CB-SG	5.09	123.16	114.00

There are no chirality outliers.

There are no planarity outliers.

## 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	8356	0	8129	922	0
1	B	8191	0	7974	740	0
1	C	8365	0	8121	1102	0
2	E	28	0	25	0	0
2	G	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	4	0
2	K	28	0	25	4	0
2	L	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	28	0	25	1	0
2	N	28	0	25	0	0
2	O	28	0	25	3	0
2	P	28	0	25	2	0
3	Q	28	0	24	2	0
4	A	140	0	129	6	0
4	B	112	0	103	1	0
4	C	98	0	91	2	0
All	All	25570	0	24821	2698	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 54.

All (2698) 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:C:118:LEU:HD22	1:C:135:PHE:CZ	1.27	1.67
1:A:87:ASN:ND2	1:A:269:TYR:CD2	1.69	1.55
1:A:33:THR:HG22	1:A:58:PHE:CD2	1.47	1.49
1:B:718:PHE:HB2	1:B:1067:TYR:CE1	1.46	1.49
1:B:1104:VAL:CG1	1:B:1119:ASN:HD21	1.27	1.48
1:B:1104:VAL:CG1	1:B:1119:ASN:ND2	1.75	1.46
1:B:599:THR:HG22	1:B:608:VAL:CG1	1.50	1.42
1:C:825:LYS:NZ	1:C:942:ALA:HB2	1.32	1.42
1:B:57:PRO:CB	1:B:273:ARG:HH12	1.33	1.38
1:C:516:GLU:HG3	1:C:519:HIS:NE2	1.35	1.38
1:B:1104:VAL:HG11	1:B:1119:ASN:ND2	1.16	1.38
1:A:89:GLY:HA3	1:A:270:LEU:N	1.38	1.37
1:C:118:LEU:CD2	1:C:135:PHE:CZ	2.04	1.37
1:A:353:TRP:CD1	1:A:466:ARG:HD3	1.57	1.36
1:A:107:GLY:CA	1:A:235:ILE:HG22	1.52	1.35
1:C:378:LYS:CG	1:C:433:VAL:HG12	1.55	1.35
1:C:87:ASN:OD1	1:C:269:TYR:CE2	1.79	1.35
1:A:885:GLY:HA2	1:A:901:GLN:NE2	1.35	1.35
1:C:453:TYR:HD1	1:C:495:TYR:CE1	1.42	1.34
1:C:36:VAL:O	1:C:223:LEU:HD21	1.27	1.34
1:C:37:TYR:CE1	1:C:55:PHE:CE1	2.15	1.33
1:C:453:TYR:CD1	1:C:495:TYR:HE1	1.46	1.33
1:A:452:LEU:HD13	1:A:493:GLN:O	1.25	1.32
1:A:797:PHE:CE1	1:A:882:ILE:HG21	1.64	1.32
1:C:289:VAL:HG23	1:C:306:PHE:CZ	1.65	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:454:ARG:NH2	1:C:467:ASP:OD2	1.59	1.31
1:C:328:ARG:NE	1:C:578:ASP:OD2	1.59	1.31
1:A:552:LEU:HD22	1:A:587:ILE:CD1	1.61	1.30
1:B:1088:HIS:CD2	1:B:1137:VAL:HG11	1.66	1.30
1:A:33:THR:HG22	1:A:58:PHE:CE2	1.64	1.29
1:A:83:VAL:HG21	1:A:237:ARG:CD	1.60	1.29
1:A:743:CYS:SG	1:A:749:CYS:C	2.12	1.27
1:A:726:ILE:HD12	1:A:944:ALA:O	1.33	1.27
1:C:220:PHE:CZ	1:C:288:ALA:N	2.02	1.27
1:A:34:ARG:NH1	1:A:217:PRO:HG2	1.49	1.27
1:C:970:PHE:CD2	1:C:999:GLY:HA3	1.67	1.26
1:A:353:TRP:CG	1:A:466:ARG:HD3	1.68	1.26
1:B:885:GLY:HA2	1:B:901:GLN:NE2	1.46	1.26
1:C:37:TYR:HE1	1:C:55:PHE:CE1	1.52	1.26
1:A:310:LYS:HB2	1:A:600:PRO:O	1.34	1.26
1:C:33:THR:HG22	1:C:58:PHE:CE2	1.70	1.26
1:B:718:PHE:CB	1:B:1067:TYR:HE1	1.50	1.24
1:A:1102:TRP:HB2	1:A:1135:ASN:ND2	1.51	1.23
1:B:118:LEU:HD22	1:B:135:PHE:CZ	1.72	1.23
1:C:607:GLN:NE2	1:C:674:TYR:OH	1.72	1.22
1:A:797:PHE:HE1	1:A:882:ILE:CG2	1.53	1.22
1:C:420:ASP:O	1:C:460:ASN:OD1	1.58	1.22
1:B:57:PRO:HB3	1:B:273:ARG:NH1	1.55	1.21
1:B:107:GLY:O	1:B:235:ILE:HG23	1.40	1.21
1:C:456:PHE:HB3	1:C:473:TYR:CE1	1.75	1.21
1:A:83:VAL:CG2	1:A:237:ARG:CD	2.19	1.21
1:A:497:PHE:CE2	1:A:507:PRO:HB3	1.74	1.21
1:A:87:ASN:ND2	1:A:269:TYR:CE2	2.07	1.21
1:A:87:ASN:ND2	1:A:269:TYR:HD2	1.11	1.21
1:A:118:LEU:HD22	1:A:135:PHE:CZ	1.75	1.20
1:C:36:VAL:O	1:C:223:LEU:CD2	1.88	1.20
1:C:360:ASN:HA	1:C:523:THR:CG2	1.70	1.20
1:A:90:VAL:HG23	1:A:238:PHE:CE2	1.75	1.20
1:C:725:GLU:OE2	1:C:1028:LYS:NZ	1.74	1.20
1:A:53:ASP:O	1:A:55:PHE:CD2	1.95	1.19
1:B:599:THR:HG22	1:B:608:VAL:HG11	1.22	1.19
1:A:353:TRP:HZ2	1:A:465:GLU:C	1.46	1.19
1:A:308:VAL:O	1:A:602:THR:HG22	1.41	1.19
1:A:905:ARG:HD3	1:A:1049:LEU:O	1.41	1.19
1:A:797:PHE:CE1	1:A:882:ILE:CG2	2.26	1.18
1:B:1039:ARG:CZ	1:B:1042:PHE:CE2	2.25	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:PRO:HD3	1:C:544:ASN:ND2	1.57	1.18
1:C:393:THR:OG1	1:C:522:ALA:HB2	1.43	1.18
1:C:106:PHE:HB3	1:C:235:ILE:HD13	1.19	1.18
1:C:37:TYR:CE1	1:C:55:PHE:HE1	1.55	1.17
1:C:598:ILE:HD11	1:C:666:ILE:CD1	1.75	1.17
1:B:372:ALA:HB1	1:B:374:PHE:CE2	1.79	1.17
1:A:64:TRP:NE1	1:A:266:TYR:CE2	2.13	1.16
1:A:724:THR:HG22	1:A:1063:LEU:HD23	1.27	1.16
1:A:34:ARG:CZ	1:A:217:PRO:HG2	1.76	1.16
1:C:393:THR:OG1	1:C:522:ALA:CB	1.93	1.16
1:A:1084:ASP:HB2	1:A:1086:LYS:HZ2	1.05	1.15
1:A:34:ARG:NH1	1:A:217:PRO:CG	2.08	1.15
1:C:105:ILE:HD11	1:C:241:LEU:CD1	1.74	1.15
1:C:615:VAL:CG2	1:C:649:CYS:HB2	1.77	1.15
1:C:1090:PRO:CA	1:C:1120:THR:HG22	1.74	1.15
1:C:462:LYS:HA	1:C:462:LYS:HE2	1.27	1.15
1:B:322:PRO:HG3	1:B:540:ASN:OD1	1.47	1.14
1:B:718:PHE:CB	1:B:1067:TYR:CE1	2.26	1.14
1:C:1090:PRO:HA	1:C:1120:THR:CG2	1.77	1.14
1:A:33:THR:CG2	1:A:58:PHE:CE2	2.29	1.14
1:C:662:CYS:SG	1:C:697:MET:HB3	1.86	1.14
1:A:453:TYR:CE2	1:A:493:GLN:HG2	1.83	1.14
1:B:298:GLU:HG2	1:B:315:THR:HG21	1.24	1.14
1:C:87:ASN:OD1	1:C:269:TYR:CD2	2.01	1.14
1:A:83:VAL:CG2	1:A:237:ARG:HD2	1.74	1.13
1:C:671:CYS:SG	1:C:697:MET:HB3	1.88	1.13
1:C:38:TYR:CE1	1:C:285:ILE:HG13	1.83	1.13
1:A:289:VAL:HG23	1:A:306:PHE:HE1	1.10	1.12
1:A:83:VAL:HG22	1:A:237:ARG:HD3	1.30	1.12
1:B:56:LEU:HD12	1:B:57:PRO:HD2	1.32	1.11
1:B:329:PHE:CE2	1:B:528:LYS:HB3	1.84	1.11
1:B:1104:VAL:HG13	1:B:1119:ASN:HD21	0.98	1.11
1:C:200:TYR:CD2	1:C:230:PRO:HA	1.83	1.11
1:C:426:PRO:HG2	1:C:464:PHE:CE2	1.83	1.11
1:C:97:LYS:NZ	1:C:180:GLU:OE1	1.83	1.11
1:C:378:LYS:CG	1:C:433:VAL:CG1	2.28	1.11
1:A:64:TRP:CD1	1:A:266:TYR:CD2	2.38	1.10
1:B:743:CYS:SG	1:B:750:SER:N	2.23	1.10
1:C:921:LYS:HE2	1:C:921:LYS:HA	1.33	1.10
1:B:826:VAL:HG23	1:B:945:LEU:HD12	1.33	1.10
1:A:299:THR:OG1	1:A:597:VAL:HG21	1.49	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:TYR:HD2	1:C:230:PRO:HA	1.06	1.10
1:C:210:ILE:HG12	1:C:212:LEU:HD21	1.30	1.10
1:C:378:LYS:HG3	1:C:433:VAL:HG12	1.17	1.10
1:A:1088:HIS:ND1	1:A:1122:VAL:CG1	2.15	1.09
1:B:770:ILE:HD11	1:B:1012:LEU:CD1	1.82	1.09
1:A:353:TRP:HZ2	1:A:465:GLU:O	1.34	1.09
1:C:353:TRP:NE1	1:C:466:ARG:HB3	1.68	1.09
1:C:337:PRO:HD2	1:C:358:ILE:HD11	1.34	1.09
1:C:1089:PHE:O	1:C:1120:THR:HB	1.53	1.09
1:B:615:VAL:HG11	1:B:620:VAL:CG1	1.82	1.09
1:C:360:ASN:HA	1:C:523:THR:HG23	1.33	1.09
1:C:87:ASN:CG	1:C:269:TYR:CD2	2.26	1.09
1:A:303:LEU:HD23	1:A:308:VAL:HG12	1.33	1.08
1:C:502:GLY:O	1:C:506:GLN:HG3	1.53	1.08
1:A:617:CYS:SG	1:A:644:GLN:HB2	1.93	1.08
1:B:599:THR:CG2	1:B:608:VAL:HG11	1.82	1.08
1:C:453:TYR:CD1	1:C:495:TYR:CE1	2.29	1.08
1:C:615:VAL:CG2	1:C:649:CYS:CB	2.31	1.08
1:C:741:TYR:CE1	1:C:966:LEU:HD21	1.88	1.08
1:A:107:GLY:N	1:A:235:ILE:CG2	2.16	1.08
1:A:105:ILE:HG13	1:A:118:LEU:HD13	1.33	1.08
1:C:289:VAL:HG23	1:C:306:PHE:CE2	1.89	1.08
1:A:90:VAL:HG12	1:A:194:PHE:O	1.54	1.08
1:A:552:LEU:HD22	1:A:587:ILE:HD13	1.09	1.08
1:B:57:PRO:HB3	1:B:273:ARG:HH12	0.91	1.08
1:B:599:THR:CG2	1:B:608:VAL:CG1	2.32	1.08
1:C:1102:TRP:HB2	1:C:1135:ASN:OD1	1.53	1.08
1:A:107:GLY:N	1:A:235:ILE:HG22	1.67	1.07
1:B:204:TYR:CE1	1:B:225:PRO:HB3	1.89	1.07
1:C:85:PRO:HG2	1:C:269:TYR:OH	1.54	1.07
1:A:89:GLY:O	1:A:269:TYR:HA	1.53	1.07
1:A:204:TYR:CD1	1:A:225:PRO:HA	1.90	1.07
1:B:1088:HIS:CE1	1:B:1122:VAL:HG23	1.89	1.07
1:C:350:VAL:HG12	1:C:422:ASN:HB3	1.33	1.07
1:A:90:VAL:HG23	1:A:238:PHE:HE2	0.96	1.07
1:C:615:VAL:HG21	1:C:649:CYS:HB3	1.37	1.07
1:B:1039:ARG:NH1	1:B:1042:PHE:CE2	2.22	1.06
1:C:186:PHE:O	1:C:211:ASN:HB3	1.53	1.06
1:C:490:PHE:HE2	1:C:492:LEU:HB2	1.17	1.06
1:C:89:GLY:C	1:C:270:LEU:HD13	1.76	1.06
1:C:581:THR:HG21	1:C:583:GLU:OE2	1.55	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:ARG:NH1	1:C:292:ALA:HB3	1.69	1.06
1:C:748:GLU:OE1	1:C:981:LEU:HG	1.56	1.06
1:B:85:PRO:HG2	1:B:269:TYR:OH	1.56	1.05
1:B:715:PRO:HA	1:B:1071:GLN:O	1.56	1.05
1:A:353:TRP:CD1	1:A:466:ARG:CD	2.39	1.05
1:A:896:ILE:HD13	1:C:712:ILE:HG13	1.32	1.05
1:C:395:VAL:HG21	1:C:524:VAL:HG11	1.33	1.05
1:A:90:VAL:HG11	1:A:194:PHE:HB2	1.37	1.05
1:A:736:VAL:HG22	1:A:858:LEU:HD22	1.37	1.05
1:C:617:CYS:SG	1:C:644:GLN:NE2	2.30	1.05
1:A:620:VAL:HB	1:A:621:PRO:HD3	1.08	1.05
1:A:353:TRP:H	1:A:466:ARG:HD2	1.13	1.05
1:B:1081:ILE:O	1:B:1088:HIS:HB2	1.58	1.04
1:B:204:TYR:HE1	1:B:225:PRO:HB3	1.19	1.04
1:B:718:PHE:CD2	1:B:1067:TYR:CE1	2.45	1.04
1:A:83:VAL:CG2	1:A:237:ARG:HD3	1.85	1.04
1:B:1043:CYS:HB2	1:B:1048:HIS:HD2	1.21	1.04
1:C:1087:ALA:O	1:C:1122:VAL:HG23	1.57	1.04
1:A:1088:HIS:ND1	1:A:1122:VAL:HG13	1.71	1.04
1:C:615:VAL:HG23	1:C:649:CYS:CB	1.87	1.04
1:A:289:VAL:HG23	1:A:306:PHE:CE1	1.92	1.03
1:C:37:TYR:CD1	1:C:55:PHE:HE1	1.75	1.03
1:A:67:ALA:HB3	1:A:263:ALA:HB3	1.40	1.03
1:A:379:CYS:HB2	1:A:384:PRO:HD3	1.40	1.03
1:B:718:PHE:CG	1:B:1067:TYR:HE1	1.76	1.03
1:A:164:ASN:ND2	2:K:1:NAG:O5	1.90	1.03
1:B:318:PHE:HE2	1:B:615:VAL:HG21	1.18	1.03
1:B:615:VAL:CG1	1:B:620:VAL:HG12	1.87	1.03
1:A:742:ILE:CD1	1:A:1001:LEU:HD23	1.88	1.03
1:B:743:CYS:O	1:B:977:LEU:HD12	1.57	1.03
1:B:105:ILE:HG13	1:B:118:LEU:HD13	1.36	1.03
1:B:1102:TRP:HB2	1:B:1135:ASN:HD22	1.19	1.03
1:A:970:PHE:CD2	1:A:999:GLY:HA3	1.92	1.02
1:B:298:GLU:CG	1:B:315:THR:HG21	1.88	1.02
1:C:598:ILE:HD11	1:C:666:ILE:HD12	1.39	1.02
1:C:490:PHE:CE2	1:C:492:LEU:HB2	1.94	1.02
1:C:615:VAL:HG23	1:C:649:CYS:HB2	1.06	1.02
1:A:90:VAL:CG1	1:A:194:PHE:HB2	1.89	1.02
1:A:328:ARG:HH22	1:A:533:LEU:HB2	1.23	1.02
1:B:92:PHE:CZ	1:B:265:TYR:HD2	1.77	1.02
1:C:87:ASN:CG	1:C:269:TYR:HD2	1.61	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:724:THR:HG22	1:B:1063:LEU:HD23	1.38	1.01
1:C:825:LYS:NZ	1:C:942:ALA:CB	2.21	1.01
1:B:298:GLU:HG2	1:B:315:THR:CG2	1.87	1.01
1:C:105:ILE:HG21	1:C:135:PHE:HE2	1.24	1.01
1:C:119:ILE:HG23	1:C:127:VAL:O	1.58	1.01
1:A:204:TYR:HD1	1:A:225:PRO:HA	1.23	1.01
1:B:826:VAL:HG23	1:B:945:LEU:CD1	1.90	1.01
1:C:516:GLU:CG	1:C:519:HIS:NE2	2.22	1.01
1:B:106:PHE:HB3	1:B:235:ILE:CD1	1.91	1.01
1:B:615:VAL:HG11	1:B:620:VAL:HG12	1.01	1.01
1:B:641:ASN:ND2	1:B:654:GLU:OE1	1.92	1.01
1:B:1039:ARG:CZ	1:B:1042:PHE:CD2	2.44	1.01
1:B:1104:VAL:HG11	1:B:1119:ASN:HD22	1.20	1.01
1:A:310:LYS:HG3	1:A:664:ILE:HD11	1.39	1.00
1:B:56:LEU:HD12	1:B:57:PRO:CD	1.90	1.00
1:B:85:PRO:O	1:B:269:TYR:OH	1.79	1.00
1:A:33:THR:CG2	1:A:58:PHE:CD2	2.44	1.00
1:A:107:GLY:HA2	1:A:235:ILE:HG22	1.41	1.00
1:C:105:ILE:HD11	1:C:241:LEU:HD11	1.43	1.00
1:C:118:LEU:HD22	1:C:135:PHE:CE2	1.94	1.00
1:A:353:TRP:CZ2	1:A:465:GLU:O	2.14	1.00
1:A:782:PHE:HE2	1:A:874:THR:CG2	1.75	1.00
1:C:712:ILE:CD1	1:C:1094:VAL:HG11	1.92	1.00
1:A:552:LEU:CD2	1:A:587:ILE:CD1	2.40	1.00
1:A:89:GLY:HA3	1:A:270:LEU:H	0.92	1.00
1:B:57:PRO:CB	1:B:273:ARG:NH1	2.15	1.00
1:B:576:VAL:HG12	1:B:587:ILE:HD11	1.42	1.00
1:A:715:PRO:HA	1:A:1071:GLN:O	1.62	0.99
1:C:321:GLN:OE1	1:C:322:PRO:HD3	1.60	0.99
1:C:454:ARG:CZ	1:C:467:ASP:OD2	2.09	0.99
1:C:726:ILE:HD12	1:C:1061:VAL:HG22	1.39	0.99
1:B:770:ILE:HD11	1:B:1012:LEU:HD12	1.00	0.99
1:C:220:PHE:CE2	1:C:288:ALA:N	2.22	0.99
1:A:90:VAL:CG2	1:A:238:PHE:CE2	2.44	0.99
1:A:620:VAL:HB	1:A:621:PRO:CD	1.91	0.99
1:B:559:PHE:CD1	1:B:584:ILE:HG12	1.98	0.99
1:A:620:VAL:CB	1:A:621:PRO:HD3	1.91	0.99
1:C:328:ARG:CZ	1:C:578:ASP:OD2	2.09	0.99
1:B:1043:CYS:HB2	1:B:1048:HIS:CD2	1.97	0.99
1:A:782:PHE:CE1	1:A:1060:VAL:HG22	1.97	0.99
1:B:107:GLY:N	1:B:235:ILE:HD13	1.78	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:662:CYS:SG	1:C:697:MET:CB	2.50	0.98
1:C:210:ILE:CG1	1:C:212:LEU:HD21	1.91	0.98
1:C:821:LEU:HD21	1:C:939:SER:HB3	1.45	0.98
1:C:429:PHE:HE1	1:C:431:GLY:O	1.47	0.98
1:A:885:GLY:CA	1:A:901:GLN:NE2	2.27	0.98
1:C:186:PHE:O	1:C:211:ASN:CB	2.11	0.98
1:C:378:LYS:HG2	1:C:433:VAL:HG12	1.44	0.98
1:C:223:LEU:N	1:C:223:LEU:HD23	1.78	0.98
1:C:612:TYR:O	1:C:615:VAL:HG22	1.64	0.98
1:A:89:GLY:CA	1:A:270:LEU:H	1.77	0.98
1:B:1102:TRP:HB2	1:B:1135:ASN:ND2	1.79	0.98
1:A:353:TRP:CZ2	1:A:465:GLU:C	2.36	0.97
1:B:533:LEU:HD11	1:B:552:LEU:HD13	1.46	0.97
1:C:220:PHE:CE2	1:C:287:ASP:HA	1.98	0.97
1:B:1081:ILE:HD12	1:B:1133:VAL:HG23	1.45	0.97
1:B:815:ARG:NH1	1:B:823:PHE:CE2	2.31	0.97
1:A:564:GLN:OE1	1:A:577:ARG:HD2	1.64	0.97
1:B:1088:HIS:HD2	1:B:1137:VAL:HG11	1.03	0.97
1:A:1102:TRP:HB2	1:A:1135:ASN:HD21	1.05	0.97
1:B:770:ILE:CD1	1:B:1012:LEU:HD12	1.95	0.97
1:C:378:LYS:HG2	1:C:433:VAL:CG1	1.93	0.96
1:C:472:ILE:HD11	1:C:482:GLY:H	1.30	0.96
1:C:220:PHE:HZ	1:C:288:ALA:CA	1.78	0.96
1:C:612:TYR:HB2	1:C:615:VAL:CG1	1.96	0.96
1:A:107:GLY:CA	1:A:235:ILE:CG2	2.44	0.96
1:A:324:GLU:O	1:A:539:VAL:HB	1.65	0.96
1:C:473:TYR:N	1:C:489:TYR:O	1.98	0.96
1:B:718:PHE:CD2	1:B:1067:TYR:HE1	1.83	0.96
1:A:797:PHE:HE1	1:A:882:ILE:HG22	1.30	0.96
1:A:1081:ILE:HG21	1:A:1135:ASN:HB3	1.44	0.96
1:C:350:VAL:CG1	1:C:422:ASN:HB3	1.95	0.96
1:A:204:TYR:HE1	1:A:225:PRO:HB3	1.31	0.96
1:C:33:THR:CG2	1:C:58:PHE:HE2	1.78	0.96
1:A:718:PHE:CD2	1:A:1109:PHE:HE2	1.84	0.96
1:A:101:ILE:HD11	1:A:263:ALA:HB1	1.44	0.96
1:A:64:TRP:CD1	1:A:266:TYR:CE2	2.54	0.95
1:B:784:GLN:HA	1:B:784:GLN:HE21	1.28	0.95
1:B:1080:ALA:O	1:B:1132:ILE:HG13	1.63	0.95
1:C:392:PHE:CE2	1:C:515:PHE:CZ	2.32	0.95
1:B:641:ASN:ND2	1:B:654:GLU:HA	1.80	0.95
1:C:392:PHE:HE2	1:C:515:PHE:CZ	1.49	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:726:ILE:CD1	1:C:1061:VAL:HG22	1.95	0.95
1:C:360:ASN:HA	1:C:523:THR:HG21	1.46	0.95
1:A:107:GLY:H	1:A:235:ILE:CG2	1.78	0.95
1:A:204:TYR:CE1	1:A:225:PRO:HB3	2.00	0.95
1:A:712:ILE:HB	1:A:1077:THR:HG21	1.47	0.95
1:C:328:ARG:HE	1:C:578:ASP:CG	1.70	0.95
1:B:57:PRO:CA	1:B:273:ARG:HH12	1.78	0.95
1:B:329:PHE:HB3	1:B:330:PRO:HD2	1.49	0.95
1:A:1084:ASP:HB2	1:A:1086:LYS:NZ	1.82	0.94
1:B:615:VAL:CG1	1:B:620:VAL:CG1	2.45	0.94
1:C:878:LEU:CD2	1:C:1053:PRO:HD2	1.97	0.94
1:B:96:GLU:OE1	1:B:101:ILE:N	2.00	0.94
1:B:119:ILE:HG12	1:B:128:ILE:HG12	1.48	0.94
1:A:278:LYS:HB2	1:A:306:PHE:CE2	2.02	0.94
1:C:33:THR:CG2	1:C:58:PHE:CE2	2.50	0.94
1:B:822:LEU:HD21	1:B:1061:VAL:HG21	1.47	0.94
1:A:96:GLU:OE1	1:A:101:ILE:N	1.99	0.94
1:A:743:CYS:SG	1:A:750:SER:N	2.40	0.94
1:C:33:THR:HG22	1:C:58:PHE:CD2	2.03	0.94
1:C:1095:PHE:CZ	1:C:1120:THR:HG21	2.02	0.94
1:C:856:ASN:O	1:C:858:LEU:HD13	1.66	0.94
1:B:322:PRO:CG	1:B:540:ASN:OD1	2.14	0.94
1:C:393:THR:CG2	1:C:522:ALA:CB	2.46	0.94
1:C:598:ILE:HD11	1:C:666:ILE:HD11	1.49	0.94
1:A:731:MET:HB2	1:A:955:ASN:HD21	1.32	0.93
1:C:220:PHE:HZ	1:C:288:ALA:N	1.56	0.93
1:C:360:ASN:CA	1:C:523:THR:HG23	1.98	0.93
1:A:822:LEU:HD22	1:A:945:LEU:HD21	1.49	0.93
1:B:91:TYR:CE1	1:B:93:ALA:HB2	2.03	0.93
1:C:581:THR:HG22	1:C:583:GLU:HG3	1.50	0.93
1:A:89:GLY:CA	1:A:270:LEU:HB2	1.97	0.93
1:A:308:VAL:N	1:A:602:THR:HG21	1.84	0.93
1:C:231:ILE:H	1:C:231:ILE:HD12	1.33	0.93
1:A:53:ASP:O	1:A:55:PHE:CE2	2.21	0.93
1:A:89:GLY:CA	1:A:270:LEU:CB	2.47	0.93
1:C:392:PHE:O	1:C:524:VAL:HB	1.68	0.93
1:C:289:VAL:CG2	1:C:306:PHE:CE2	2.52	0.93
1:C:289:VAL:CG2	1:C:306:PHE:CZ	2.51	0.93
1:C:495:TYR:HD2	1:C:497:PHE:HE2	1.13	0.93
1:B:106:PHE:HB3	1:B:235:ILE:HD13	1.48	0.93
1:B:906:PHE:CD2	1:B:916:LEU:HB2	2.03	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:374:PHE:HD2	1:C:436:TRP:CD1	1.86	0.93
1:B:1039:ARG:CZ	1:B:1042:PHE:HE2	1.74	0.93
1:C:210:ILE:CB	1:C:212:LEU:HD21	1.99	0.93
1:A:322:PRO:HG2	1:A:540:ASN:OD1	1.67	0.93
1:C:87:ASN:ND2	1:C:269:TYR:CD2	2.37	0.93
1:C:128:ILE:HG22	1:C:129:LYS:N	1.83	0.93
1:B:543:PHE:HE2	1:B:578:ASP:HB3	1.32	0.92
1:C:87:ASN:OD1	1:C:269:TYR:HE2	1.36	0.92
1:C:102:ARG:HD2	1:C:141:LEU:HD13	1.51	0.92
1:C:905:ARG:HE	1:C:1050:MET:HE2	1.33	0.92
1:C:342:PHE:HE1	1:C:511:VAL:HG11	1.33	0.92
1:C:33:THR:HG22	1:C:58:PHE:HE2	1.13	0.92
1:C:655:HIS:HB2	1:C:694:ALA:O	1.67	0.92
1:C:378:LYS:HD2	1:C:433:VAL:HG11	1.52	0.92
1:C:380:TYR:CE2	1:C:412:PRO:CD	2.52	0.92
1:A:310:LYS:CB	1:A:600:PRO:O	2.16	0.92
1:A:718:PHE:HD2	1:A:1109:PHE:HE2	1.16	0.92
1:A:885:GLY:HA2	1:A:901:GLN:HE22	1.28	0.92
1:C:102:ARG:CD	1:C:141:LEU:HD13	2.00	0.92
1:A:736:VAL:HG22	1:A:858:LEU:CD2	2.00	0.92
1:A:89:GLY:HA2	1:A:270:LEU:HB2	1.50	0.92
1:A:896:ILE:CD1	1:C:712:ILE:HG13	1.99	0.92
1:A:33:THR:CB	1:A:58:PHE:CE2	2.53	0.92
1:A:83:VAL:HG21	1:A:237:ARG:HD2	0.92	0.92
1:A:598:ILE:HG23	1:A:664:ILE:HG21	1.51	0.91
1:A:617:CYS:HA	1:A:649:CYS:SG	2.11	0.91
1:C:203:ILE:CG2	1:C:227:VAL:HG22	2.00	0.91
1:C:615:VAL:HG21	1:C:649:CYS:CB	1.97	0.91
1:A:452:LEU:CD1	1:A:493:GLN:O	2.18	0.91
1:B:725:GLU:OE1	1:B:1028:LYS:NZ	2.01	0.91
1:C:380:TYR:HE2	1:C:412:PRO:CD	1.83	0.91
1:C:490:PHE:CE2	1:C:492:LEU:HD23	2.05	0.91
1:A:278:LYS:HB2	1:A:306:PHE:HE2	1.34	0.91
1:B:1072:GLU:HG2	1:C:894:LEU:CD2	2.00	0.91
1:C:100:ILE:HD12	1:C:243:ALA:O	1.70	0.91
1:C:393:THR:HG23	1:C:522:ALA:CB	2.00	0.91
1:C:347:PHE:CD1	1:C:509:ARG:NH1	2.39	0.91
1:C:497:PHE:HD1	1:C:507:PRO:HD3	1.35	0.91
1:A:976:VAL:HG13	1:A:979:ASP:HB3	1.51	0.91
1:A:1096:VAL:HG21	1:A:1105:THR:HG22	1.48	0.91
1:A:231:ILE:HG22	1:A:233:ILE:H	1.34	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:970:PHE:CD2	1:C:999:GLY:CA	2.53	0.91
1:B:1095:PHE:CZ	1:B:1120:THR:HG21	2.06	0.91
1:C:367:VAL:HG23	1:C:368:LEU:HD12	1.53	0.91
1:C:404:GLY:HA2	1:C:508:TYR:HD2	1.34	0.91
1:C:107:GLY:O	1:C:235:ILE:HG23	1.71	0.91
1:C:970:PHE:HD2	1:C:999:GLY:HA3	1.06	0.91
1:C:1089:PHE:O	1:C:1120:THR:CB	2.17	0.91
1:A:330:PRO:HA	1:A:580:GLN:HE22	1.35	0.90
1:B:318:PHE:CE2	1:B:615:VAL:HG21	2.05	0.90
1:B:718:PHE:HD2	1:B:1067:TYR:CE1	1.84	0.90
1:B:1080:ALA:HB2	1:B:1089:PHE:CE1	2.07	0.90
1:C:825:LYS:HZ1	1:C:942:ALA:HB2	0.85	0.90
1:A:241:LEU:HD12	1:A:242:LEU:N	1.87	0.90
1:C:37:TYR:HE1	1:C:55:PHE:CD1	1.89	0.90
1:A:89:GLY:HA2	1:A:270:LEU:CB	2.01	0.90
1:A:736:VAL:CG2	1:A:858:LEU:HD22	1.99	0.90
1:B:773:GLU:OE2	1:B:1019:ARG:NH1	2.04	0.90
1:A:308:VAL:H	1:A:602:THR:HG21	1.35	0.90
1:A:552:LEU:CD2	1:A:587:ILE:HD13	1.97	0.90
1:B:1039:ARG:NH2	1:B:1042:PHE:HE2	1.70	0.90
1:A:128:ILE:HG22	1:A:129:LYS:N	1.86	0.90
1:B:826:VAL:HG13	1:B:949:GLN:OE1	1.71	0.90
1:C:366:SER:O	1:C:370:ASN:N	2.04	0.90
1:A:89:GLY:HA3	1:A:270:LEU:CA	2.00	0.90
1:A:204:TYR:HD1	1:A:225:PRO:CA	1.84	0.90
1:A:1087:ALA:HB2	1:A:1126:CYS:HB3	1.50	0.90
1:C:1090:PRO:HA	1:C:1120:THR:HG22	0.91	0.90
1:C:210:ILE:HB	1:C:212:LEU:HD21	1.50	0.90
1:A:453:TYR:CE2	1:A:493:GLN:CG	2.55	0.90
1:A:673:SER:O	1:A:693:ILE:HD13	1.72	0.90
1:A:119:ILE:HG12	1:A:128:ILE:HG12	1.52	0.90
1:A:353:TRP:H	1:A:466:ARG:CD	1.85	0.90
1:A:896:ILE:HD13	1:C:712:ILE:CG1	2.01	0.89
1:C:220:PHE:HZ	1:C:288:ALA:CB	1.83	0.89
1:C:970:PHE:HE2	1:C:999:GLY:C	1.75	0.89
1:A:805:ILE:O	1:A:816:SER:OG	1.90	0.89
1:A:541:PHE:CE2	1:A:587:ILE:HD12	2.07	0.89
1:B:190:ARG:HE	1:B:207:HIS:CE1	1.89	0.89
1:A:34:ARG:HH12	1:A:217:PRO:CG	1.79	0.89
1:B:128:ILE:HG22	1:B:129:LYS:N	1.87	0.89
1:B:599:THR:HG22	1:B:608:VAL:HG12	1.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:SER:O	1:C:370:ASN:CB	2.21	0.89
1:C:1082:CYS:HG	1:C:1126:CYS:HG	0.91	0.89
1:C:1095:PHE:HZ	1:C:1120:THR:HG21	1.38	0.89
1:A:89:GLY:HA2	1:A:270:LEU:CG	2.03	0.89
1:C:971:GLY:O	1:C:995:ARG:HD2	1.73	0.89
1:A:105:ILE:HG13	1:A:118:LEU:CD1	2.02	0.89
1:A:729:VAL:HG21	1:A:1060:VAL:HG23	1.54	0.89
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.53	0.89
1:A:64:TRP:HD1	1:A:266:TYR:CD2	1.87	0.89
1:C:456:PHE:HB3	1:C:473:TYR:CD1	2.07	0.89
1:B:906:PHE:CE2	1:B:916:LEU:HB2	2.08	0.88
1:B:559:PHE:CE1	1:B:584:ILE:HG21	2.08	0.88
1:C:612:TYR:CB	1:C:615:VAL:CG1	2.51	0.88
1:A:742:ILE:HD13	1:A:1001:LEU:CD2	2.02	0.88
1:B:53:ASP:HB3	1:B:55:PHE:CE2	2.09	0.88
1:B:885:GLY:HA2	1:B:901:GLN:HE21	1.14	0.88
1:C:107:GLY:H	1:C:235:ILE:HG23	1.38	0.88
1:C:365:TYR:HA	1:C:368:LEU:HD13	1.56	0.88
1:A:328:ARG:HD3	1:A:531:THR:O	1.73	0.88
1:B:105:ILE:HG13	1:B:118:LEU:CD1	2.02	0.88
1:B:324:GLU:O	1:B:539:VAL:CG2	2.21	0.88
1:B:767:LEU:HD21	1:B:1008:VAL:HG22	1.55	0.88
1:C:611:LEU:HB2	1:C:650:LEU:HD13	1.55	0.88
1:B:1039:ARG:NH2	1:B:1042:PHE:CE2	2.41	0.88
1:B:718:PHE:HZ	1:B:923:ILE:HD11	1.39	0.88
1:B:776:LYS:HZ2	1:B:780:GLU:HG2	1.39	0.88
1:B:574:ASP:O	1:B:587:ILE:HB	1.74	0.88
1:C:89:GLY:C	1:C:270:LEU:CD1	2.41	0.88
1:C:115:GLN:O	1:C:233:ILE:HD11	1.73	0.88
1:C:119:ILE:CG1	1:C:128:ILE:HG12	2.04	0.88
1:C:495:TYR:HD2	1:C:497:PHE:CE2	1.91	0.88
1:A:742:ILE:HD13	1:A:1001:LEU:HD23	1.56	0.87
1:B:738:CYS:SG	1:B:760:CYS:O	2.31	0.87
1:A:420:ASP:HB3	1:A:460:ASN:OD1	1.74	0.87
1:C:490:PHE:HE2	1:C:492:LEU:CB	1.87	0.87
1:C:763:LEU:HD13	1:C:1004:LEU:HD22	1.56	0.87
1:C:712:ILE:HD13	1:C:1094:VAL:HG11	1.53	0.87
1:A:204:TYR:CD1	1:A:225:PRO:CA	2.57	0.87
1:B:1079:PRO:HG2	1:B:1131:GLY:O	1.74	0.87
1:C:290:ASP:O	1:C:297:SER:HB3	1.74	0.87
1:A:1080:ALA:O	1:A:1132:ILE:HG13	1.75	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:815:ARG:NH1	1:B:823:PHE:CD2	2.40	0.87
1:C:105:ILE:HG21	1:C:135:PHE:CE2	2.09	0.87
1:C:383:SER:HB3	1:C:386:LYS:HB2	1.56	0.87
1:C:395:VAL:CG2	1:C:524:VAL:HG11	2.04	0.87
1:A:718:PHE:HD2	1:A:1109:PHE:CE2	1.91	0.87
1:C:503:VAL:HA	1:C:506:GLN:CD	1.95	0.87
1:C:748:GLU:HG3	1:C:981:LEU:HD21	1.57	0.86
1:A:379:CYS:CB	1:A:384:PRO:HD3	2.04	0.86
1:C:336:CYS:SG	1:C:361:CYS:C	2.53	0.86
1:B:204:TYR:CD1	1:B:225:PRO:HA	2.10	0.86
1:C:612:TYR:CB	1:C:615:VAL:HG13	2.05	0.86
1:B:815:ARG:NH1	1:B:823:PHE:CZ	2.43	0.86
1:C:756:TYR:HB3	1:C:759:PHE:CD2	2.11	0.86
1:A:90:VAL:CG1	1:A:194:PHE:O	2.23	0.86
1:A:642:VAL:HG13	1:A:651:ILE:HG12	1.55	0.86
1:A:1102:TRP:CB	1:A:1135:ASN:ND2	2.37	0.86
1:B:800:PHE:HD2	1:B:927:PHE:CD2	1.93	0.86
1:C:342:PHE:CE1	1:C:511:VAL:HG11	2.10	0.86
1:C:392:PHE:HE2	1:C:515:PHE:CE1	1.93	0.86
1:B:719:THR:CG2	1:B:1070:ALA:HB2	2.06	0.86
1:B:1095:PHE:HZ	1:B:1120:THR:HG21	1.41	0.86
1:B:970:PHE:CD2	1:B:999:GLY:HA3	2.11	0.86
1:A:453:TYR:CZ	1:A:493:GLN:HG3	2.10	0.85
1:A:104:TRP:O	1:A:118:LEU:HD12	1.76	0.85
1:B:57:PRO:HB3	1:B:273:ARG:CZ	2.06	0.85
1:A:782:PHE:CE2	1:A:874:THR:CG2	2.59	0.85
1:C:350:VAL:HG12	1:C:422:ASN:CB	2.06	0.85
1:C:433:VAL:HG23	1:C:512:VAL:HG22	1.58	0.85
1:C:128:ILE:CG2	1:C:129:LYS:N	2.40	0.85
1:C:210:ILE:HB	1:C:212:LEU:CD2	2.06	0.85
1:C:1081:ILE:O	1:C:1088:HIS:HB2	1.77	0.85
1:A:724:THR:CG2	1:A:1063:LEU:HD23	2.06	0.85
1:B:89:GLY:C	1:B:270:LEU:CD1	2.45	0.85
1:A:66:HIS:HD2	1:A:68:ILE:CG2	1.90	0.85
1:A:742:ILE:HD11	1:A:1001:LEU:HD23	1.55	0.85
1:C:878:LEU:HD23	1:C:1053:PRO:HD2	1.57	0.85
1:C:825:LYS:HZ1	1:C:942:ALA:CB	1.81	0.85
1:C:748:GLU:CD	1:C:981:LEU:HG	1.97	0.84
1:A:43:PHE:HE2	1:A:282:ASN:O	1.59	0.84
1:A:895:GLN:NE2	1:C:713:ALA:HB2	1.91	0.84
1:B:37:TYR:OH	1:B:195:LYS:NZ	2.10	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:TRP:O	1:B:118:LEU:HD12	1.77	0.84
1:C:220:PHE:CZ	1:C:288:ALA:CB	2.60	0.84
1:C:328:ARG:NH2	1:C:578:ASP:OD2	2.10	0.84
1:C:429:PHE:CE1	1:C:431:GLY:N	2.43	0.84
1:B:1090:PRO:HA	1:B:1120:THR:HG22	1.57	0.84
1:C:1115:ILE:HD12	1:C:1115:ILE:H	1.42	0.84
1:B:1081:ILE:HD12	1:B:1133:VAL:CG2	2.07	0.84
1:B:675:GLN:HE21	1:B:675:GLN:HA	1.41	0.84
1:C:916:LEU:HD13	1:C:923:ILE:CD1	2.08	0.84
1:C:921:LYS:HA	1:C:921:LYS:CE	2.08	0.84
1:A:724:THR:HG22	1:A:1063:LEU:CD2	2.06	0.84
1:A:1088:HIS:CE1	1:A:1122:VAL:CG1	2.61	0.84
1:B:599:THR:HG22	1:B:608:VAL:CB	2.06	0.84
1:B:275:PHE:CD1	1:B:290:ASP:HA	2.13	0.84
1:A:712:ILE:HB	1:A:1077:THR:CG2	2.07	0.83
1:C:393:THR:CG2	1:C:522:ALA:HB2	2.08	0.83
1:C:426:PRO:HG2	1:C:464:PHE:CD2	2.12	0.83
1:C:741:TYR:CZ	1:C:966:LEU:HD21	2.13	0.83
1:A:34:ARG:NH2	1:A:217:PRO:HG2	1.93	0.83
1:B:713:ALA:HA	1:B:1073:LYS:O	1.78	0.83
1:A:308:VAL:H	1:A:602:THR:CG2	1.89	0.83
1:A:815:ARG:NH1	1:A:823:PHE:CD1	2.45	0.83
1:A:895:GLN:OE1	1:A:895:GLN:N	2.11	0.83
1:C:599:THR:HB	1:C:608:VAL:HG12	1.60	0.83
1:A:92:PHE:CE1	1:A:94:SER:HB3	2.13	0.83
1:B:719:THR:HG23	1:B:1070:ALA:HB2	1.59	0.83
1:C:612:TYR:HB3	1:C:615:VAL:HG13	1.60	0.83
1:C:452:LEU:HD23	1:C:492:LEU:HB3	1.58	0.83
1:A:620:VAL:HG23	1:A:621:PRO:HD2	1.61	0.83
1:B:107:GLY:H	1:B:235:ILE:CG2	1.90	0.83
1:C:495:TYR:CD2	1:C:497:PHE:CE2	2.67	0.83
1:C:972:ALA:HB3	1:C:996:LEU:HD11	1.57	0.83
1:A:620:VAL:CB	1:A:621:PRO:CD	2.55	0.83
1:C:328:ARG:NH2	1:C:581:THR:OG1	2.12	0.83
1:C:350:VAL:CG1	1:C:422:ASN:CB	2.56	0.83
1:A:391:CYS:HA	1:A:525:CYS:HB3	1.59	0.83
1:B:715:PRO:CA	1:B:1071:GLN:O	2.27	0.83
1:B:718:PHE:HB2	1:B:1067:TYR:CZ	2.12	0.83
1:C:210:ILE:C	1:C:212:LEU:HD22	1.98	0.83
1:C:581:THR:HG21	1:C:583:GLU:CD	1.98	0.83
1:A:31:SER:CB	1:A:216:LEU:HD22	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:VAL:CG2	1:A:238:PHE:HE2	1.82	0.82
1:A:107:GLY:C	1:A:235:ILE:HG22	1.99	0.82
1:A:290:ASP:O	1:A:297:SER:HB3	1.79	0.82
1:A:1096:VAL:CG2	1:A:1105:THR:HG22	2.09	0.82
1:B:726:ILE:HD12	1:B:1061:VAL:HG22	1.61	0.82
1:B:885:GLY:CA	1:B:901:GLN:HE21	1.91	0.82
1:C:1103:PHE:HE1	1:C:1114:ILE:CD1	1.92	0.82
1:B:327:VAL:HG11	1:B:529:LYS:O	1.78	0.82
1:B:805:ILE:HG22	1:B:878:LEU:HD13	1.61	0.82
1:C:273:ARG:NH1	1:C:292:ALA:CB	2.41	0.82
1:C:273:ARG:HH11	1:C:292:ALA:HB3	1.43	0.82
1:B:204:TYR:HD1	1:B:225:PRO:HA	1.42	0.82
1:C:87:ASN:CG	1:C:269:TYR:CE2	2.50	0.82
1:A:128:ILE:CG2	1:A:129:LYS:N	2.42	0.82
1:C:393:THR:HG23	1:C:522:ALA:HB1	1.57	0.82
1:C:204:TYR:CD1	1:C:225:PRO:HB3	2.14	0.82
1:C:326:ILE:HG21	1:C:534:VAL:HG12	1.62	0.82
1:A:985:ASP:OD1	1:A:986:PRO:CD	2.26	0.82
1:B:1142:GLN:HA	1:B:1142:GLN:HE21	1.42	0.82
1:A:299:THR:OG1	1:A:597:VAL:CG2	2.27	0.82
1:C:773:GLU:OE2	1:C:1019:ARG:HD2	1.80	0.82
1:C:105:ILE:HG13	1:C:118:LEU:HD13	1.59	0.82
1:C:429:PHE:CE1	1:C:431:GLY:O	2.32	0.82
1:A:353:TRP:CE2	1:A:466:ARG:HB2	2.14	0.82
1:A:357:ARG:HG2	1:A:357:ARG:HH11	1.44	0.82
1:C:1102:TRP:O	1:C:1115:ILE:CD1	2.28	0.82
1:A:353:TRP:CD2	1:A:466:ARG:HD3	2.15	0.82
1:B:885:GLY:CA	1:B:901:GLN:NE2	2.39	0.82
1:C:581:THR:CG2	1:C:583:GLU:OE2	2.27	0.82
1:C:612:TYR:HB2	1:C:615:VAL:HG11	1.61	0.82
1:A:55:PHE:HB3	1:A:275:PHE:CE2	2.15	0.81
1:A:600:PRO:HD3	1:A:692:ILE:HD11	1.61	0.81
1:A:985:ASP:OD1	1:A:986:PRO:HD2	1.80	0.81
1:B:1088:HIS:ND1	1:B:1122:VAL:HG23	1.93	0.81
1:C:555:SER:OG	1:C:584:ILE:HG22	1.79	0.81
1:C:353:TRP:HE1	1:C:466:ARG:HB3	1.45	0.81
1:C:970:PHE:CE2	1:C:999:GLY:C	2.53	0.81
1:A:31:SER:HB2	1:A:216:LEU:HD22	1.61	0.81
1:A:350:VAL:HG12	1:A:452:LEU:O	1.79	0.81
1:A:675:GLN:HA	1:A:675:GLN:HE21	1.45	0.81
1:B:128:ILE:CG2	1:B:129:LYS:N	2.43	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:ASN:HD22	1:C:737:ASP:HB2	1.46	0.81
1:A:782:PHE:HE1	1:A:1060:VAL:HG22	1.45	0.81
1:B:902:MET:HB3	1:B:916:LEU:HD21	1.62	0.81
1:C:48:LEU:HD12	1:C:48:LEU:H	1.44	0.81
1:C:330:PRO:HD3	1:C:544:ASN:HD21	1.45	0.81
1:C:1102:TRP:O	1:C:1115:ILE:HD11	1.80	0.81
1:A:1078:ALA:N	1:A:1102:TRP:HH2	1.78	0.81
1:C:128:ILE:O	1:C:129:LYS:HG2	1.81	0.81
1:C:456:PHE:CB	1:C:473:TYR:CD1	2.64	0.81
1:C:497:PHE:CD1	1:C:507:PRO:HD3	2.15	0.81
1:C:128:ILE:CG2	1:C:129:LYS:H	1.93	0.81
1:C:970:PHE:CE2	1:C:999:GLY:CA	2.63	0.81
1:B:617:CYS:HG	1:B:649:CYS:HG	0.83	0.81
1:C:393:THR:CB	1:C:522:ALA:HB2	2.11	0.81
1:C:970:PHE:HE2	1:C:999:GLY:O	1.64	0.81
1:A:308:VAL:HG22	1:A:602:THR:HB	1.61	0.81
1:C:825:LYS:CE	1:C:942:ALA:HB2	2.11	0.81
1:C:905:ARG:HD3	1:C:1049:LEU:O	1.81	0.81
1:C:922:LEU:HD11	1:C:926:GLN:HE21	1.44	0.81
1:A:984:LEU:HD13	1:A:988:GLU:HG3	1.64	0.80
1:C:340:GLU:OE2	1:C:356:LYS:NZ	2.14	0.80
1:A:825:LYS:HB2	1:A:945:LEU:CD1	2.11	0.80
1:C:85:PRO:HG2	1:C:269:TYR:HH	1.45	0.80
1:C:105:ILE:HG13	1:C:118:LEU:CD1	2.11	0.80
1:C:931:ILE:O	1:C:934:ILE:HG23	1.81	0.80
1:A:33:THR:HB	1:A:58:PHE:CE2	2.17	0.80
1:C:203:ILE:CG2	1:C:227:VAL:CG2	2.59	0.80
1:C:1031:GLU:O	1:C:1035:GLY:O	2.00	0.80
1:C:119:ILE:HG12	1:C:128:ILE:HG12	1.62	0.80
1:C:654:GLU:OE1	1:C:654:GLU:N	2.14	0.80
1:B:1116:THR:HG22	1:B:1140:PRO:HD3	1.63	0.80
1:A:1088:HIS:CE1	1:A:1122:VAL:HG11	2.17	0.80
1:C:118:LEU:HD23	1:C:135:PHE:CZ	2.14	0.80
1:C:36:VAL:C	1:C:223:LEU:HD21	2.02	0.80
1:C:393:THR:CB	1:C:522:ALA:CB	2.59	0.79
1:A:118:LEU:CD2	1:A:135:PHE:CZ	2.62	0.79
1:A:954:GLN:HG2	1:A:1014:ARG:NH1	1.97	0.79
1:B:563:GLN:NE2	1:C:43:PHE:HB2	1.97	0.79
1:A:107:GLY:N	1:A:235:ILE:HG21	1.95	0.79
1:C:324:GLU:O	1:C:539:VAL:HB	1.82	0.79
1:C:462:LYS:HA	1:C:462:LYS:CE	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:LEU:CD2	1:C:135:PHE:HZ	1.60	0.79
1:A:353:TRP:CZ2	1:A:466:ARG:HB2	2.16	0.79
1:C:1033:VAL:CG2	1:C:1062:PHE:HE1	1.95	0.79
1:A:403:ARG:HG3	1:A:495:TYR:OH	1.83	0.79
1:C:34:ARG:CZ	1:C:221:SER:OG	2.30	0.79
1:A:106:PHE:HZ	1:A:194:PHE:CD2	2.01	0.79
1:B:555:SER:CB	1:B:586:ASP:OD1	2.30	0.79
1:B:555:SER:HB2	1:B:586:ASP:OD1	1.83	0.79
1:C:611:LEU:HB2	1:C:650:LEU:CD1	2.12	0.79
1:B:546:LEU:HD22	1:B:565:PHE:CE2	2.17	0.78
1:B:597:VAL:HG22	1:B:610:VAL:HG12	1.65	0.78
1:B:718:PHE:CZ	1:B:923:ILE:HD11	2.18	0.78
1:C:791:THR:HG22	1:C:792:PRO:HD2	1.65	0.78
1:A:453:TYR:CZ	1:A:493:GLN:CG	2.67	0.78
1:B:576:VAL:CG1	1:B:587:ILE:HD11	2.13	0.78
1:B:1088:HIS:CE1	1:B:1122:VAL:CG2	2.64	0.78
1:C:380:TYR:HE2	1:C:412:PRO:HD3	1.47	0.78
1:A:235:ILE:H	1:A:235:ILE:HD12	1.46	0.78
1:C:599:THR:CB	1:C:608:VAL:HG12	2.12	0.78
1:A:552:LEU:HD22	1:A:587:ILE:HD11	1.60	0.78
1:A:697:MET:CE	1:B:869:MET:SD	2.71	0.78
1:A:718:PHE:CD2	1:A:1109:PHE:CE2	2.68	0.78
1:B:800:PHE:CD2	1:B:927:PHE:HD2	2.02	0.78
1:A:89:GLY:CA	1:A:270:LEU:N	2.34	0.78
1:A:885:GLY:HA2	1:A:901:GLN:CD	2.03	0.78
1:B:106:PHE:HZ	1:B:194:PHE:CD2	2.01	0.78
1:B:324:GLU:O	1:B:539:VAL:HG22	1.83	0.78
1:B:324:GLU:O	1:B:539:VAL:HG23	1.83	0.78
1:C:692:ILE:HD12	1:C:692:ILE:H	1.49	0.78
1:A:970:PHE:HE1	1:B:756:TYR:O	1.66	0.78
1:B:763:LEU:HD22	1:B:1008:VAL:HG21	1.65	0.78
1:C:203:ILE:HG21	1:C:227:VAL:HG22	1.63	0.78
1:C:220:PHE:CZ	1:C:288:ALA:HB3	2.17	0.78
1:C:456:PHE:CB	1:C:473:TYR:CE1	2.61	0.78
1:C:517:LEU:H	1:C:517:LEU:HD12	1.49	0.78
1:C:970:PHE:CE2	1:C:999:GLY:HA3	2.17	0.78
1:B:190:ARG:HE	1:B:207:HIS:HE1	1.28	0.78
1:C:1072:GLU:OE1	1:C:1072:GLU:N	2.17	0.78
1:A:328:ARG:HH22	1:A:533:LEU:CB	1.97	0.78
1:A:570:ALA:HB1	1:B:963:VAL:HG11	1.64	0.78
1:C:210:ILE:O	1:C:212:LEU:CD2	2.32	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:374:PHE:CD2	1:C:436:TRP:CD1	2.72	0.78
1:C:36:VAL:O	1:C:223:LEU:HD23	1.82	0.77
1:C:360:ASN:CA	1:C:523:THR:CG2	2.55	0.77
1:A:89:GLY:HA3	1:A:270:LEU:CB	2.13	0.77
1:A:617:CYS:SG	1:A:644:GLN:CB	2.72	0.77
1:B:118:LEU:CD2	1:B:135:PHE:CZ	2.62	0.77
1:B:736:VAL:HG13	1:B:858:LEU:HD23	1.65	0.77
1:C:726:ILE:HD12	1:C:1061:VAL:CG2	2.13	0.77
1:A:85:PRO:HG2	1:A:269:TYR:OH	1.83	0.77
1:B:1080:ALA:HB2	1:B:1089:PHE:HE1	1.46	0.77
1:A:85:PRO:O	1:A:269:TYR:OH	2.01	0.77
1:A:712:ILE:CD1	1:A:1094:VAL:HG21	2.15	0.77
1:B:767:LEU:CD2	1:B:1008:VAL:HG22	2.15	0.77
1:A:557:LYS:NZ	1:A:574:ASP:OD2	2.17	0.77
1:B:351:TYR:HB3	1:B:422:ASN:ND2	2.00	0.77
1:A:743:CYS:SG	1:A:749:CYS:O	2.42	0.77
1:C:878:LEU:HD21	1:C:1053:PRO:HD2	1.66	0.77
1:A:203:ILE:HG22	1:A:227:VAL:HG23	1.65	0.77
1:B:200:TYR:HB3	1:B:230:PRO:HA	1.67	0.77
1:B:107:GLY:O	1:B:235:ILE:CG2	2.29	0.77
1:B:902:MET:HB3	1:B:916:LEU:CD2	2.15	0.77
1:C:118:LEU:CD2	1:C:135:PHE:CE1	2.67	0.77
1:C:203:ILE:HG22	1:C:227:VAL:CG2	2.15	0.77
1:A:353:TRP:NE1	1:A:466:ARG:HD3	1.98	0.76
1:A:742:ILE:CD1	1:A:1001:LEU:CD2	2.61	0.76
1:A:1048:HIS:ND1	1:A:1048:HIS:O	2.19	0.76
1:B:351:TYR:HB3	1:B:422:ASN:HD22	1.51	0.76
1:C:495:TYR:CD2	1:C:497:PHE:HE2	1.99	0.76
1:C:729:VAL:H	1:C:1059:GLY:HA2	1.49	0.76
1:A:321:GLN:HA	1:A:321:GLN:HE21	1.50	0.76
1:A:1089:PHE:HB2	1:A:1121:PHE:CE1	2.20	0.76
1:B:746:SER:O	1:B:749:CYS:SG	2.42	0.76
1:B:1089:PHE:O	1:B:1120:THR:HB	1.85	0.76
1:C:105:ILE:CG2	1:C:135:PHE:HE2	1.95	0.76
1:B:743:CYS:SG	1:B:749:CYS:C	2.63	0.76
1:B:725:GLU:CD	1:B:1028:LYS:NZ	2.39	0.76
1:B:1088:HIS:CD2	1:B:1137:VAL:CG1	2.61	0.76
1:A:308:VAL:N	1:A:602:THR:CG2	2.48	0.76
1:A:403:ARG:CG	1:A:495:TYR:CE1	2.68	0.76
1:A:1081:ILE:CG2	1:A:1135:ASN:HB3	2.16	0.76
1:B:543:PHE:CE2	1:B:578:ASP:HB3	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:605:SER:OG	1:C:607:GLN:HG2	1.86	0.76
1:A:119:ILE:CG1	1:A:128:ILE:HG12	2.15	0.76
1:A:1096:VAL:HG21	1:A:1105:THR:CG2	2.15	0.76
1:B:204:TYR:HD1	1:B:225:PRO:CA	1.99	0.76
1:C:229:LEU:HB3	1:C:231:ILE:HD13	1.66	0.76
1:A:353:TRP:NE1	1:A:466:ARG:CG	2.48	0.76
1:C:118:LEU:C	1:C:119:ILE:HD12	2.06	0.76
1:C:599:THR:HB	1:C:608:VAL:CG1	2.15	0.76
1:A:34:ARG:HH12	1:A:217:PRO:HG2	1.37	0.76
1:C:822:LEU:HD11	1:C:1061:VAL:HG21	1.68	0.76
1:A:220:PHE:HZ	1:A:288:ALA:HB3	1.51	0.75
1:B:92:PHE:CZ	1:B:265:TYR:CD2	2.69	0.75
1:B:106:PHE:HB3	1:B:235:ILE:HD12	1.68	0.75
1:B:800:PHE:CD2	1:B:927:PHE:CD2	2.74	0.75
1:C:38:TYR:OH	1:C:284:THR:HA	1.84	0.75
1:C:168:PHE:CZ	1:C:231:ILE:HD11	2.21	0.75
1:C:546:LEU:CD1	1:C:565:PHE:HE1	1.99	0.75
1:A:976:VAL:HG13	1:A:979:ASP:CB	2.16	0.75
1:B:805:ILE:HG22	1:B:878:LEU:CD1	2.16	0.75
1:C:101:ILE:HD11	1:C:263:ALA:HB1	1.68	0.75
1:A:673:SER:O	1:A:693:ILE:CD1	2.35	0.75
1:C:281:GLU:HB3	2:P:1:NAG:H82	1.67	0.75
1:C:1103:PHE:HE1	1:C:1114:ILE:HD13	1.52	0.75
1:B:565:PHE:HB2	1:C:42:VAL:HG12	1.66	0.75
1:C:37:TYR:HB3	1:C:223:LEU:HD11	1.69	0.75
1:C:204:TYR:CE1	1:C:225:PRO:HB3	2.21	0.75
1:C:320:VAL:HG21	1:C:619:GLU:OE2	1.86	0.75
1:C:1083:HIS:HB2	1:C:1137:VAL:CG2	2.16	0.75
1:C:715:PRO:HA	1:C:1071:GLN:O	1.85	0.75
1:C:330:PRO:CD	1:C:544:ASN:ND2	2.46	0.75
1:A:34:ARG:HH12	1:A:217:PRO:HG3	1.52	0.75
1:A:222:VAL:HG21	1:A:285:ILE:HB	1.66	0.75
1:C:34:ARG:NH1	1:C:221:SER:OG	2.20	0.75
1:A:289:VAL:CG2	1:A:306:PHE:CE1	2.70	0.75
1:C:294:ASP:OD2	1:C:296:LEU:HB3	1.87	0.75
1:C:1080:ALA:O	1:C:1132:ILE:HG13	1.87	0.75
1:B:89:GLY:O	1:B:270:LEU:CD1	2.34	0.74
1:B:316:SER:O	1:B:595:VAL:HG22	1.87	0.74
1:B:577:ARG:HB2	1:B:584:ILE:HG13	1.69	0.74
1:B:730:SER:O	1:B:1058:HIS:HB3	1.87	0.74
1:C:426:PRO:CG	1:C:464:PHE:CE2	2.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:ILE:CG2	1:B:129:LYS:H	2.01	0.74
1:B:388:ASN:ND2	1:B:527:PRO:HG2	2.02	0.74
1:A:128:ILE:CG2	1:A:129:LYS:H	2.00	0.74
1:A:782:PHE:CE2	1:A:874:THR:HG22	2.22	0.74
1:C:643:PHE:HZ	1:C:655:HIS:ND1	1.84	0.74
1:C:825:LYS:CE	1:C:942:ALA:CB	2.65	0.74
1:B:119:ILE:CG1	1:B:128:ILE:HG12	2.15	0.74
1:B:743:CYS:SG	1:B:750:SER:CA	2.75	0.74
1:B:1090:PRO:HD3	1:B:1095:PHE:HE1	1.50	0.74
1:C:88:ASP:OD1	1:C:88:ASP:N	2.15	0.74
1:C:498:GLN:CG	1:C:499:PRO:HD2	2.17	0.74
1:C:756:TYR:HB3	1:C:759:PHE:HD2	1.49	0.74
1:C:200:TYR:HD2	1:C:230:PRO:CA	1.95	0.74
1:C:414:GLN:HE21	1:C:414:GLN:HA	1.52	0.74
1:C:105:ILE:CG1	1:C:118:LEU:HD13	2.17	0.74
1:C:612:TYR:CB	1:C:615:VAL:HG11	2.17	0.74
1:C:643:PHE:CE1	1:C:655:HIS:CG	2.75	0.74
1:C:791:THR:CG2	1:C:792:PRO:HD2	2.16	0.74
1:A:758:SER:OG	1:C:965:GLN:OE1	2.06	0.74
1:B:584:ILE:H	1:B:584:ILE:HD12	1.51	0.74
1:B:718:PHE:HD2	1:B:1067:TYR:CD1	2.05	0.74
1:C:220:PHE:HE2	1:C:288:ALA:H	1.27	0.74
1:B:270:LEU:H	1:B:270:LEU:HD12	1.51	0.74
1:A:55:PHE:CB	1:A:275:PHE:CE2	2.71	0.74
1:A:299:THR:HG1	1:A:597:VAL:HG21	1.50	0.74
1:C:973:ILE:HG13	1:C:980:ILE:HD12	1.69	0.74
1:A:89:GLY:CA	1:A:270:LEU:HG	2.18	0.74
1:C:97:LYS:HB2	1:C:186:PHE:HA	1.69	0.74
1:C:105:ILE:HG23	1:C:118:LEU:HD13	1.69	0.74
1:C:822:LEU:HD21	1:C:945:LEU:HD22	1.70	0.74
1:A:497:PHE:CD2	1:A:507:PRO:HB3	2.23	0.73
1:A:1082:CYS:HB2	1:A:1132:ILE:CD1	2.18	0.73
1:B:534:VAL:O	1:B:552:LEU:HD12	1.88	0.73
1:C:490:PHE:CG	1:C:491:PRO:HD2	2.23	0.73
1:B:91:TYR:HE1	1:B:93:ALA:HB2	1.52	0.73
1:B:329:PHE:CZ	1:B:528:LYS:HB3	2.22	0.73
1:B:645:THR:O	1:B:648:GLY:N	2.21	0.73
1:B:1031:GLU:OE2	1:B:1039:ARG:HD3	1.87	0.73
1:C:83:VAL:HG11	1:C:237:ARG:HH21	1.52	0.73
1:C:118:LEU:HD22	1:C:135:PHE:HZ	1.05	0.73
1:C:916:LEU:CD1	1:C:923:ILE:HD12	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:TYR:CE1	1:A:225:PRO:CB	2.71	0.73
1:A:308:VAL:C	1:A:602:THR:HG22	2.07	0.73
1:B:89:GLY:C	1:B:270:LEU:HD13	2.08	0.73
1:C:497:PHE:CE1	1:C:507:PRO:HA	2.24	0.73
1:C:560:LEU:HD12	1:C:562:PHE:CZ	2.23	0.73
1:C:822:LEU:HD21	1:C:945:LEU:CD2	2.19	0.73
1:B:1082:CYS:SG	1:B:1087:ALA:HA	2.29	0.73
1:C:598:ILE:CD1	1:C:666:ILE:HD11	2.18	0.73
1:C:825:LYS:HZ3	1:C:942:ALA:HB2	1.49	0.73
1:A:193:VAL:HG13	1:A:270:LEU:HD11	1.69	0.73
1:A:497:PHE:CZ	1:A:507:PRO:HB3	2.23	0.73
1:C:643:PHE:CZ	1:C:655:HIS:CG	2.77	0.73
1:C:644:GLN:NE2	1:C:644:GLN:HA	2.02	0.73
1:A:555:SER:HB2	1:A:586:ASP:HB2	1.69	0.73
1:B:599:THR:CB	1:B:608:VAL:HG12	2.19	0.73
1:B:1081:ILE:CD1	1:B:1133:VAL:CG2	2.67	0.73
1:A:88:ASP:OD1	1:A:88:ASP:N	2.16	0.73
1:A:92:PHE:CZ	1:A:94:SER:HB3	2.23	0.73
1:A:782:PHE:CE1	1:A:1060:VAL:CG2	2.70	0.73
1:B:718:PHE:HZ	1:B:923:ILE:CD1	2.01	0.73
1:C:210:ILE:C	1:C:212:LEU:CD2	2.57	0.73
1:A:108:THR:OG1	1:A:234:ASN:O	2.08	0.72
1:A:131:CYS:HG	1:A:166:CYS:HG	1.34	0.72
1:A:353:TRP:CG	1:A:466:ARG:CD	2.63	0.72
1:A:782:PHE:CZ	1:A:1060:VAL:HG22	2.25	0.72
1:C:555:SER:OG	1:C:584:ILE:C	2.27	0.72
1:C:610:VAL:O	1:C:651:ILE:HG12	1.89	0.72
1:C:660:TYR:HB2	1:C:695:TYR:CE2	2.24	0.72
1:C:1029:MET:O	1:C:1033:VAL:HB	1.90	0.72
1:A:326:ILE:HG21	1:A:534:VAL:HG22	1.70	0.72
1:C:231:ILE:HD12	1:C:231:ILE:N	2.05	0.72
1:C:294:ASP:OD1	1:C:297:SER:N	2.19	0.72
1:C:380:TYR:CE2	1:C:412:PRO:HD2	2.24	0.72
1:C:426:PRO:CG	1:C:464:PHE:CD2	2.73	0.72
1:C:429:PHE:CZ	1:C:431:GLY:CA	2.73	0.72
2:O:2:NAG:O7	2:O:2:NAG:O3	2.07	0.72
1:C:337:PRO:CD	1:C:358:ILE:HD11	2.17	0.72
1:A:56:LEU:HD12	1:A:57:PRO:HD2	1.72	0.72
1:A:729:VAL:CG2	1:A:1060:VAL:HG23	2.19	0.72
1:B:327:VAL:HG11	1:B:329:PHE:CE2	2.24	0.72
1:C:916:LEU:HD13	1:C:923:ILE:HD12	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1004:LEU:O	1:C:1004:LEU:HD23	1.90	0.72
1:A:912:THR:OG1	1:A:914:ASN:OD1	2.03	0.72
1:B:99:ASN:O	1:B:102:ARG:NE	2.20	0.72
1:B:204:TYR:CD1	1:B:225:PRO:CA	2.72	0.72
1:B:559:PHE:HA	1:B:563:GLN:OE1	1.89	0.72
1:C:395:VAL:HG23	1:C:524:VAL:HG21	1.70	0.72
1:C:411:ALA:C	1:C:425:LEU:HD12	2.10	0.72
1:A:204:TYR:HE1	1:A:225:PRO:CB	2.01	0.72
1:B:53:ASP:O	1:B:55:PHE:CD2	2.42	0.72
1:A:34:ARG:NH1	1:A:217:PRO:HG3	1.99	0.72
1:B:329:PHE:CD2	1:B:528:LYS:HB3	2.23	0.72
1:B:1090:PRO:CD	1:B:1095:PHE:HE1	2.03	0.72
1:C:46:SER:HA	1:C:279:TYR:O	1.90	0.72
1:C:328:ARG:NE	1:C:578:ASP:CG	2.34	0.72
1:C:729:VAL:HG23	1:C:1059:GLY:HA2	1.72	0.72
1:A:731:MET:HB2	1:A:955:ASN:ND2	2.04	0.71
1:A:556:ASN:OD1	1:A:556:ASN:N	2.24	0.71
1:B:1118:ASP:OD1	1:B:1119:ASN:N	2.24	0.71
1:B:712:ILE:O	1:B:1075:PHE:N	2.21	0.71
1:C:33:THR:HA	1:C:58:PHE:CE2	2.25	0.71
1:C:343:ASN:HD21	3:Q:1:NDG:C1	2.03	0.71
1:C:429:PHE:CE1	1:C:431:GLY:CA	2.73	0.71
1:A:693:ILE:HD13	1:A:693:ILE:H	1.54	0.71
1:A:1089:PHE:HB2	1:A:1121:PHE:HE1	1.54	0.71
1:B:335:LEU:H	1:B:335:LEU:HD12	1.56	0.71
1:C:200:TYR:CD2	1:C:230:PRO:CA	2.69	0.71
1:B:55:PHE:CB	1:B:275:PHE:HE2	2.03	0.71
1:C:37:TYR:CD1	1:C:55:PHE:CE1	2.65	0.71
1:C:37:TYR:HB3	1:C:223:LEU:CD1	2.20	0.71
1:C:1030:SER:O	1:C:1034:LEU:HB2	1.90	0.71
1:A:896:ILE:HD13	1:C:712:ILE:CD1	2.21	0.71
1:B:89:GLY:O	1:B:270:LEU:HD12	1.91	0.71
1:C:220:PHE:HE2	1:C:287:ASP:OD1	1.72	0.71
1:C:296:LEU:O	1:C:296:LEU:HD12	1.91	0.71
1:C:366:SER:O	1:C:370:ASN:HB3	1.89	0.71
1:C:429:PHE:CE1	1:C:431:GLY:C	2.64	0.71
1:C:503:VAL:HA	1:C:506:GLN:OE1	1.90	0.71
1:C:516:GLU:HG3	1:C:519:HIS:CD2	2.25	0.71
1:A:55:PHE:CG	1:A:275:PHE:CE2	2.79	0.71
1:B:200:TYR:CB	1:B:230:PRO:HA	2.20	0.71
1:B:461:LEU:HD21	1:B:467:ASP:HB2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:800:PHE:HD2	1:B:927:PHE:HD2	1.34	0.71
1:B:1090:PRO:CB	1:B:1093:GLY:O	2.39	0.71
1:C:337:PRO:HD2	1:C:358:ILE:CD1	2.18	0.71
1:A:53:ASP:O	1:A:55:PHE:HD2	1.73	0.70
1:A:203:ILE:CG2	1:A:227:VAL:HG23	2.20	0.70
1:C:916:LEU:HD13	1:C:923:ILE:HD13	1.73	0.70
1:A:29:THR:O	1:A:62:VAL:CG1	2.39	0.70
1:A:597:VAL:HG12	1:A:610:VAL:HG22	1.74	0.70
1:A:1095:PHE:HB3	1:A:1102:TRP:CZ3	2.26	0.70
1:B:85:PRO:CG	1:B:269:TYR:OH	2.36	0.70
1:C:426:PRO:HG2	1:C:464:PHE:HE2	1.55	0.70
1:A:266:TYR:N	1:A:266:TYR:CD1	2.60	0.70
1:A:570:ALA:HB3	1:B:855:PHE:CZ	2.26	0.70
1:A:617:CYS:SG	1:A:644:GLN:OE1	2.50	0.70
1:B:533:LEU:CD1	1:B:552:LEU:HD13	2.20	0.70
1:C:378:LYS:CD	1:C:433:VAL:HG11	2.21	0.70
1:C:654:GLU:OE1	1:C:692:ILE:O	2.08	0.70
1:A:66:HIS:CD2	1:A:68:ILE:CG2	2.75	0.70
1:A:89:GLY:CA	1:A:270:LEU:CG	2.68	0.70
1:A:353:TRP:NE1	1:A:466:ARG:HG3	2.07	0.70
1:A:675:GLN:HA	1:A:675:GLN:NE2	2.07	0.70
1:B:878:LEU:HD21	1:B:1052:PHE:HB3	1.73	0.70
1:C:380:TYR:CE2	1:C:412:PRO:HD3	2.24	0.70
1:C:393:THR:CG2	1:C:522:ALA:HB1	2.18	0.70
1:C:799:GLY:O	1:C:924:ALA:HB1	1.91	0.70
1:A:896:ILE:CD1	1:C:712:ILE:CG1	2.64	0.70
1:B:388:ASN:OD1	1:B:527:PRO:O	2.08	0.70
1:B:641:ASN:HD22	1:B:654:GLU:HA	1.57	0.70
1:B:724:THR:HG22	1:B:1063:LEU:CD2	2.17	0.70
1:B:742:ILE:HD11	1:B:1004:LEU:HD12	1.73	0.70
1:B:1142:GLN:HA	1:B:1142:GLN:NE2	2.05	0.70
1:C:32:PHE:HB3	1:C:59:PHE:CD2	2.26	0.70
1:A:67:ALA:HB3	1:A:263:ALA:CB	2.19	0.70
1:C:497:PHE:CE1	1:C:507:PRO:CA	2.75	0.70
1:C:643:PHE:CZ	1:C:655:HIS:ND1	2.60	0.70
1:A:774:GLN:HE21	1:A:774:GLN:HA	1.56	0.70
1:B:654:GLU:O	1:B:693:ILE:HA	1.92	0.70
1:B:1105:THR:HB	1:B:1111:GLU:O	1.92	0.70
1:C:404:GLY:HA2	1:C:508:TYR:CD2	2.23	0.70
1:A:552:LEU:N	1:A:552:LEU:HD23	2.06	0.69
1:C:100:ILE:HA	1:C:243:ALA:HB3	1.71	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:914:ASN:OD1	1:B:915:VAL:N	2.25	0.69
1:C:378:LYS:CD	1:C:433:VAL:CG1	2.70	0.69
1:C:546:LEU:CD1	1:C:565:PHE:CE1	2.76	0.69
1:C:733:LYS:HD3	1:C:775:ASP:OD1	1.92	0.69
1:A:33:THR:CG2	1:A:58:PHE:HE2	2.05	0.69
1:A:342:PHE:CE1	1:A:511:VAL:HG11	2.27	0.69
1:C:105:ILE:HD11	1:C:241:LEU:HD13	1.70	0.69
1:C:414:GLN:HA	1:C:414:GLN:NE2	2.07	0.69
1:C:931:ILE:O	1:C:934:ILE:CG2	2.40	0.69
1:A:551:VAL:C	1:A:552:LEU:HD23	2.12	0.69
1:A:774:GLN:HA	1:A:774:GLN:NE2	2.07	0.69
1:C:33:THR:CB	1:C:58:PHE:CE2	2.75	0.69
1:A:33:THR:HG22	1:A:58:PHE:HD2	1.48	0.69
1:A:1094:VAL:HG23	1:B:900:MET:CE	2.22	0.69
1:B:815:ARG:NH1	1:B:823:PHE:CG	2.60	0.69
1:B:1039:ARG:NH1	1:B:1042:PHE:HE2	1.76	0.69
1:C:607:GLN:NE2	1:C:674:TYR:CZ	2.55	0.69
1:B:599:THR:CG2	1:B:608:VAL:HG12	2.15	0.69
1:C:86:PHE:CD2	1:C:90:VAL:HG21	2.28	0.69
1:C:374:PHE:HA	1:C:436:TRP:HB3	1.74	0.69
1:C:351:TYR:O	1:C:467:ASP:O	2.10	0.69
1:C:490:PHE:CD1	1:C:491:PRO:HD2	2.28	0.69
1:C:662:CYS:SG	1:C:697:MET:HB2	2.32	0.69
1:A:220:PHE:HE2	1:A:288:ALA:H	1.36	0.69
1:A:643:PHE:CD2	1:A:655:HIS:HB2	2.28	0.69
1:B:50:SER:HA	1:B:275:PHE:O	1.92	0.69
1:B:275:PHE:HD1	1:B:290:ASP:HA	1.58	0.69
1:B:289:VAL:HG23	1:B:306:PHE:CE2	2.28	0.69
1:B:298:GLU:CD	1:B:315:THR:HG21	2.13	0.69
1:C:107:GLY:N	1:C:235:ILE:HG23	2.05	0.69
1:C:348:ALA:O	1:C:400:PHE:HA	1.92	0.69
1:C:490:PHE:CZ	1:C:492:LEU:HD23	2.27	0.69
1:C:692:ILE:HD12	1:C:692:ILE:N	2.07	0.69
1:C:1115:ILE:HD12	1:C:1115:ILE:N	2.06	0.69
1:C:360:ASN:N	1:C:523:THR:HG23	2.07	0.69
1:A:329:PHE:CE2	1:A:391:CYS:SG	2.86	0.69
1:C:409:GLN:HG3	1:C:415:THR:O	1.92	0.69
1:A:403:ARG:HD3	1:A:495:TYR:HE1	1.55	0.68
1:B:641:ASN:HD21	1:B:654:GLU:HA	1.56	0.68
1:A:220:PHE:CZ	1:A:288:ALA:HB3	2.27	0.68
1:A:280:ASN:ND2	1:A:286:THR:HG21	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1127:ASP:N	1:B:1127:ASP:OD1	2.26	0.68
1:B:882:ILE:HG23	1:B:898:PHE:CD2	2.28	0.68
1:C:102:ARG:HD3	1:C:141:LEU:HD13	1.74	0.68
1:C:718:PHE:HZ	1:C:923:ILE:CG1	2.06	0.68
1:C:1093:GLY:HA3	1:C:1105:THR:O	1.94	0.68
1:C:380:TYR:HE2	1:C:412:PRO:HD2	1.57	0.68
1:A:797:PHE:CD1	1:A:882:ILE:HG21	2.26	0.68
1:B:372:ALA:CB	1:B:374:PHE:CE2	2.68	0.68
1:C:48:LEU:HD12	1:C:48:LEU:N	2.08	0.68
1:C:223:LEU:HD23	1:C:223:LEU:H	1.58	0.68
1:A:357:ARG:HG3	1:A:396:TYR:CE1	2.28	0.68
1:A:817:PHE:HE2	1:A:935:GLN:HG3	1.56	0.68
1:B:666:ILE:HD11	1:B:672:ALA:HB2	1.74	0.68
1:C:203:ILE:HG22	1:C:227:VAL:HG23	1.73	0.68
1:C:347:PHE:CZ	1:C:509:ARG:HD3	2.27	0.68
1:C:555:SER:OG	1:C:584:ILE:O	2.10	0.68
1:A:664:ILE:HB	1:A:672:ALA:O	1.94	0.68
1:B:1105:THR:CB	1:B:1111:GLU:O	2.42	0.68
1:C:203:ILE:HG21	1:C:227:VAL:CG2	2.24	0.68
1:C:825:LYS:HE2	1:C:942:ALA:HA	1.76	0.68
1:A:659:SER:CB	1:A:698:SER:HB3	2.23	0.68
1:A:817:PHE:CE2	1:A:935:GLN:CD	2.68	0.68
1:A:1033:VAL:HG12	1:A:1034:LEU:HD23	1.76	0.68
1:C:87:ASN:OD1	1:C:87:ASN:N	2.24	0.68
1:A:220:PHE:CE2	1:A:288:ALA:N	2.62	0.68
1:B:372:ALA:HB1	1:B:374:PHE:CD2	2.28	0.68
1:C:581:THR:CG2	1:C:583:GLU:HG3	2.23	0.68
1:A:90:VAL:HG13	1:A:194:PHE:HB2	1.74	0.68
1:B:326:ILE:HD11	1:B:552:LEU:HD11	1.74	0.68
1:B:743:CYS:O	1:B:749:CYS:SG	2.52	0.68
1:C:90:VAL:N	1:C:270:LEU:HD13	2.09	0.68
1:C:218:GLN:OE1	1:C:218:GLN:N	2.23	0.68
1:C:541:PHE:HZ	1:C:587:ILE:HD13	1.59	0.68
1:B:275:PHE:CE1	1:B:290:ASP:HA	2.29	0.67
1:C:220:PHE:CE2	1:C:287:ASP:CA	2.77	0.67
1:C:541:PHE:CZ	1:C:587:ILE:HD13	2.29	0.67
1:A:1081:ILE:HG21	1:A:1135:ASN:CB	2.22	0.67
1:B:118:LEU:HD22	1:B:135:PHE:CE1	2.27	0.67
1:C:741:TYR:CE1	1:C:966:LEU:CD2	2.72	0.67
1:C:611:LEU:O	1:C:611:LEU:HD23	1.94	0.67
1:C:786:LYS:N	1:C:786:LYS:HE3	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:724:THR:CG2	1:A:1063:LEU:CD2	2.70	0.67
1:A:970:PHE:CE1	1:B:756:TYR:O	2.48	0.67
1:A:992:GLN:HA	1:A:992:GLN:NE2	2.10	0.67
1:B:909:ILE:HD13	1:B:1049:LEU:HD21	1.76	0.67
1:C:100:ILE:HG23	1:C:243:ALA:H	1.59	0.67
1:C:334:ASN:N	1:C:334:ASN:OD1	2.25	0.67
1:C:387:LEU:HD23	1:C:390:LEU:HD11	1.76	0.67
1:C:503:VAL:HA	1:C:506:GLN:CG	2.25	0.67
1:A:86:PHE:HB3	1:A:237:ARG:HA	1.75	0.67
1:A:97:LYS:HD3	1:A:98:SER:OG	1.94	0.67
1:A:321:GLN:HA	1:A:321:GLN:NE2	2.09	0.67
1:C:659:SER:HB3	1:C:698:SER:HB3	1.76	0.67
1:C:1089:PHE:C	1:C:1120:THR:HB	2.14	0.67
1:A:726:ILE:CD1	1:A:944:ALA:O	2.27	0.67
1:B:1039:ARG:NE	1:B:1042:PHE:CD2	2.63	0.67
1:C:115:GLN:C	1:C:233:ILE:HD11	2.15	0.67
1:C:226:LEU:HG	1:C:227:VAL:HG13	1.75	0.67
1:C:448:ASN:O	1:C:449:TYR:CD1	2.47	0.67
1:C:497:PHE:CD1	1:C:507:PRO:CD	2.77	0.67
1:A:203:ILE:CG2	1:A:227:VAL:CG2	2.73	0.67
1:A:329:PHE:O	1:A:580:GLN:NE2	2.27	0.67
1:A:1105:THR:CB	1:A:1111:GLU:O	2.43	0.67
1:B:56:LEU:CD1	1:B:57:PRO:HD2	2.17	0.67
1:B:737:ASP:N	1:B:737:ASP:OD1	2.28	0.67
1:C:43:PHE:CD1	1:C:43:PHE:C	2.67	0.67
1:C:126:VAL:HG13	1:C:175:PHE:CZ	2.30	0.67
1:A:403:ARG:HG3	1:A:495:TYR:CZ	2.30	0.67
1:A:817:PHE:HE2	1:A:935:GLN:CD	1.98	0.67
1:B:91:TYR:HE1	1:B:93:ALA:CB	2.07	0.67
1:C:118:LEU:HD12	1:C:119:ILE:H	1.58	0.67
1:B:388:ASN:CG	1:B:527:PRO:HG2	2.15	0.67
1:C:90:VAL:N	1:C:270:LEU:CD1	2.58	0.67
1:C:429:PHE:CZ	1:C:431:GLY:HA3	2.30	0.67
1:C:462:LYS:HE2	1:C:462:LYS:CA	2.16	0.67
1:A:66:HIS:HD2	1:A:68:ILE:HG22	1.61	0.66
1:A:797:PHE:CE1	1:A:882:ILE:HG22	2.13	0.66
1:B:57:PRO:CA	1:B:273:ARG:NH1	2.51	0.66
1:C:392:PHE:CE2	1:C:515:PHE:CE1	2.75	0.66
1:C:660:TYR:O	1:C:695:TYR:HE2	1.79	0.66
1:C:709:ASN:OD1	1:C:709:ASN:N	2.25	0.66
1:C:765:ARG:HA	1:C:768:THR:HG22	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:HIS:CD2	1:A:68:ILE:HG22	2.31	0.66
1:A:642:VAL:CG1	1:A:651:ILE:HG12	2.25	0.66
1:A:895:GLN:HE22	1:C:713:ALA:HB2	1.59	0.66
1:C:321:GLN:OE1	1:C:322:PRO:CD	2.40	0.66
1:A:782:PHE:HE1	1:A:1060:VAL:CG2	2.06	0.66
1:A:1031:GLU:OE1	1:C:1039:ARG:NE	2.22	0.66
1:B:97:LYS:HD3	1:B:98:SER:OG	1.94	0.66
1:B:584:ILE:HD12	1:B:584:ILE:N	2.10	0.66
1:C:48:LEU:HB3	1:C:276:LEU:HD21	1.77	0.66
1:C:673:SER:O	1:C:693:ILE:HG12	1.95	0.66
1:A:117:LEU:HD13	1:A:201:PHE:CE2	2.30	0.66
1:A:1090:PRO:CB	1:A:1093:GLY:O	2.43	0.66
1:B:919:ASN:N	1:B:919:ASN:OD1	2.28	0.66
1:C:95:THR:HG23	1:C:186:PHE:CD2	2.30	0.66
1:C:896:ILE:HG13	1:C:897:PRO:HD2	1.76	0.66
1:C:83:VAL:HG21	1:C:237:ARG:NH2	2.10	0.66
1:C:972:ALA:CB	1:C:996:LEU:CD1	2.73	0.66
1:B:106:PHE:HB2	1:B:117:LEU:HB3	1.76	0.66
1:A:817:PHE:HE2	1:A:935:GLN:CG	2.09	0.66
1:B:726:ILE:HG21	1:B:948:LEU:HG	1.78	0.66
1:C:972:ALA:CB	1:C:996:LEU:HD11	2.25	0.66
1:A:201:PHE:HD1	1:A:202:LYS:N	1.93	0.66
1:A:328:ARG:NH1	1:A:578:ASP:OD2	2.29	0.66
1:C:922:LEU:HD12	1:C:922:LEU:O	1.95	0.66
1:A:1002:GLN:HA	1:A:1002:GLN:NE2	2.11	0.66
1:A:1102:TRP:CB	1:A:1135:ASN:HD21	1.96	0.66
1:A:29:THR:O	1:A:62:VAL:HG12	1.96	0.66
1:C:770:ILE:O	1:C:774:GLN:HG2	1.96	0.66
1:A:118:LEU:HD22	1:A:135:PHE:CE1	2.29	0.65
1:C:472:ILE:CD1	1:C:482:GLY:H	2.07	0.65
1:A:353:TRP:CE2	1:A:466:ARG:HD3	2.31	0.65
1:A:1095:PHE:HB3	1:A:1102:TRP:HZ3	1.60	0.65
1:A:1127:ASP:OD1	1:A:1127:ASP:N	2.27	0.65
1:B:611:LEU:HD22	1:B:666:ILE:HG23	1.76	0.65
1:B:1043:CYS:CB	1:B:1048:HIS:CD2	2.76	0.65
1:C:210:ILE:H	1:C:210:ILE:CD1	2.09	0.65
1:A:888:PHE:CZ	1:A:1034:LEU:HD22	2.31	0.65
1:A:1078:ALA:N	1:A:1102:TRP:CH2	2.63	0.65
1:B:658:ASN:OD1	1:B:658:ASN:N	2.22	0.65
1:C:210:ILE:HG12	1:C:212:LEU:CD2	2.19	0.65
1:C:805:ILE:HG22	1:C:878:LEU:HD13	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1024:LEU:HD12	1:C:1024:LEU:O	1.95	0.65
1:A:336:CYS:N	1:A:361:CYS:HB2	2.12	0.65
1:B:204:TYR:CE1	1:B:225:PRO:CB	2.75	0.65
1:B:280:ASN:HB3	1:B:286:THR:HG23	1.77	0.65
1:B:776:LYS:NZ	1:B:780:GLU:HG2	2.11	0.65
1:B:877:LEU:HD13	1:B:1029:MET:SD	2.36	0.65
1:C:210:ILE:H	1:C:210:ILE:HD13	1.61	0.65
1:A:424:LYS:O	1:A:463:PRO:HA	1.97	0.65
1:A:659:SER:HB3	1:A:698:SER:HB3	1.78	0.65
1:C:224:GLU:N	1:C:224:GLU:OE1	2.29	0.65
1:C:718:PHE:HD2	1:C:1109:PHE:HE1	1.44	0.65
1:C:912:THR:HG23	1:C:1106:GLN:OE1	1.97	0.65
1:A:729:VAL:HG21	1:A:1060:VAL:CG2	2.25	0.65
1:B:1090:PRO:HD3	1:B:1095:PHE:CE1	2.31	0.65
1:B:718:PHE:CG	1:B:1067:TYR:CE1	2.65	0.65
1:A:96:GLU:OE2	1:A:101:ILE:O	2.14	0.64
1:A:541:PHE:HE2	1:A:587:ILE:HD12	1.59	0.64
1:A:743:CYS:O	1:A:977:LEU:CD2	2.45	0.64
1:B:784:GLN:HA	1:B:784:GLN:NE2	2.07	0.64
1:C:87:ASN:ND2	1:C:269:TYR:CE2	2.65	0.64
1:C:352:ALA:CB	1:C:468:ILE:HG22	2.27	0.64
1:A:1044:GLY:N	1:A:1064:HIS:ND1	2.45	0.64
1:B:726:ILE:CD1	1:B:1061:VAL:HG22	2.27	0.64
1:B:1011:GLN:HE21	1:B:1011:GLN:HA	1.61	0.64
1:C:581:THR:O	1:C:582:LEU:HB3	1.96	0.64
1:C:718:PHE:CZ	1:C:923:ILE:HG12	2.33	0.64
1:A:1082:CYS:HB2	1:A:1132:ILE:HD11	1.80	0.64
1:B:980:ILE:HD11	1:B:984:LEU:HD12	1.78	0.64
1:C:314:GLN:O	1:C:314:GLN:HG3	1.96	0.64
1:C:1091:ARG:HB2	1:C:1119:ASN:O	1.97	0.64
1:A:1088:HIS:HB3	1:A:1120:THR:HB	1.80	0.64
1:B:748:GLU:CD	1:B:981:LEU:HD11	2.18	0.64
1:C:55:PHE:O	1:C:270:LEU:HB3	1.98	0.64
1:C:168:PHE:CZ	1:C:229:LEU:HD12	2.32	0.64
1:C:326:ILE:HG13	1:C:326:ILE:O	1.96	0.64
1:A:1141:LEU:HD13	1:C:1141:LEU:HD11	1.79	0.64
1:A:322:PRO:HB3	1:A:539:VAL:HA	1.80	0.64
1:A:371:SER:HA	2:J:2:NAG:H82	1.80	0.64
1:B:107:GLY:H	1:B:235:ILE:HG21	1.62	0.64
1:B:1102:TRP:CB	1:B:1135:ASN:HD22	2.03	0.64
1:C:453:TYR:CD1	1:C:495:TYR:CD1	2.86	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:PHE:CZ	1:A:620:VAL:HG21	2.32	0.64
1:B:335:LEU:HD12	1:B:335:LEU:N	2.12	0.64
1:B:422:ASN:HD21	1:B:454:ARG:H	1.46	0.64
1:B:613:GLN:HG2	1:C:861:LEU:HD12	1.79	0.64
1:C:287:ASP:OD2	1:C:306:PHE:CE2	2.51	0.64
1:C:347:PHE:CE1	1:C:509:ARG:HD3	2.33	0.64
1:C:502:GLY:C	1:C:506:GLN:HG3	2.17	0.64
1:A:106:PHE:HB2	1:A:117:LEU:HB3	1.79	0.64
1:A:452:LEU:HD13	1:A:493:GLN:C	2.14	0.64
1:B:617:CYS:SG	1:B:642:VAL:HG12	2.38	0.64
1:C:461:LEU:HD21	1:C:465:GLU:OE1	1.98	0.64
1:B:119:ILE:HG23	1:B:127:VAL:O	1.98	0.63
1:B:725:GLU:CD	1:B:1028:LYS:HZ2	2.00	0.63
1:B:776:LYS:NZ	1:B:780:GLU:CG	2.61	0.63
1:B:909:ILE:HG23	1:B:1036:GLN:HE22	1.63	0.63
1:C:106:PHE:HZ	1:C:194:PHE:CD2	2.16	0.63
1:C:758:SER:HB2	1:C:761:THR:HB	1.81	0.63
1:B:57:PRO:HB3	1:B:273:ARG:NH2	2.13	0.63
1:C:498:GLN:HG2	1:C:499:PRO:HD2	1.80	0.63
1:A:620:VAL:HG23	1:A:621:PRO:CD	2.28	0.63
1:A:1078:ALA:HB3	1:A:1102:TRP:CH2	2.34	0.63
1:B:107:GLY:H	1:B:235:ILE:HD13	1.58	0.63
1:B:128:ILE:O	1:B:129:LYS:HG2	1.98	0.63
1:C:83:VAL:HG21	1:C:237:ARG:CZ	2.29	0.63
1:C:560:LEU:HD12	1:C:562:PHE:HZ	1.62	0.63
1:C:1029:MET:SD	1:C:1033:VAL:HG21	2.39	0.63
1:A:89:GLY:HA2	1:A:270:LEU:HG	1.74	0.63
1:A:620:VAL:CG2	1:A:621:PRO:CD	2.77	0.63
1:B:563:GLN:HE22	1:C:43:PHE:HB2	1.63	0.63
1:B:909:ILE:CG2	1:B:1036:GLN:NE2	2.61	0.63
1:B:1102:TRP:CZ2	1:B:1133:VAL:HG21	2.33	0.63
1:C:558:LYS:N	1:C:558:LYS:HD2	2.12	0.63
1:C:857:GLY:O	1:C:858:LEU:HD12	1.98	0.63
1:B:216:LEU:HD12	1:B:216:LEU:O	1.99	0.63
1:B:804:GLN:HB3	1:B:818:ILE:HG13	1.78	0.63
1:C:411:ALA:CA	1:C:425:LEU:HD12	2.28	0.63
1:A:985:ASP:OD1	1:A:986:PRO:HD3	1.96	0.63
1:A:1081:ILE:CG2	1:A:1135:ASN:CB	2.76	0.63
1:B:905:ARG:NH1	1:B:1049:LEU:O	2.32	0.63
1:C:1033:VAL:HG23	1:C:1062:PHE:HE1	1.62	0.63
1:C:1103:PHE:CE1	1:C:1114:ILE:HD13	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:GLY:H	1:B:235:ILE:HG23	1.62	0.63
1:B:675:GLN:HA	1:B:675:GLN:NE2	2.12	0.63
1:B:815:ARG:NH1	1:B:823:PHE:CE1	2.64	0.63
1:A:238:PHE:CD1	1:A:238:PHE:C	2.72	0.63
1:B:33:THR:HA	1:B:58:PHE:CE2	2.34	0.63
1:B:53:ASP:HB3	1:B:55:PHE:HE2	1.62	0.63
1:C:91:TYR:N	1:C:268:GLY:O	2.27	0.63
1:C:368:LEU:HD12	1:C:368:LEU:H	1.63	0.63
1:A:119:ILE:HG23	1:A:127:VAL:O	1.99	0.63
1:A:277:LEU:HD23	1:A:288:ALA:CB	2.28	0.63
1:A:453:TYR:HE2	1:A:493:GLN:HG2	1.59	0.63
1:B:826:VAL:CG2	1:B:945:LEU:CD1	2.73	0.63
1:C:393:THR:CB	1:C:522:ALA:HB1	2.28	0.63
1:C:472:ILE:HA	1:C:491:PRO:HD3	1.80	0.63
1:A:319:ARG:NH2	1:A:319:ARG:HB3	2.14	0.62
1:A:417:LYS:NZ	1:A:455:LEU:O	2.30	0.62
4:A:1307:NAG:C1	4:A:1307:NAG:C8	2.77	0.62
1:B:825:LYS:NZ	1:B:938:LEU:O	2.31	0.62
1:B:1011:GLN:HA	1:B:1011:GLN:NE2	2.14	0.62
1:C:293:LEU:HD12	1:C:293:LEU:O	1.99	0.62
1:A:90:VAL:CG1	1:A:194:PHE:CB	2.72	0.62
1:C:343:ASN:ND2	3:Q:1:NDG:C1	2.63	0.62
1:C:671:CYS:SG	1:C:697:MET:CB	2.80	0.62
1:A:675:GLN:HE21	1:A:675:GLN:CA	2.12	0.62
1:B:654:GLU:HB3	1:B:693:ILE:HG22	1.81	0.62
1:C:119:ILE:HG13	1:C:128:ILE:HG12	1.81	0.62
1:C:128:ILE:C	1:C:129:LYS:CG	2.66	0.62
1:A:289:VAL:HG11	1:A:300:LYS:HD2	1.81	0.62
1:A:982:SER:O	1:C:386:LYS:HE2	1.98	0.62
1:B:826:VAL:HG23	1:B:945:LEU:HD13	1.80	0.62
1:C:89:GLY:O	1:C:270:LEU:HD12	2.00	0.62
1:C:411:ALA:HB1	1:C:412:PRO:HD2	1.81	0.62
1:A:55:PHE:CG	1:A:275:PHE:CD2	2.87	0.62
1:C:86:PHE:CE2	1:C:106:PHE:CE2	2.88	0.62
1:C:748:GLU:OE1	1:C:981:LEU:CG	2.42	0.62
1:A:54:LEU:H	1:A:54:LEU:HD12	1.63	0.62
1:B:560:LEU:H	1:B:563:GLN:CD	2.03	0.62
1:C:472:ILE:HD13	1:C:482:GLY:HA2	1.82	0.62
1:A:697:MET:HE2	1:B:869:MET:SD	2.40	0.62
1:A:817:PHE:O	1:A:821:LEU:HD13	1.99	0.62
1:A:329:PHE:CD2	1:A:391:CYS:SG	2.93	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:TRP:CE2	1:A:466:ARG:CB	2.82	0.62
1:A:675:GLN:O	1:A:693:ILE:CD1	2.48	0.62
1:A:886:TRP:HB2	1:A:1035:GLY:HA2	1.81	0.62
1:B:96:GLU:OE2	1:B:101:ILE:O	2.16	0.62
1:B:658:ASN:HB2	1:B:660:TYR:CE1	2.34	0.62
1:B:1122:VAL:O	1:B:1122:VAL:HG22	2.00	0.62
1:C:89:GLY:CA	1:C:270:LEU:HD13	2.29	0.62
1:C:461:LEU:CD2	1:C:465:GLU:OE1	2.48	0.62
1:C:905:ARG:NE	1:C:1050:MET:HE2	2.10	0.62
1:B:53:ASP:O	1:B:55:PHE:HD2	1.83	0.62
1:B:574:ASP:O	1:B:587:ILE:CB	2.47	0.62
1:C:220:PHE:HZ	1:C:288:ALA:HB3	1.53	0.62
1:A:231:ILE:CG2	1:A:233:ILE:HG23	2.30	0.62
1:A:371:SER:CB	2:J:2:NAG:H82	2.30	0.62
1:B:275:PHE:HE1	1:B:290:ASP:CB	2.13	0.62
1:B:533:LEU:HD11	1:B:552:LEU:CD1	2.26	0.62
1:C:229:LEU:HB3	1:C:231:ILE:CD1	2.30	0.62
1:C:584:ILE:C	1:C:585:LEU:HD23	2.19	0.62
1:A:90:VAL:CG2	1:A:238:PHE:CD2	2.83	0.61
1:B:106:PHE:CB	1:B:235:ILE:HD13	2.24	0.61
1:C:194:PHE:CD1	1:C:203:ILE:HG13	2.34	0.61
1:C:735:SER:HB3	1:C:861:LEU:HD21	1.82	0.61
1:A:567:ARG:HE	1:B:42:VAL:HG11	1.65	0.61
1:A:611:LEU:HD22	1:A:666:ILE:HG23	1.81	0.61
1:A:660:TYR:O	1:A:695:TYR:CE2	2.53	0.61
1:A:707:TYR:CD1	1:A:708:SER:N	2.67	0.61
1:B:54:LEU:HD12	1:B:54:LEU:H	1.65	0.61
1:B:165:ASN:HD21	4:B:1305:NAG:C7	2.13	0.61
1:C:231:ILE:H	1:C:231:ILE:CD1	2.09	0.61
1:C:454:ARG:HD3	1:C:457:ARG:HB2	1.82	0.61
1:C:738:CYS:SG	1:C:760:CYS:O	2.58	0.61
1:C:739:THR:N	1:C:760:CYS:SG	2.73	0.61
1:A:404:GLY:HA2	1:A:508:TYR:CD2	2.34	0.61
1:A:471:GLU:OE1	1:A:471:GLU:HA	2.00	0.61
1:B:57:PRO:CG	1:B:273:ARG:NH1	2.64	0.61
1:C:534:VAL:CG1	1:C:539:VAL:HG21	2.30	0.61
1:C:1043:CYS:HB2	1:C:1048:HIS:CD2	2.35	0.61
1:A:335:LEU:HD12	1:A:335:LEU:O	2.00	0.61
1:A:403:ARG:HG3	1:A:495:TYR:CE1	2.35	0.61
1:A:895:GLN:O	1:C:712:ILE:HA	2.00	0.61
1:A:1029:MET:HB2	1:A:1062:PHE:CZ	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:THR:CA	1:C:58:PHE:CE2	2.84	0.61
1:C:194:PHE:HD1	1:C:203:ILE:HG13	1.66	0.61
1:C:321:GLN:OE1	1:C:321:GLN:HA	2.01	0.61
1:A:741:TYR:OH	1:A:962:LEU:HD12	2.01	0.61
1:B:55:PHE:HB2	1:B:275:PHE:HE2	1.65	0.61
1:B:327:VAL:CG1	1:B:529:LYS:O	2.49	0.61
1:C:327:VAL:H	1:C:531:THR:CG2	2.13	0.61
1:A:437:ASN:HA	1:A:508:TYR:CD1	2.35	0.61
1:B:55:PHE:HB2	1:B:275:PHE:CE2	2.36	0.61
1:B:1050:MET:O	1:B:1065:VAL:HG23	2.00	0.61
1:C:334:ASN:O	1:C:361:CYS:HB2	2.00	0.61
1:C:916:LEU:CD1	1:C:923:ILE:CD1	2.78	0.61
1:A:92:PHE:CE1	1:A:94:SER:CB	2.84	0.61
1:A:1105:THR:HB	1:A:1111:GLU:O	2.00	0.61
1:B:130:VAL:HG21	1:B:231:ILE:CD1	2.30	0.61
1:B:676:THR:HA	1:B:690:GLN:HA	1.83	0.61
1:B:976:VAL:O	1:B:980:ILE:HG22	2.01	0.61
1:C:120:VAL:HG21	1:C:157:PHE:HZ	1.64	0.61
1:A:33:THR:HB	1:A:58:PHE:CZ	2.34	0.61
1:A:353:TRP:N	1:A:466:ARG:HD2	1.99	0.61
1:A:725:GLU:OE2	1:A:1028:LYS:NZ	2.33	0.61
1:A:954:GLN:HG2	1:A:1014:ARG:CZ	2.31	0.61
1:C:722:VAL:HA	1:C:1064:HIS:O	2.00	0.61
1:A:770:ILE:HD11	1:A:1012:LEU:HG	1.82	0.61
1:B:718:PHE:CB	1:B:1067:TYR:CZ	2.78	0.61
1:C:107:GLY:H	1:C:235:ILE:CG2	2.13	0.61
1:C:318:PHE:CE2	1:C:612:TYR:CD1	2.89	0.61
1:C:456:PHE:HB2	1:C:473:TYR:CD1	2.36	0.61
1:A:749:CYS:SG	1:A:977:LEU:HD21	2.41	0.60
1:A:1002:GLN:HA	1:A:1002:GLN:HE21	1.66	0.60
1:C:497:PHE:HE1	1:C:507:PRO:HA	1.64	0.60
1:A:335:LEU:HD12	1:A:335:LEU:C	2.20	0.60
1:B:553:THR:HG23	1:B:586:ASP:HB2	1.83	0.60
1:C:194:PHE:HE1	1:C:203:ILE:HD11	1.66	0.60
1:B:317:ASN:ND2	1:C:737:ASP:HB2	2.13	0.60
1:B:329:PHE:CE2	1:B:528:LYS:CB	2.75	0.60
1:C:106:PHE:CB	1:C:235:ILE:HD13	2.13	0.60
1:C:107:GLY:O	1:C:235:ILE:CG2	2.48	0.60
1:A:715:PRO:CA	1:A:1071:GLN:O	2.43	0.60
1:C:102:ARG:HH12	1:C:179:LEU:HD22	1.65	0.60
1:C:393:THR:HG1	1:C:522:ALA:HB2	1.60	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LEU:H	1:A:54:LEU:CD1	2.14	0.60
1:A:128:ILE:O	1:A:129:LYS:HG2	2.01	0.60
1:B:332:ILE:HG22	1:B:334:ASN:OD1	2.02	0.60
1:C:377:PHE:CD1	1:C:434:ILE:HG13	2.36	0.60
1:C:453:TYR:O	1:C:493:GLN:HB3	2.01	0.60
1:C:965:GLN:HG2	1:C:1003:SER:OG	2.01	0.60
4:C:1305:NAG:O7	4:C:1305:NAG:H3	2.00	0.60
1:B:802:PHE:HE1	1:B:1052:PHE:CE2	2.19	0.60
1:C:106:PHE:HB3	1:C:235:ILE:CD1	2.12	0.60
1:A:318:PHE:CE1	1:A:620:VAL:HG11	2.36	0.60
1:A:1012:LEU:HB3	1:C:1013:ILE:HD13	1.82	0.60
1:B:164:ASN:OD1	1:B:165:ASN:CG	2.39	0.60
1:B:597:VAL:HG12	1:B:599:THR:HG23	1.82	0.60
1:C:105:ILE:HD12	1:C:105:ILE:N	2.16	0.60
1:C:309:GLU:OE1	1:C:309:GLU:HA	2.02	0.60
1:C:378:LYS:HD2	1:C:433:VAL:CG1	2.25	0.60
1:C:423:TYR:CE2	1:C:425:LEU:HD21	2.36	0.60
1:A:128:ILE:C	1:A:129:LYS:CG	2.70	0.60
1:A:709:ASN:OD1	1:A:709:ASN:N	2.34	0.60
1:B:1088:HIS:NE2	1:B:1137:VAL:HG21	2.16	0.60
1:A:330:PRO:CA	1:A:580:GLN:HE22	2.13	0.60
1:A:612:TYR:HB3	1:A:615:VAL:CG2	2.31	0.60
1:A:1082:CYS:HB2	1:A:1132:ILE:HD13	1.83	0.60
1:A:330:PRO:HA	1:A:580:GLN:NE2	2.12	0.60
1:A:896:ILE:CD1	1:C:712:ILE:CD1	2.80	0.60
1:B:738:CYS:SG	1:B:760:CYS:C	2.80	0.60
1:B:1139:ASP:OD1	1:B:1141:LEU:HB3	2.01	0.60
1:C:86:PHE:CE2	1:C:106:PHE:HE2	2.20	0.60
1:C:774:GLN:OE1	1:C:774:GLN:HA	2.02	0.60
1:A:31:SER:HB3	1:A:216:LEU:HD22	1.82	0.59
1:A:353:TRP:HZ2	1:A:466:ARG:N	1.99	0.59
1:A:919:ASN:O	1:A:923:ILE:HG13	2.02	0.59
1:C:366:SER:O	1:C:370:ASN:HB2	2.01	0.59
1:A:369:TYR:OH	1:A:384:PRO:HB2	2.02	0.59
1:B:128:ILE:C	1:B:129:LYS:CG	2.70	0.59
1:B:327:VAL:CG1	1:B:329:PHE:CE2	2.84	0.59
1:B:676:THR:HA	1:B:690:GLN:HG2	1.84	0.59
1:C:105:ILE:CG2	1:C:118:LEU:HD13	2.31	0.59
1:C:546:LEU:HD12	1:C:565:PHE:CE1	2.36	0.59
1:A:403:ARG:HD3	1:A:495:TYR:CE1	2.37	0.59
1:A:403:ARG:CD	1:A:495:TYR:HE1	2.14	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:718:PHE:HZ	1:B:923:ILE:CG1	2.14	0.59
1:B:722:VAL:HG12	1:B:934:ILE:HG13	1.83	0.59
1:C:273:ARG:HH12	1:C:292:ALA:CB	2.13	0.59
1:C:610:VAL:HB	1:C:651:ILE:HD11	1.83	0.59
1:A:104:TRP:O	1:A:118:LEU:CD1	2.49	0.59
1:A:203:ILE:HG21	1:A:227:VAL:CG2	2.33	0.59
1:C:741:TYR:CZ	1:C:966:LEU:CD2	2.84	0.59
1:A:755:GLN:O	1:C:968:SER:OG	2.20	0.59
1:A:800:PHE:CE2	1:A:927:PHE:HD2	2.21	0.59
1:C:95:THR:OG1	1:C:186:PHE:HB3	2.03	0.59
1:C:118:LEU:CA	1:C:119:ILE:HD12	2.32	0.59
1:C:718:PHE:HZ	1:C:923:ILE:HG12	1.68	0.59
1:C:718:PHE:HD2	1:C:1109:PHE:CE1	2.20	0.59
1:C:729:VAL:HG21	1:C:782:PHE:HE1	1.67	0.59
1:C:856:ASN:O	1:C:858:LEU:CD1	2.48	0.59
1:A:825:LYS:HB2	1:A:945:LEU:HD12	1.83	0.59
1:B:226:LEU:CD1	1:B:227:VAL:HG13	2.33	0.59
1:C:103:GLY:HA2	1:C:104:TRP:CE3	2.37	0.59
1:A:93:ALA:O	1:A:266:TYR:HD1	1.85	0.59
1:A:314:GLN:HG3	1:A:314:GLN:O	2.03	0.59
1:A:900:MET:CE	1:C:1094:VAL:HG23	2.33	0.59
1:B:106:PHE:C	1:B:235:ILE:HD13	2.23	0.59
1:C:119:ILE:HG13	1:C:128:ILE:HA	1.85	0.59
1:C:716:THR:N	1:C:1071:GLN:O	2.36	0.59
1:A:1043:CYS:HA	1:A:1064:HIS:HE1	1.68	0.59
1:B:275:PHE:HE1	1:B:290:ASP:HB2	1.68	0.59
1:B:584:ILE:H	1:B:584:ILE:CD1	2.16	0.59
1:C:37:TYR:CB	1:C:223:LEU:HG	2.32	0.59
1:C:382:VAL:HG13	1:C:390:LEU:HD21	1.85	0.59
1:A:541:PHE:CE2	1:A:587:ILE:CD1	2.84	0.59
1:A:598:ILE:HD12	1:A:598:ILE:N	2.17	0.59
1:C:123:ALA:O	1:C:175:PHE:O	2.21	0.59
1:A:107:GLY:HA2	1:A:235:ILE:CG2	2.19	0.59
1:A:437:ASN:HA	1:A:508:TYR:HD1	1.68	0.59
1:B:654:GLU:OE1	1:B:654:GLU:HA	2.02	0.59
1:C:726:ILE:HD13	1:C:1061:VAL:HG22	1.82	0.59
1:A:322:PRO:HB3	1:A:539:VAL:CA	2.33	0.58
1:B:822:LEU:HD23	1:B:1056:ALA:HB2	1.84	0.58
1:C:43:PHE:HE1	1:C:45:SER:HB3	1.67	0.58
1:C:186:PHE:O	1:C:211:ASN:ND2	2.36	0.58
1:C:360:ASN:H	1:C:523:THR:HG23	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:805:ILE:HD11	1:C:1063:LEU:HD12	1.84	0.58
4:A:1308:NAG:O7	4:A:1308:NAG:O3	2.20	0.58
1:B:1054:GLN:OE1	1:B:1054:GLN:HA	2.03	0.58
1:C:442:ASP:OD2	1:C:507:PRO:HB2	2.03	0.58
1:A:117:LEU:HD13	1:A:201:PHE:CD2	2.39	0.58
1:A:552:LEU:CD2	1:A:587:ILE:HD11	2.25	0.58
1:A:981:LEU:HD21	1:A:993:ILE:HD11	1.84	0.58
1:B:104:TRP:O	1:B:118:LEU:CD1	2.49	0.58
1:B:645:THR:O	1:B:646:ARG:C	2.42	0.58
1:B:708:SER:HB2	1:B:711:SER:OG	2.02	0.58
1:C:404:GLY:CA	1:C:508:TYR:HD2	2.11	0.58
1:A:741:TYR:CE2	1:A:962:LEU:HG	2.38	0.58
1:A:970:PHE:CD2	1:A:999:GLY:CA	2.79	0.58
1:B:85:PRO:O	1:B:269:TYR:CZ	2.56	0.58
1:B:599:THR:HA	1:B:608:VAL:HG12	1.84	0.58
1:B:1080:ALA:O	1:B:1132:ILE:CG1	2.46	0.58
1:C:497:PHE:CE1	1:C:507:PRO:HB3	2.39	0.58
1:A:791:THR:CG2	1:A:792:PRO:HD2	2.34	0.58
1:B:356:LYS:HB3	1:B:397:ALA:HB3	1.86	0.58
1:C:401:VAL:HG22	1:C:509:ARG:HA	1.86	0.58
1:C:490:PHE:CE2	1:C:492:LEU:CD2	2.84	0.58
1:C:805:ILE:CG2	1:C:878:LEU:HD13	2.34	0.58
1:A:353:TRP:CD1	1:A:466:ARG:CG	2.87	0.58
1:A:1054:GLN:OE1	1:A:1054:GLN:HA	2.04	0.58
1:A:1102:TRP:CZ2	1:A:1133:VAL:HG21	2.38	0.58
1:B:277:LEU:HD23	1:B:288:ALA:CB	2.34	0.58
1:B:559:PHE:CG	1:B:584:ILE:HG12	2.39	0.58
1:A:29:THR:O	1:A:62:VAL:HG13	2.03	0.58
1:A:804:GLN:OE1	1:A:931:ILE:HG22	2.03	0.58
1:B:58:PHE:CD1	1:B:290:ASP:HB2	2.38	0.58
1:B:1126:CYS:SG	1:B:1132:ILE:HD13	2.44	0.58
1:C:37:TYR:CD2	1:C:204:TYR:CE2	2.91	0.58
1:C:360:ASN:HD22	1:C:523:THR:CG2	2.16	0.58
1:C:409:GLN:HE21	1:C:409:GLN:H	1.51	0.58
1:A:123:ALA:O	1:A:175:PHE:O	2.20	0.58
1:A:536:ASN:HD22	1:A:536:ASN:N	2.02	0.58
1:A:612:TYR:HB3	1:A:615:VAL:HG22	1.86	0.58
1:A:695:TYR:H	1:A:695:TYR:HD1	1.47	0.58
1:A:1101:HIS:HB2	1:A:1103:PHE:CZ	2.39	0.58
1:C:220:PHE:CD2	1:C:287:ASP:HA	2.38	0.58
1:C:352:ALA:HB1	1:C:468:ILE:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:521:PRO:HG3	1:C:564:GLN:HG3	1.83	0.58
1:A:931:ILE:O	1:A:934:ILE:CG2	2.51	0.58
1:B:321:GLN:CD	1:B:321:GLN:H	2.08	0.58
1:B:329:PHE:CD2	1:B:528:LYS:CB	2.86	0.58
1:B:600:PRO:HD3	1:B:692:ILE:HD11	1.86	0.58
1:C:210:ILE:O	1:C:212:LEU:HD23	2.02	0.58
1:C:417:LYS:O	1:C:421:TYR:HB2	2.03	0.58
1:C:1115:ILE:H	1:C:1115:ILE:CD1	2.14	0.58
1:A:55:PHE:HB3	1:A:275:PHE:HE2	1.67	0.58
1:A:216:LEU:HD12	1:A:216:LEU:N	2.18	0.58
1:B:123:ALA:O	1:B:175:PHE:O	2.20	0.58
1:B:1104:VAL:CG1	1:B:1119:ASN:HD22	1.83	0.58
1:C:615:VAL:CG2	1:C:649:CYS:H	2.16	0.58
1:C:1102:TRP:CB	1:C:1135:ASN:OD1	2.42	0.58
1:B:119:ILE:CG2	1:B:120:VAL:N	2.66	0.57
1:B:555:SER:HB2	1:B:586:ASP:N	2.19	0.57
1:B:922:LEU:HD12	1:B:922:LEU:O	2.04	0.57
1:C:534:VAL:HG11	1:C:539:VAL:HG21	1.86	0.57
1:A:927:PHE:O	1:A:927:PHE:HD1	1.86	0.57
1:B:274:THR:O	1:B:291:CYS:HB2	2.04	0.57
1:B:1072:GLU:HG2	1:C:894:LEU:HD22	1.83	0.57
1:C:97:LYS:C	1:C:97:LYS:HD3	2.23	0.57
1:C:106:PHE:CZ	1:C:194:PHE:CD2	2.92	0.57
1:C:210:ILE:CB	1:C:212:LEU:CD2	2.72	0.57
1:A:86:PHE:CE1	1:A:235:ILE:HD13	2.39	0.57
1:A:985:ASP:CG	1:A:986:PRO:HD2	2.24	0.57
1:B:718:PHE:HB3	1:B:1067:TYR:OH	2.04	0.57
1:B:1142:GLN:HB3	1:B:1143:PRO:HD3	1.87	0.57
1:C:185:ASN:ND2	1:C:211:ASN:HD21	2.01	0.57
1:A:357:ARG:HG2	1:A:357:ARG:NH1	2.19	0.57
1:A:487:ASN:HA	1:A:489:TYR:HE1	1.68	0.57
1:A:914:ASN:O	1:A:918:GLU:HG3	2.04	0.57
1:A:1029:MET:HE1	1:A:1053:PRO:HG3	1.87	0.57
1:C:453:TYR:OH	1:C:493:GLN:NE2	2.38	0.57
1:B:1081:ILE:CD1	1:B:1133:VAL:HG23	2.25	0.57
1:C:390:LEU:HD12	1:C:390:LEU:O	2.04	0.57
1:A:87:ASN:ND2	1:A:269:TYR:HE2	1.92	0.57
1:A:896:ILE:HD12	1:A:897:PRO:CD	2.34	0.57
1:B:560:LEU:N	1:B:563:GLN:OE1	2.34	0.57
1:C:318:PHE:HZ	1:C:615:VAL:HG12	1.70	0.57
2:O:1:NAG:H2	2:O:1:NAG:O6	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ILE:CG2	1:A:120:VAL:N	2.67	0.57
1:C:328:ARG:HH21	1:C:578:ASP:CG	2.07	0.57
1:C:498:GLN:HG3	1:C:499:PRO:HD2	1.85	0.57
1:A:329:PHE:HB3	1:A:330:PRO:HD2	1.86	0.57
1:A:421:TYR:HB3	1:A:454:ARG:HD2	1.86	0.57
1:B:119:ILE:HG22	1:B:120:VAL:N	2.20	0.57
1:B:805:ILE:CG2	1:B:878:LEU:CD1	2.82	0.57
1:B:815:ARG:NH1	1:B:823:PHE:CD1	2.73	0.57
1:C:523:THR:HG23	1:C:523:THR:O	2.04	0.57
1:C:817:PHE:CE1	1:C:935:GLN:HG3	2.39	0.57
1:A:36:VAL:HG21	1:A:220:PHE:CE1	2.40	0.57
1:A:619:GLU:OE1	1:A:619:GLU:HA	2.05	0.57
1:B:277:LEU:HD23	1:B:288:ALA:HB2	1.87	0.57
1:B:325:SER:HA	1:B:540:ASN:O	2.04	0.57
1:B:533:LEU:CD1	1:B:552:LEU:CD1	2.83	0.57
1:B:770:ILE:CD1	1:B:1012:LEU:CD1	2.71	0.57
1:B:826:VAL:CG2	1:B:945:LEU:HD13	2.34	0.57
1:C:212:LEU:HD22	1:C:212:LEU:N	2.19	0.57
1:C:490:PHE:CE2	1:C:492:LEU:CB	2.73	0.57
1:A:472:ILE:HA	1:A:491:PRO:HD3	1.85	0.57
1:B:422:ASN:HD21	1:B:453:TYR:HA	1.69	0.57
1:C:391:CYS:HB3	1:C:545:GLY:HA3	1.87	0.57
1:A:277:LEU:HD23	1:A:288:ALA:HB1	1.86	0.56
1:A:886:TRP:HB2	1:A:1035:GLY:N	2.20	0.56
1:A:993:ILE:O	1:A:997:ILE:HG13	2.05	0.56
1:B:776:LYS:HZ2	1:B:780:GLU:CG	2.12	0.56
1:B:909:ILE:CG2	1:B:1036:GLN:HE22	2.18	0.56
1:C:276:LEU:HD23	1:C:276:LEU:C	2.25	0.56
1:C:429:PHE:HE2	1:C:514:SER:HB2	1.70	0.56
1:C:1078:ALA:N	1:C:1102:TRP:HH2	2.02	0.56
1:A:353:TRP:NE1	1:A:466:ARG:CD	2.61	0.56
1:A:890:ALA:HA	1:C:1046:GLY:CA	2.35	0.56
1:B:57:PRO:HA	1:B:273:ARG:NH1	2.18	0.56
1:B:1094:VAL:HG23	1:C:900:MET:HE2	1.87	0.56
1:C:36:VAL:HG21	1:C:220:PHE:HE1	1.69	0.56
1:C:472:ILE:HD11	1:C:482:GLY:N	2.12	0.56
1:A:119:ILE:HG22	1:A:120:VAL:N	2.21	0.56
1:A:408:ARG:O	1:A:414:GLN:NE2	2.38	0.56
1:A:611:LEU:HB2	1:A:650:LEU:HD12	1.85	0.56
1:A:741:TYR:OH	1:A:962:LEU:CD1	2.53	0.56
1:A:797:PHE:CD1	1:A:882:ILE:CG2	2.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:800:PHE:HE2	1:A:927:PHE:HD2	1.53	0.56
1:A:864:LEU:HD13	1:C:665:PRO:HB2	1.87	0.56
1:C:37:TYR:CE2	1:C:204:TYR:CE2	2.93	0.56
1:C:434:ILE:N	1:C:434:ILE:HD12	2.21	0.56
1:A:800:PHE:CD2	1:A:927:PHE:CD2	2.93	0.56
1:B:103:GLY:H	1:B:241:LEU:HB2	1.70	0.56
1:B:273:ARG:HH11	1:B:273:ARG:HG3	1.70	0.56
1:B:804:GLN:OE1	1:B:804:GLN:N	2.37	0.56
1:B:900:MET:HG2	1:B:917:TYR:OH	2.06	0.56
1:C:204:TYR:HD1	1:C:225:PRO:HB3	1.65	0.56
1:A:164:ASN:ND2	2:K:1:NAG:C6	2.69	0.56
1:A:203:ILE:HG22	1:A:227:VAL:CG2	2.32	0.56
1:A:238:PHE:C	1:A:238:PHE:HD1	2.09	0.56
1:A:825:LYS:CB	1:A:945:LEU:HD12	2.36	0.56
1:A:905:ARG:CD	1:A:1049:LEU:O	2.35	0.56
1:B:645:THR:O	1:B:647:ALA:N	2.38	0.56
1:B:714:ILE:CG2	1:B:1110:TYR:HB2	2.35	0.56
1:B:1039:ARG:NH2	1:B:1042:PHE:CD2	2.70	0.56
1:C:393:THR:HG23	1:C:522:ALA:CA	2.35	0.56
1:C:1090:PRO:HD3	1:C:1095:PHE:CE2	2.40	0.56
1:B:44:ARG:NH1	1:B:279:TYR:OH	2.38	0.56
1:A:611:LEU:HG	1:A:611:LEU:O	2.06	0.56
1:A:1081:ILE:HD12	1:A:1133:VAL:HG23	1.88	0.56
1:B:1090:PRO:HB2	1:B:1093:GLY:O	2.04	0.56
1:C:882:ILE:HA	1:C:898:PHE:HE1	1.71	0.56
1:A:353:TRP:CZ2	1:A:466:ARG:N	2.73	0.56
1:A:697:MET:HE3	1:B:869:MET:SD	2.45	0.56
1:A:896:ILE:CD1	1:C:712:ILE:HD12	2.36	0.56
1:B:31:SER:OG	1:B:60:SER:O	2.16	0.56
1:C:817:PHE:HE1	1:C:935:GLN:CG	2.18	0.56
1:A:402:ILE:HD11	1:A:418:ILE:HG21	1.87	0.56
1:A:890:ALA:HA	1:C:1046:GLY:HA3	1.87	0.56
1:B:422:ASN:ND2	1:B:454:ARG:H	2.03	0.56
1:B:1088:HIS:HE1	1:B:1122:VAL:CG2	2.18	0.56
1:C:581:THR:HG22	1:C:583:GLU:CG	2.31	0.56
1:C:817:PHE:HE1	1:C:935:GLN:HG3	1.71	0.56
1:C:1103:PHE:HE1	1:C:1114:ILE:HD12	1.66	0.56
1:A:141:LEU:N	1:A:241:LEU:HD11	2.20	0.55
1:A:654:GLU:HG3	1:A:693:ILE:HG22	1.87	0.55
1:C:452:LEU:HD22	1:C:492:LEU:HD12	1.87	0.55
1:C:988:GLU:HA	1:C:988:GLU:OE2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:675:GLN:O	1:A:693:ILE:HD12	2.05	0.55
1:A:690:GLN:OE1	1:A:690:GLN:HA	2.06	0.55
1:A:725:GLU:OE2	1:A:1028:LYS:CE	2.54	0.55
1:B:240:THR:HG22	1:B:241:LEU:N	2.20	0.55
1:B:909:ILE:HG22	1:B:1036:GLN:NE2	2.20	0.55
1:A:296:LEU:HD12	1:A:296:LEU:O	2.06	0.55
1:A:324:GLU:H	1:A:539:VAL:HG12	1.71	0.55
1:A:976:VAL:CG1	1:A:979:ASP:CB	2.84	0.55
1:C:230:PRO:HD2	1:C:231:ILE:HD12	1.88	0.55
1:C:330:PRO:CD	1:C:544:ASN:HD21	2.15	0.55
1:C:1028:LYS:HG2	1:C:1042:PHE:CE2	2.41	0.55
1:A:90:VAL:CG1	1:A:194:PHE:C	2.75	0.55
1:A:1081:ILE:HG23	1:A:1133:VAL:O	2.06	0.55
1:A:1085:GLY:C	1:A:1126:CYS:SG	2.84	0.55
1:B:726:ILE:HD13	1:B:1061:VAL:HG13	1.87	0.55
1:B:743:CYS:SG	1:B:750:SER:HA	2.46	0.55
1:C:270:LEU:HD12	1:C:270:LEU:N	2.20	0.55
1:A:43:PHE:CE2	1:A:282:ASN:O	2.51	0.55
1:A:92:PHE:HE1	1:A:94:SER:CB	2.19	0.55
1:C:128:ILE:C	1:C:129:LYS:HG2	2.26	0.55
1:C:558:LYS:HD2	1:C:558:LYS:H	1.72	0.55
1:C:733:LYS:CD	1:C:775:ASP:OD1	2.55	0.55
1:C:931:ILE:HA	1:C:934:ILE:CG2	2.36	0.55
1:C:1091:ARG:CB	1:C:1119:ASN:O	2.54	0.55
1:A:296:LEU:HB2	1:A:608:VAL:HG11	1.89	0.55
1:B:64:TRP:HD1	1:B:65:PHE:H	1.52	0.55
1:C:451:TYR:C	1:C:452:LEU:HD12	2.26	0.55
1:C:1102:TRP:C	1:C:1115:ILE:HD11	2.27	0.55
1:A:201:PHE:CD1	1:A:202:LYS:N	2.73	0.55
1:A:318:PHE:HE1	1:A:620:VAL:HG11	1.70	0.55
1:A:886:TRP:HB2	1:A:1035:GLY:H	1.72	0.55
1:B:34:ARG:HH12	1:B:189:LEU:HD21	1.72	0.55
1:B:773:GLU:OE2	1:B:1019:ARG:CZ	2.54	0.55
1:B:1102:TRP:CH2	1:B:1133:VAL:HG21	2.41	0.55
1:C:992:GLN:OE1	1:C:992:GLN:HA	2.07	0.55
1:A:322:PRO:HG3	1:A:549:THR:CG2	2.37	0.55
1:A:697:MET:O	1:A:697:MET:HG2	2.05	0.55
1:A:741:TYR:CZ	1:A:966:LEU:HD21	2.42	0.55
1:A:822:LEU:CD2	1:A:945:LEU:HD21	2.29	0.55
1:B:1039:ARG:NE	1:C:1031:GLU:OE2	2.36	0.55
1:C:33:THR:CB	1:C:58:PHE:HE2	2.15	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:ARG:O	1:C:56:LEU:HD23	2.05	0.55
1:C:644:GLN:HA	1:C:644:GLN:HE21	1.69	0.55
1:A:802:PHE:CD2	1:A:882:ILE:HD13	2.42	0.55
1:A:902:MET:HG3	1:A:916:LEU:HD11	1.88	0.55
1:C:741:TYR:OH	1:C:962:LEU:HD12	2.07	0.55
1:A:471:GLU:O	1:A:491:PRO:HG3	2.06	0.55
1:A:535:LYS:C	1:A:536:ASN:HD22	2.10	0.55
1:A:886:TRP:HB2	1:A:1035:GLY:CA	2.37	0.55
1:A:962:LEU:O	1:A:965:GLN:HB2	2.07	0.55
1:A:1047:TYR:HD1	1:A:1067:TYR:O	1.90	0.55
1:B:64:TRP:HD1	1:B:65:PHE:N	2.05	0.55
1:C:101:ILE:HD12	1:C:101:ILE:N	2.22	0.55
1:C:102:ARG:NE	1:C:141:LEU:HD22	2.22	0.55
1:C:905:ARG:HD2	1:C:1050:MET:HE3	1.88	0.55
1:A:34:ARG:CZ	1:A:217:PRO:CG	2.66	0.54
1:A:90:VAL:HG13	1:A:194:PHE:CB	2.34	0.54
1:A:381:GLY:O	1:B:983:ARG:NH1	2.40	0.54
1:B:560:LEU:O	1:B:563:GLN:HG2	2.06	0.54
1:C:89:GLY:O	1:C:270:LEU:CD1	2.52	0.54
1:C:277:LEU:HD22	1:C:285:ILE:HG21	1.89	0.54
1:C:423:TYR:CE2	1:C:425:LEU:CD2	2.90	0.54
1:A:663:ASP:N	1:A:695:TYR:OH	2.41	0.54
1:A:963:VAL:CG1	1:C:570:ALA:HB1	2.37	0.54
1:C:454:ARG:NH2	1:C:467:ASP:CG	2.51	0.54
1:C:581:THR:CG2	1:C:583:GLU:CD	2.72	0.54
1:C:915:VAL:HG23	1:C:1111:GLU:OE2	2.08	0.54
1:C:1001:LEU:O	1:C:1001:LEU:HD13	2.07	0.54
1:A:546:LEU:CD2	1:A:565:PHE:CE1	2.91	0.54
1:B:107:GLY:C	1:B:235:ILE:HG23	2.24	0.54
1:B:240:THR:CG2	1:B:241:LEU:N	2.70	0.54
1:B:905:ARG:HD2	1:B:1049:LEU:O	2.08	0.54
1:C:328:ARG:HB2	1:C:543:PHE:HD1	1.71	0.54
1:C:972:ALA:HB3	1:C:996:LEU:CD1	2.29	0.54
1:A:302:THR:HG21	1:A:315:THR:HA	1.89	0.54
1:A:804:GLN:O	1:A:816:SER:HB3	2.08	0.54
1:A:931:ILE:O	1:A:934:ILE:HG23	2.07	0.54
1:B:226:LEU:HG	1:B:227:VAL:HG22	1.88	0.54
1:B:454:ARG:NH1	1:B:469:SER:OG	2.40	0.54
1:B:866:THR:HG22	1:B:869:MET:SD	2.48	0.54
1:B:882:ILE:HG23	1:B:898:PHE:HD2	1.72	0.54
1:B:1140:PRO:C	1:B:1143:PRO:HD2	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1141:LEU:HD23	1:B:1141:LEU:C	2.28	0.54
1:C:643:PHE:HE1	1:C:655:HIS:CD2	2.26	0.54
1:A:357:ARG:HG3	1:A:396:TYR:HE1	1.71	0.54
1:B:718:PHE:CZ	1:B:923:ILE:HG12	2.43	0.54
1:B:874:THR:HG21	1:B:1055:SER:HB3	1.89	0.54
1:C:741:TYR:CZ	1:C:962:LEU:HD11	2.43	0.54
1:C:896:ILE:HG13	1:C:897:PRO:CD	2.37	0.54
1:A:101:ILE:HG13	1:A:242:LEU:HD13	1.90	0.54
1:A:1102:TRP:CE2	1:A:1133:VAL:HG21	2.42	0.54
1:C:490:PHE:HE2	1:C:492:LEU:CG	2.19	0.54
1:C:497:PHE:CE1	1:C:507:PRO:CB	2.91	0.54
1:C:560:LEU:CD1	1:C:562:PHE:CZ	2.89	0.54
1:A:235:ILE:HD12	1:A:235:ILE:N	2.18	0.54
1:A:1029:MET:HB2	1:A:1062:PHE:CE2	2.43	0.54
1:C:725:GLU:CD	1:C:1028:LYS:NZ	2.60	0.54
1:A:229:LEU:HD12	1:A:229:LEU:N	2.23	0.54
1:A:659:SER:HB2	1:A:698:SER:HB3	1.89	0.54
1:A:712:ILE:HD13	1:A:1094:VAL:HG21	1.90	0.54
1:A:726:ILE:CG2	1:A:948:LEU:HG	2.38	0.54
1:A:1081:ILE:HG13	1:A:1095:PHE:CE2	2.43	0.54
1:B:1090:PRO:N	1:B:1095:PHE:HE1	2.05	0.54
1:B:1125:ASN:OD1	1:B:1125:ASN:N	2.41	0.54
1:C:353:TRP:CD1	1:C:466:ARG:HB3	2.41	0.54
1:C:480:CYS:HA	1:C:483:VAL:HG12	1.89	0.54
1:C:1054:GLN:OE1	1:C:1054:GLN:HA	2.08	0.54
1:A:661:GLU:O	1:A:695:TYR:CE2	2.61	0.54
1:A:1090:PRO:HG3	1:A:1093:GLY:O	2.08	0.54
1:B:318:PHE:HE2	1:B:615:VAL:CG2	2.04	0.54
1:B:882:ILE:HG23	1:B:898:PHE:CE2	2.42	0.54
1:C:692:ILE:H	1:C:692:ILE:CD1	2.19	0.54
1:C:930:ALA:O	1:C:934:ILE:HG22	2.08	0.54
1:B:774:GLN:OE1	1:B:774:GLN:HA	2.08	0.54
1:C:404:GLY:CA	1:C:508:TYR:CD2	2.90	0.54
1:C:409:GLN:H	1:C:409:GLN:NE2	2.05	0.54
1:C:915:VAL:CG2	1:C:1111:GLU:OE2	2.56	0.54
1:C:1068:VAL:O	1:C:1068:VAL:HG23	2.08	0.54
1:A:426:PRO:HD2	1:A:429:PHE:HB2	1.88	0.53
1:A:662:CYS:SG	1:A:697:MET:SD	3.06	0.53
1:B:43:PHE:CD1	1:B:43:PHE:C	2.80	0.53
1:B:976:VAL:HB	1:B:979:ASP:HB3	1.90	0.53
1:B:1105:THR:OG1	1:B:1111:GLU:O	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:ASN:O	1:C:361:CYS:HB3	2.07	0.53
1:C:1033:VAL:CG2	1:C:1062:PHE:CE1	2.85	0.53
1:A:1043:CYS:CA	1:A:1064:HIS:CE1	2.91	0.53
1:B:280:ASN:HB3	1:B:286:THR:CG2	2.39	0.53
1:B:726:ILE:CG2	1:B:948:LEU:HG	2.37	0.53
1:C:861:LEU:HD22	1:C:861:LEU:H	1.74	0.53
1:A:693:ILE:CD1	1:A:693:ILE:H	2.19	0.53
1:B:48:LEU:HD12	1:B:48:LEU:N	2.24	0.53
1:C:365:TYR:HD2	1:C:387:LEU:HD13	1.73	0.53
1:C:429:PHE:CZ	1:C:431:GLY:C	2.82	0.53
1:C:857:GLY:C	1:C:858:LEU:HD12	2.29	0.53
1:B:289:VAL:HG23	1:B:306:PHE:HE2	1.70	0.53
1:B:722:VAL:CG1	1:B:934:ILE:HG13	2.38	0.53
1:C:410:ILE:O	1:C:410:ILE:HG22	2.08	0.53
1:C:742:ILE:HD12	1:C:753:LEU:HD21	1.89	0.53
1:B:712:ILE:HD12	1:C:896:ILE:HD12	1.90	0.53
1:B:885:GLY:HA2	1:B:901:GLN:HE22	1.64	0.53
1:C:104:TRP:CE3	1:C:104:TRP:N	2.77	0.53
1:C:168:PHE:CE2	1:C:231:ILE:HD11	2.43	0.53
1:B:29:THR:HG23	1:B:62:VAL:HG12	1.89	0.53
1:B:57:PRO:HB3	1:B:273:ARG:HH22	1.74	0.53
1:B:563:GLN:NE2	1:C:43:PHE:CB	2.71	0.53
1:B:1011:GLN:HE21	1:B:1011:GLN:CA	2.19	0.53
1:B:1078:ALA:CB	1:B:1133:VAL:HG22	2.38	0.53
1:C:612:TYR:HB2	1:C:615:VAL:HG13	1.74	0.53
1:C:660:TYR:N	1:C:660:TYR:CD1	2.77	0.53
1:B:707:TYR:HE1	1:C:897:PRO:HA	1.74	0.53
1:B:1039:ARG:CZ	1:B:1042:PHE:HD2	2.16	0.53
1:B:1072:GLU:HG2	1:C:894:LEU:HD21	1.87	0.53
1:A:712:ILE:HG13	1:B:896:ILE:HG13	1.90	0.53
1:C:524:VAL:O	1:C:524:VAL:HG12	2.09	0.53
1:C:729:VAL:HG13	1:C:781:VAL:HG21	1.91	0.53
1:A:67:ALA:CB	1:A:263:ALA:HB3	2.27	0.53
1:A:273:ARG:HH21	1:A:292:ALA:CB	2.22	0.53
1:A:357:ARG:HG3	1:A:396:TYR:CD1	2.44	0.53
1:B:353:TRP:O	1:B:466:ARG:NH2	2.42	0.53
1:C:185:ASN:ND2	1:C:211:ASN:ND2	2.56	0.53
1:C:452:LEU:CD2	1:C:492:LEU:HB3	2.34	0.53
1:C:494:SER:OG	1:C:495:TYR:N	2.41	0.53
1:C:611:LEU:HD23	1:C:611:LEU:C	2.28	0.53
1:A:570:ALA:HB1	1:B:963:VAL:CG1	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:817:PHE:CZ	1:A:935:GLN:NE2	2.77	0.53
1:A:922:LEU:HD11	1:A:926:GLN:HE21	1.72	0.53
1:C:353:TRP:CD1	1:C:466:ARG:HD3	2.43	0.53
1:C:442:ASP:OD2	1:C:507:PRO:CB	2.57	0.53
1:C:719:THR:HG23	1:C:1070:ALA:HB2	1.90	0.53
1:A:241:LEU:HD12	1:A:241:LEU:C	2.26	0.52
1:A:612:TYR:HE1	1:A:651:ILE:HD12	1.74	0.52
1:A:779:GLN:HE21	1:A:864:LEU:HD23	1.73	0.52
1:B:351:TYR:CE1	1:B:452:LEU:HB2	2.44	0.52
1:C:269:TYR:CD1	1:C:269:TYR:N	2.77	0.52
1:A:472:ILE:HG23	1:A:489:TYR:O	2.09	0.52
1:A:722:VAL:HA	1:A:1064:HIS:O	2.08	0.52
1:A:782:PHE:HE2	1:A:874:THR:HG21	1.71	0.52
1:A:895:GLN:H	1:A:895:GLN:CD	2.06	0.52
1:B:195:LYS:HG2	1:B:202:LYS:HB2	1.90	0.52
1:B:599:THR:HG22	1:B:608:VAL:HB	1.87	0.52
1:B:1101:HIS:HB3	1:B:1103:PHE:CZ	2.45	0.52
1:C:318:PHE:HE2	1:C:612:TYR:HB3	1.74	0.52
1:C:328:ARG:NH2	1:C:578:ASP:CG	2.62	0.52
1:C:355:ARG:NH2	1:C:396:TYR:CG	2.77	0.52
1:C:546:LEU:HD23	1:C:546:LEU:C	2.29	0.52
1:C:770:ILE:HG23	1:C:774:GLN:HE21	1.73	0.52
1:A:403:ARG:CG	1:A:495:TYR:HE1	2.22	0.52
1:A:799:GLY:O	1:A:924:ALA:HB1	2.10	0.52
1:B:599:THR:CA	1:B:608:VAL:HG12	2.39	0.52
1:B:733:LYS:HD3	1:B:775:ASP:OD1	2.10	0.52
1:B:1116:THR:CG2	1:B:1140:PRO:HD3	2.36	0.52
1:C:220:PHE:CE1	1:C:288:ALA:HB3	2.44	0.52
1:C:368:LEU:HD12	1:C:368:LEU:N	2.25	0.52
1:B:55:PHE:CB	1:B:275:PHE:CE2	2.88	0.52
1:B:1095:PHE:CZ	1:B:1120:THR:CG2	2.88	0.52
1:C:328:ARG:HB2	1:C:543:PHE:CD1	2.44	0.52
1:C:360:ASN:HD22	1:C:523:THR:HG22	1.75	0.52
1:A:582:LEU:HD22	1:A:582:LEU:N	2.24	0.52
1:A:800:PHE:CE2	1:A:927:PHE:CD2	2.98	0.52
1:A:922:LEU:CD1	1:A:926:GLN:HE21	2.22	0.52
1:A:1088:HIS:ND1	1:A:1122:VAL:HG12	2.19	0.52
1:B:63:THR:O	1:B:63:THR:OG1	2.27	0.52
1:B:1134:ASN:OD1	1:B:1134:ASN:N	2.42	0.52
1:C:388:ASN:HD22	1:C:388:ASN:N	2.07	0.52
1:C:490:PHE:CD2	1:C:492:LEU:N	2.76	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:660:TYR:HB2	1:C:695:TYR:CZ	2.44	0.52
1:C:660:TYR:H	1:C:695:TYR:HE2	1.54	0.52
1:C:661:GLU:OE1	1:C:661:GLU:N	2.25	0.52
1:A:712:ILE:CB	1:A:1077:THR:HG21	2.29	0.52
1:A:896:ILE:HD12	1:A:897:PRO:HD3	1.92	0.52
1:B:103:GLY:O	1:B:240:THR:HG23	2.09	0.52
1:B:204:TYR:HE1	1:B:225:PRO:CB	2.08	0.52
1:B:949:GLN:OE1	1:B:949:GLN:HA	2.10	0.52
1:C:87:ASN:ND2	1:C:269:TYR:HD2	1.92	0.52
1:C:360:ASN:N	1:C:360:ASN:HD22	2.05	0.52
1:C:718:PHE:CZ	1:C:923:ILE:CG1	2.89	0.52
1:A:318:PHE:CE1	1:A:620:VAL:HG21	2.45	0.52
1:A:805:ILE:O	1:A:816:SER:CB	2.57	0.52
1:B:763:LEU:HD22	1:B:1008:VAL:CG2	2.39	0.52
1:B:805:ILE:CG2	1:B:878:LEU:HD11	2.40	0.52
1:B:1090:PRO:HB3	1:B:1093:GLY:O	2.10	0.52
1:C:378:LYS:HG3	1:C:433:VAL:CG1	2.09	0.52
1:C:825:LYS:NZ	1:C:942:ALA:CA	2.73	0.52
1:C:1089:PHE:O	1:C:1120:THR:CA	2.57	0.52
1:A:106:PHE:CZ	1:A:194:PHE:CD2	2.90	0.52
1:A:273:ARG:NH2	1:A:292:ALA:CB	2.72	0.52
1:A:280:ASN:HB2	1:A:286:THR:HG23	1.91	0.52
1:A:521:PRO:HG3	1:A:564:GLN:CB	2.40	0.52
1:A:712:ILE:HD12	1:A:1094:VAL:HG21	1.90	0.52
1:A:1041:ASP:HB3	1:B:1030:SER:OG	2.09	0.52
1:B:65:PHE:HB2	1:B:265:TYR:CE1	2.45	0.52
1:B:265:TYR:N	1:B:265:TYR:HD1	2.08	0.52
1:B:749:CYS:HB3	1:B:977:LEU:HD13	1.92	0.52
1:C:393:THR:OG1	1:C:522:ALA:HB1	2.04	0.52
1:C:825:LYS:HZ3	1:C:942:ALA:CA	2.23	0.52
1:C:1033:VAL:HG23	1:C:1062:PHE:CE1	2.45	0.52
1:A:91:TYR:CE1	1:A:93:ALA:HB2	2.44	0.52
1:A:327:VAL:HG23	1:A:529:LYS:O	2.10	0.52
1:A:371:SER:CA	2:J:2:NAG:H82	2.40	0.52
1:B:37:TYR:CD1	1:B:37:TYR:C	2.83	0.52
1:B:107:GLY:N	1:B:235:ILE:CD1	2.62	0.52
1:B:718:PHE:CZ	1:B:923:ILE:CG1	2.93	0.52
1:C:119:ILE:CG2	1:C:120:VAL:N	2.73	0.52
1:C:226:LEU:CD1	1:C:227:VAL:HG13	2.40	0.52
1:C:380:TYR:CE2	1:C:412:PRO:CG	2.93	0.52
1:A:329:PHE:HE2	1:A:391:CYS:SG	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:PRO:CG	1:A:674:TYR:HD1	2.23	0.52
1:A:1079:PRO:HB3	1:B:917:TYR:CZ	2.45	0.52
1:A:1103:PHE:N	1:A:1103:PHE:CD1	2.77	0.52
1:B:369:TYR:HA	1:B:372:ALA:HB3	1.91	0.52
1:C:330:PRO:HD3	1:C:544:ASN:HD22	1.64	0.52
1:C:423:TYR:HE2	1:C:425:LEU:HD21	1.75	0.52
1:C:429:PHE:CE2	1:C:514:SER:HB2	2.44	0.52
1:C:577:ARG:HB2	1:C:584:ILE:HD13	1.92	0.52
1:C:581:THR:CG2	1:C:583:GLU:CG	2.87	0.52
1:C:654:GLU:OE2	1:C:693:ILE:HG22	2.10	0.52
1:C:718:PHE:CZ	1:C:923:ILE:HD11	2.45	0.52
1:A:643:PHE:CE2	1:A:655:HIS:HB2	2.45	0.51
1:B:617:CYS:SG	1:B:642:VAL:CG1	2.97	0.51
1:B:1078:ALA:HB3	1:B:1133:VAL:HG22	1.92	0.51
1:C:43:PHE:CE1	1:C:45:SER:HB3	2.46	0.51
1:C:280:ASN:OD1	1:C:284:THR:N	2.42	0.51
1:C:280:ASN:ND2	1:C:284:THR:OG1	2.43	0.51
1:C:813:SER:O	1:C:868:GLU:OE1	2.28	0.51
1:C:825:LYS:CE	1:C:942:ALA:HA	2.39	0.51
1:A:294:ASP:HB2	1:A:297:SER:OG	2.10	0.51
1:A:353:TRP:CD1	1:A:353:TRP:N	2.78	0.51
1:C:197:ILE:O	1:C:197:ILE:HG13	2.10	0.51
1:C:294:ASP:OD1	1:C:297:SER:OG	2.16	0.51
1:A:211:ASN:ND2	1:A:211:ASN:O	2.43	0.51
1:A:273:ARG:HH21	1:A:292:ALA:HB3	1.75	0.51
1:B:64:TRP:CD1	1:B:65:PHE:N	2.79	0.51
1:B:101:ILE:HD11	1:B:263:ALA:HB1	1.93	0.51
1:B:916:LEU:HD12	1:B:923:ILE:HD12	1.92	0.51
1:A:313:TYR:N	1:A:313:TYR:CD1	2.78	0.51
1:A:992:GLN:HA	1:A:992:GLN:HE21	1.76	0.51
1:B:106:PHE:CZ	1:B:194:PHE:CD2	2.91	0.51
1:B:293:LEU:O	1:B:293:LEU:HD12	2.11	0.51
1:C:220:PHE:CZ	1:C:288:ALA:CA	2.66	0.51
1:C:374:PHE:N	1:C:374:PHE:CD1	2.79	0.51
1:C:452:LEU:HG	1:C:494:SER:HA	1.92	0.51
1:C:515:PHE:CD1	1:C:515:PHE:N	2.79	0.51
1:C:974:SER:HB3	1:C:980:ILE:HD11	1.91	0.51
1:A:90:VAL:HG22	1:A:90:VAL:O	2.10	0.51
1:A:1102:TRP:HB2	1:A:1135:ASN:HD22	1.65	0.51
1:B:92:PHE:HZ	1:B:265:TYR:CD2	2.24	0.51
1:B:296:LEU:HD12	1:B:296:LEU:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:ARG:HG3	1:B:497:PHE:HE1	1.75	0.51
1:B:599:THR:CB	1:B:608:VAL:CG1	2.82	0.51
1:B:896:ILE:HG12	1:B:897:PRO:HD2	1.92	0.51
1:B:1142:GLN:N	1:B:1143:PRO:CD	2.74	0.51
1:C:126:VAL:HG13	1:C:175:PHE:HZ	1.74	0.51
1:C:377:PHE:CE1	1:C:434:ILE:HG13	2.45	0.51
1:C:454:ARG:HH22	1:C:467:ASP:CG	2.12	0.51
1:A:299:THR:HA	1:A:315:THR:HG21	1.92	0.51
1:A:317:ASN:HD21	1:B:737:ASP:HB3	1.75	0.51
1:A:894:LEU:HB3	1:C:713:ALA:HB3	1.91	0.51
1:A:903:ALA:HA	1:A:916:LEU:HD13	1.92	0.51
1:A:1029:MET:HE2	1:A:1062:PHE:CE2	2.46	0.51
1:A:1043:CYS:HA	1:A:1064:HIS:CE1	2.44	0.51
1:B:118:LEU:HD12	1:B:119:ILE:H	1.76	0.51
1:B:164:ASN:OD1	1:B:165:ASN:ND2	2.43	0.51
1:C:303:LEU:HD12	1:C:308:VAL:HG22	1.93	0.51
1:A:903:ALA:CA	1:A:916:LEU:HD13	2.40	0.51
1:A:950:ASP:OD1	1:A:954:GLN:NE2	2.43	0.51
1:A:1043:CYS:CB	1:A:1064:HIS:CE1	2.94	0.51
1:A:1094:VAL:HG23	1:B:900:MET:HE1	1.93	0.51
1:B:238:PHE:C	1:B:238:PHE:CD1	2.84	0.51
1:B:265:TYR:N	1:B:265:TYR:CD1	2.79	0.51
1:B:565:PHE:CB	1:C:42:VAL:HG12	2.37	0.51
1:B:1018:ILE:O	1:B:1022:ALA:N	2.34	0.51
1:B:1039:ARG:NE	1:B:1042:PHE:HD2	2.07	0.51
1:C:34:ARG:HG3	1:C:91:TYR:OH	2.09	0.51
1:C:226:LEU:CG	1:C:227:VAL:HG13	2.40	0.51
1:C:599:THR:OG1	1:C:608:VAL:HG12	2.11	0.51
1:C:695:TYR:N	1:C:695:TYR:CD1	2.76	0.51
1:A:1029:MET:HE2	1:A:1062:PHE:HE2	1.75	0.51
1:B:91:TYR:O	1:B:91:TYR:HD1	1.93	0.51
1:B:329:PHE:CE2	1:B:529:LYS:O	2.64	0.51
1:B:577:ARG:HA	1:B:584:ILE:HA	1.91	0.51
1:B:641:ASN:ND2	1:B:654:GLU:CA	2.64	0.51
1:B:915:VAL:O	1:B:919:ASN:OD1	2.28	0.51
1:C:100:ILE:CG2	1:C:243:ALA:H	2.23	0.51
1:C:366:SER:O	1:C:370:ASN:CA	2.59	0.51
1:A:273:ARG:NH2	1:A:292:ALA:HB1	2.26	0.51
1:A:1013:ILE:HD13	1:B:1012:LEU:HB3	1.93	0.51
1:A:1084:ASP:CB	1:A:1086:LYS:NZ	2.65	0.51
1:B:44:ARG:HB2	1:B:279:TYR:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:ILE:HD12	1:C:239:GLN:O	2.11	0.51
1:C:118:LEU:HD23	1:C:135:PHE:CE1	2.42	0.51
1:C:738:CYS:SG	1:C:760:CYS:C	2.86	0.51
1:C:1083:HIS:HB2	1:C:1137:VAL:HG23	1.92	0.51
1:A:403:ARG:HG2	1:A:495:TYR:CE1	2.44	0.51
1:A:521:PRO:HG3	1:A:564:GLN:HG2	1.93	0.51
1:A:560:LEU:HD12	1:A:560:LEU:N	2.26	0.51
1:B:718:PHE:CZ	1:B:923:ILE:CD1	2.84	0.51
1:B:1089:PHE:HB2	1:B:1121:PHE:CE1	2.46	0.51
1:C:735:SER:CB	1:C:861:LEU:HD21	2.40	0.51
1:C:791:THR:HG22	1:C:792:PRO:CD	2.38	0.51
1:A:118:LEU:HD12	1:A:119:ILE:H	1.77	0.50
1:A:241:LEU:HD12	1:A:242:LEU:H	1.69	0.50
1:A:490:PHE:CE2	1:A:492:LEU:HB2	2.47	0.50
1:B:324:GLU:HG3	1:B:539:VAL:HG23	1.93	0.50
1:C:90:VAL:C	1:C:270:LEU:HD11	2.31	0.50
1:C:204:TYR:HD1	1:C:225:PRO:CB	2.23	0.50
1:C:317:ASN:HB3	1:C:593:GLY:O	2.11	0.50
1:A:37:TYR:HD1	1:A:37:TYR:H	1.59	0.50
1:A:353:TRP:NE1	1:A:466:ARG:CB	2.74	0.50
1:A:671:CYS:O	1:A:694:ALA:HA	2.12	0.50
1:A:896:ILE:CD1	1:A:897:PRO:HD2	2.41	0.50
1:B:615:VAL:CG1	1:B:620:VAL:HG13	2.38	0.50
1:B:909:ILE:HG23	1:B:1036:GLN:NE2	2.25	0.50
1:B:1017:GLU:OE2	1:C:1019:ARG:NH1	2.44	0.50
1:C:655:HIS:CB	1:C:694:ALA:O	2.51	0.50
1:C:671:CYS:O	1:C:695:TYR:CD1	2.65	0.50
1:C:719:THR:OG1	1:C:1068:VAL:CG2	2.59	0.50
1:C:990:GLU:OE1	1:C:990:GLU:HA	2.11	0.50
1:A:93:ALA:O	1:A:266:TYR:CD1	2.65	0.50
1:A:521:PRO:HG3	1:A:564:GLN:HB3	1.93	0.50
1:A:743:CYS:SG	1:A:750:SER:CA	3.00	0.50
1:A:1090:PRO:CG	1:A:1093:GLY:O	2.58	0.50
1:B:712:ILE:HG12	1:B:713:ALA:N	2.26	0.50
1:B:776:LYS:NZ	1:B:780:GLU:OE2	2.31	0.50
1:B:1054:GLN:HB2	1:B:1061:VAL:O	2.11	0.50
1:C:119:ILE:HD12	1:C:119:ILE:N	2.26	0.50
1:A:64:TRP:NE1	1:A:266:TYR:CZ	2.44	0.50
1:A:817:PHE:CE2	1:A:935:GLN:HG3	2.43	0.50
1:A:1105:THR:OG1	1:A:1111:GLU:N	2.43	0.50
1:B:347:PHE:HB2	1:B:401:VAL:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:743:CYS:O	1:B:977:LEU:CD1	2.45	0.50
1:C:86:PHE:CD2	1:C:106:PHE:HE2	2.30	0.50
1:C:118:LEU:HD12	1:C:119:ILE:N	2.25	0.50
1:C:817:PHE:HD1	1:C:818:ILE:HD13	1.75	0.50
1:A:310:LYS:CG	1:A:664:ILE:HD11	2.28	0.50
1:A:885:GLY:CA	1:A:901:GLN:CD	2.73	0.50
1:B:164:ASN:OD1	1:B:165:ASN:OD1	2.29	0.50
1:B:229:LEU:N	1:B:229:LEU:HD22	2.26	0.50
1:B:675:GLN:HE21	1:B:675:GLN:CA	2.10	0.50
1:B:916:LEU:CD1	1:B:923:ILE:HD12	2.41	0.50
1:B:1040:VAL:HG12	1:B:1041:ASP:OD1	2.11	0.50
1:C:734:THR:O	1:C:767:LEU:HD12	2.11	0.50
1:A:927:PHE:HE1	1:A:931:ILE:CG1	2.24	0.50
1:C:365:TYR:N	1:C:365:TYR:HD1	2.10	0.50
1:C:462:LYS:HB3	1:C:463:PRO:HD2	1.94	0.50
1:C:612:TYR:HB2	1:C:615:VAL:CG2	2.41	0.50
1:A:200:TYR:OH	1:C:394:ASN:ND2	2.45	0.50
1:A:1030:SER:OG	1:C:1041:ASP:HB3	2.12	0.50
1:A:1043:CYS:C	1:A:1064:HIS:ND1	2.65	0.50
1:B:105:ILE:HB	1:B:239:GLN:HB3	1.93	0.50
1:B:332:ILE:CG2	1:B:334:ASN:OD1	2.60	0.50
1:B:714:ILE:HG22	1:B:1110:TYR:HB2	1.94	0.50
1:C:119:ILE:HG22	1:C:120:VAL:N	2.27	0.50
1:C:168:PHE:CD2	1:C:231:ILE:HG13	2.47	0.50
1:C:353:TRP:HD1	1:C:353:TRP:O	1.94	0.50
1:A:55:PHE:CD1	1:A:275:PHE:CD2	2.99	0.50
1:B:395:VAL:HG22	1:B:515:PHE:HB3	1.93	0.50
1:B:560:LEU:O	1:B:561:PRO:C	2.50	0.50
1:B:1056:ALA:HB1	1:B:1057:PRO:HD2	1.94	0.50
1:C:365:TYR:CD2	1:C:387:LEU:HD13	2.47	0.50
1:C:738:CYS:C	1:C:760:CYS:SG	2.89	0.50
1:A:33:THR:HA	1:A:58:PHE:CZ	2.46	0.50
1:A:64:TRP:HD1	1:A:266:TYR:CG	2.29	0.50
1:A:168:PHE:CE2	1:A:230:PRO:HD2	2.47	0.50
1:A:353:TRP:CZ2	1:A:466:ARG:CB	2.93	0.50
1:A:411:ALA:HB3	1:A:414:GLN:HE21	1.77	0.50
1:A:736:VAL:CG2	1:A:858:LEU:CD2	2.73	0.50
1:B:970:PHE:CD2	1:B:999:GLY:CA	2.90	0.50
1:B:1062:PHE:HB3	1:B:1064:HIS:CE1	2.47	0.50
1:C:204:TYR:CD1	1:C:225:PRO:CB	2.92	0.50
1:C:310:LYS:HB2	1:C:600:PRO:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:ARG:CZ	1:C:578:ASP:CG	2.79	0.50
1:C:560:LEU:HB3	1:C:562:PHE:CE1	2.47	0.50
1:C:612:TYR:CG	1:C:615:VAL:HG11	2.47	0.50
1:A:87:ASN:CG	1:A:269:TYR:CE2	2.84	0.49
1:B:126:VAL:HG13	1:B:175:PHE:CZ	2.47	0.49
1:B:914:ASN:OD1	1:B:915:VAL:HG23	2.11	0.49
1:C:37:TYR:HB3	1:C:223:LEU:HG	1.93	0.49
1:C:353:TRP:CH2	1:C:423:TYR:HA	2.47	0.49
1:C:825:LYS:HZ3	1:C:942:ALA:CB	2.14	0.49
1:A:278:LYS:HB3	1:A:287:ASP:O	2.12	0.49
1:A:741:TYR:CZ	1:A:962:LEU:HD11	2.47	0.49
1:B:273:ARG:NH1	1:B:273:ARG:HG3	2.26	0.49
1:B:277:LEU:CD2	1:B:288:ALA:HB2	2.42	0.49
1:B:294:ASP:HB3	1:B:295:PRO:HD2	1.94	0.49
1:B:1140:PRO:O	1:B:1143:PRO:HD2	2.11	0.49
1:C:68:ILE:HD12	1:C:262:ALA:CB	2.42	0.49
1:C:365:TYR:N	1:C:365:TYR:CD1	2.79	0.49
1:C:671:CYS:O	1:C:695:TYR:CE1	2.65	0.49
1:C:1083:HIS:HB3	1:C:1088:HIS:CE1	2.46	0.49
2:O:2:NAG:HO3	2:O:2:NAG:C7	2.15	0.49
1:C:355:ARG:HA	1:C:397:ALA:O	2.12	0.49
1:C:516:GLU:OE1	1:C:516:GLU:HA	2.12	0.49
1:C:585:LEU:HD23	1:C:585:LEU:N	2.26	0.49
1:C:973:ILE:HD11	1:C:980:ILE:HG23	1.93	0.49
1:A:430:THR:HG21	1:A:517:LEU:HG	1.94	0.49
1:C:336:CYS:SG	1:C:362:VAL:N	2.84	0.49
1:C:712:ILE:HG22	1:C:1077:THR:HB	1.95	0.49
1:A:126:VAL:HG13	1:A:175:PHE:CZ	2.48	0.49
1:B:107:GLY:HA2	1:B:235:ILE:HG12	1.95	0.49
1:B:1080:ALA:CB	1:B:1089:PHE:CE1	2.91	0.49
1:C:672:ALA:HA	1:C:693:ILE:O	2.12	0.49
1:B:350:VAL:HB	1:B:402:ILE:HG22	1.93	0.49
1:B:749:CYS:CB	1:B:977:LEU:HD13	2.42	0.49
1:C:763:LEU:HD22	1:C:1008:VAL:CG2	2.34	0.49
1:A:641:ASN:OD1	1:A:641:ASN:N	2.46	0.49
1:A:1078:ALA:CB	1:A:1102:TRP:CH2	2.96	0.49
1:B:57:PRO:HG3	1:B:273:ARG:NH1	2.26	0.49
1:B:1114:ILE:HD12	1:B:1114:ILE:N	2.28	0.49
1:C:230:PRO:HD2	1:C:231:ILE:CD1	2.43	0.49
1:C:868:GLU:OE1	1:C:868:GLU:HA	2.13	0.49
1:A:90:VAL:HG21	1:A:238:PHE:CD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:VAL:HG21	1:A:231:ILE:HD11	1.94	0.49
1:A:612:TYR:CE1	1:A:651:ILE:HD12	2.47	0.49
1:A:974:SER:OG	1:A:980:ILE:HG12	2.12	0.49
1:C:658:ASN:OD1	1:C:658:ASN:N	2.35	0.49
1:C:934:ILE:O	1:C:934:ILE:HD12	2.13	0.49
1:C:1095:PHE:CE1	1:C:1120:THR:HG21	2.44	0.49
1:A:89:GLY:HA2	1:A:270:LEU:CD1	2.43	0.49
1:A:403:ARG:CG	1:A:495:TYR:CZ	2.94	0.49
1:A:916:LEU:O	1:A:916:LEU:HD23	2.12	0.49
1:A:1039:ARG:CZ	1:A:1042:PHE:CD2	2.95	0.49
1:B:62:VAL:HG21	1:B:266:TYR:HB3	1.94	0.49
1:B:328:ARG:NH2	1:B:580:GLN:CB	2.75	0.49
1:C:287:ASP:CG	1:C:306:PHE:CE2	2.86	0.49
1:C:797:PHE:HE2	1:C:882:ILE:HB	1.78	0.49
1:A:1035:GLY:HA3	1:C:1040:VAL:HG21	1.94	0.49
1:B:317:ASN:HD22	1:C:737:ASP:CB	2.21	0.49
1:B:1078:ALA:CB	1:B:1102:TRP:CH2	2.95	0.49
1:C:424:LYS:O	1:C:463:PRO:HA	2.12	0.49
1:C:659:SER:CB	1:C:698:SER:HB3	2.43	0.49
1:B:615:VAL:HG12	1:B:620:VAL:HG13	1.95	0.48
1:C:368:LEU:H	1:C:368:LEU:CD1	2.26	0.48
1:C:822:LEU:HD21	1:C:945:LEU:HD21	1.95	0.48
1:C:1060:VAL:HG13	1:C:1060:VAL:O	2.13	0.48
1:A:33:THR:HA	1:A:58:PHE:CE1	2.48	0.48
1:A:805:ILE:HD12	1:A:878:LEU:HD11	1.96	0.48
1:A:57:PRO:HB3	1:A:273:ARG:HE	1.77	0.48
1:A:276:LEU:HD23	1:A:276:LEU:C	2.34	0.48
1:A:984:LEU:CD1	1:A:988:GLU:HG3	2.37	0.48
1:B:329:PHE:HB3	1:B:330:PRO:CD	2.32	0.48
1:C:281:GLU:CB	2:P:1:NAG:H82	2.42	0.48
1:A:455:LEU:HG	1:A:456:PHE:CD2	2.48	0.48
1:A:1080:ALA:C	1:A:1132:ILE:HG13	2.31	0.48
1:B:96:GLU:OE1	1:B:100:ILE:N	2.46	0.48
1:B:405:ASP:N	1:B:504:GLY:O	2.46	0.48
1:C:277:LEU:HD13	1:C:285:ILE:HD13	1.95	0.48
1:A:650:LEU:HD11	1:A:666:ILE:HD13	1.96	0.48
1:C:931:ILE:HA	1:C:934:ILE:HG22	1.95	0.48
1:C:1001:LEU:HD13	1:C:1001:LEU:C	2.34	0.48
1:A:96:GLU:OE1	1:A:100:ILE:N	2.46	0.48
1:A:204:TYR:CE1	1:A:225:PRO:CA	2.96	0.48
1:A:277:LEU:HD23	1:A:288:ALA:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:ASN:HB2	1:A:497:PHE:HB2	1.96	0.48
1:B:190:ARG:NE	1:B:207:HIS:HE1	2.05	0.48
1:C:241:LEU:CD1	1:C:241:LEU:N	2.76	0.48
1:C:555:SER:HG	1:C:584:ILE:C	2.07	0.48
1:C:661:GLU:O	1:C:695:TYR:OH	2.31	0.48
1:A:299:THR:HA	1:A:315:THR:CG2	2.44	0.48
1:A:903:ALA:HA	1:A:916:LEU:CD1	2.43	0.48
1:B:1088:HIS:HD1	1:B:1122:VAL:HG23	1.76	0.48
1:C:33:THR:HA	1:C:58:PHE:CZ	2.48	0.48
1:C:598:ILE:O	1:C:598:ILE:HG22	2.13	0.48
1:C:660:TYR:N	1:C:660:TYR:HD1	2.11	0.48
1:C:1090:PRO:CA	1:C:1120:THR:CG2	2.60	0.48
1:B:130:VAL:CG2	1:B:231:ILE:CD1	2.92	0.48
1:C:37:TYR:CD1	1:C:37:TYR:N	2.81	0.48
1:C:456:PHE:CD2	1:C:473:TYR:CE2	3.02	0.48
1:C:825:LYS:CE	1:C:942:ALA:CA	2.92	0.48
1:A:55:PHE:CD1	1:A:275:PHE:CE2	3.01	0.48
1:A:736:VAL:HG22	1:A:858:LEU:HD23	1.92	0.48
1:B:54:LEU:HD12	1:B:54:LEU:N	2.29	0.48
1:B:396:TYR:N	1:B:514:SER:O	2.43	0.48
1:B:1141:LEU:HD23	1:B:1141:LEU:O	2.14	0.48
1:C:453:TYR:CE2	1:C:493:GLN:CD	2.87	0.48
1:C:643:PHE:CE1	1:C:655:HIS:CD2	3.02	0.48
1:A:379:CYS:HB3	1:A:382:VAL:O	2.14	0.48
1:A:1031:GLU:OE2	1:A:1042:PHE:HE2	1.97	0.48
1:C:742:ILE:HG22	1:C:743:CYS:SG	2.54	0.48
1:A:353:TRP:N	1:A:466:ARG:CD	2.67	0.47
1:A:401:VAL:HG11	1:A:451:TYR:CE2	2.49	0.47
1:A:600:PRO:HG2	1:A:674:TYR:CD1	2.49	0.47
1:A:660:TYR:O	1:A:695:TYR:HE2	1.97	0.47
1:A:782:PHE:CE2	1:A:874:THR:HG23	2.49	0.47
1:A:886:TRP:HE3	1:A:886:TRP:O	1.97	0.47
1:B:902:MET:CB	1:B:916:LEU:HD21	2.39	0.47
1:B:1110:TYR:HD1	1:B:1111:GLU:N	2.11	0.47
1:C:32:PHE:CE1	1:C:218:GLN:HB3	2.49	0.47
1:C:69:HIS:HA	1:C:78:ARG:O	2.13	0.47
1:C:406:GLU:OE1	1:C:406:GLU:N	2.47	0.47
1:C:1001:LEU:HD13	1:C:1005:GLN:HG3	1.95	0.47
1:A:981:LEU:CD2	1:A:993:ILE:HD11	2.43	0.47
1:B:326:ILE:CD1	1:B:552:LEU:HD11	2.43	0.47
1:B:805:ILE:HD13	1:B:1052:PHE:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:ASN:N	1:C:211:ASN:OD1	2.47	0.47
1:C:517:LEU:HD12	1:C:517:LEU:N	2.14	0.47
1:C:532:ASN:HD22	1:C:532:ASN:N	2.11	0.47
1:C:1004:LEU:HD23	1:C:1004:LEU:C	2.34	0.47
1:C:1083:HIS:HB2	1:C:1137:VAL:HG21	1.95	0.47
1:A:225:PRO:HG2	1:C:562:PHE:CG	2.50	0.47
1:A:472:ILE:HD12	1:A:472:ILE:N	2.30	0.47
1:A:954:GLN:HG2	1:A:1014:ARG:HH12	1.74	0.47
1:A:963:VAL:HG11	1:C:570:ALA:HB1	1.94	0.47
1:C:100:ILE:HG23	1:C:243:ALA:N	2.26	0.47
1:C:392:PHE:CD1	1:C:392:PHE:N	2.82	0.47
1:A:914:ASN:OD1	1:A:914:ASN:N	2.45	0.47
1:B:97:LYS:HB2	1:B:186:PHE:HA	1.97	0.47
1:B:719:THR:O	1:B:1068:VAL:HG22	2.15	0.47
1:B:962:LEU:O	1:B:965:GLN:HB2	2.15	0.47
1:B:973:ILE:HD11	1:B:984:LEU:HD11	1.97	0.47
1:B:1110:TYR:CD1	1:B:1111:GLU:N	2.83	0.47
1:C:555:SER:OG	1:C:585:LEU:N	2.46	0.47
1:C:773:GLU:OE2	1:C:1019:ARG:CD	2.55	0.47
1:C:922:LEU:HD12	1:C:922:LEU:C	2.34	0.47
1:C:1033:VAL:HG21	1:C:1062:PHE:HE1	1.77	0.47
1:A:105:ILE:O	1:A:238:PHE:HB2	2.15	0.47
1:A:617:CYS:CA	1:A:649:CYS:SG	2.94	0.47
1:A:719:THR:HG23	1:A:1070:ALA:HB2	1.97	0.47
4:A:1307:NAG:N2	4:A:1307:NAG:H5	2.28	0.47
1:B:643:PHE:CZ	1:B:655:HIS:CG	3.03	0.47
1:B:1101:HIS:HB3	1:B:1103:PHE:CE2	2.48	0.47
1:C:905:ARG:CD	1:C:1049:LEU:O	2.59	0.47
1:A:37:TYR:O	1:A:38:TYR:C	2.52	0.47
1:A:521:PRO:HG3	1:A:564:GLN:CG	2.44	0.47
1:A:600:PRO:HG2	1:A:674:TYR:HD1	1.78	0.47
1:B:549:THR:HG22	1:B:590:CYS:SG	2.55	0.47
1:B:1083:HIS:CE1	1:B:1136:THR:OG1	2.67	0.47
1:C:195:LYS:HD2	1:C:204:TYR:CE2	2.50	0.47
1:C:336:CYS:HB2	1:C:363:ALA:HB2	1.97	0.47
1:C:607:GLN:NE2	1:C:674:TYR:CE1	2.83	0.47
1:C:662:CYS:SG	1:C:697:MET:CE	3.03	0.47
1:A:128:ILE:HG22	1:A:129:LYS:H	1.64	0.47
1:A:231:ILE:CG2	1:A:233:ILE:H	2.17	0.47
1:A:318:PHE:CZ	1:A:620:VAL:CG2	2.98	0.47
1:A:453:TYR:OH	1:A:493:GLN:HG3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:TYR:CE1	1:B:222:VAL:HG12	2.50	0.47
1:B:91:TYR:CE1	1:B:93:ALA:CB	2.81	0.47
1:B:641:ASN:HD22	1:B:654:GLU:CA	2.26	0.47
1:B:712:ILE:O	1:B:1074:ASN:HA	2.14	0.47
1:B:822:LEU:HD13	1:B:938:LEU:HD13	1.97	0.47
1:C:37:TYR:HB3	1:C:223:LEU:CG	2.45	0.47
1:C:105:ILE:HD13	1:C:239:GLN:HB3	1.96	0.47
1:A:515:PHE:N	1:A:515:PHE:CD1	2.79	0.47
1:A:555:SER:O	1:A:584:ILE:CD1	2.63	0.47
1:B:89:GLY:CA	1:B:270:LEU:HD13	2.45	0.47
1:B:728:PRO:HB3	1:B:951:VAL:HG21	1.97	0.47
1:C:92:PHE:CD1	1:C:92:PHE:C	2.88	0.47
1:C:309:GLU:O	1:C:313:TYR:OH	2.21	0.47
1:C:326:ILE:HD13	1:C:534:VAL:HG12	1.96	0.47
1:C:615:VAL:HG23	1:C:649:CYS:H	1.80	0.47
1:C:741:TYR:CD1	1:C:966:LEU:HD21	2.44	0.47
1:A:353:TRP:CE2	1:A:466:ARG:CD	2.98	0.47
1:A:541:PHE:O	1:A:541:PHE:CD1	2.68	0.47
1:A:781:VAL:HG11	1:A:1060:VAL:HG21	1.97	0.47
1:A:1031:GLU:OE2	1:A:1042:PHE:CE2	2.68	0.47
1:C:99:ASN:N	1:C:99:ASN:ND2	2.62	0.47
1:C:707:TYR:C	1:C:707:TYR:CD1	2.88	0.47
1:C:1080:ALA:C	1:C:1132:ILE:HG13	2.34	0.47
1:A:97:LYS:HB2	1:A:186:PHE:HA	1.97	0.47
1:A:280:ASN:HD22	1:A:286:THR:HG21	1.80	0.47
1:C:55:PHE:C	1:C:270:LEU:HB3	2.34	0.47
1:C:541:PHE:C	1:C:541:PHE:CD1	2.87	0.47
1:C:724:THR:OG1	1:C:934:ILE:HD13	2.15	0.47
1:C:916:LEU:HD12	1:C:923:ILE:HD12	1.96	0.47
1:C:921:LYS:HE2	1:C:921:LYS:CA	2.22	0.47
1:A:90:VAL:HG13	1:A:194:PHE:CA	2.45	0.46
1:A:92:PHE:C	1:A:92:PHE:CD1	2.88	0.46
1:A:353:TRP:HE1	1:A:466:ARG:HG3	1.80	0.46
1:B:324:GLU:HG3	1:B:539:VAL:CG2	2.44	0.46
1:B:794:ILE:HG22	1:B:796:ASP:H	1.80	0.46
1:B:888:PHE:CD1	1:B:888:PHE:C	2.88	0.46
1:C:216:LEU:HD12	1:C:216:LEU:O	2.15	0.46
1:C:902:MET:HB3	1:C:916:LEU:HD21	1.97	0.46
1:A:164:ASN:HD21	2:K:1:NAG:C6	2.28	0.46
1:A:457:ARG:NH1	1:A:460:ASN:O	2.48	0.46
1:A:546:LEU:HD23	1:A:565:PHE:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:984:LEU:HD23	1:A:984:LEU:HA	1.75	0.46
1:B:130:VAL:HG21	1:B:231:ILE:HD11	1.98	0.46
1:B:396:TYR:HB2	1:B:514:SER:HB3	1.96	0.46
1:B:715:PRO:CB	1:B:1071:GLN:O	2.64	0.46
1:B:866:THR:HG23	1:B:869:MET:H	1.79	0.46
1:C:326:ILE:HG21	1:C:534:VAL:CG1	2.40	0.46
1:A:33:THR:CB	1:A:58:PHE:CZ	2.96	0.46
1:A:203:ILE:CG2	1:A:227:VAL:HG22	2.46	0.46
1:A:675:GLN:O	1:A:693:ILE:HD11	2.15	0.46
1:A:896:ILE:HD12	1:A:897:PRO:HD2	1.97	0.46
1:B:101:ILE:HG13	1:B:242:LEU:HD13	1.97	0.46
1:B:130:VAL:HG21	1:B:231:ILE:HD13	1.96	0.46
1:B:130:VAL:CG2	1:B:231:ILE:HD13	2.44	0.46
1:B:1111:GLU:O	1:B:1111:GLU:HG3	2.13	0.46
1:C:902:MET:HB3	1:C:916:LEU:CD2	2.46	0.46
1:A:58:PHE:HB2	1:A:293:LEU:HD22	1.97	0.46
1:A:353:TRP:CD1	1:A:466:ARG:HG3	2.49	0.46
1:C:337:PRO:HB2	1:C:340:GLU:CG	2.45	0.46
1:C:588:THR:HG22	1:C:589:PRO:HD2	1.96	0.46
1:A:489:TYR:N	1:A:489:TYR:CD1	2.83	0.46
1:C:210:ILE:CD1	1:C:210:ILE:N	2.78	0.46
1:C:540:ASN:HA	1:C:549:THR:HG23	1.96	0.46
1:C:555:SER:OG	1:C:585:LEU:CA	2.63	0.46
1:C:660:TYR:N	1:C:695:TYR:CE2	2.79	0.46
1:C:1045:LYS:H	1:C:1066:THR:HG21	1.81	0.46
1:A:403:ARG:CD	1:A:495:TYR:CE1	2.95	0.46
1:A:555:SER:OG	1:A:557:LYS:HG3	2.16	0.46
1:B:270:LEU:HD12	1:B:270:LEU:N	2.25	0.46
1:B:718:PHE:CB	1:B:1067:TYR:OH	2.63	0.46
1:C:204:TYR:HD1	1:C:225:PRO:HA	1.80	0.46
1:C:414:GLN:HE21	1:C:414:GLN:CA	2.16	0.46
1:C:886:TRP:CD1	1:C:886:TRP:C	2.88	0.46
1:C:949:GLN:OE1	1:C:949:GLN:HA	2.16	0.46
1:C:1122:VAL:HG13	1:C:1122:VAL:O	2.15	0.46
2:L:2:NAG:O7	2:L:2:NAG:O3	2.32	0.46
1:A:64:TRP:CD1	1:A:266:TYR:CG	3.02	0.46
1:A:131:CYS:HB2	1:A:133:PHE:CE2	2.50	0.46
1:A:569:ILE:HG12	1:B:47:VAL:CG1	2.46	0.46
1:A:1047:TYR:O	1:A:1066:THR:HA	2.16	0.46
1:B:1090:PRO:CD	1:B:1095:PHE:CE1	2.92	0.46
1:B:1097:SER:HB3	1:B:1102:TRP:CG	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:SER:O	1:C:59:PHE:HA	2.15	0.46
1:C:168:PHE:CG	1:C:231:ILE:HG12	2.51	0.46
1:C:825:LYS:HZ3	1:C:942:ALA:N	2.14	0.46
1:C:826:VAL:HG12	1:C:826:VAL:O	2.16	0.46
1:A:91:TYR:CZ	1:A:93:ALA:HB2	2.50	0.46
1:A:328:ARG:HH22	1:A:533:LEU:CA	2.28	0.46
1:A:497:PHE:CE2	1:A:507:PRO:CB	2.70	0.46
1:A:707:TYR:CD1	1:A:707:TYR:C	2.89	0.46
1:A:825:LYS:HD2	1:A:938:LEU:O	2.16	0.46
1:B:1137:VAL:HG23	1:B:1137:VAL:O	2.15	0.46
1:C:241:LEU:N	1:C:241:LEU:HD12	2.31	0.46
1:C:317:ASN:OD1	1:C:317:ASN:N	2.49	0.46
1:C:661:GLU:H	1:C:661:GLU:CD	2.13	0.46
1:A:490:PHE:HE2	1:A:492:LEU:HB2	1.80	0.46
1:A:1096:VAL:HG23	1:A:1096:VAL:O	2.16	0.46
1:B:86:PHE:C	1:B:86:PHE:CD1	2.88	0.46
1:B:562:PHE:CE1	1:C:224:GLU:HG3	2.51	0.46
1:B:659:SER:CB	1:B:698:SER:HB3	2.46	0.46
1:C:315:THR:O	1:C:595:VAL:HB	2.15	0.46
1:C:1067:TYR:CD1	1:C:1067:TYR:C	2.88	0.46
1:A:86:PHE:CD1	1:A:86:PHE:C	2.89	0.46
1:A:866:THR:H	1:A:869:MET:HE3	1.81	0.46
1:A:931:ILE:O	1:A:934:ILE:HG22	2.15	0.46
1:B:107:GLY:N	1:B:235:ILE:HG23	2.29	0.46
1:B:599:THR:HG21	1:B:608:VAL:HG11	1.85	0.46
1:B:784:GLN:HE21	1:B:784:GLN:CA	2.05	0.46
1:B:1027:THR:O	1:B:1031:GLU:HB2	2.16	0.46
1:B:1031:GLU:OE2	1:B:1039:ARG:CD	2.60	0.46
1:B:1077:THR:CG2	1:C:900:MET:SD	3.04	0.46
1:C:168:PHE:CE1	1:C:231:ILE:HD11	2.50	0.46
1:C:220:PHE:CE2	1:C:287:ASP:C	2.85	0.46
1:A:328:ARG:NH2	1:A:533:LEU:N	2.64	0.45
1:A:620:VAL:CG2	1:A:621:PRO:HD3	2.42	0.45
1:A:650:LEU:HD23	1:A:653:ALA:HB3	1.98	0.45
1:B:356:LYS:N	1:B:397:ALA:O	2.44	0.45
1:B:884:SER:CB	1:B:893:ALA:HB1	2.46	0.45
1:C:119:ILE:CG2	1:C:127:VAL:O	2.48	0.45
1:C:318:PHE:CD1	1:C:318:PHE:C	2.89	0.45
1:C:350:VAL:CG1	1:C:422:ASN:HB2	2.45	0.45
1:C:434:ILE:HB	1:C:511:VAL:CG1	2.46	0.45
1:C:763:LEU:HD21	1:C:1005:GLN:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:986:PRO:O	1:C:990:GLU:HG2	2.16	0.45
1:C:1085:GLY:C	1:C:1126:CYS:SG	2.94	0.45
1:C:1098:ASN:OD1	1:C:1098:ASN:N	2.48	0.45
1:A:819:GLU:OE2	1:A:1054:GLN:OE1	2.34	0.45
1:A:1010:GLN:OE1	1:A:1010:GLN:HA	2.15	0.45
1:B:298:GLU:HG2	1:B:315:THR:HG23	1.88	0.45
1:B:726:ILE:CD1	1:B:1061:VAL:HG13	2.46	0.45
1:C:392:PHE:O	1:C:524:VAL:CB	2.52	0.45
1:C:395:VAL:HG21	1:C:524:VAL:CG1	2.24	0.45
1:C:643:PHE:CE1	1:C:655:HIS:HB3	2.51	0.45
1:A:422:ASN:HD21	1:A:454:ARG:H	1.64	0.45
1:A:791:THR:HG21	1:A:806:LEU:HD11	1.99	0.45
1:A:1002:GLN:HE21	1:A:1002:GLN:CA	2.27	0.45
1:B:131:CYS:HB2	1:B:133:PHE:CE2	2.51	0.45
1:B:805:ILE:CD1	1:B:1052:PHE:CD2	2.99	0.45
1:B:822:LEU:HD11	1:B:945:LEU:HD21	1.97	0.45
1:C:318:PHE:CD2	1:C:612:TYR:CD1	3.04	0.45
1:C:350:VAL:HG11	1:C:422:ASN:CB	2.45	0.45
1:C:360:ASN:N	1:C:360:ASN:ND2	2.64	0.45
1:C:1076:THR:OG1	1:C:1097:SER:OG	2.33	0.45
1:C:1087:ALA:O	1:C:1122:VAL:CG2	2.48	0.45
1:A:976:VAL:CG1	1:A:979:ASP:HB2	2.46	0.45
1:A:37:TYR:HD2	1:A:204:TYR:CE2	2.34	0.45
1:A:695:TYR:CD1	1:A:695:TYR:N	2.76	0.45
1:A:1067:TYR:C	1:A:1067:TYR:CD1	2.89	0.45
1:B:200:TYR:HB2	1:B:230:PRO:HA	1.96	0.45
1:C:220:PHE:CE1	1:C:288:ALA:CB	2.99	0.45
1:C:409:GLN:NE2	1:C:409:GLN:N	2.65	0.45
1:C:422:ASN:O	1:C:461:LEU:HD13	2.17	0.45
1:C:555:SER:OG	1:C:585:LEU:HA	2.16	0.45
1:A:357:ARG:NH1	1:A:357:ARG:CG	2.80	0.45
1:B:55:PHE:HB3	1:B:275:PHE:HE2	1.78	0.45
1:B:448:ASN:HB3	1:B:497:PHE:HB2	1.97	0.45
1:B:729:VAL:H	1:B:1059:GLY:HA2	1.82	0.45
1:B:961:THR:O	1:B:965:GLN:HG2	2.16	0.45
1:B:1081:ILE:CD1	1:B:1133:VAL:HG22	2.43	0.45
1:C:353:TRP:HD1	1:C:466:ARG:HD3	1.80	0.45
1:C:358:ILE:HG22	1:C:395:VAL:HB	1.99	0.45
1:C:490:PHE:CD2	1:C:491:PRO:HD2	2.51	0.45
1:A:107:GLY:H	1:A:235:ILE:HG21	1.61	0.45
1:A:201:PHE:CD1	1:A:201:PHE:C	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ILE:HG12	1:A:217:PRO:HB3	1.99	0.45
1:A:572:THR:HG1	1:B:855:PHE:HZ	1.62	0.45
1:A:1078:ALA:CB	1:A:1102:TRP:HH2	2.29	0.45
1:B:613:GLN:O	1:B:647:ALA:O	2.34	0.45
1:C:68:ILE:HD12	1:C:262:ALA:HB2	1.98	0.45
1:C:230:PRO:CD	1:C:231:ILE:HD12	2.47	0.45
1:C:320:VAL:HG23	1:C:591:SER:HB2	1.99	0.45
1:C:1089:PHE:O	1:C:1120:THR:CG2	2.64	0.45
1:A:128:ILE:C	1:A:129:LYS:HG3	2.37	0.45
1:A:815:ARG:NH1	1:A:823:PHE:CE1	2.71	0.45
1:A:902:MET:CG	1:A:916:LEU:HD11	2.47	0.45
1:A:970:PHE:HD2	1:A:999:GLY:HA3	1.65	0.45
1:B:92:PHE:HE1	1:B:94:SER:HB3	1.82	0.45
1:C:97:LYS:HD3	1:C:97:LYS:O	2.17	0.45
1:C:659:SER:C	1:C:660:TYR:CD1	2.91	0.45
1:A:204:TYR:HD1	1:A:225:PRO:N	2.13	0.45
1:A:216:LEU:HD12	1:A:216:LEU:H	1.82	0.45
1:A:1043:CYS:SG	1:A:1064:HIS:HE1	2.40	0.45
1:B:265:TYR:HD1	1:B:265:TYR:H	1.64	0.45
1:B:800:PHE:HD2	1:B:927:PHE:CE2	2.34	0.45
1:C:186:PHE:O	1:C:211:ASN:CG	2.55	0.45
1:C:294:ASP:OD1	1:C:297:SER:CB	2.64	0.45
1:C:655:HIS:CD2	1:C:655:HIS:C	2.90	0.45
1:A:413:GLY:HA2	1:C:987:PRO:HG3	1.98	0.45
1:A:752:LEU:HD11	1:A:990:GLU:HG3	1.99	0.45
1:A:791:THR:HG23	1:A:792:PRO:HD2	1.99	0.45
1:A:794:ILE:HG22	1:A:796:ASP:H	1.82	0.45
1:B:612:TYR:CD2	1:B:620:VAL:HG11	2.52	0.45
1:B:805:ILE:HG21	1:B:878:LEU:CD2	2.47	0.45
1:B:1138:TYR:O	1:B:1139:ASP:C	2.50	0.45
1:C:480:CYS:HB3	1:C:483:VAL:HG12	1.99	0.45
1:C:734:THR:HG23	1:C:767:LEU:CD1	2.47	0.45
1:A:302:THR:HG21	1:A:315:THR:CA	2.46	0.44
1:A:675:GLN:NE2	1:A:675:GLN:CA	2.74	0.44
1:A:896:ILE:HG13	1:A:897:PRO:HD2	1.99	0.44
1:B:617:CYS:HA	1:B:649:CYS:SG	2.57	0.44
1:B:785:VAL:HG13	1:B:877:LEU:HD21	1.99	0.44
1:C:453:TYR:CZ	1:C:493:GLN:NE2	2.85	0.44
1:C:497:PHE:CD1	1:C:507:PRO:CG	3.00	0.44
1:C:666:ILE:O	1:C:666:ILE:HG22	2.16	0.44
1:C:718:PHE:CD1	1:C:718:PHE:C	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1043:CYS:CB	1:C:1048:HIS:CD2	2.99	0.44
1:C:1116:THR:HA	1:C:1138:TYR:O	2.16	0.44
2:J:2:NAG:O7	2:J:2:NAG:O3	2.29	0.44
1:A:303:LEU:CD2	1:A:308:VAL:HG12	2.24	0.44
1:A:741:TYR:HE2	1:A:962:LEU:HG	1.79	0.44
1:B:90:VAL:HG11	1:B:238:PHE:CE2	2.52	0.44
1:B:92:PHE:CE2	1:B:265:TYR:HD2	2.28	0.44
1:B:743:CYS:C	1:B:749:CYS:SG	2.96	0.44
1:C:328:ARG:NH1	1:C:580:GLN:OE1	2.50	0.44
1:C:709:ASN:HD22	4:C:1304:NAG:C7	2.28	0.44
1:C:729:VAL:HG23	1:C:1059:GLY:CA	2.45	0.44
1:C:1097:SER:HB3	1:C:1102:TRP:CD2	2.53	0.44
1:A:563:GLN:CD	1:B:43:PHE:HB2	2.37	0.44
1:A:600:PRO:CG	1:A:674:TYR:CD1	3.00	0.44
1:A:718:PHE:CD1	1:A:718:PHE:C	2.91	0.44
1:A:800:PHE:HD2	1:A:927:PHE:CD2	2.33	0.44
1:B:190:ARG:HG2	1:B:207:HIS:CE1	2.52	0.44
1:B:296:LEU:HB2	1:B:608:VAL:HG21	2.00	0.44
1:B:588:THR:CG2	1:B:589:PRO:HD2	2.47	0.44
1:C:44:ARG:O	1:C:279:TYR:HB3	2.18	0.44
1:C:97:LYS:H	1:C:186:PHE:HD1	1.64	0.44
1:C:238:PHE:HZ	1:C:267:VAL:HG21	1.83	0.44
1:C:392:PHE:CE2	1:C:515:PHE:CD1	2.94	0.44
1:C:521:PRO:CG	1:C:564:GLN:HG3	2.47	0.44
1:C:660:TYR:O	1:C:695:TYR:CE2	2.64	0.44
1:C:807:PRO:CG	1:C:875:SER:HB2	2.48	0.44
1:C:984:LEU:HD12	1:C:984:LEU:HA	1.82	0.44
1:A:612:TYR:CB	1:A:615:VAL:CG2	2.95	0.44
1:A:743:CYS:SG	1:A:750:SER:HA	2.57	0.44
1:A:963:VAL:HG11	1:C:570:ALA:CB	2.48	0.44
1:C:497:PHE:CD1	1:C:507:PRO:CB	3.01	0.44
1:C:503:VAL:HG22	1:C:506:GLN:OE1	2.18	0.44
1:C:660:TYR:C	1:C:695:TYR:HE2	2.20	0.44
1:A:56:LEU:HD11	1:A:60:SER:HB3	2.00	0.44
1:A:331:ASN:ND2	4:A:1306:NAG:O7	2.51	0.44
1:A:660:TYR:O	1:A:695:TYR:CD2	2.70	0.44
1:A:864:LEU:HA	1:C:667:GLY:HA2	1.99	0.44
1:A:906:PHE:O	1:A:909:ILE:HG12	2.17	0.44
1:A:1028:LYS:HG2	1:A:1042:PHE:CE1	2.52	0.44
1:B:30:ASN:HA	1:B:61:ASN:HA	1.99	0.44
1:B:133:PHE:CE1	1:B:163:ALA:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:866:THR:O	1:B:869:MET:N	2.50	0.44
1:C:27:ALA:HB3	1:C:64:TRP:HB3	1.98	0.44
1:C:38:TYR:HE1	1:C:285:ILE:HG13	1.67	0.44
1:C:194:PHE:HE1	1:C:203:ILE:CD1	2.29	0.44
1:C:338:PHE:CD2	1:C:363:ALA:HB1	2.53	0.44
1:A:37:TYR:CD2	1:A:204:TYR:CE2	3.05	0.44
1:A:84:LEU:O	1:A:237:ARG:HB2	2.18	0.44
1:A:617:CYS:HG	1:A:644:GLN:CD	2.17	0.44
1:A:1024:LEU:O	1:A:1024:LEU:HD12	2.18	0.44
1:B:38:TYR:CE1	1:B:222:VAL:CG1	3.01	0.44
1:C:285:ILE:HG22	1:C:285:ILE:O	2.18	0.44
1:C:491:PRO:HG2	1:C:492:LEU:CD2	2.48	0.44
1:C:712:ILE:HD12	1:C:1094:VAL:HG11	1.87	0.44
1:A:56:LEU:HD12	1:A:57:PRO:CD	2.44	0.44
1:A:89:GLY:N	1:A:270:LEU:HB2	2.32	0.44
1:A:200:TYR:CE1	1:A:230:PRO:HB3	2.52	0.44
1:A:379:CYS:HB2	1:A:384:PRO:CD	2.29	0.44
1:A:600:PRO:HB3	1:A:674:TYR:HB2	1.99	0.44
1:A:716:THR:N	1:A:1071:GLN:O	2.46	0.44
1:B:91:TYR:O	1:B:91:TYR:CD1	2.70	0.44
1:B:309:GLU:HA	1:B:309:GLU:OE2	2.18	0.44
1:B:1080:ALA:C	1:B:1132:ILE:HG13	2.32	0.44
1:C:64:TRP:HD1	1:C:65:PHE:H	1.64	0.44
1:C:411:ALA:HA	1:C:425:LEU:CD1	2.48	0.44
1:C:472:ILE:CD1	1:C:482:GLY:N	2.75	0.44
1:C:1019:ARG:O	1:C:1023:ASN:OD1	2.35	0.44
1:A:332:ILE:HD12	1:A:332:ILE:N	2.33	0.44
1:A:564:GLN:OE1	1:A:564:GLN:HA	2.18	0.44
1:A:895:GLN:CD	1:C:713:ALA:HB2	2.36	0.44
1:B:553:THR:O	1:B:586:ASP:N	2.51	0.44
1:B:728:PRO:CB	1:B:951:VAL:HG21	2.48	0.44
1:B:1110:TYR:CD1	1:B:1110:TYR:C	2.90	0.44
1:C:107:GLY:C	1:C:235:ILE:HG23	2.37	0.44
1:C:659:SER:C	1:C:660:TYR:HD1	2.20	0.44
1:A:54:LEU:HD12	1:A:54:LEU:N	2.30	0.44
1:A:130:VAL:HG21	1:A:231:ILE:CD1	2.48	0.44
1:A:752:LEU:HD23	1:A:752:LEU:HA	1.81	0.44
1:A:874:THR:HG21	1:A:1055:SER:HB3	2.00	0.44
1:B:38:TYR:N	1:B:38:TYR:CD1	2.86	0.44
1:B:236:THR:O	1:B:236:THR:HG22	2.17	0.44
1:B:884:SER:OG	1:B:888:PHE:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1097:SER:HB3	1:B:1102:TRP:CD2	2.53	0.44
1:C:318:PHE:CZ	1:C:615:VAL:HG12	2.50	0.44
1:C:472:ILE:CD1	1:C:482:GLY:CA	2.96	0.44
1:C:541:PHE:CZ	1:C:587:ILE:CD1	2.99	0.44
1:C:741:TYR:OH	1:C:962:LEU:CD1	2.64	0.44
1:A:741:TYR:CD1	1:A:741:TYR:C	2.91	0.43
1:B:67:ALA:HB3	1:B:263:ALA:HB3	1.99	0.43
1:B:955:ASN:HD22	1:B:955:ASN:HA	1.61	0.43
1:C:96:GLU:HB3	1:C:99:ASN:HA	2.00	0.43
1:C:320:VAL:HG21	1:C:619:GLU:CG	2.48	0.43
1:C:643:PHE:HZ	1:C:655:HIS:CE1	2.36	0.43
1:C:795:LYS:HB3	1:C:797:PHE:HE1	1.82	0.43
1:C:962:LEU:HD12	1:C:962:LEU:O	2.18	0.43
1:C:1142:GLN:HB3	1:C:1143:PRO:HD3	1.99	0.43
1:A:231:ILE:HG22	1:A:232:GLY:N	2.34	0.43
1:A:909:ILE:HD13	1:A:1049:LEU:HD21	2.00	0.43
1:B:615:VAL:O	1:B:649:CYS:HB2	2.19	0.43
1:C:591:SER:OG	1:C:619:GLU:HG2	2.18	0.43
1:A:29:THR:HG23	1:A:62:VAL:CG1	2.48	0.43
1:A:375:SER:OG	1:A:435:ALA:O	2.36	0.43
1:A:528:LYS:HD3	1:A:528:LYS:HA	1.85	0.43
1:A:620:VAL:CG2	1:A:621:PRO:HD2	2.34	0.43
1:B:215:ASP:N	1:B:215:ASP:OD1	2.51	0.43
1:B:1041:ASP:HB2	1:C:1030:SER:HB3	2.01	0.43
1:B:1134:ASN:ND2	2:M:1:NAG:O7	2.51	0.43
1:C:210:ILE:HB	1:C:212:LEU:HD22	1.96	0.43
1:C:853:GLN:CB	1:C:859:THR:HG22	2.49	0.43
1:C:1094:VAL:HG13	1:C:1094:VAL:O	2.18	0.43
1:A:141:LEU:HB2	1:A:241:LEU:HD11	2.00	0.43
1:A:967:SER:O	1:A:975:SER:HB2	2.19	0.43
1:A:992:GLN:NE2	1:A:992:GLN:CA	2.76	0.43
1:B:714:ILE:HG23	1:B:715:PRO:HD2	1.99	0.43
1:C:564:GLN:OE1	1:C:564:GLN:HA	2.19	0.43
1:C:1081:ILE:HD13	1:C:1133:VAL:HG22	1.98	0.43
1:A:133:PHE:CE1	1:A:163:ALA:HB2	2.54	0.43
1:A:322:PRO:CG	1:A:540:ASN:OD1	2.54	0.43
1:A:438:SER:HB2	1:A:442:ASP:HB2	2.00	0.43
1:B:218:GLN:NE2	1:B:218:GLN:O	2.52	0.43
1:B:462:LYS:HA	1:B:462:LYS:HD2	1.85	0.43
1:B:555:SER:OG	1:B:586:ASP:OD1	2.37	0.43
1:B:748:GLU:OE2	1:B:981:LEU:HD11	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:805:ILE:HG21	1:B:878:LEU:HD21	2.00	0.43
1:B:945:LEU:O	1:B:947:LYS:N	2.50	0.43
1:C:328:ARG:HG3	1:C:543:PHE:HE1	1.84	0.43
1:C:461:LEU:HD23	1:C:465:GLU:OE1	2.19	0.43
1:A:118:LEU:CD2	1:A:135:PHE:CE1	2.99	0.43
1:A:128:ILE:O	1:A:129:LYS:CG	2.66	0.43
1:A:409:GLN:NE2	1:A:418:ILE:HG22	2.33	0.43
1:B:126:VAL:HG13	1:B:175:PHE:HZ	1.83	0.43
1:B:785:VAL:HG12	1:B:888:PHE:HE1	1.83	0.43
1:C:245:HIS:HB3	1:C:259:THR:O	2.18	0.43
1:C:453:TYR:CE1	1:C:495:TYR:CD1	3.07	0.43
1:A:126:VAL:HG13	1:A:175:PHE:HZ	1.84	0.43
1:B:353:TRP:CZ3	1:B:423:TYR:HD1	2.37	0.43
1:B:819:GLU:OE2	1:B:1054:GLN:OE1	2.37	0.43
1:B:965:GLN:NE2	1:B:965:GLN:HA	2.34	0.43
1:C:101:ILE:N	1:C:101:ILE:CD1	2.82	0.43
1:C:1102:TRP:O	1:C:1115:ILE:HD13	2.16	0.43
1:C:1124:GLY:C	1:C:1125:ASN:HD22	2.22	0.43
1:A:201:PHE:HD1	1:A:201:PHE:C	2.22	0.43
1:B:108:THR:OG1	1:B:234:ASN:O	2.34	0.43
1:B:541:PHE:CD1	1:B:541:PHE:C	2.92	0.43
1:B:1078:ALA:N	1:B:1102:TRP:HH2	2.17	0.43
1:C:223:LEU:CD2	1:C:223:LEU:N	2.59	0.43
1:C:916:LEU:HD12	1:C:916:LEU:O	2.19	0.43
1:A:600:PRO:CD	1:A:692:ILE:HD11	2.43	0.43
1:A:1090:PRO:HD3	1:A:1095:PHE:CE1	2.54	0.43
1:A:1102:TRP:CB	1:A:1135:ASN:HD22	2.25	0.43
1:B:108:THR:HG22	1:B:109:THR:HG23	2.00	0.43
1:C:411:ALA:CA	1:C:425:LEU:CD1	2.95	0.43
1:C:577:ARG:HB2	1:C:584:ILE:CD1	2.48	0.43
1:C:959:LEU:HA	1:C:959:LEU:HD12	1.76	0.43
1:C:1042:PHE:HD2	1:C:1043:CYS:SG	2.42	0.43
1:A:128:ILE:HG23	1:A:129:LYS:H	1.81	0.43
1:A:560:LEU:N	1:A:560:LEU:CD1	2.82	0.43
1:A:1080:ALA:O	1:A:1132:ILE:CG1	2.57	0.43
1:B:38:TYR:H	1:B:38:TYR:HD1	1.66	0.43
1:B:674:TYR:HD1	1:B:692:ILE:HD13	1.83	0.43
1:B:785:VAL:HG12	1:B:888:PHE:CE1	2.54	0.43
1:B:1142:GLN:HE21	1:B:1142:GLN:CA	2.12	0.43
1:C:490:PHE:CD2	1:C:492:LEU:HB2	2.47	0.43
1:C:970:PHE:HD2	1:C:999:GLY:CA	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:SER:HB2	1:A:216:LEU:CD2	2.43	0.42
1:A:89:GLY:HA2	1:A:270:LEU:HD12	2.01	0.42
1:A:767:LEU:HD23	1:A:767:LEU:HA	1.79	0.42
1:A:1019:ARG:HG2	1:A:1019:ARG:HH11	1.84	0.42
1:B:529:LYS:HA	1:B:529:LYS:HE3	2.01	0.42
1:B:675:GLN:NE2	1:B:675:GLN:CA	2.74	0.42
1:C:738:CYS:HB3	1:C:1004:LEU:HD11	2.01	0.42
1:A:29:THR:HG23	1:A:62:VAL:HG13	2.01	0.42
1:A:66:HIS:CD2	1:A:68:ILE:HG21	2.52	0.42
1:A:349:SER:O	1:A:352:ALA:O	2.38	0.42
1:A:804:GLN:H	1:A:804:GLN:HG2	1.51	0.42
1:A:896:ILE:HD11	1:C:712:ILE:HD12	2.00	0.42
1:A:1095:PHE:HD2	1:A:1102:TRP:HE3	1.67	0.42
1:B:226:LEU:HD12	1:B:227:VAL:HG13	2.00	0.42
1:B:498:GLN:N	1:B:501:ASN:OD1	2.46	0.42
1:B:977:LEU:HA	1:B:980:ILE:HG22	2.01	0.42
1:C:335:LEU:HD22	1:C:335:LEU:N	2.34	0.42
1:C:860:VAL:HG23	1:C:860:VAL:O	2.19	0.42
2:K:2:NAG:O7	2:K:2:NAG:O3	2.37	0.42
1:A:280:ASN:HD22	1:A:286:THR:CG2	2.32	0.42
1:A:492:LEU:HD12	1:A:492:LEU:N	2.34	0.42
1:A:693:ILE:CD1	1:A:693:ILE:N	2.81	0.42
1:A:1097:SER:HB2	1:A:1102:TRP:CG	2.54	0.42
1:C:204:TYR:HD1	1:C:225:PRO:CA	2.32	0.42
1:C:948:LEU:HD21	1:C:1059:GLY:HA3	2.01	0.42
1:A:216:LEU:N	1:A:216:LEU:CD1	2.82	0.42
1:A:350:VAL:HG13	1:A:422:ASN:ND2	2.34	0.42
1:A:488:CYS:C	1:A:489:TYR:CD1	2.93	0.42
1:A:802:PHE:HE1	1:A:927:PHE:CZ	2.38	0.42
1:A:967:SER:O	1:A:975:SER:CB	2.67	0.42
1:B:118:LEU:CD2	1:B:135:PHE:CE1	2.99	0.42
1:B:1098:ASN:OD1	1:B:1098:ASN:N	2.51	0.42
1:C:128:ILE:HG22	1:C:129:LYS:H	1.55	0.42
1:C:192:PHE:HA	1:C:204:TYR:O	2.20	0.42
1:C:785:VAL:O	1:C:785:VAL:HG13	2.19	0.42
1:A:92:PHE:CE1	1:A:104:TRP:HZ2	2.37	0.42
1:B:855:PHE:CD1	1:B:855:PHE:C	2.91	0.42
1:C:100:ILE:CD1	1:C:243:ALA:HB3	2.50	0.42
1:C:328:ARG:NE	1:C:578:ASP:OD1	2.52	0.42
1:C:338:PHE:CE2	1:C:363:ALA:CB	3.02	0.42
1:C:658:ASN:ND2	1:C:660:TYR:OH	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:660:TYR:CB	1:C:695:TYR:CE2	2.97	0.42
1:A:25:PRO:HA	1:A:26:PRO:HD3	1.94	0.42
1:A:192:PHE:HA	1:A:204:TYR:O	2.20	0.42
1:A:426:PRO:HG3	1:A:463:PRO:HB2	2.02	0.42
1:A:472:ILE:HA	1:A:491:PRO:CD	2.49	0.42
1:B:128:ILE:HG23	1:B:129:LYS:H	1.81	0.42
1:C:314:GLN:HE21	1:C:314:GLN:HB2	1.73	0.42
1:C:882:ILE:HA	1:C:898:PHE:CE1	2.52	0.42
1:C:1096:VAL:O	1:C:1096:VAL:HG23	2.19	0.42
1:A:328:ARG:NH2	1:A:533:LEU:CA	2.83	0.42
1:A:347:PHE:CE2	1:A:399:SER:HB2	2.54	0.42
1:A:884:SER:O	1:A:884:SER:OG	2.38	0.42
1:A:1047:TYR:CD1	1:A:1047:TYR:N	2.79	0.42
1:B:88:ASP:OD1	1:B:88:ASP:N	2.53	0.42
1:B:354:ASN:O	1:B:398:ASP:HA	2.19	0.42
1:B:715:PRO:HG3	1:B:1069:PRO:HB3	2.01	0.42
1:B:1081:ILE:O	1:B:1088:HIS:CB	2.48	0.42
1:C:558:LYS:N	1:C:558:LYS:CD	2.82	0.42
1:C:782:PHE:CD2	1:C:870:ILE:HG23	2.54	0.42
1:A:266:TYR:HD1	1:A:266:TYR:H	1.68	0.42
1:A:426:PRO:HG3	1:A:463:PRO:CB	2.49	0.42
1:A:954:GLN:CG	1:A:1014:ARG:CZ	2.97	0.42
1:B:37:TYR:C	1:B:37:TYR:HD1	2.22	0.42
1:B:724:THR:CG2	1:B:1063:LEU:CD2	2.93	0.42
1:B:822:LEU:CD1	1:B:938:LEU:HD13	2.50	0.42
1:B:1078:ALA:HB3	1:B:1102:TRP:CH2	2.55	0.42
1:C:90:VAL:CA	1:C:270:LEU:CD1	2.98	0.42
1:C:168:PHE:CG	1:C:231:ILE:CG1	3.02	0.42
1:C:817:PHE:CD1	1:C:817:PHE:C	2.93	0.42
1:A:37:TYR:N	1:A:37:TYR:CD1	2.83	0.42
1:A:369:TYR:OH	1:A:384:PRO:CB	2.67	0.42
1:A:617:CYS:SG	1:A:644:GLN:CA	3.08	0.42
1:A:662:CYS:HA	1:A:695:TYR:OH	2.20	0.42
1:A:736:VAL:HG21	1:A:858:LEU:HD22	1.91	0.42
1:A:741:TYR:CZ	1:A:962:LEU:CD1	3.03	0.42
1:B:805:ILE:HG23	1:B:1054:GLN:NE2	2.34	0.42
1:C:43:PHE:O	1:C:43:PHE:CG	2.69	0.42
1:C:117:LEU:O	1:C:118:LEU:HB2	2.20	0.42
1:C:378:LYS:HG2	1:C:433:VAL:HG13	1.93	0.42
1:C:541:PHE:CD1	1:C:541:PHE:O	2.72	0.42
1:C:738:CYS:N	1:C:760:CYS:SG	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:821:LEU:CD2	1:C:939:SER:HB3	2.34	0.42
1:A:91:TYR:CD1	1:A:91:TYR:C	2.93	0.42
1:A:266:TYR:N	1:A:266:TYR:HD1	2.14	0.42
1:A:704:SER:HB2	1:B:790:LYS:HB2	2.01	0.42
1:B:17:ASN:O	1:B:255:SER:HA	2.20	0.42
1:B:806:LEU:HD22	1:B:807:PRO:HD2	2.02	0.42
1:B:868:GLU:OE1	1:B:868:GLU:HA	2.20	0.42
1:B:911:VAL:HG21	1:B:1067:TYR:CE2	2.55	0.42
1:B:1039:ARG:HB2	1:B:1042:PHE:HB2	2.02	0.42
1:C:99:ASN:N	1:C:99:ASN:HD22	2.17	0.42
1:C:290:ASP:O	1:C:297:SER:CB	2.59	0.42
1:C:358:ILE:CG2	1:C:395:VAL:HB	2.50	0.42
1:C:433:VAL:CG2	1:C:512:VAL:HG22	2.40	0.42
1:C:521:PRO:HD3	1:C:564:GLN:HG3	2.01	0.42
1:A:302:THR:HG21	1:A:315:THR:CB	2.50	0.41
1:A:336:CYS:HA	1:A:337:PRO:HD3	1.93	0.41
1:B:231:ILE:HG22	1:B:233:ILE:H	1.85	0.41
1:B:312:ILE:O	1:B:312:ILE:HG23	2.20	0.41
1:B:388:ASN:OD1	1:B:527:PRO:HG2	2.20	0.41
1:B:658:ASN:HB2	1:B:660:TYR:HE1	1.85	0.41
1:C:326:ILE:HA	1:C:531:THR:HG21	2.02	0.41
1:C:327:VAL:H	1:C:531:THR:HG22	1.85	0.41
1:C:660:TYR:N	1:C:695:TYR:HE2	2.16	0.41
1:A:90:VAL:CG1	1:A:194:PHE:CA	2.98	0.41
1:A:269:TYR:N	1:A:269:TYR:CD1	2.88	0.41
1:A:671:CYS:HB2	1:A:695:TYR:CZ	2.55	0.41
1:A:1090:PRO:HD3	1:A:1095:PHE:CD1	2.54	0.41
1:B:48:LEU:HB3	1:B:276:LEU:HD21	2.02	0.41
1:C:317:ASN:HA	1:C:593:GLY:O	2.20	0.41
1:C:317:ASN:CA	1:C:593:GLY:O	2.68	0.41
1:C:806:LEU:HA	1:C:806:LEU:HD23	1.82	0.41
1:A:103:GLY:H	1:A:241:LEU:HB3	1.85	0.41
1:A:106:PHE:HB3	1:A:235:ILE:HG21	2.02	0.41
1:A:216:LEU:H	1:A:216:LEU:CD1	2.34	0.41
1:A:309:GLU:H	1:A:309:GLU:CD	2.18	0.41
1:A:350:VAL:HG11	1:A:418:ILE:HD11	2.02	0.41
1:A:1043:CYS:CA	1:A:1064:HIS:HE1	2.27	0.41
1:B:560:LEU:CB	1:B:562:PHE:CE1	3.03	0.41
1:B:577:ARG:HE	1:B:584:ILE:HD11	1.85	0.41
1:C:337:PRO:HB2	1:C:340:GLU:HG2	2.02	0.41
1:C:513:LEU:HD12	1:C:513:LEU:HA	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:PRO:CG	1:A:564:GLN:HG2	2.49	0.41
1:A:878:LEU:HD23	1:A:878:LEU:C	2.40	0.41
1:B:334:ASN:O	1:B:362:VAL:HB	2.20	0.41
1:B:383:SER:H	1:B:386:LYS:HZ3	1.68	0.41
1:B:1095:PHE:HZ	1:B:1120:THR:CG2	2.20	0.41
1:C:108:THR:OG1	1:C:234:ASN:O	2.39	0.41
1:C:313:TYR:CD1	1:C:313:TYR:N	2.88	0.41
1:C:1086:LYS:HE2	1:C:1122:VAL:HG21	2.02	0.41
1:A:17:ASN:O	1:A:255:SER:HA	2.20	0.41
1:A:556:ASN:O	1:A:557:LYS:C	2.59	0.41
1:A:886:TRP:O	1:A:886:TRP:CE3	2.73	0.41
1:A:1004:LEU:HD23	1:A:1004:LEU:HA	1.75	0.41
1:B:107:GLY:CA	1:B:235:ILE:HG12	2.49	0.41
1:B:350:VAL:HG13	1:B:422:ASN:ND2	2.35	0.41
1:B:410:ILE:HG23	1:B:425:LEU:HD11	2.03	0.41
1:B:945:LEU:HD22	1:B:948:LEU:HD12	2.02	0.41
1:C:349:SER:OG	1:C:451:TYR:HA	2.20	0.41
1:C:352:ALA:HB2	1:C:468:ILE:HG22	1.99	0.41
1:C:380:TYR:CE2	1:C:412:PRO:HG3	2.55	0.41
1:C:612:TYR:HB3	1:C:615:VAL:CG1	2.30	0.41
1:C:751:ASN:N	1:C:751:ASN:HD22	2.18	0.41
1:C:1103:PHE:HA	1:C:1115:ILE:HD11	2.02	0.41
1:A:48:LEU:N	1:A:48:LEU:CD1	2.84	0.41
1:A:230:PRO:HG2	1:C:357:ARG:CZ	2.51	0.41
1:A:743:CYS:O	1:A:977:LEU:HD21	2.21	0.41
1:A:864:LEU:CD1	1:C:665:PRO:HB2	2.49	0.41
1:A:917:TYR:CZ	1:C:1079:PRO:HB3	2.56	0.41
1:B:185:ASN:HB2	1:B:213:VAL:HG21	2.03	0.41
1:B:417:LYS:O	1:B:421:TYR:HB2	2.20	0.41
1:B:453:TYR:CE2	1:B:493:GLN:HB2	2.55	0.41
1:C:32:PHE:HB3	1:C:59:PHE:CE2	2.54	0.41
1:C:37:TYR:HA	1:C:223:LEU:HG	2.03	0.41
1:C:312:ILE:HD11	1:C:596:SER:HB3	2.01	0.41
1:C:312:ILE:O	1:C:312:ILE:HG23	2.21	0.41
1:C:534:VAL:HG13	1:C:539:VAL:HG21	2.00	0.41
1:C:1144:GLU:OE1	1:C:1144:GLU:HA	2.20	0.41
1:A:117:LEU:O	1:A:118:LEU:HB2	2.20	0.41
1:A:319:ARG:HB3	1:A:319:ARG:HH21	1.84	0.41
1:A:357:ARG:CD	1:A:396:TYR:HE1	2.34	0.41
1:A:670:ILE:CG2	1:A:694:ALA:HB1	2.51	0.41
1:B:275:PHE:CE1	1:B:290:ASP:CA	3.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:900:MET:HA	1:B:917:TYR:OH	2.20	0.41
1:C:490:PHE:HE2	1:C:492:LEU:CD2	2.30	0.41
1:C:655:HIS:CD2	1:C:655:HIS:O	2.73	0.41
1:C:1083:HIS:CG	1:C:1137:VAL:HB	2.56	0.41
1:A:141:LEU:H	1:A:241:LEU:HD11	1.85	0.41
1:A:403:ARG:HB2	1:A:406:GLU:OE1	2.20	0.41
1:A:726:ILE:HG12	1:A:1061:VAL:HG22	2.03	0.41
1:A:795:LYS:HE2	1:A:795:LYS:HA	2.02	0.41
1:A:805:ILE:HB	1:A:878:LEU:HD11	2.03	0.41
1:A:1007:TYR:CE1	1:A:1011:GLN:OE1	2.74	0.41
1:B:34:ARG:NH1	1:B:189:LEU:HD21	2.34	0.41
1:B:91:TYR:CD1	1:B:91:TYR:C	2.93	0.41
1:B:289:VAL:CG2	1:B:306:PHE:CE2	3.01	0.41
1:B:712:ILE:CG1	1:B:713:ALA:N	2.84	0.41
1:B:718:PHE:CG	1:B:718:PHE:O	2.73	0.41
1:B:726:ILE:HD12	1:B:1061:VAL:CG2	2.41	0.41
1:B:763:LEU:HD23	1:B:763:LEU:HA	1.95	0.41
1:C:226:LEU:O	1:C:226:LEU:HD12	2.21	0.41
1:C:320:VAL:CG2	1:C:619:GLU:HG3	2.51	0.41
1:C:452:LEU:CD2	1:C:492:LEU:HD12	2.51	0.41
1:C:856:ASN:HD22	1:C:856:ASN:HA	1.70	0.41
1:A:384:PRO:HA	1:A:387:LEU:CD1	2.51	0.41
1:A:536:ASN:N	1:A:536:ASN:ND2	2.68	0.41
1:A:597:VAL:HG23	1:A:597:VAL:O	2.21	0.41
1:A:822:LEU:HD13	1:A:1061:VAL:HG21	2.02	0.41
4:A:1307:NAG:O5	4:A:1307:NAG:H83	2.21	0.41
1:B:381:GLY:HA3	1:B:430:THR:HG23	2.01	0.41
1:B:574:ASP:O	1:B:587:ILE:N	2.54	0.41
1:B:715:PRO:HG2	1:B:1108:ASN:O	2.19	0.41
1:B:813:SER:O	1:B:813:SER:OG	2.37	0.41
1:B:976:VAL:HG12	1:B:979:ASP:H	1.86	0.41
1:C:68:ILE:HD12	1:C:262:ALA:HA	2.01	0.41
1:C:105:ILE:CD1	1:C:239:GLN:O	2.68	0.41
1:C:203:ILE:HG21	1:C:203:ILE:HD13	1.85	0.41
1:C:358:ILE:O	1:C:358:ILE:HG23	2.21	0.41
1:C:927:PHE:HZ	1:C:1052:PHE:CE2	2.38	0.41
1:C:931:ILE:CA	1:C:934:ILE:HG22	2.51	0.41
1:A:326:ILE:HG21	1:A:534:VAL:CG2	2.45	0.41
1:A:541:PHE:HB2	1:A:543:PHE:HE1	1.84	0.41
1:A:1048:HIS:O	1:A:1048:HIS:CG	2.73	0.41
1:A:1085:GLY:HA2	1:A:1126:CYS:SG	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:866:THR:O	1:B:867:ASP:C	2.59	0.41
1:B:1102:TRP:CZ2	1:B:1133:VAL:HG11	2.56	0.41
1:C:472:ILE:CD1	1:C:482:GLY:HA2	2.50	0.41
1:C:715:PRO:CA	1:C:1071:GLN:O	2.63	0.41
1:C:882:ILE:HG22	1:C:898:PHE:CE1	2.55	0.41
1:A:559:PHE:CZ	1:B:43:PHE:HD2	2.39	0.40
1:A:560:LEU:HD22	1:A:563:GLN:NE2	2.37	0.40
1:A:927:PHE:CE1	1:A:931:ILE:CG1	3.04	0.40
1:A:1084:ASP:OD2	1:A:1086:LYS:NZ	2.54	0.40
1:B:212:LEU:HD13	1:B:213:VAL:N	2.36	0.40
1:B:661:GLU:OE1	1:B:661:GLU:HA	2.21	0.40
1:B:817:PHE:CD1	1:B:817:PHE:C	2.94	0.40
1:B:937:SER:O	1:B:941:THR:OG1	2.36	0.40
1:C:105:ILE:CB	1:C:118:LEU:HD13	2.50	0.40
1:C:393:THR:HG21	1:C:522:ALA:HB2	1.98	0.40
1:C:752:LEU:HD21	1:C:990:GLU:OE1	2.21	0.40
1:C:754:LEU:HD23	1:C:754:LEU:C	2.41	0.40
1:A:280:ASN:ND2	1:A:286:THR:CG2	2.83	0.40
1:A:881:THR:O	1:A:885:GLY:N	2.55	0.40
1:A:922:LEU:HG	1:A:926:GLN:HE21	1.86	0.40
1:A:927:PHE:C	1:A:927:PHE:CD1	2.94	0.40
1:B:365:TYR:O	1:B:368:LEU:HB2	2.21	0.40
1:B:695:TYR:CD1	1:B:695:TYR:O	2.75	0.40
1:C:342:PHE:HE1	1:C:511:VAL:CG1	2.18	0.40
1:C:601:GLY:O	1:C:605:SER:O	2.39	0.40
1:A:731:MET:HG2	1:A:774:GLN:OE1	2.20	0.40
1:A:976:VAL:CG1	1:A:979:ASP:HB3	2.34	0.40
1:B:659:SER:HB2	1:B:698:SER:HB3	2.03	0.40
1:B:712:ILE:CD1	1:C:896:ILE:HD12	2.51	0.40
1:B:822:LEU:HD21	1:B:1061:VAL:CG2	2.33	0.40
1:C:497:PHE:CD1	1:C:507:PRO:HB3	2.55	0.40
1:A:405:ASP:OD1	1:A:405:ASP:N	2.53	0.40
1:A:1019:ARG:HG2	1:A:1019:ARG:NH1	2.36	0.40
1:A:1029:MET:HE2	1:A:1033:VAL:HG21	2.04	0.40
1:A:1085:GLY:CA	1:A:1126:CYS:SG	3.10	0.40
4:A:1307:NAG:N2	4:A:1307:NAG:C5	2.84	0.40
1:B:560:LEU:HB2	1:B:562:PHE:CE1	2.56	0.40
1:B:612:TYR:O	1:B:648:GLY:HA3	2.21	0.40
1:B:736:VAL:HG13	1:B:858:LEU:CD2	2.45	0.40
1:C:480:CYS:CA	1:C:483:VAL:HG12	2.51	0.40
1:C:520:ALA:HB1	1:C:521:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:560:LEU:CB	1:C:562:PHE:CE1	3.04	0.40
1:C:1004:LEU:C	1:C:1004:LEU:CD2	2.90	0.40
1:A:131:CYS:HG	1:A:166:CYS:CB	2.33	0.40
1:C:37:TYR:CD2	1:C:204:TYR:CD2	3.09	0.40
1:C:102:ARG:O	1:C:104:TRP:CZ3	2.74	0.40
1:C:269:TYR:N	1:C:269:TYR:HD1	2.19	0.40
1:C:718:PHE:CE1	1:C:923:ILE:HG12	2.56	0.40
1:C:782:PHE:CZ	1:C:1060:VAL:HB	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1060/1250 (85%)	1001 (94%)	52 (5%)	7 (1%)	19	47
1	B	1035/1250 (83%)	986 (95%)	45 (4%)	4 (0%)	30	60
1	C	1064/1250 (85%)	1015 (95%)	48 (4%)	1 (0%)	48	78
All	All	3159/3750 (84%)	3002 (95%)	145 (5%)	12 (0%)	32	60

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	620	VAL
1	B	946	GLY
1	A	347	PHE
1	A	501	ASN
1	A	643	PHE
1	B	646	ARG
1	A	337	PRO
1	A	1053	PRO
1	C	665	PRO

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Mol	Chain	Res	Type
1	B	1112	PRO
1	A	1112	PRO
1	B	728	PRO

### 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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	933/1090 (86%)	874 (94%)	59 (6%)	15	40
1	B	915/1090 (84%)	870 (95%)	45 (5%)	21	48
1	C	929/1090 (85%)	864 (93%)	65 (7%)	12	37
All	All	2777/3270 (85%)	2608 (94%)	169 (6%)	18	40

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

Mol	Chain	Res	Type
1	A	32	PHE
1	A	37	TYR
1	A	43	PHE
1	A	64	TRP
1	A	86	PHE
1	A	88	ASP
1	A	117	LEU
1	A	201	PHE
1	A	211	ASN
1	A	220	PHE
1	A	227	VAL
1	A	235	ILE
1	A	238	PHE
1	A	240	THR
1	A	266	TYR
1	A	301	CYS
1	A	304	LYS
1	A	318	PHE
1	A	335	LEU

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Mol	Chain	Res	Type
1	A	345	THR
1	A	353	TRP
1	A	382	VAL
1	A	515	PHE
1	A	536	ASN
1	A	544	ASN
1	A	546	LEU
1	A	552	LEU
1	A	556	ASN
1	A	559	PHE
1	A	602	THR
1	A	607	GLN
1	A	611	LEU
1	A	642	VAL
1	A	643	PHE
1	A	650	LEU
1	A	654	GLU
1	A	661	GLU
1	A	693	ILE
1	A	695	TYR
1	A	696	THR
1	A	709	ASN
1	A	738	CYS
1	A	751	ASN
1	A	760	CYS
1	A	804	GLN
1	A	927	PHE
1	A	954	GLN
1	A	959	LEU
1	A	1019	ARG
1	A	1034	LEU
1	A	1048	HIS
1	A	1067	TYR
1	A	1072	GLU
1	A	1103	PHE
1	A	1106	GLN
1	A	1107	ARG
1	A	1115	ILE
1	A	1121	PHE
1	A	1127	ASP
1	B	37	TYR
1	B	43	PHE

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Mol	Chain	Res	Type
1	B	86	PHE
1	B	88	ASP
1	B	164	ASN
1	B	198	ASP
1	B	212	LEU
1	B	215	ASP
1	B	216	LEU
1	B	218	GLN
1	B	220	PHE
1	B	226	LEU
1	B	234	ASN
1	B	238	PHE
1	B	265	TYR
1	B	270	LEU
1	B	291	CYS
1	B	301	CYS
1	B	318	PHE
1	B	328	ARG
1	B	335	LEU
1	B	546	LEU
1	B	553	THR
1	B	613	GLN
1	B	617	CYS
1	B	620	VAL
1	B	658	ASN
1	B	674	TYR
1	B	695	TYR
1	B	737	ASP
1	B	740	MET
1	B	747	THR
1	B	784	GLN
1	B	820	ASP
1	B	888	PHE
1	B	895	GLN
1	B	941	THR
1	B	950	ASP
1	B	955	ASN
1	B	959	LEU
1	B	1065	VAL
1	B	1088	HIS
1	B	1116	THR
1	B	1127	ASP

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Mol	Chain	Res	Type
1	B	1134	ASN
1	C	32	PHE
1	C	43	PHE
1	C	48	LEU
1	C	51	THR
1	C	55	PHE
1	C	87	ASN
1	C	88	ASP
1	C	96	GLU
1	C	99	ASN
1	C	104	TRP
1	C	105	ILE
1	C	171	VAL
1	C	201	PHE
1	C	210	ILE
1	C	212	LEU
1	C	213	VAL
1	C	216	LEU
1	C	220	PHE
1	C	223	LEU
1	C	226	LEU
1	C	266	TYR
1	C	269	TYR
1	C	270	LEU
1	C	314	GLN
1	C	317	ASN
1	C	334	ASN
1	C	340	GLU
1	C	345	THR
1	C	353	TRP
1	C	365	TYR
1	C	388	ASN
1	C	392	PHE
1	C	409	GLN
1	C	445	VAL
1	C	461	LEU
1	C	483	VAL
1	C	515	PHE
1	C	517	LEU
1	C	531	THR
1	C	546	LEU
1	C	556	ASN

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Mol	Chain	Res	Type
1	C	559	PHE
1	C	585	LEU
1	C	611	LEU
1	C	618	THR
1	C	655	HIS
1	C	660	TYR
1	C	671	CYS
1	C	709	ASN
1	C	736	VAL
1	C	786	LYS
1	C	861	LEU
1	C	896	ILE
1	C	902	MET
1	C	916	LEU
1	C	922	LEU
1	C	934	ILE
1	C	981	LEU
1	C	1083	HIS
1	C	1092	GLU
1	C	1098	ASN
1	C	1101	HIS
1	C	1134	ASN
1	C	1135	ASN
1	C	1139	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	164	ASN
1	A	211	ASN
1	A	317	ASN
1	A	321	GLN
1	A	409	GLN
1	A	501	ASN
1	A	536	ASN
1	A	580	GLN
1	A	613	GLN
1	A	641	ASN
1	A	675	GLN
1	A	751	ASN
1	A	755	GLN

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Mol	Chain	Res	Type
1	A	764	ASN
1	A	779	GLN
1	A	901	GLN
1	A	926	GLN
1	A	954	GLN
1	A	955	ASN
1	A	965	GLN
1	A	978	ASN
1	A	992	GLN
1	A	1002	GLN
1	A	1108	ASN
1	B	165	ASN
1	B	207	HIS
1	B	211	ASN
1	B	218	GLN
1	B	314	GLN
1	B	317	ASN
1	B	360	ASN
1	B	422	ASN
1	B	564	GLN
1	B	606	ASN
1	B	675	GLN
1	B	784	GLN
1	B	913	GLN
1	B	955	ASN
1	B	965	GLN
1	B	1011	GLN
1	B	1036	GLN
1	B	1083	HIS
1	B	1119	ASN
1	B	1142	GLN
1	C	99	ASN
1	C	165	ASN
1	C	185	ASN
1	C	207	HIS
1	C	314	GLN
1	C	343	ASN
1	C	360	ASN
1	C	388	ASN
1	C	394	ASN
1	C	409	GLN
1	C	414	GLN

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Mol	Chain	Res	Type
1	C	493	GLN
1	C	532	ASN
1	C	544	ASN
1	C	607	GLN
1	C	644	GLN
1	C	751	ASN
1	C	779	GLN
1	C	824	ASN
1	C	856	ASN
1	C	901	GLN
1	C	1002	GLN
1	C	1088	HIS
1	C	1125	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

22 monosaccharides are modelled in this entry.

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	E	1	1,2	14,14,15	0.96	1 (7%)	17,19,21	2.33	4 (23%)
2	NAG	E	2	2	14,14,15	0.75	0	17,19,21	1.10	2 (11%)
2	NAG	G	1	1,2	14,14,15	1.02	1 (7%)	17,19,21	1.89	4 (23%)
2	NAG	G	2	2	14,14,15	0.76	1 (7%)	17,19,21	1.09	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	I	1	1,2	14,14,15	1.12	2 (14%)	17,19,21	2.23	6 (35%)
2	NAG	I	2	2	14,14,15	0.89	1 (7%)	17,19,21	1.68	3 (17%)
2	NAG	J	1	1,2	14,14,15	0.76	0	17,19,21	1.08	1 (5%)
2	NAG	J	2	2	14,14,15	0.73	0	17,19,21	1.66	4 (23%)
2	NAG	K	1	1,2	14,14,15	0.66	0	17,19,21	1.33	2 (11%)
2	NAG	K	2	2	14,14,15	0.91	0	17,19,21	1.79	4 (23%)
2	NAG	L	1	1,2	14,14,15	0.69	0	17,19,21	1.26	1 (5%)
2	NAG	L	2	2	14,14,15	0.72	1 (7%)	17,19,21	1.54	3 (17%)
2	NAG	M	1	1,2	14,14,15	0.61	0	17,19,21	1.26	2 (11%)
2	NAG	M	2	2	14,14,15	0.28	0	17,19,21	0.63	0
2	NAG	N	1	1,2	14,14,15	1.24	2 (14%)	17,19,21	2.14	5 (29%)
2	NAG	N	2	2	14,14,15	0.24	0	17,19,21	0.78	0
2	NAG	O	1	1,2	14,14,15	2.10	4 (28%)	17,19,21	3.85	8 (47%)
2	NAG	O	2	2	14,14,15	0.86	1 (7%)	17,19,21	1.72	3 (17%)
2	NAG	P	1	1,2	14,14,15	1.12	1 (7%)	17,19,21	2.26	6 (35%)
2	NAG	P	2	2	14,14,15	0.93	0	17,19,21	1.66	2 (11%)
3	NDG	Q	1	3	14,14,15	1.17	2 (14%)	17,19,21	2.12	6 (35%)
3	NAG	Q	2	3	14,14,15	0.90	2 (14%)	17,19,21	1.82	3 (17%)

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	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	1/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	O	2	2	-	3/6/23/26	0/1/1/1
2	NAG	P	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	P	2	2	-	1/6/23/26	0/1/1/1
3	NDG	Q	1	3	-	0/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	1/6/23/26	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	1	NAG	C2-N2	-5.83	1.36	1.46
2	N	1	NAG	C2-N2	-3.29	1.40	1.46
2	N	1	NAG	C8-C7	-2.86	1.44	1.50
2	I	2	NAG	C8-C7	-2.85	1.44	1.50
3	Q	1	NDG	C2-N2	-2.57	1.41	1.46
2	O	2	NAG	C8-C7	-2.49	1.45	1.50
2	I	1	NAG	C8-C7	-2.48	1.45	1.50
2	G	2	NAG	O5-C1	-2.48	1.39	1.43
2	P	1	NAG	C2-N2	-2.48	1.42	1.46
2	O	1	NAG	C8-C7	-2.40	1.45	1.50
2	I	1	NAG	C2-N2	-2.38	1.42	1.46
3	Q	2	NAG	C8-C7	-2.28	1.45	1.50
3	Q	1	NDG	C8-C7	-2.24	1.45	1.50
2	E	1	NAG	O5-C1	-2.15	1.40	1.43
2	O	1	NAG	C3-C2	-2.10	1.48	1.52
3	Q	2	NAG	C2-N2	-2.09	1.42	1.46
2	G	1	NAG	C2-N2	-2.07	1.42	1.46
2	L	2	NAG	C8-C7	-2.07	1.46	1.50
2	O	1	NAG	O5-C1	-2.02	1.40	1.43

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	1	NAG	O7-C7-N2	9.64	139.67	121.95
2	E	1	NAG	C1-O5-C5	-7.86	101.54	112.19
2	O	1	NAG	C8-C7-N2	-6.85	104.50	116.10
2	O	1	NAG	C1-O5-C5	6.30	120.72	112.19
2	N	1	NAG	C8-C7-N2	-6.07	105.83	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1	NAG	C8-C7-N2	-5.77	106.33	116.10
2	O	1	NAG	O3-C3-C4	-5.37	97.94	110.35
3	Q	1	NDG	C8-C7-N2	-5.31	107.10	116.10
2	P	2	NAG	C1-O5-C5	5.26	119.32	112.19
3	Q	2	NAG	C8-C7-N2	-5.13	107.42	116.10
2	P	1	NAG	O5-C1-C2	-5.06	103.30	111.29
2	P	1	NAG	C1-O5-C5	5.04	119.02	112.19
2	K	2	NAG	C8-C7-N2	-4.54	108.41	116.10
2	J	2	NAG	C2-N2-C7	-4.44	116.58	122.90
2	I	1	NAG	C1-C2-N2	-4.41	102.96	110.49
2	I	2	NAG	C2-N2-C7	-4.15	116.99	122.90
3	Q	1	NDG	C1-C2-N2	-3.90	103.82	110.49
2	K	1	NAG	C1-O5-C5	3.89	117.46	112.19
2	L	2	NAG	C2-N2-C7	-3.72	117.61	122.90
2	G	1	NAG	C1-C2-N2	-3.71	104.14	110.49
2	G	1	NAG	C8-C7-N2	-3.64	109.93	116.10
3	Q	2	NAG	O7-C7-N2	3.63	128.63	121.95
2	N	1	NAG	O7-C7-N2	3.58	128.54	121.95
2	E	1	NAG	O5-C1-C2	3.53	116.86	111.29
2	O	2	NAG	C2-N2-C7	-3.48	117.95	122.90
2	I	2	NAG	O7-C7-N2	3.37	128.15	121.95
2	I	2	NAG	C8-C7-N2	-3.37	110.40	116.10
2	O	1	NAG	O7-C7-C8	-3.35	115.83	122.06
2	P	1	NAG	C8-C7-N2	-3.29	110.53	116.10
2	G	1	NAG	C3-C4-C5	3.28	116.09	110.24
2	L	2	NAG	O7-C7-N2	3.12	127.69	121.95
2	O	1	NAG	C2-N2-C7	3.11	127.33	122.90
2	K	2	NAG	O7-C7-N2	3.04	127.55	121.95
2	K	2	NAG	C1-O5-C5	3.02	116.28	112.19
3	Q	2	NAG	C2-N2-C7	-3.02	118.61	122.90
2	I	1	NAG	O7-C7-C8	3.01	127.66	122.06
2	G	1	NAG	C1-O5-C5	2.99	116.24	112.19
2	I	1	NAG	O5-C5-C6	-2.96	102.57	107.20
2	L	2	NAG	C8-C7-N2	-2.92	111.16	116.10
3	Q	1	NDG	O5-C1-C2	-2.90	106.70	111.29
2	N	1	NAG	O5-C1-C2	-2.89	106.73	111.29
2	O	1	NAG	C1-C2-N2	-2.86	105.60	110.49
2	P	1	NAG	C1-C2-N2	-2.85	105.62	110.49
2	M	1	NAG	C4-C3-C2	-2.81	106.90	111.02
2	M	1	NAG	C1-O5-C5	-2.77	108.43	112.19
3	Q	1	NDG	O7-C7-N2	2.73	126.97	121.95
2	K	2	NAG	C2-N2-C7	-2.69	119.07	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	2	NAG	C4-C3-C2	2.63	114.87	111.02
2	P	1	NAG	O7-C7-N2	2.59	126.70	121.95
2	J	2	NAG	O7-C7-N2	2.57	126.68	121.95
2	E	2	NAG	C2-N2-C7	-2.57	119.25	122.90
2	E	1	NAG	C2-N2-C7	2.56	126.55	122.90
2	J	2	NAG	C1-O5-C5	2.52	115.60	112.19
2	G	2	NAG	C1-O5-C5	2.49	115.56	112.19
2	P	2	NAG	C1-C2-N2	-2.48	106.26	110.49
2	P	1	NAG	C4-C3-C2	-2.41	107.48	111.02
2	K	1	NAG	C4-C3-C2	2.38	114.51	111.02
2	E	2	NAG	C1-C2-N2	-2.35	106.48	110.49
2	O	1	NAG	O4-C4-C3	-2.33	104.96	110.35
2	N	1	NAG	C1-O5-C5	2.29	115.30	112.19
2	G	2	NAG	C2-N2-C7	-2.22	119.75	122.90
2	N	1	NAG	C2-N2-C7	-2.19	119.78	122.90
2	E	1	NAG	C1-C2-N2	-2.13	106.86	110.49
2	J	1	NAG	C8-C7-N2	-2.11	112.52	116.10
3	Q	1	NDG	C3-C4-C5	2.08	113.95	110.24
2	I	1	NAG	O7-C7-N2	2.08	125.77	121.95
2	L	1	NAG	O5-C1-C2	-2.08	108.01	111.29
2	J	2	NAG	O7-C7-C8	-2.08	118.20	122.06
3	Q	1	NDG	O7-C7-C8	2.07	125.90	122.06
2	O	2	NAG	C3-C4-C5	2.05	113.89	110.24
2	I	1	NAG	C3-C4-C5	2.02	113.85	110.24

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	O	1	NAG	C3-C2-N2-C7
2	O	2	NAG	C1-C2-N2-C7
2	J	2	NAG	C1-C2-N2-C7
2	L	2	NAG	C1-C2-N2-C7
2	G	2	NAG	C1-C2-N2-C7
2	I	2	NAG	C1-C2-N2-C7
2	E	2	NAG	C1-C2-N2-C7
2	M	1	NAG	C3-C2-N2-C7
2	N	2	NAG	C1-C2-N2-C7
2	K	2	NAG	C1-C2-N2-C7
2	P	2	NAG	C1-C2-N2-C7
3	Q	2	NAG	C1-C2-N2-C7
2	J	2	NAG	C3-C2-N2-C7

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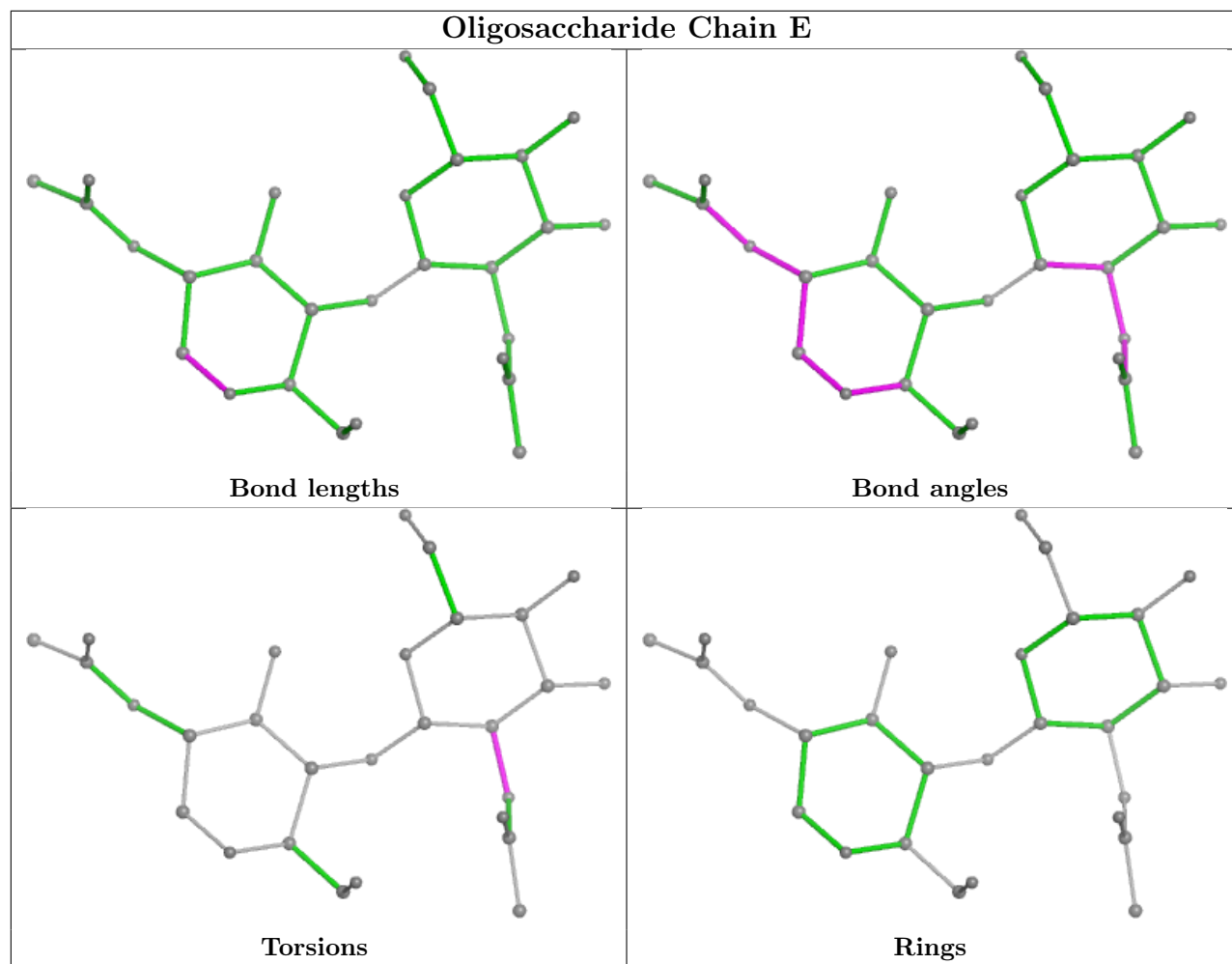
Mol	Chain	Res	Type	Atoms
2	L	2	NAG	C3-C2-N2-C7
2	O	2	NAG	C3-C2-N2-C7
2	O	1	NAG	O5-C5-C6-O6
2	O	1	NAG	C4-C5-C6-O6
2	E	2	NAG	C3-C2-N2-C7
2	K	2	NAG	C3-C2-N2-C7
2	G	2	NAG	C3-C2-N2-C7
2	N	2	NAG	C3-C2-N2-C7
2	O	2	NAG	O5-C5-C6-O6

There are no ring outliers.

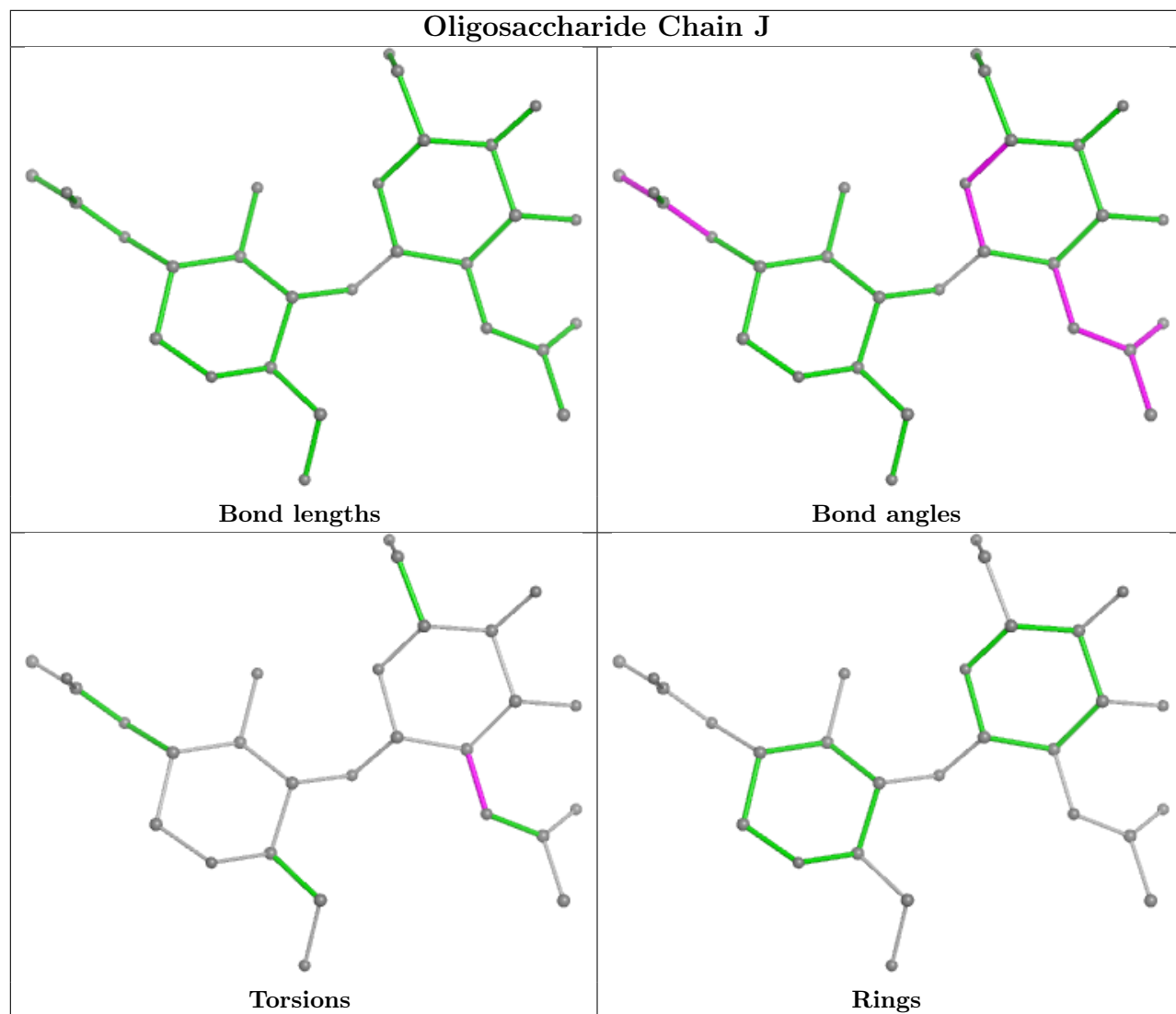
9 monomers are involved in 17 short contacts:

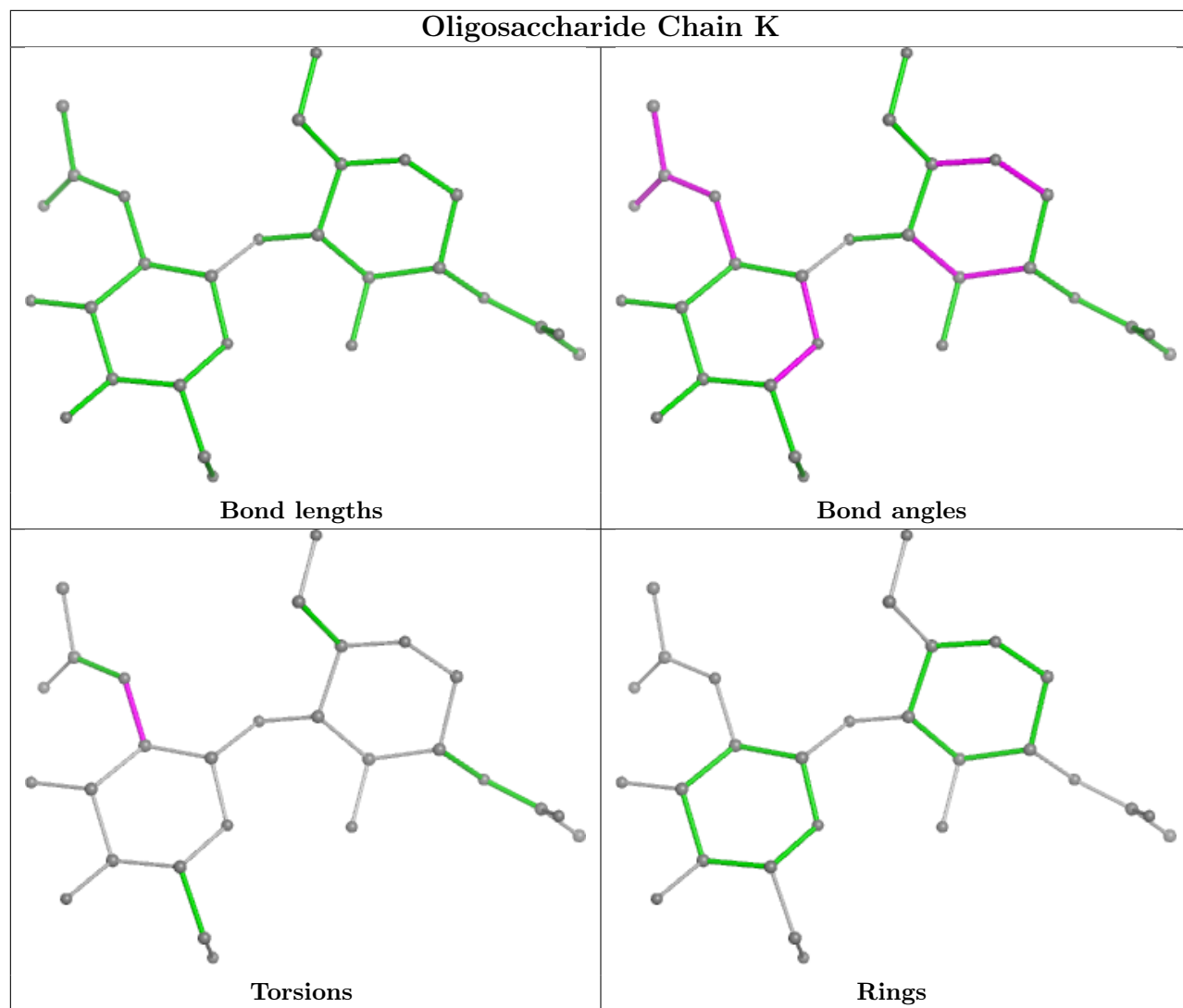
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	1	NAG	1	0
2	P	1	NAG	2	0
3	Q	1	NDG	2	0
2	O	2	NAG	2	0
2	K	2	NAG	1	0
2	L	2	NAG	1	0
2	J	2	NAG	4	0
2	M	1	NAG	1	0
2	K	1	NAG	3	0

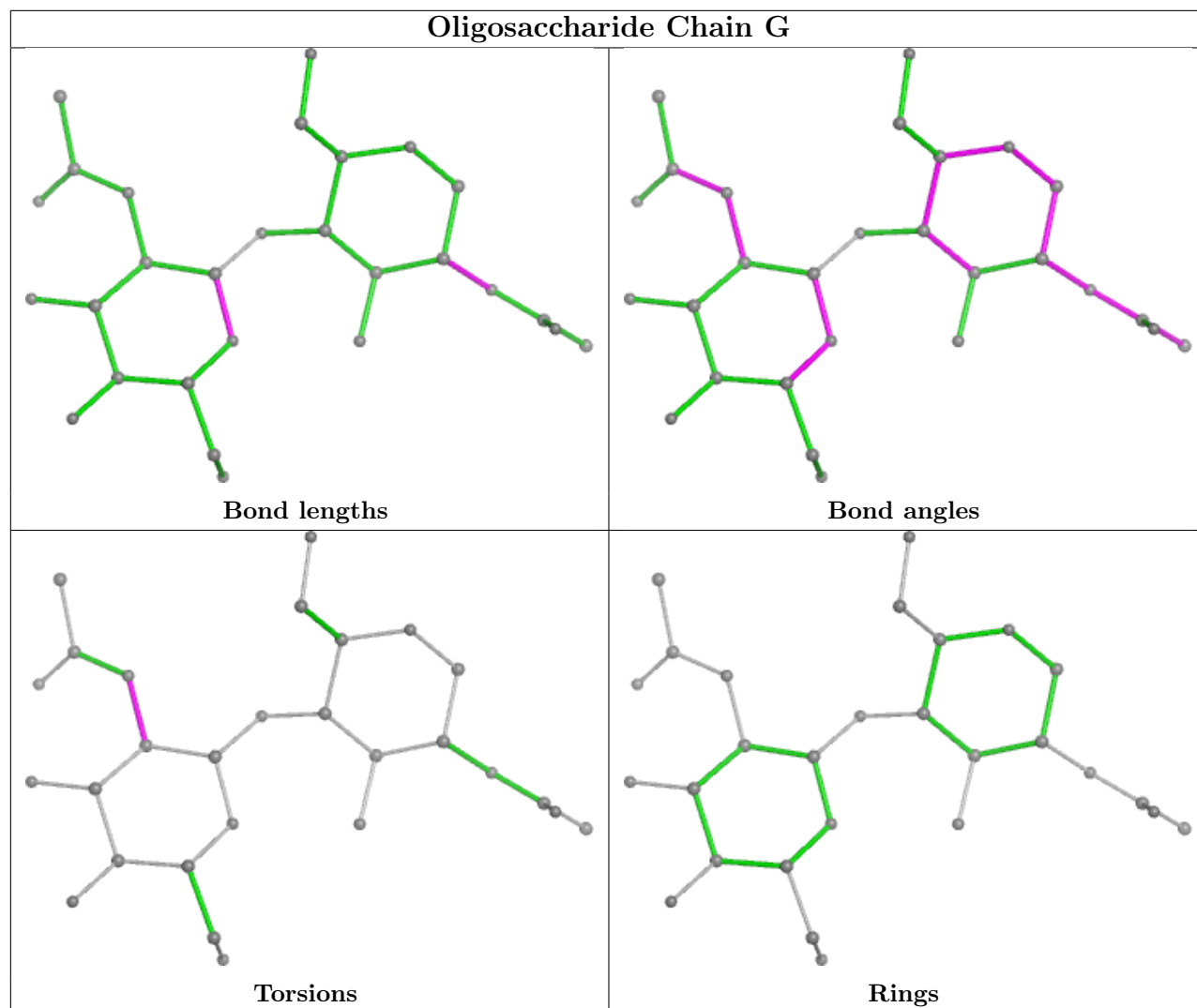
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



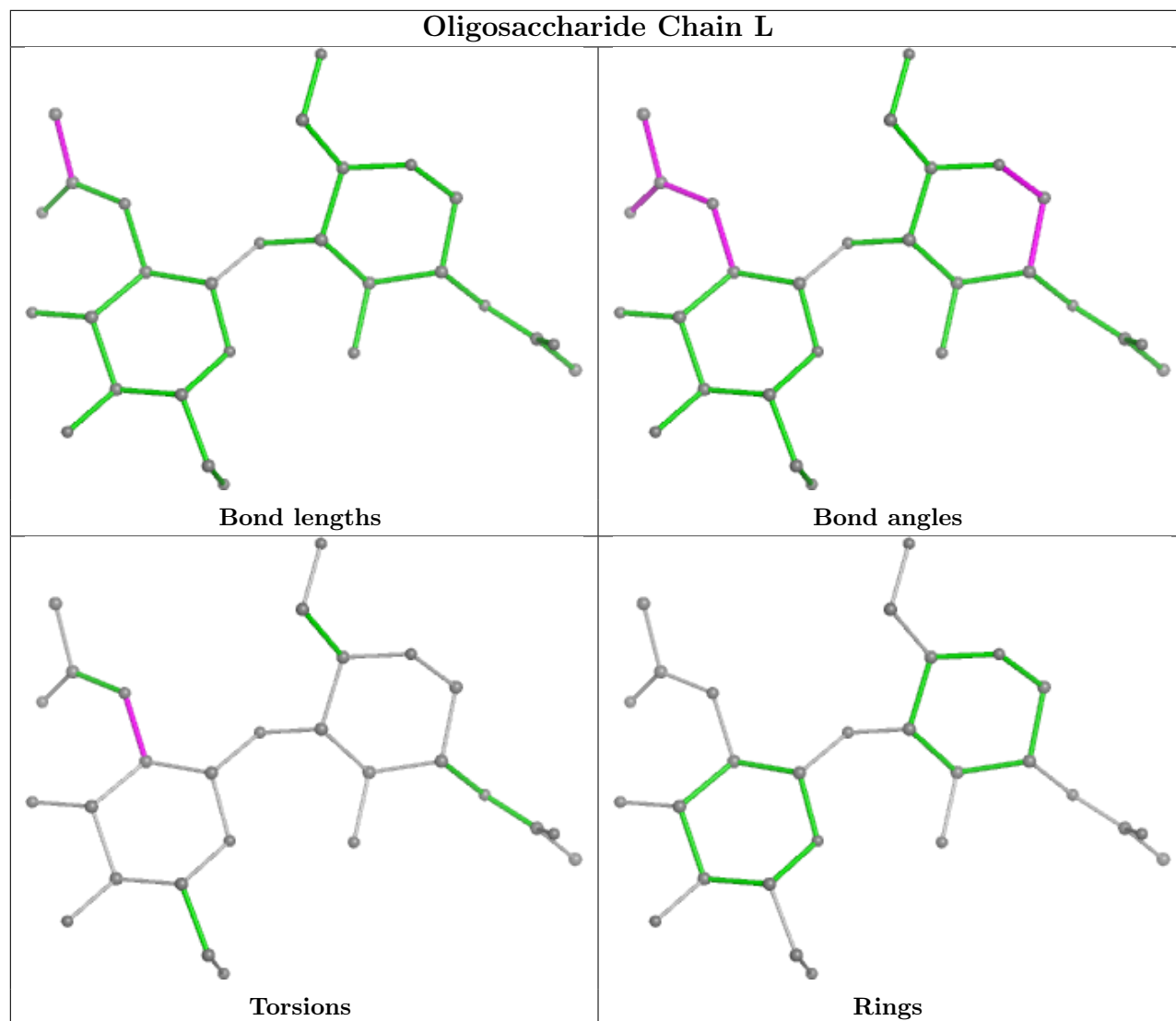
## Oligosaccharide Chain J

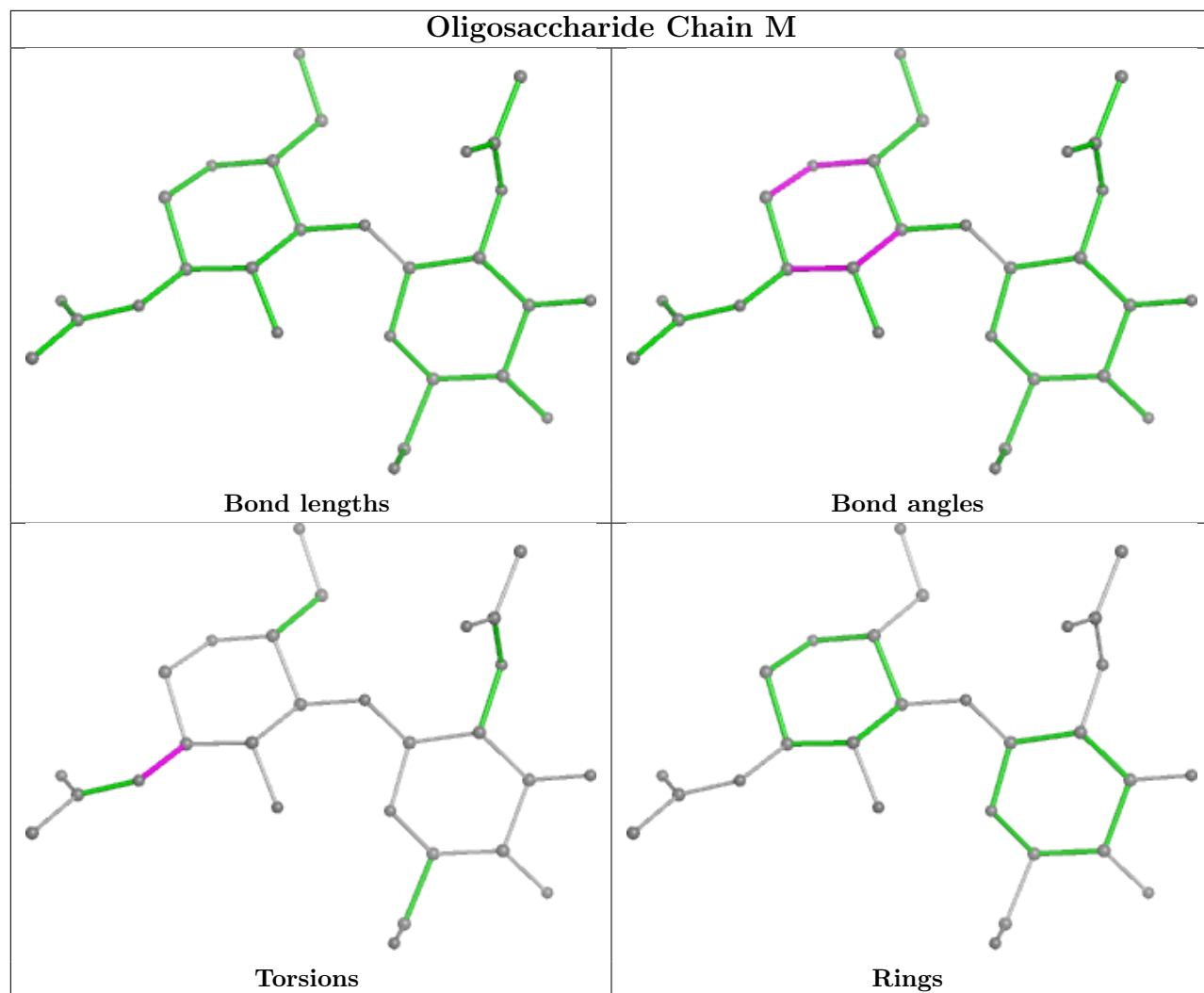


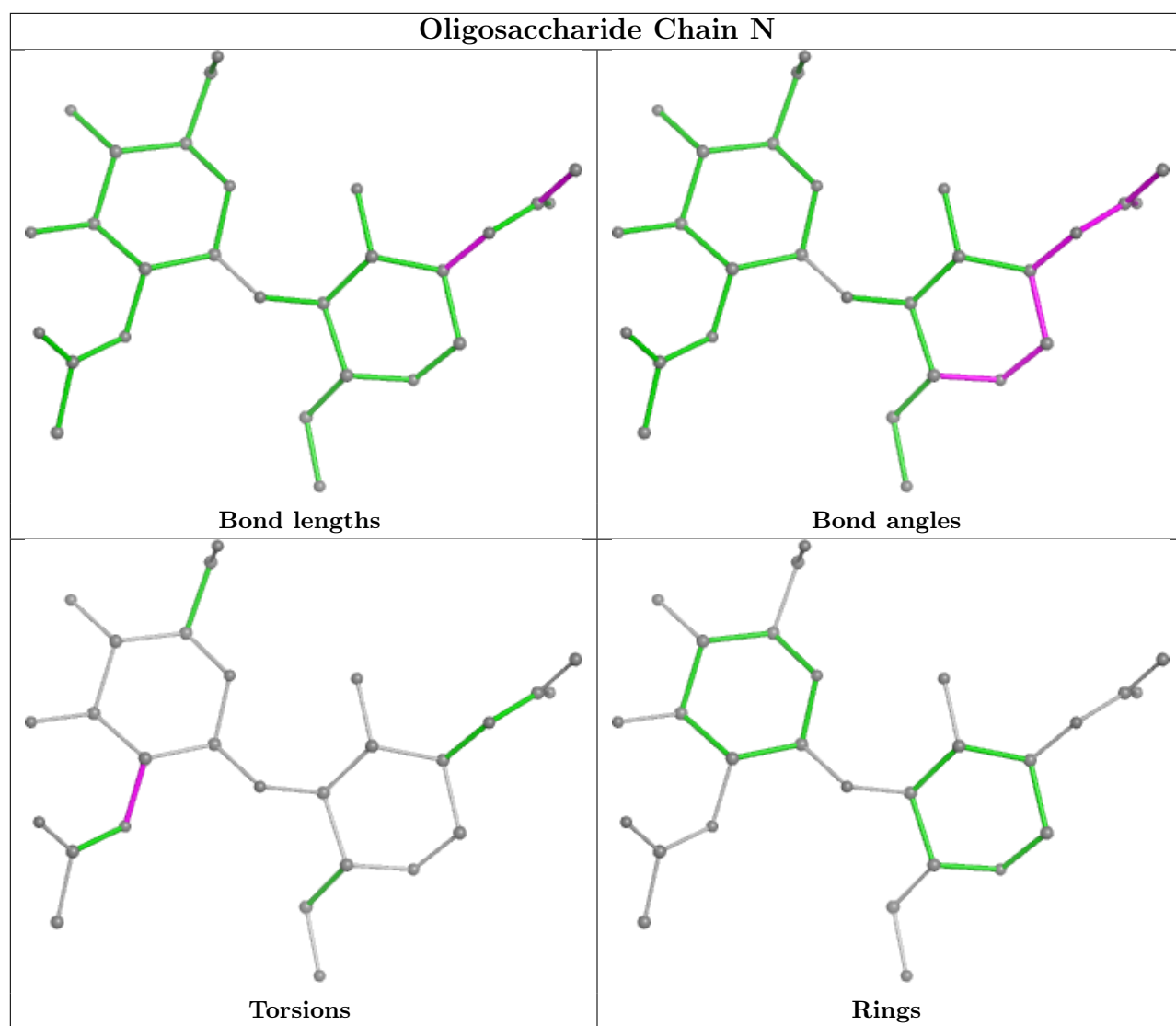


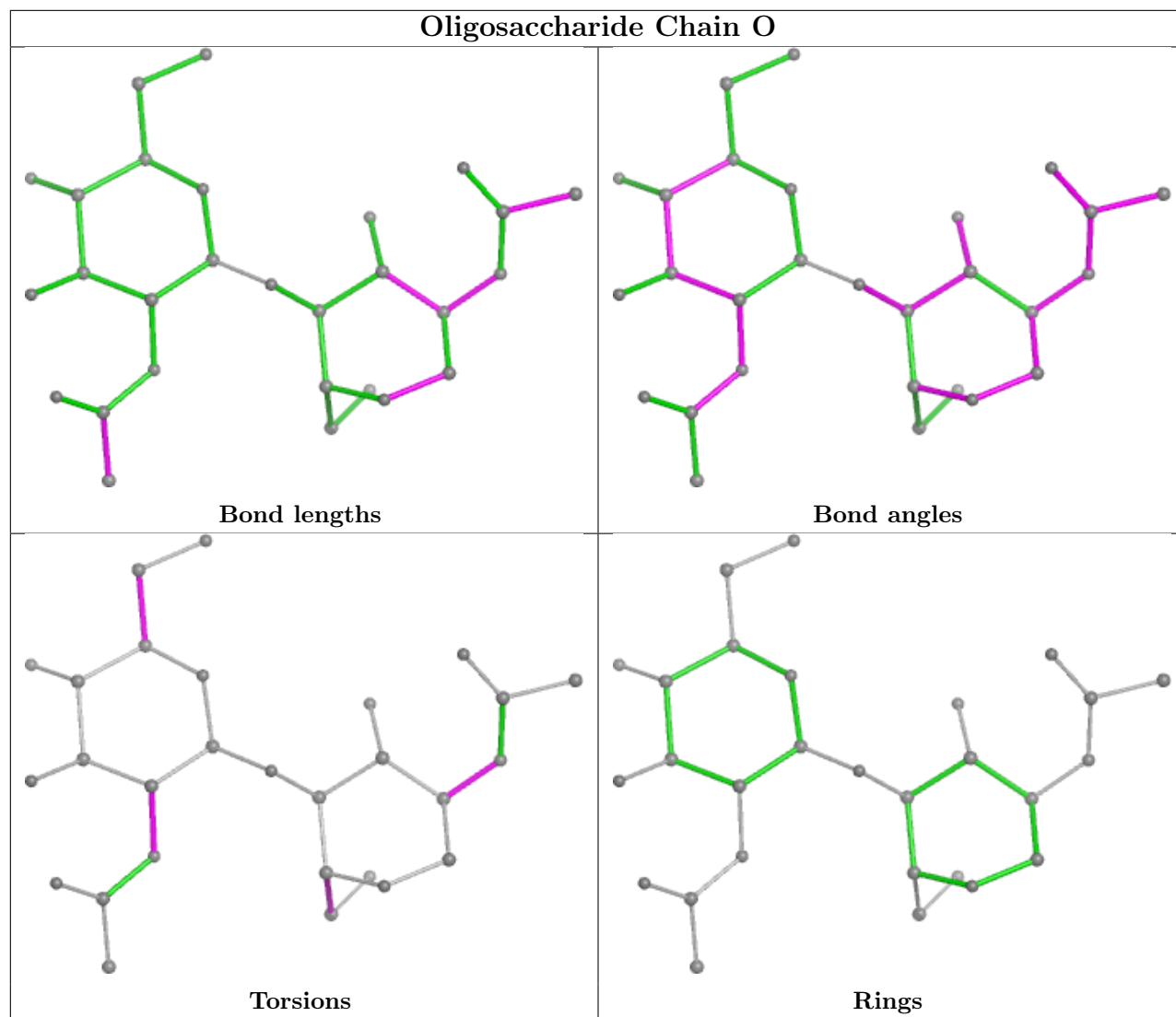


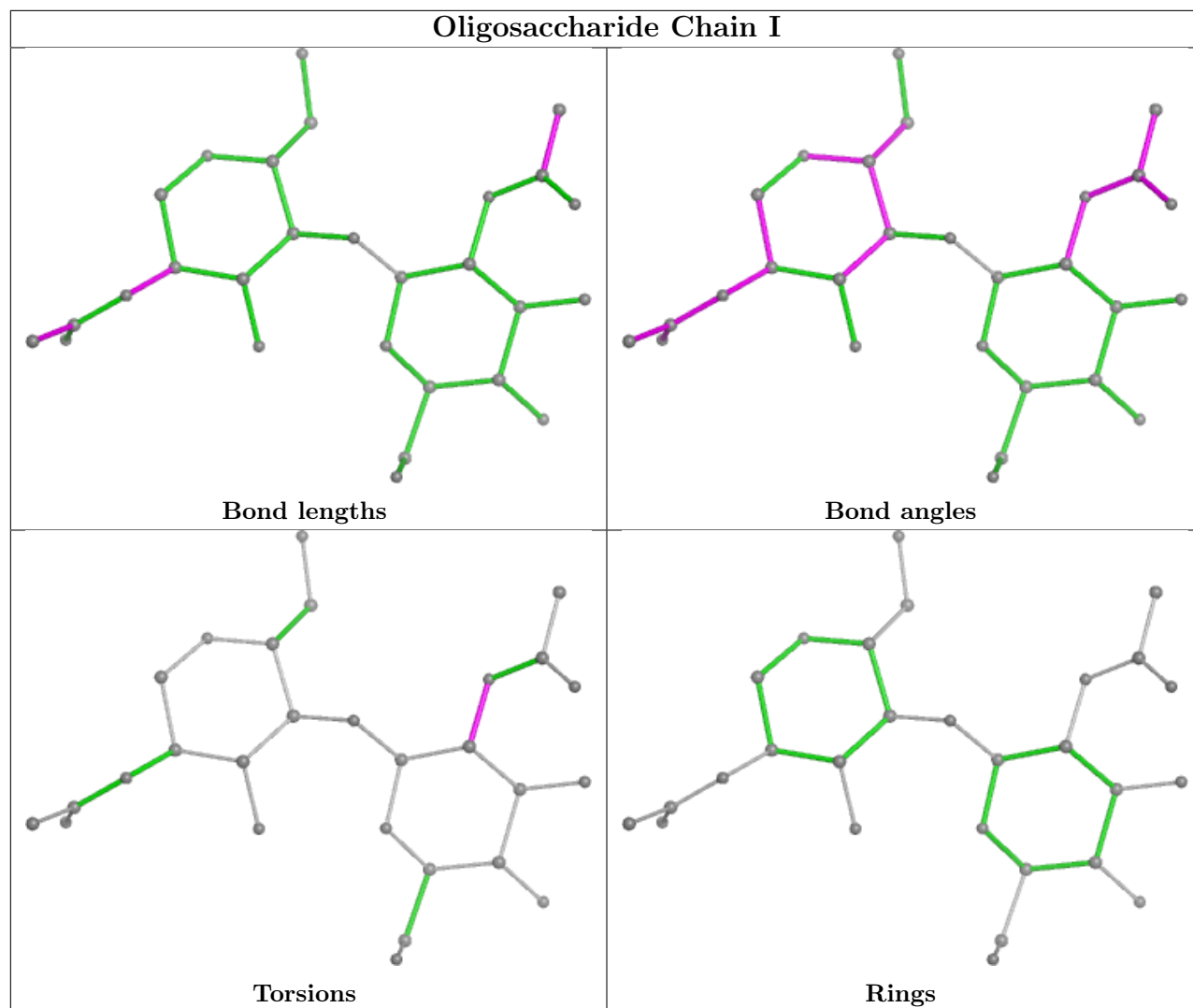


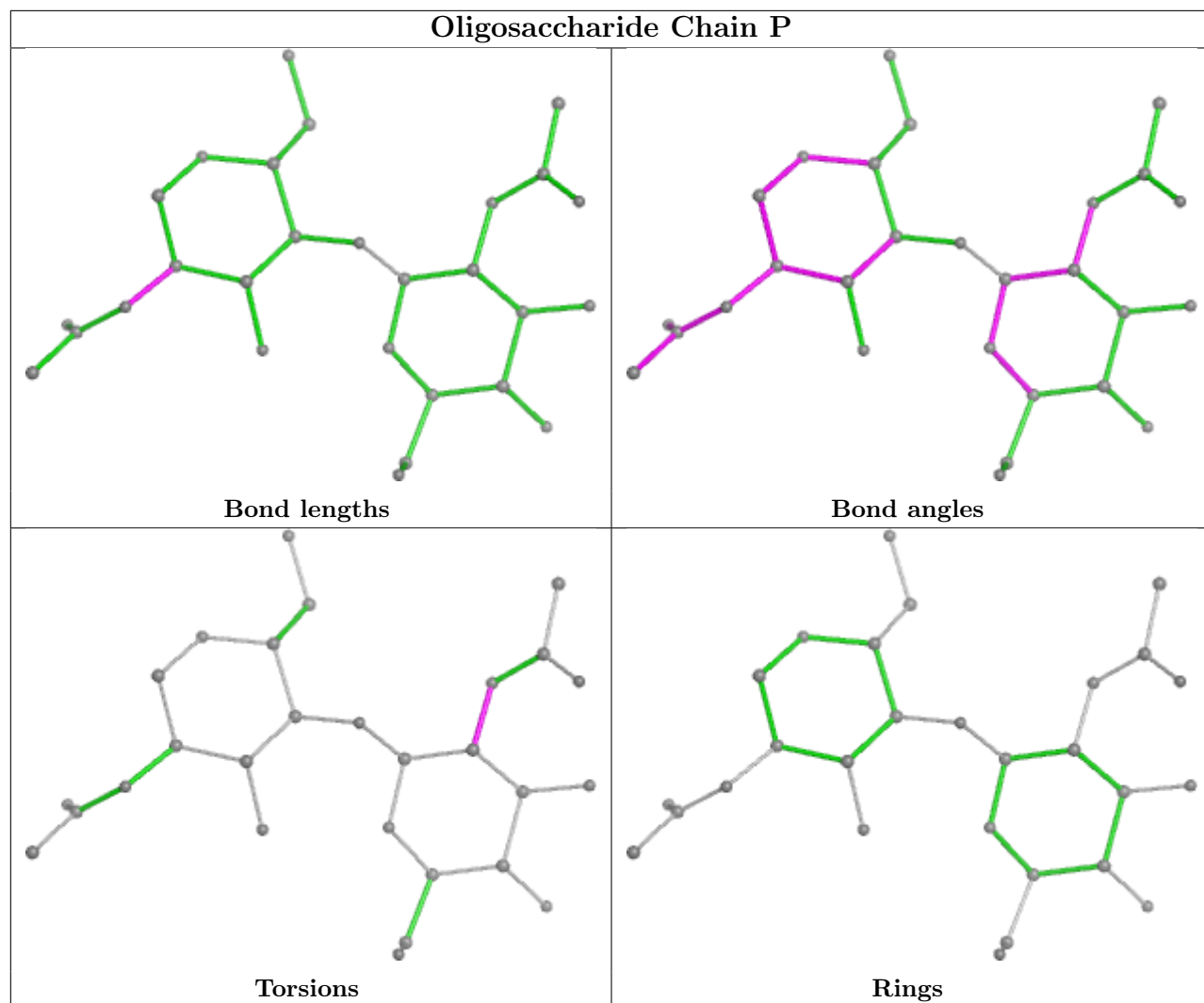


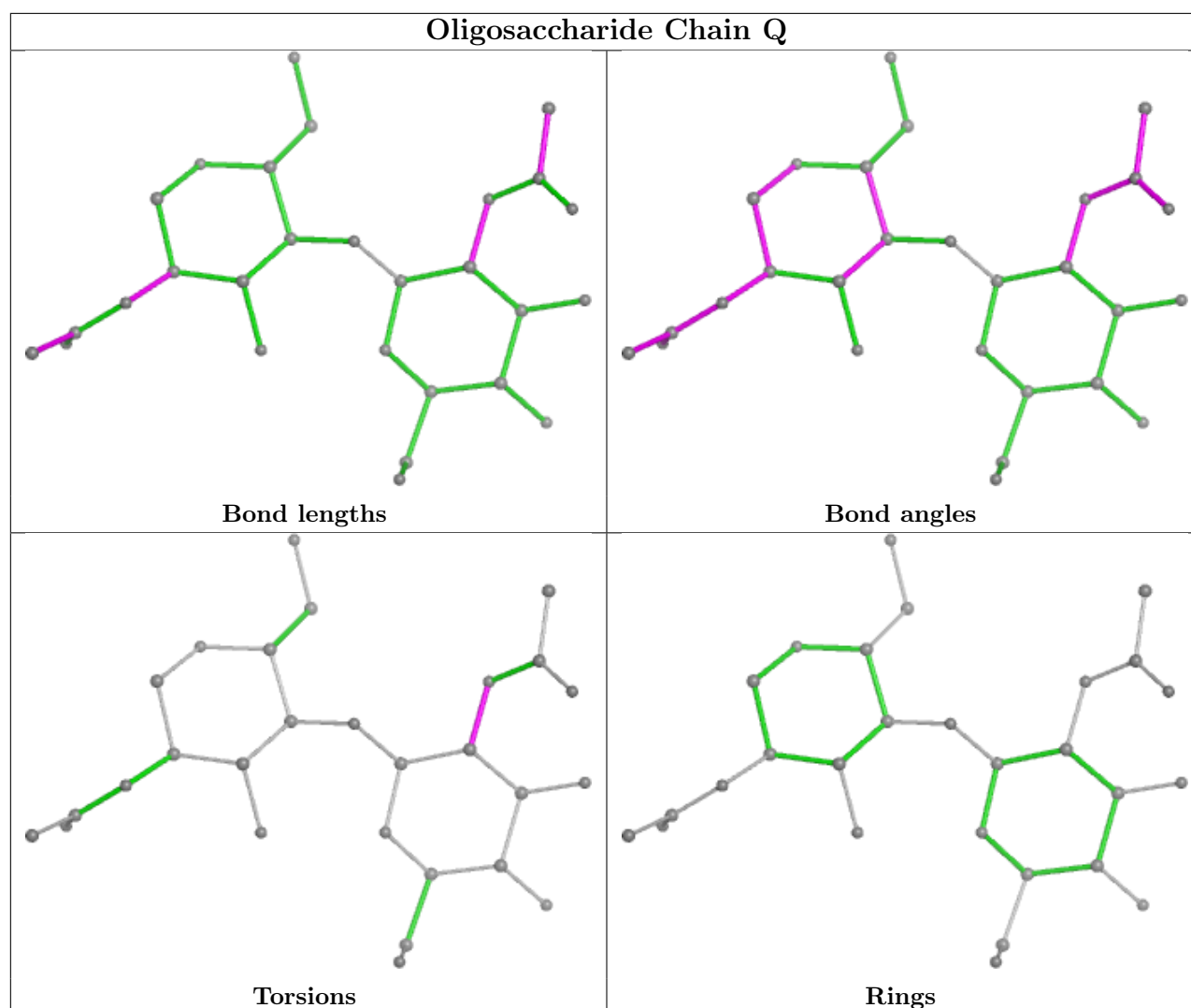












## 5.6 Ligand geometry [i](#)

25 ligands are modelled in this entry.

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	$\# Z  > 2$
4	NAG	A	1306	1	14,14,15	1.12	1 (7%)	17,19,21	1.51	3 (17%)
4	NAG	B	1303	1	14,14,15	0.43	0	17,19,21	0.86	1 (5%)
4	NAG	C	1305	1	14,14,15	0.62	0	17,19,21	0.88	1 (5%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	B	1302	1	14,14,15	0.33	0	17,19,21	1.26	1 (5%)
4	NAG	A	1305	1	14,14,15	0.45	0	17,19,21	1.28	1 (5%)
4	NAG	B	1301	1	14,14,15	0.53	0	17,19,21	1.04	0
4	NAG	A	1309	1	14,14,15	1.52	3 (21%)	17,19,21	5.15	7 (41%)
4	NAG	A	1308	1	14,14,15	0.65	1 (7%)	17,19,21	1.22	3 (17%)
4	NAG	C	1302	1	14,14,15	0.80	0	17,19,21	3.66	8 (47%)
4	NAG	B	1306	1	14,14,15	0.77	0	17,19,21	1.79	3 (17%)
4	NAG	B	1304	1	14,14,15	0.83	0	17,19,21	3.53	7 (41%)
4	NAG	B	1305	1	14,14,15	0.85	0	17,19,21	3.85	9 (52%)
4	NAG	C	1301	-	14,14,15	0.77	0	17,19,21	0.99	0
4	NAG	A	1303	1	14,14,15	0.48	0	17,19,21	0.66	0
4	NAG	A	1304	1	14,14,15	0.66	0	17,19,21	1.87	3 (17%)
4	NAG	C	1303	1	14,14,15	0.80	1 (7%)	17,19,21	1.53	1 (5%)
4	NAG	C	1307	1	14,14,15	0.53	0	17,19,21	2.42	7 (41%)
4	NAG	A	1310	1	14,14,15	0.50	0	17,19,21	0.96	1 (5%)
4	NAG	A	1302	1	14,14,15	0.83	0	17,19,21	3.45	9 (52%)
4	NAG	C	1304	1	14,14,15	0.63	0	17,19,21	1.56	3 (17%)
4	NAG	A	1301	1	14,14,15	1.15	0	17,19,21	4.29	9 (52%)
4	NAG	B	1308	1	14,14,15	1.30	3 (21%)	17,19,21	3.38	5 (29%)
4	NAG	B	1307	1	14,14,15	0.98	0	17,19,21	4.36	5 (29%)
4	NAG	C	1306	1	14,14,15	0.59	0	17,19,21	3.23	5 (29%)
4	NAG	A	1307	1	14,14,15	1.14	1 (7%)	17,19,21	3.61	7 (41%)

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
4	NAG	A	1306	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1301	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1310	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	5/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1309	NAG	O5-C1	-3.83	1.37	1.43
4	B	1308	NAG	C2-N2	-3.51	1.40	1.46
4	A	1306	NAG	O5-C1	-3.35	1.38	1.43
4	A	1307	NAG	O7-C7	-3.31	1.15	1.23
4	C	1303	NAG	C1-C2	2.61	1.56	1.52
4	A	1309	NAG	C8-C7	-2.42	1.45	1.50
4	B	1308	NAG	C7-N2	-2.42	1.26	1.34
4	B	1308	NAG	C8-C7	-2.18	1.46	1.50
4	A	1309	NAG	C2-N2	-2.08	1.42	1.46
4	A	1308	NAG	C1-C2	2.03	1.55	1.52

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1309	NAG	C2-N2-C7	14.13	143.03	122.90
4	C	1306	NAG	C1-O5-C5	11.61	127.92	112.19
4	A	1301	NAG	C8-C7-N2	-11.49	96.64	116.10
4	B	1307	NAG	C8-C7-N2	-11.45	96.71	116.10
4	A	1307	NAG	C8-C7-N2	10.38	133.67	116.10
4	B	1307	NAG	C2-N2-C7	10.05	137.22	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1309	NAG	C8-C7-N2	-9.49	100.03	116.10
4	C	1302	NAG	C8-C7-N2	-9.14	100.62	116.10
4	A	1309	NAG	O7-C7-N2	9.06	138.61	121.95
4	B	1305	NAG	C8-C7-N2	-8.72	101.33	116.10
4	B	1304	NAG	C8-C7-N2	-8.69	101.39	116.10
4	A	1302	NAG	C8-C7-N2	-8.65	101.46	116.10
4	B	1308	NAG	C8-C7-N2	-8.45	101.79	116.10
4	B	1305	NAG	C2-N2-C7	8.19	134.57	122.90
4	B	1304	NAG	C2-N2-C7	8.02	134.32	122.90
4	B	1308	NAG	C1-C2-N2	-7.23	98.13	110.49
4	A	1301	NAG	C2-N2-C7	7.12	133.04	122.90
4	A	1309	NAG	C1-C2-N2	6.50	121.59	110.49
4	A	1304	NAG	C2-N2-C7	6.48	132.14	122.90
4	B	1308	NAG	O7-C7-N2	6.24	133.43	121.95
4	B	1307	NAG	O7-C7-C8	6.22	133.62	122.06
4	B	1306	NAG	C2-N2-C7	-5.58	114.95	122.90
4	C	1302	NAG	O5-C1-C2	-5.49	102.63	111.29
4	A	1302	NAG	C2-N2-C7	5.35	130.52	122.90
4	C	1302	NAG	C2-N2-C7	5.34	130.51	122.90
4	B	1307	NAG	C1-C2-N2	-5.34	101.37	110.49
4	A	1301	NAG	O7-C7-N2	5.29	131.69	121.95
4	A	1307	NAG	C2-N2-C7	5.28	130.43	122.90
4	A	1307	NAG	O7-C7-N2	-5.28	112.24	121.95
4	C	1302	NAG	C1-C2-N2	5.21	119.39	110.49
4	A	1301	NAG	O7-C7-C8	5.18	131.68	122.06
4	A	1302	NAG	O7-C7-N2	5.14	131.39	121.95
4	B	1305	NAG	O5-C1-C2	-5.02	103.36	111.29
4	C	1303	NAG	O5-C1-C2	-4.97	103.44	111.29
4	A	1302	NAG	C1-C2-N2	4.67	118.46	110.49
4	C	1307	NAG	O5-C1-C2	-4.37	104.39	111.29
4	C	1302	NAG	O7-C7-N2	4.33	129.91	121.95
4	A	1307	NAG	O7-C7-C8	-4.30	114.07	122.06
4	B	1304	NAG	O7-C7-N2	4.29	129.84	121.95
4	A	1301	NAG	O5-C5-C6	4.25	113.87	107.20
4	C	1307	NAG	C1-C2-N2	4.19	117.64	110.49
4	B	1305	NAG	O7-C7-C8	4.17	129.80	122.06
4	A	1306	NAG	C2-N2-C7	4.15	128.82	122.90
4	B	1307	NAG	O7-C7-N2	4.15	129.58	121.95
4	A	1309	NAG	O5-C1-C2	-4.15	104.74	111.29
4	A	1301	NAG	C1-O5-C5	4.09	117.73	112.19
4	B	1302	NAG	C1-O5-C5	4.04	117.67	112.19
4	B	1305	NAG	C1-C2-N2	3.97	117.27	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1302	NAG	O7-C7-C8	3.95	129.40	122.06
4	C	1307	NAG	C8-C7-N2	-3.89	109.51	116.10
4	B	1305	NAG	O7-C7-N2	3.75	128.85	121.95
4	A	1307	NAG	O5-C5-C6	3.71	113.02	107.20
4	A	1302	NAG	O5-C1-C2	-3.66	105.51	111.29
4	A	1307	NAG	C1-C2-N2	-3.62	104.31	110.49
4	B	1304	NAG	O7-C7-C8	3.62	128.77	122.06
4	B	1308	NAG	C2-N2-C7	3.61	128.04	122.90
4	C	1307	NAG	O7-C7-N2	3.60	128.58	121.95
4	B	1304	NAG	O5-C5-C6	3.53	112.73	107.20
4	C	1307	NAG	C2-N2-C7	3.52	127.92	122.90
4	A	1301	NAG	O5-C1-C2	-3.47	105.80	111.29
4	C	1306	NAG	C2-N2-C7	3.46	127.84	122.90
4	A	1305	NAG	O5-C1-C2	3.44	116.72	111.29
4	C	1304	NAG	O7-C7-N2	3.42	128.25	121.95
4	B	1304	NAG	O5-C1-C2	-3.41	105.91	111.29
4	C	1306	NAG	O5-C1-C2	-3.39	105.93	111.29
4	C	1304	NAG	C8-C7-N2	-3.35	110.43	116.10
4	A	1301	NAG	C1-C2-N2	3.09	115.77	110.49
4	B	1305	NAG	O5-C5-C6	3.06	112.00	107.20
4	A	1308	NAG	O5-C1-C2	-3.03	106.50	111.29
4	A	1302	NAG	C1-O5-C5	2.96	116.20	112.19
4	B	1305	NAG	C3-C4-C5	-2.84	105.18	110.24
4	C	1307	NAG	C1-O5-C5	2.82	116.01	112.19
4	A	1307	NAG	O5-C1-C2	2.81	115.72	111.29
4	A	1309	NAG	C1-O5-C5	2.80	115.99	112.19
4	B	1308	NAG	C1-O5-C5	2.75	115.91	112.19
4	A	1302	NAG	O7-C7-C8	2.73	127.13	122.06
4	B	1304	NAG	C1-C2-N2	2.72	115.14	110.49
4	B	1305	NAG	C1-O5-C5	2.67	115.80	112.19
4	A	1304	NAG	O5-C1-C2	-2.66	107.08	111.29
4	C	1302	NAG	C1-O5-C5	2.65	115.79	112.19
4	A	1306	NAG	C1-C2-N2	2.60	114.92	110.49
4	A	1302	NAG	O5-C5-C6	2.58	111.25	107.20
4	A	1308	NAG	C1-O5-C5	2.45	115.50	112.19
4	A	1306	NAG	O5-C5-C6	-2.38	103.47	107.20
4	C	1305	NAG	C2-N2-C7	-2.35	119.56	122.90
4	A	1302	NAG	C3-C4-C5	-2.32	106.10	110.24
4	A	1301	NAG	C3-C4-C5	-2.31	106.13	110.24
4	C	1307	NAG	C3-C4-C5	-2.30	106.13	110.24
4	C	1306	NAG	O7-C7-C8	-2.24	117.89	122.06
4	A	1310	NAG	C1-O5-C5	-2.19	109.22	112.19

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1304	NAG	O5-C5-C6	2.19	110.64	107.20
4	C	1306	NAG	C1-C2-N2	2.18	114.21	110.49
4	B	1306	NAG	C1-O5-C5	2.17	115.13	112.19
4	A	1309	NAG	O3-C3-C4	-2.16	105.35	110.35
4	C	1302	NAG	C3-C4-C5	-2.15	106.40	110.24
4	A	1308	NAG	C2-N2-C7	-2.15	119.85	122.90
4	B	1303	NAG	O5-C1-C2	-2.04	108.07	111.29
4	A	1304	NAG	O7-C7-C8	-2.03	118.29	122.06
4	B	1306	NAG	O5-C5-C6	2.03	110.38	107.20

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1304	NAG	C3-C2-N2-C7
4	A	1306	NAG	C1-C2-N2-C7
4	A	1307	NAG	C1-C2-N2-C7
4	A	1309	NAG	C3-C2-N2-C7
4	A	1307	NAG	O5-C5-C6-O6
4	A	1307	NAG	C8-C7-N2-C2
4	A	1307	NAG	O7-C7-N2-C2
4	C	1306	NAG	C8-C7-N2-C2
4	C	1306	NAG	O7-C7-N2-C2
4	B	1308	NAG	O5-C5-C6-O6
4	B	1301	NAG	O5-C5-C6-O6
4	C	1305	NAG	O5-C5-C6-O6
4	A	1305	NAG	C4-C5-C6-O6
4	A	1303	NAG	O5-C5-C6-O6
4	A	1307	NAG	C4-C5-C6-O6
4	A	1309	NAG	C1-C2-N2-C7
4	C	1306	NAG	O5-C5-C6-O6
4	A	1305	NAG	O5-C5-C6-O6
4	A	1310	NAG	O5-C5-C6-O6
4	A	1308	NAG	C1-C2-N2-C7
4	B	1308	NAG	C4-C5-C6-O6
4	C	1305	NAG	C3-C2-N2-C7
4	C	1305	NAG	C4-C5-C6-O6
4	A	1308	NAG	C3-C2-N2-C7
4	C	1306	NAG	C4-C5-C6-O6
4	C	1307	NAG	C4-C5-C6-O6
4	B	1301	NAG	C4-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1306	NAG	1	0
4	C	1305	NAG	1	0
4	A	1308	NAG	1	0
4	B	1305	NAG	1	0
4	C	1304	NAG	1	0
4	A	1307	NAG	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13916. These allow visual inspection of the internal detail of the map and identification of artifacts.

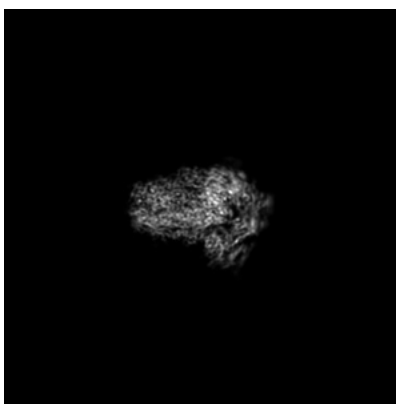
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

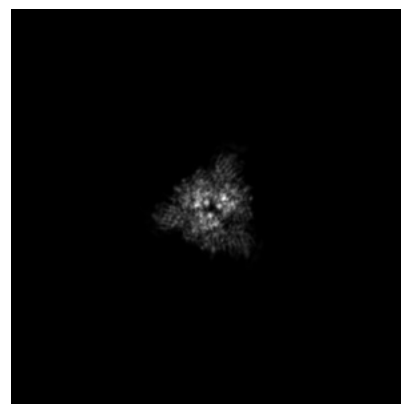
#### 6.1.1 Primary map



X

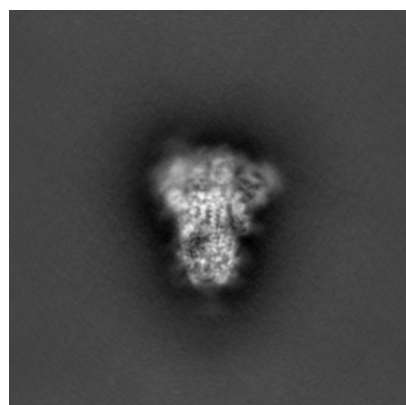


Y

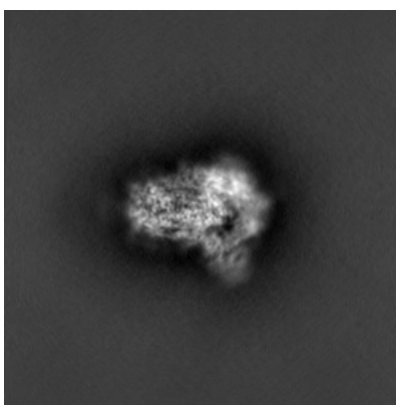


Z

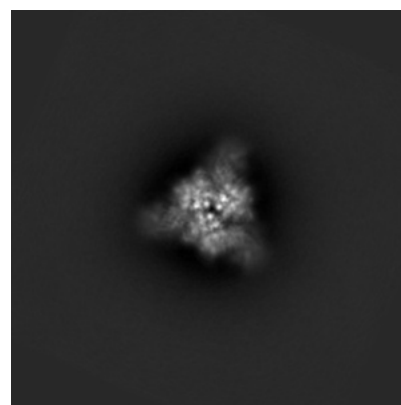
#### 6.1.2 Raw map



X



Y

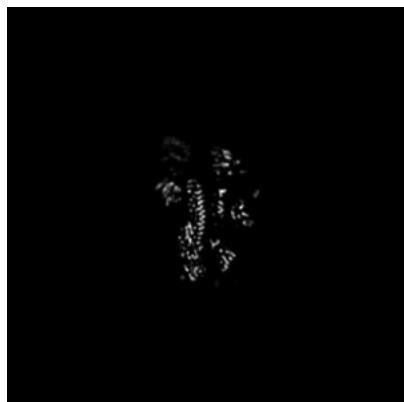


Z

The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 150

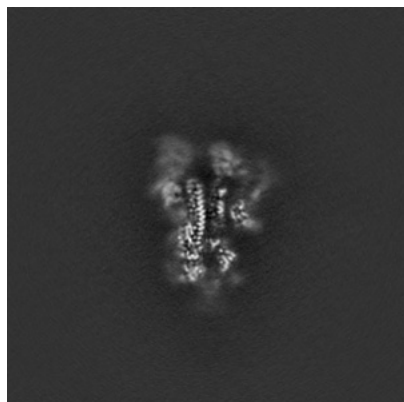


Y Index: 150

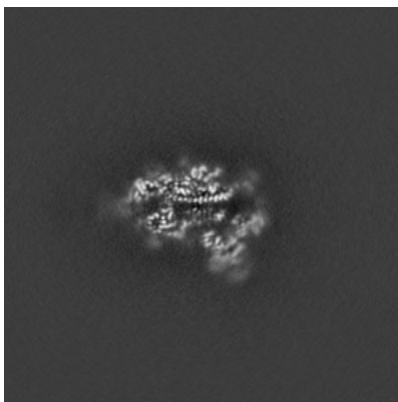


Z Index: 150

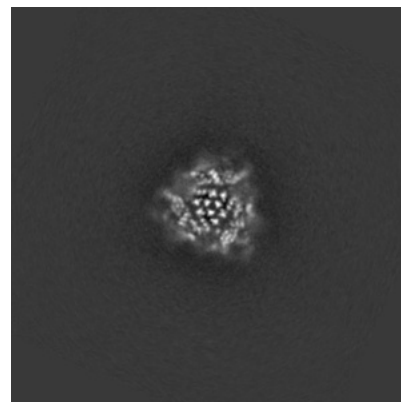
### 6.2.2 Raw map



X Index: 150



Y Index: 150



Z Index: 150

The images above show central slices of the map in three orthogonal directions.



## 6.3 Largest variance slices [i](#)

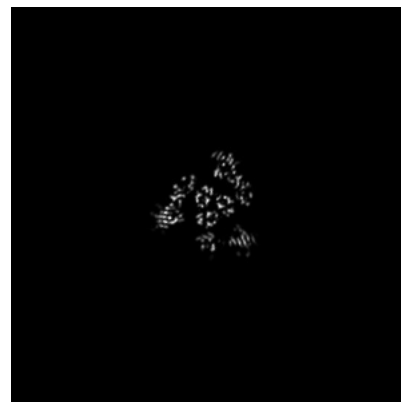
### 6.3.1 Primary map



X Index: 159

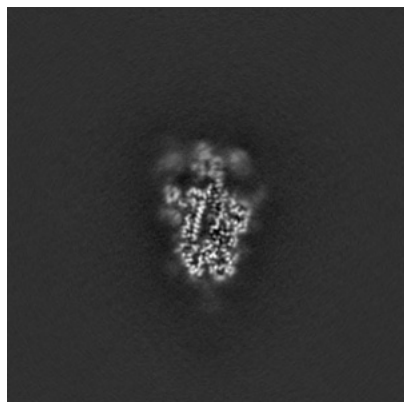


Y Index: 153

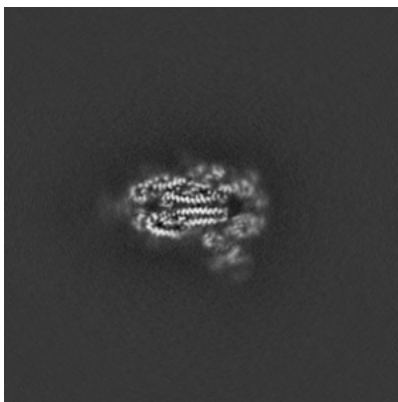


Z Index: 162

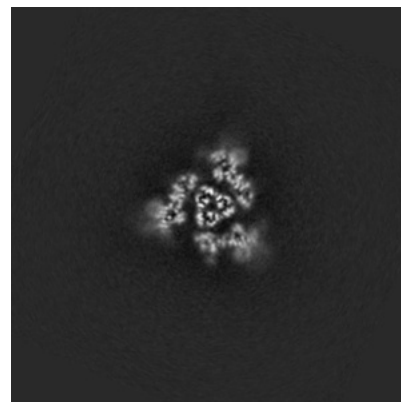
### 6.3.2 Raw map



X Index: 142



Y Index: 153

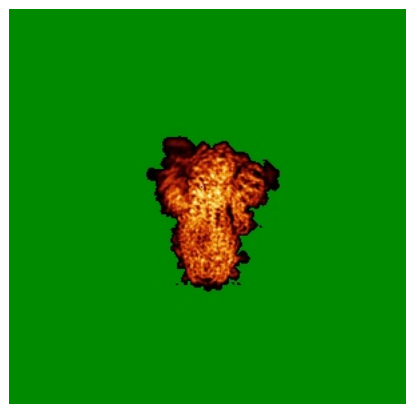


Z Index: 161

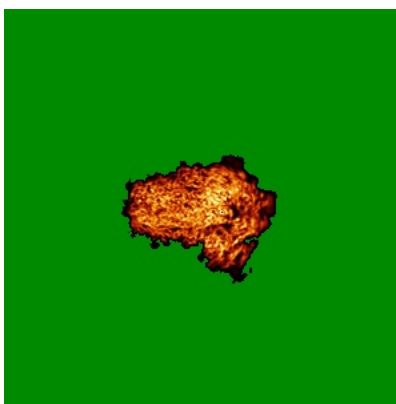
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

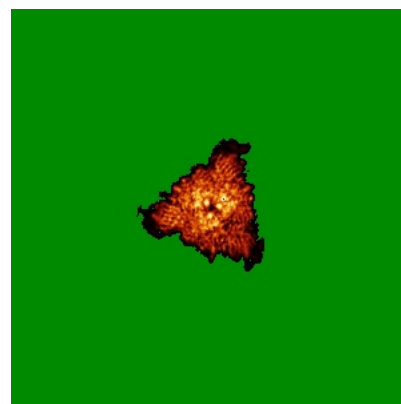
### 6.4.1 Primary map



X

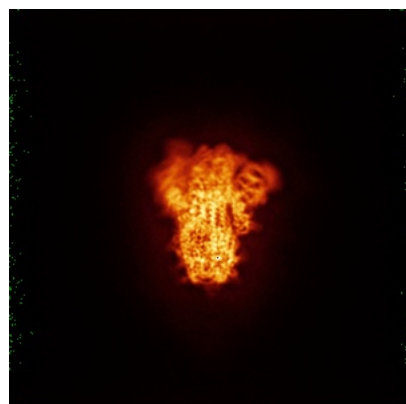


Y

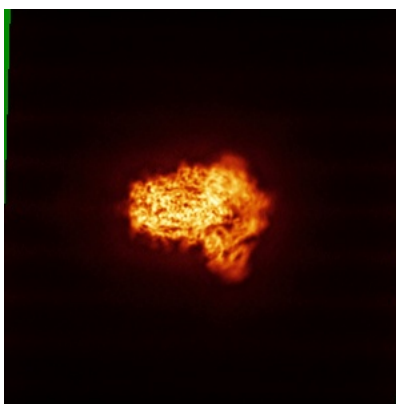


Z

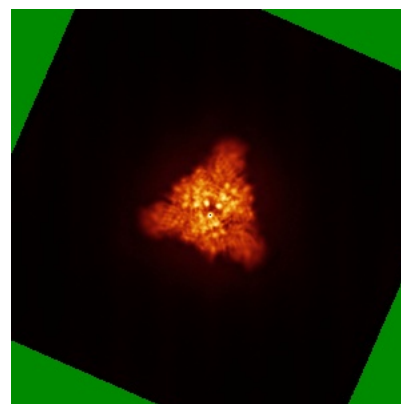
### 6.4.2 Raw map



X



Y

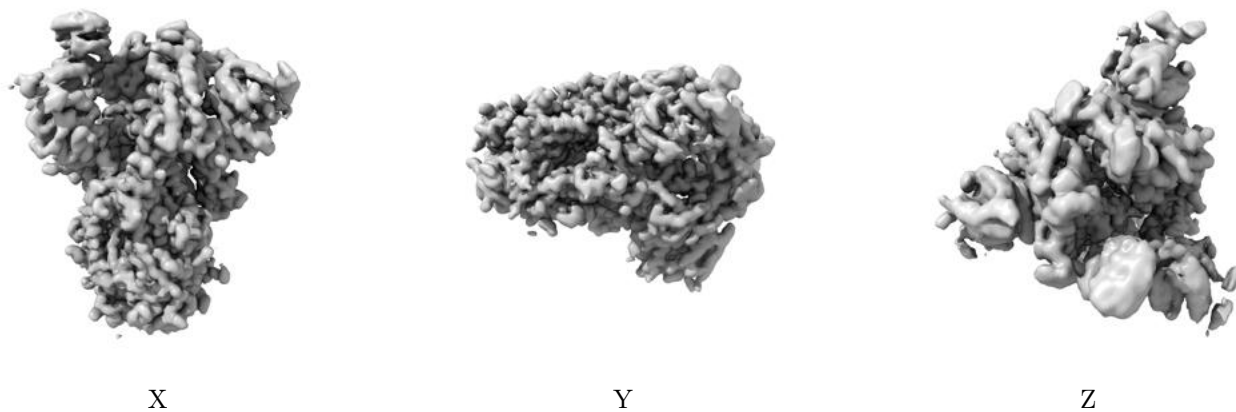


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.048. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

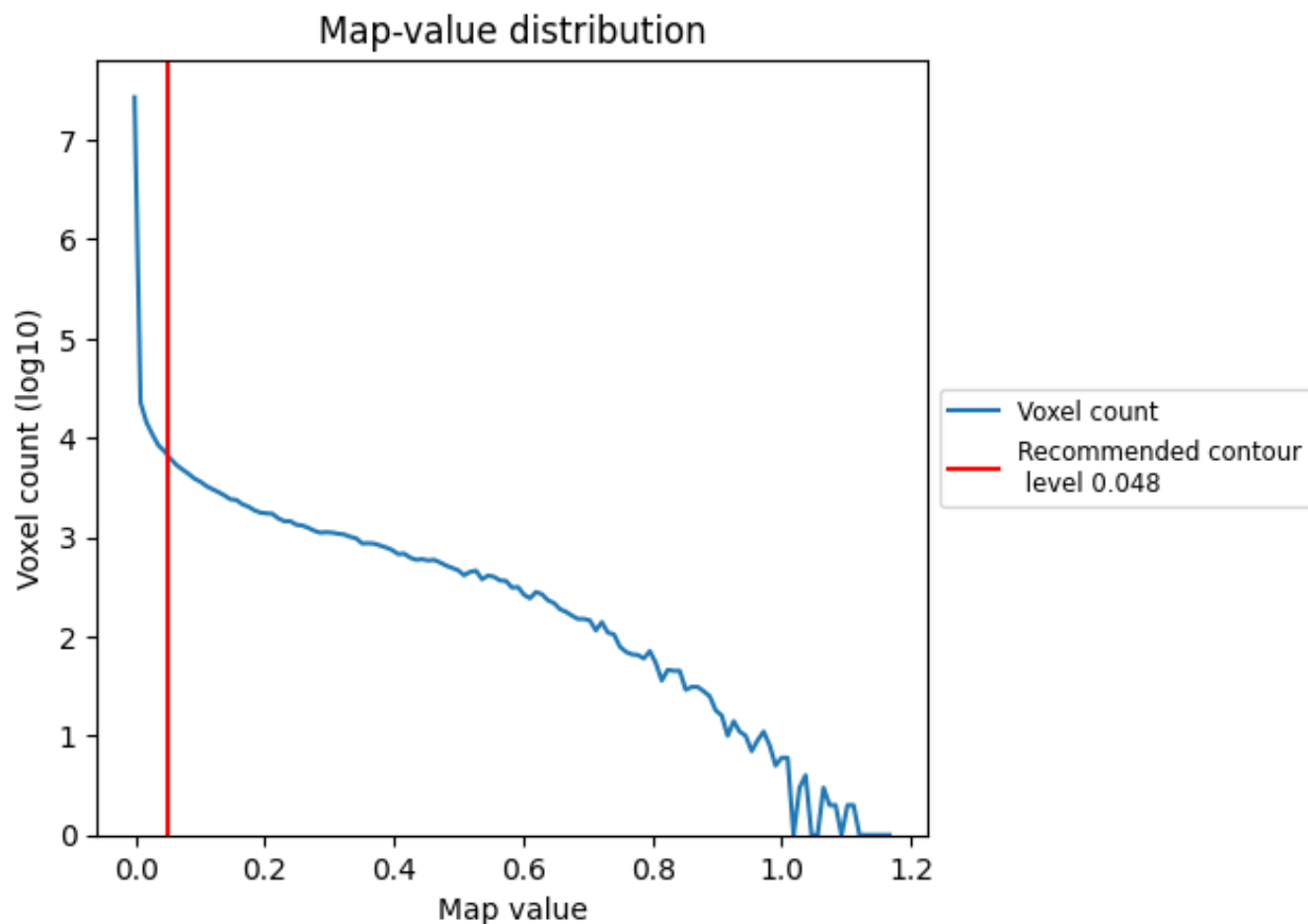
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

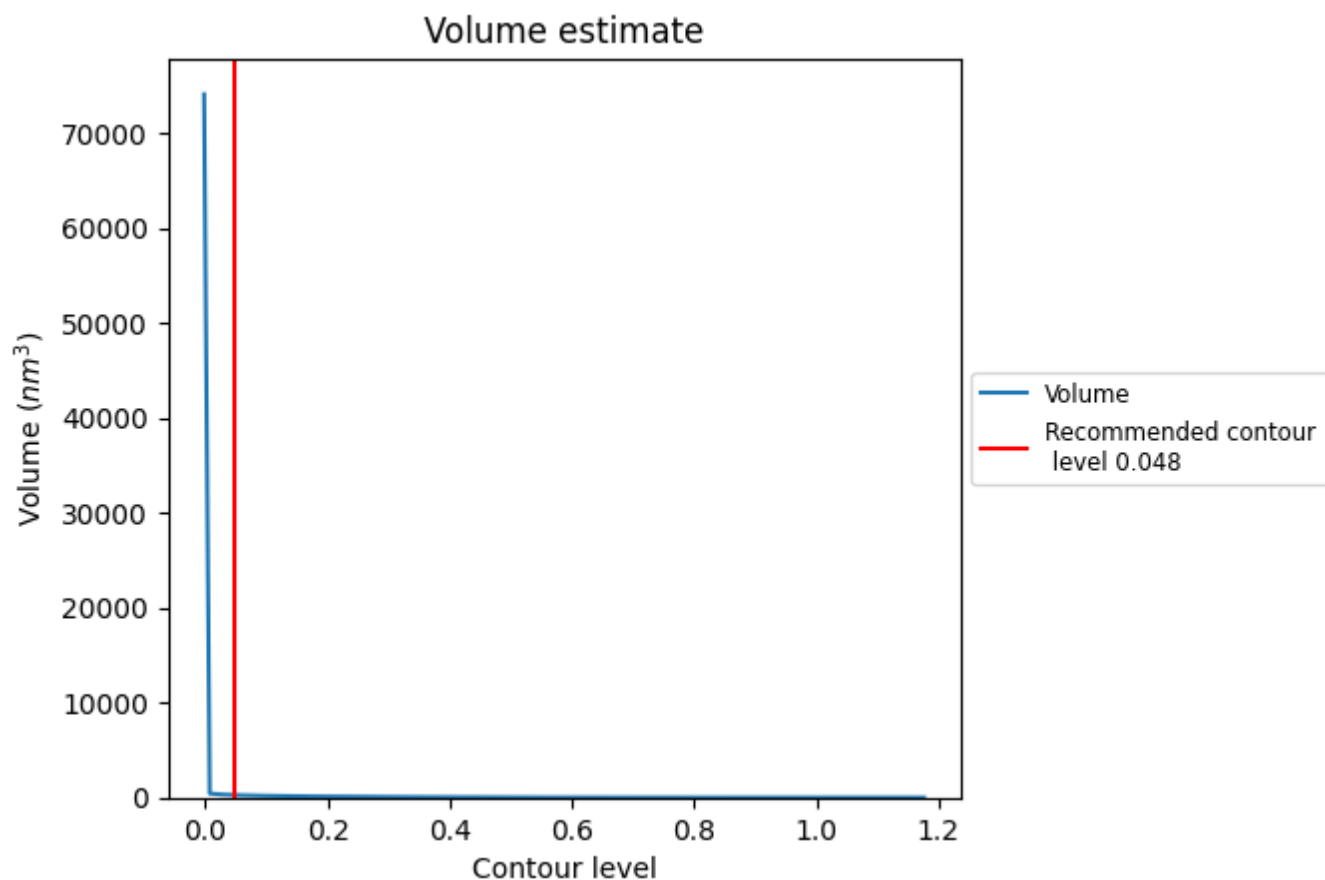
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

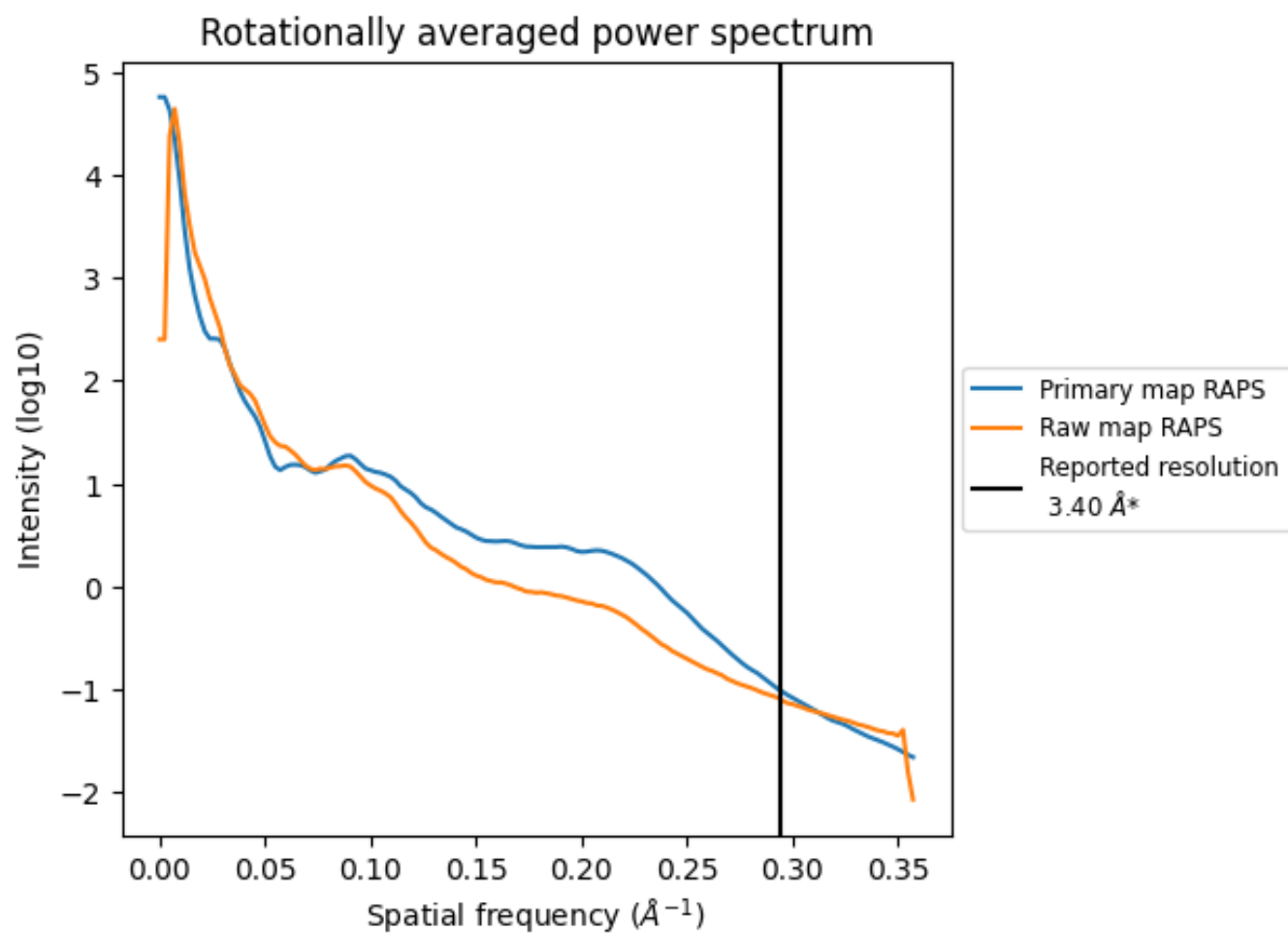
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 265 nm<sup>3</sup>; this corresponds to an approximate mass of 239 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

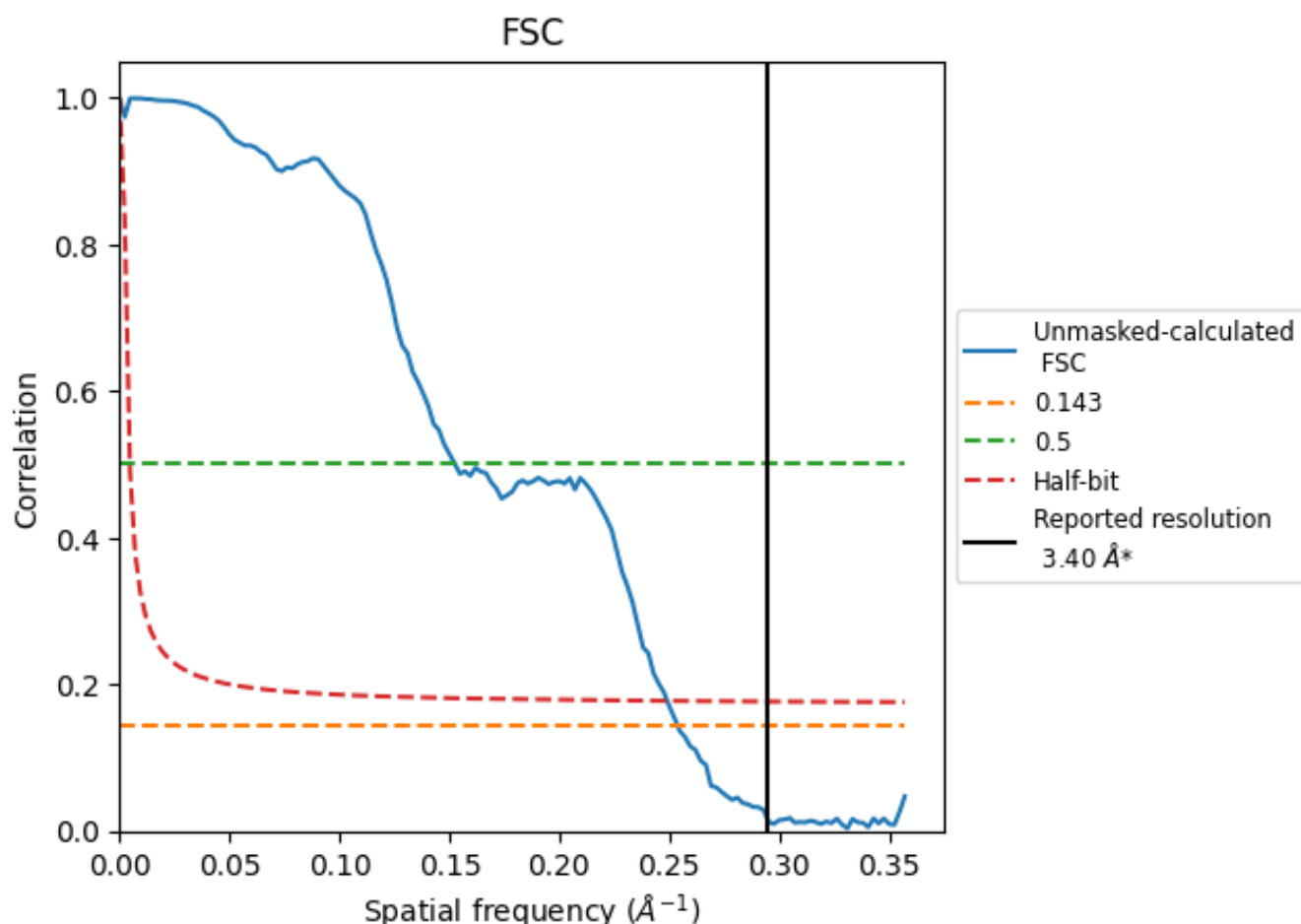


\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.294  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.94	6.55	4.01

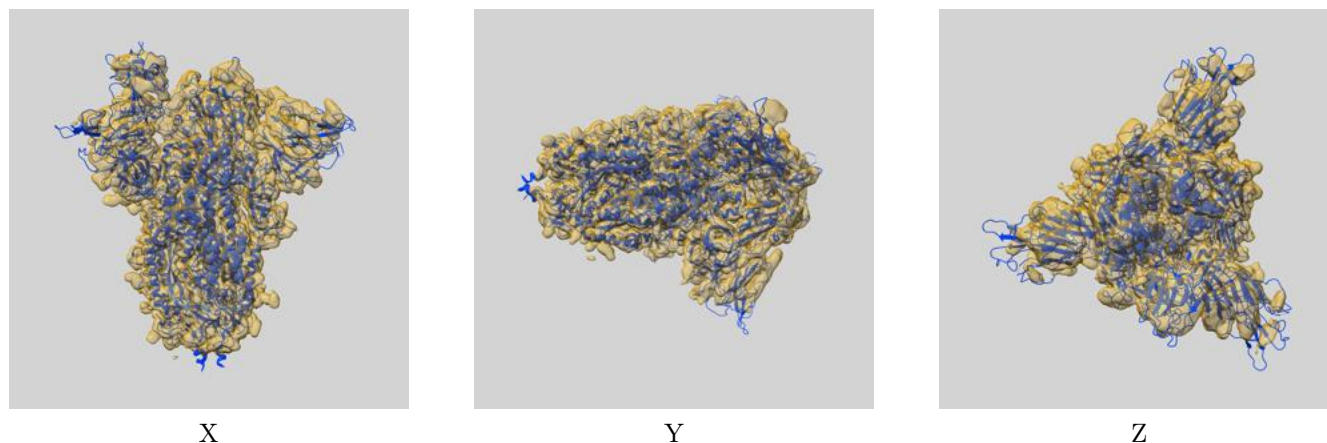
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.94 differs from the reported value 3.4 by more than 10 %



## 9 Map-model fit [i](#)

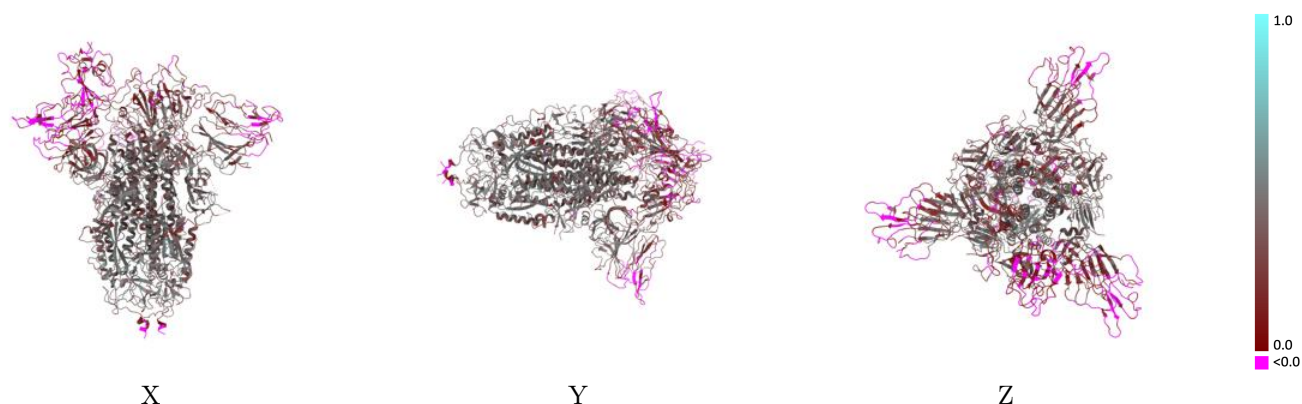
This section contains information regarding the fit between EMDB map EMD-13916 and PDB model 7QDG. Per-residue inclusion information can be found in section [3](#) on page [10](#).

### 9.1 Map-model overlay [i](#)



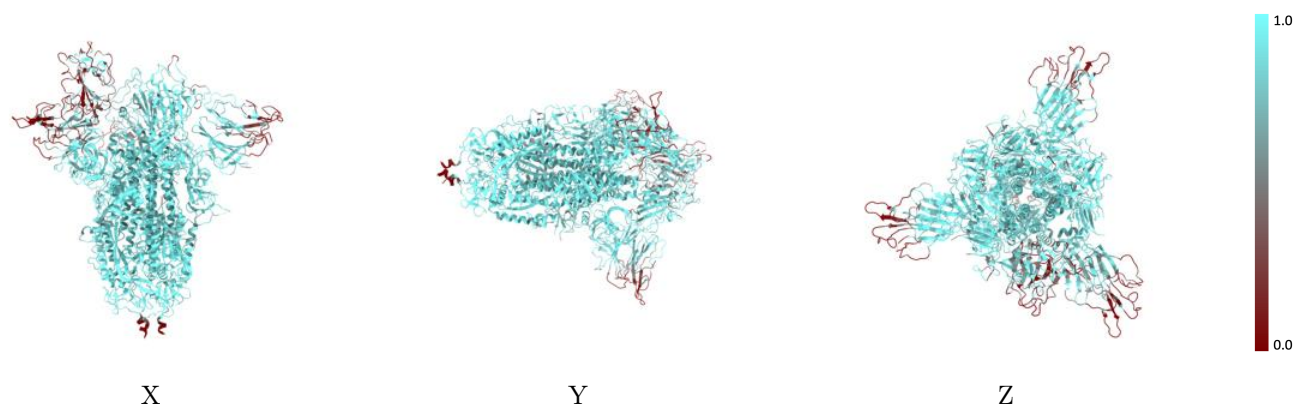
The images above show the 3D surface view of the map at the recommended contour level 0.048 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



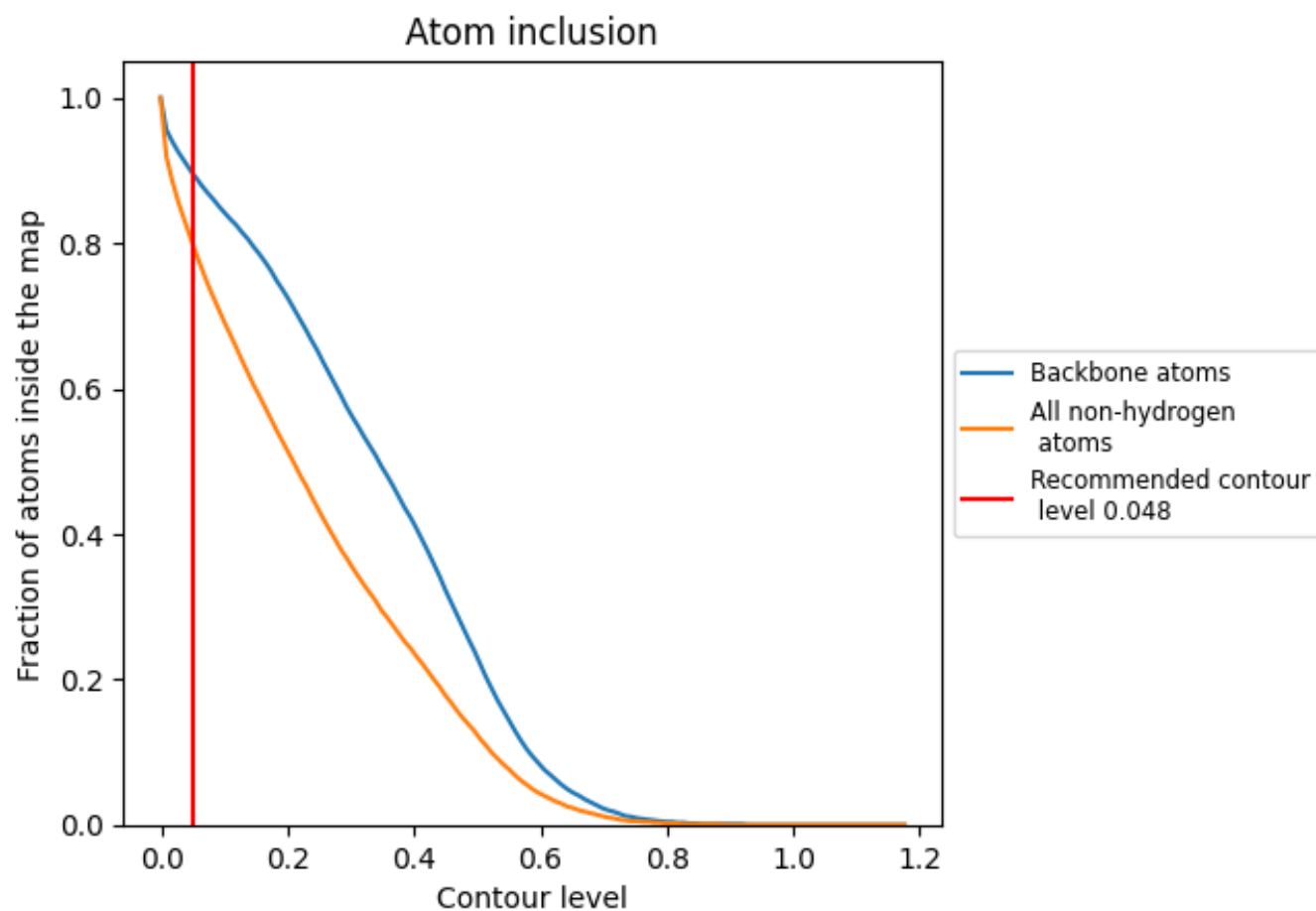
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.048).































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 90% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.048) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8020	 0.3100
A	 0.8380	 0.3210
B	 0.7640	 0.2940
C	 0.8110	 0.3170
E	 0.8930	 0.4040
G	 0.7140	 0.2580
I	 0.6790	 0.3310
J	 0.7140	 0.2020
K	 0.5710	 0.2560
L	 0.6430	 0.2520
M	 0.3930	 0.1580
N	 0.0000	 0.0930
O	 0.6430	 0.2920
P	 0.4290	 0.0380
Q	 0.6430	 0.2010

