



Full wwPDB EM Validation Report ⓘ

Oct 14, 2024 – 12:26 PM JST

PDB ID : 5X0M
EMDB ID : EMD-6698
Title : Structure of a eukaryotic voltage-gated sodium channel at near atomic resolution
Authors : Shen, H.; Zhou, Q.; Pan, X.; Li, Z.; Wu, J.; Yan, N.
Deposited on : 2017-01-21
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), 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)
Validation Pipeline (wwPDB-VP) : 2.39

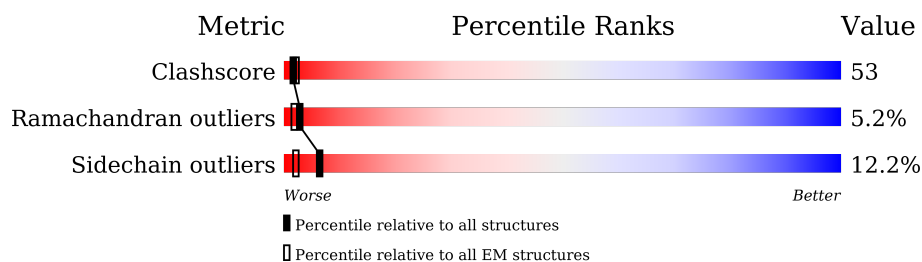
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1596	<div> <div>12%</div> <div>31%</div> <div>40%</div> <div>10%</div> <div>•</div> <div>17%</div> </div>
2	B	5	<div>100%</div>
3	C	3	<div>67%</div> <div>33%</div> <div>67%</div>
3	D	3	<div>67%</div> <div>33%</div> <div>67%</div>
3	E	3	<div>67%</div> <div>33%</div> <div>33%</div> <div>33%</div>
3	F	3	<div>67%</div> <div>100%</div>
4	G	2	<div>50%</div> <div>100%</div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10654 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 Sodium channel protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1323	Total	C	N	O	S	0	0
			10395	6885	1670	1778	62		

There are 43 discrepancies between the modelled and reference sequences:

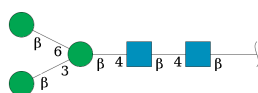
Chain	Residue	Modelled	Actual	Comment	Reference
A	-42	MET	-	initiating methionine	UNP D0E0C2
A	-41	ALA	-	expression tag	UNP D0E0C2
A	-40	SER	-	expression tag	UNP D0E0C2
A	-39	TRP	-	expression tag	UNP D0E0C2
A	-38	SER	-	expression tag	UNP D0E0C2
A	-37	HIS	-	expression tag	UNP D0E0C2
A	-36	PRO	-	expression tag	UNP D0E0C2
A	-35	GLN	-	expression tag	UNP D0E0C2
A	-34	PHE	-	expression tag	UNP D0E0C2
A	-33	GLU	-	expression tag	UNP D0E0C2
A	-32	LYS	-	expression tag	UNP D0E0C2
A	-31	GLY	-	expression tag	UNP D0E0C2
A	-30	GLY	-	expression tag	UNP D0E0C2
A	-29	GLY	-	expression tag	UNP D0E0C2
A	-28	ALA	-	expression tag	UNP D0E0C2
A	-27	ARG	-	expression tag	UNP D0E0C2
A	-26	GLY	-	expression tag	UNP D0E0C2
A	-25	GLY	-	expression tag	UNP D0E0C2
A	-24	SER	-	expression tag	UNP D0E0C2
A	-23	GLY	-	expression tag	UNP D0E0C2
A	-22	GLY	-	expression tag	UNP D0E0C2
A	-21	GLY	-	expression tag	UNP D0E0C2
A	-20	SER	-	expression tag	UNP D0E0C2
A	-19	TRP	-	expression tag	UNP D0E0C2
A	-18	SER	-	expression tag	UNP D0E0C2
A	-17	HIS	-	expression tag	UNP D0E0C2
A	-16	PRO	-	expression tag	UNP D0E0C2
A	-15	GLN	-	expression tag	UNP D0E0C2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	PHE	-	expression tag	UNP D0E0C2
A	-13	GLU	-	expression tag	UNP D0E0C2
A	-12	LYS	-	expression tag	UNP D0E0C2
A	-11	GLY	-	expression tag	UNP D0E0C2
A	-10	PHE	-	expression tag	UNP D0E0C2
A	-9	ASP	-	expression tag	UNP D0E0C2
A	-8	TYR	-	expression tag	UNP D0E0C2
A	-7	LYS	-	expression tag	UNP D0E0C2
A	-6	ASP	-	expression tag	UNP D0E0C2
A	-5	ASP	-	expression tag	UNP D0E0C2
A	-4	ASP	-	expression tag	UNP D0E0C2
A	-3	ASP	-	expression tag	UNP D0E0C2
A	-2	LYS	-	expression tag	UNP D0E0C2
A	-1	GLY	-	expression tag	UNP D0E0C2
A	0	THR	-	expression tag	UNP D0E0C2

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	5	Total	C	N	O	0	0
			61	34	2	25		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	3	Total	C	N	O	0	0
			39	22	2	15		
3	D	3	Total	C	N	O	0	0
			39	22	2	15		
3	E	3	Total	C	N	O	0	0
			39	22	2	15		

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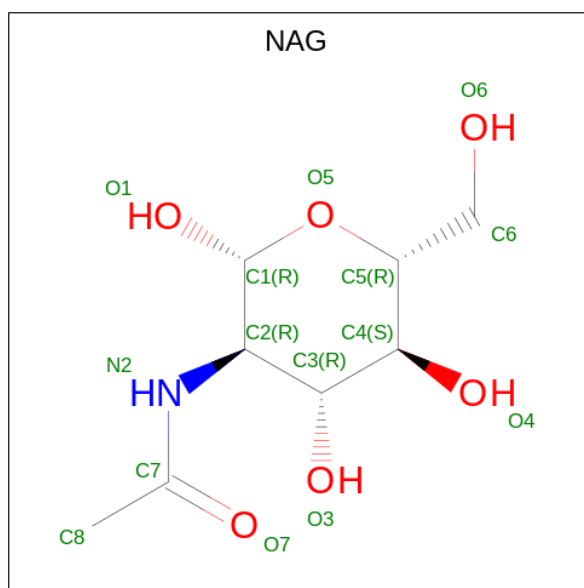
Mol	Chain	Residues	Atoms				AltConf	Trace
3	F	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 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
4	G	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

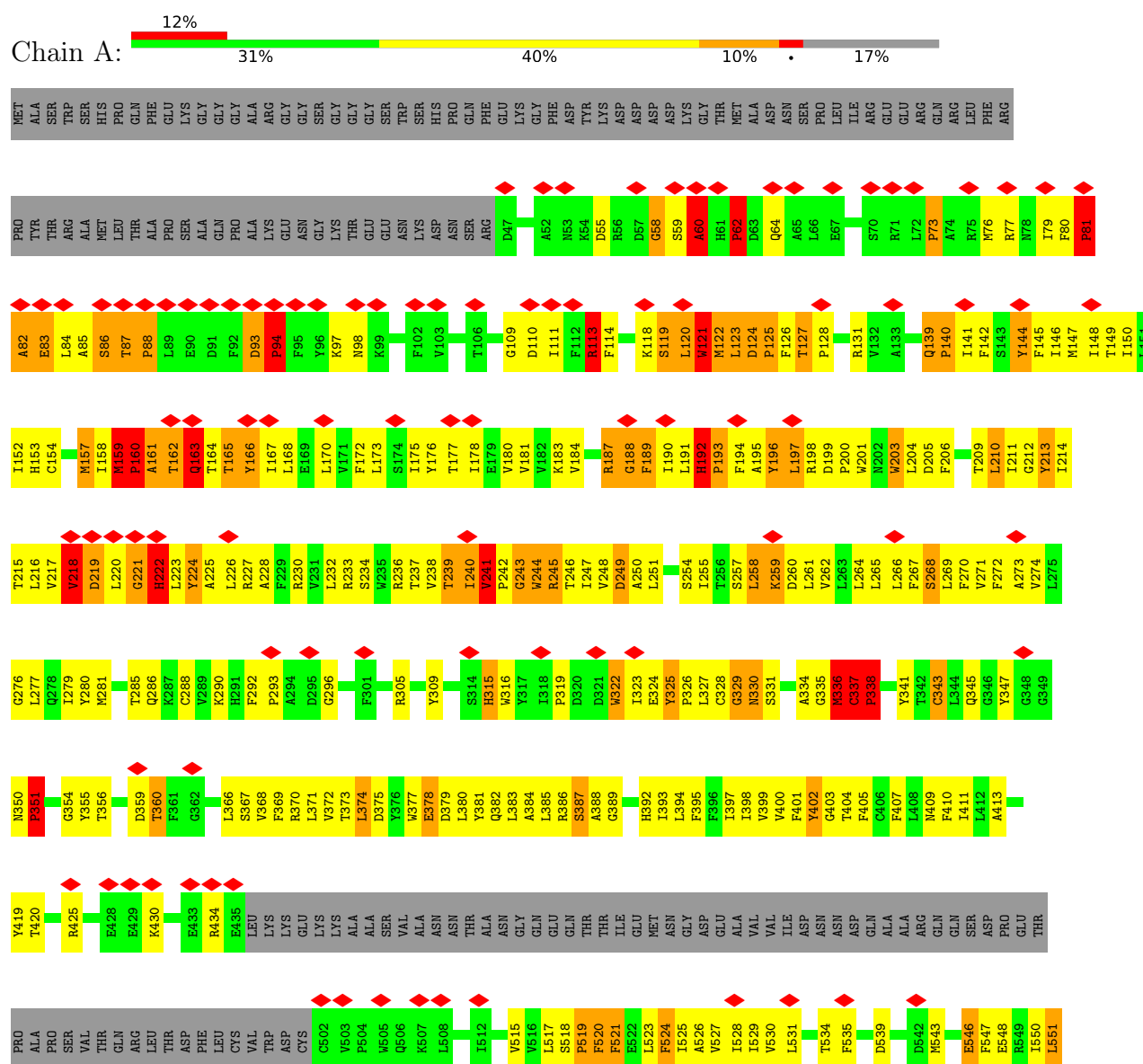


Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	

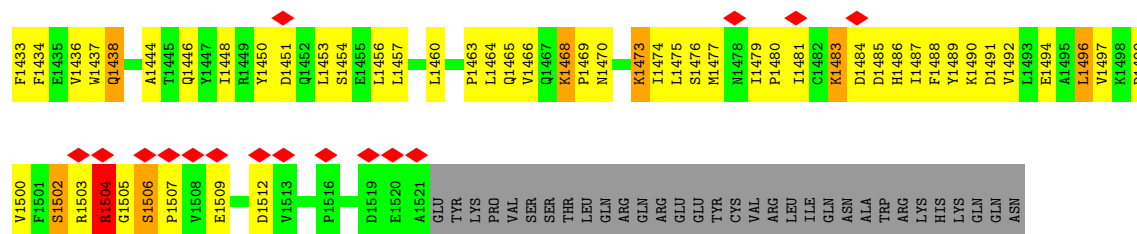
3 Residue-property plots

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: Sodium channel protein







- Molecule 2: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 100%



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

Chain C: 67%



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

Chain D: 67%



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

Chain E: 67%



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

Chain F: 67%



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1373581	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.5625	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.392	Depositor
Minimum map value	-0.264	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.0465	Depositor
Map size (Å)	258.0, 258.0, 258.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.29, 1.29, 1.29	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: BMA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.46	7/10668 (0.1%)	0.60	33/14522 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	124

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1072	ASP	C-N	10.34	1.57	1.34
1	A	674	PHE	C-N	8.18	1.49	1.34
1	A	935	LEU	C-N	6.49	1.49	1.34
1	A	1047	VAL	C-N	-5.28	1.23	1.33
1	A	980	PRO	N-CD	5.20	1.55	1.47
1	A	961	PRO	N-CD	5.14	1.55	1.47
1	A	193	PRO	N-CD	5.12	1.55	1.47

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1047	VAL	O-C-N	-9.29	107.40	123.20
1	A	519	PRO	CA-N-CD	-8.52	99.57	111.50
1	A	1072	ASP	O-C-N	7.31	134.39	122.70
1	A	1047	VAL	CA-C-N	7.24	130.68	116.20
1	A	62	PRO	N-CA-CB	6.89	111.56	103.30
1	A	1152	ILE	C-N-CD	6.78	142.63	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	574	SER	C-N-CD	6.75	142.59	128.40
1	A	1158	HIS	C-N-CD	6.63	142.32	128.40
1	A	337	CYS	C-N-CD	6.62	142.30	128.40
1	A	159	MET	C-N-CD	6.61	142.28	128.40
1	A	241	VAL	C-N-CD	6.61	142.28	128.40
1	A	338	PRO	C-N-CD	6.61	142.28	128.40
1	A	1147	LYS	C-N-CD	6.61	142.28	128.40
1	A	624	TRP	C-N-CD	6.61	142.28	128.40
1	A	139	GLN	C-N-CD	6.61	142.27	128.40
1	A	1260	SER	C-N-CD	6.59	142.25	128.40
1	A	1154	LYS	C-N-CD	6.57	142.19	128.40
1	A	880	LEU	C-N-CD	6.27	141.57	128.40
1	A	960	ARG	C-N-CD	6.17	141.36	128.40
1	A	192	HIS	C-N-CD	6.17	141.36	128.40
1	A	1090	LEU	CA-CB-CG	6.09	129.30	115.30
1	A	1089	TYR	CA-CB-CG	6.04	124.87	113.40
1	A	88	PRO	N-CA-CB	5.98	110.47	103.30
1	A	125	PRO	N-CA-CB	5.95	110.44	103.30
1	A	73	PRO	N-CA-CB	5.94	110.43	103.30
1	A	81	PRO	N-CA-CB	5.92	110.40	103.30
1	A	94	PRO	N-CA-CB	5.90	110.38	103.30
1	A	1072	ASP	CA-C-N	-5.73	104.60	117.20
1	A	979	VAL	C-N-CD	5.63	140.23	128.40
1	A	935	LEU	O-C-N	-5.31	114.20	122.70
1	A	1451	ASP	CB-CG-OD2	5.17	122.96	118.30
1	A	581	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	268	SER	CB-CA-C	-5.10	100.41	110.10

There are no chirality outliers.

All (124) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1019	LEU	Peptide
1	A	1024	THR	Peptide
1	A	1033	GLU	Peptide
1	A	1034	ASN	Peptide
1	A	1035	TYR	Peptide
1	A	1071	ILE	Peptide
1	A	109	GLY	Peptide
1	A	110	ASP	Peptide
1	A	1122	ALA	Peptide
1	A	1123	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	A	113	ARG	Peptide
1	A	1130	SER	Peptide
1	A	1147	LYS	Peptide
1	A	1151	ARG	Peptide
1	A	1152	ILE	Peptide
1	A	1154	LYS	Peptide
1	A	1156	THR	Peptide
1	A	1157	CYS	Peptide
1	A	1158	HIS	Peptide
1	A	119	SER	Peptide
1	A	1192	TYR	Peptide
1	A	1193	GLY	Peptide
1	A	120	LEU	Peptide
1	A	121	TRP	Peptide
1	A	122	MET	Peptide
1	A	123	LEU	Peptide
1	A	124	ASP	Peptide
1	A	1247	GLY	Peptide
1	A	1250	LEU	Peptide
1	A	1252	ASP	Peptide
1	A	1253	VAL	Peptide
1	A	1255	GLU	Peptide
1	A	1256	LYS	Peptide
1	A	1258	PHE	Peptide
1	A	126	PHE	Peptide
1	A	1260	SER	Peptide
1	A	127	THR	Peptide
1	A	1282	ALA	Peptide
1	A	1321	PHE	Peptide
1	A	1325	ARG	Peptide
1	A	1327	ALA	Peptide
1	A	1330	ILE	Peptide
1	A	1376	GLY	Peptide
1	A	1381	CYS	Peptide
1	A	139	GLN	Peptide
1	A	1423	GLU	Peptide
1	A	1504	ARG	Peptide
1	A	1506	SER	Peptide
1	A	159	MET	Peptide
1	A	160	PRO	Peptide
1	A	161	ALA	Peptide
1	A	162	THR	Peptide

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Mol	Chain	Res	Type	Group
1	A	163	GLN	Peptide
1	A	164	THR	Peptide
1	A	165	THR	Peptide
1	A	187	ARG	Peptide
1	A	188	GLY	Peptide
1	A	192	HIS	Peptide
1	A	197	LEU	Peptide
1	A	199	ASP	Peptide
1	A	218	VAL	Peptide
1	A	219	ASP	Peptide
1	A	221	GLY	Peptide
1	A	222	HIS	Peptide
1	A	239	THR	Peptide
1	A	240	ILE	Peptide
1	A	241	VAL	Peptide
1	A	243	GLY	Peptide
1	A	244	TRP	Peptide
1	A	245	ARG	Sidechain
1	A	292	PHE	Peptide
1	A	315	HIS	Peptide
1	A	316	TRP	Peptide
1	A	322	TRP	Peptide
1	A	325	TYR	Peptide
1	A	327	LEU	Peptide
1	A	329	GLY	Peptide
1	A	330	ASN	Peptide
1	A	335	GLY	Peptide
1	A	336	MET	Peptide
1	A	337	CYS	Peptide
1	A	338	PRO	Peptide
1	A	351	PRO	Peptide
1	A	360	THR	Peptide
1	A	517	LEU	Peptide
1	A	520	PHE	Peptide
1	A	573	LEU	Peptide
1	A	58	GLY	Peptide
1	A	60	ALA	Peptide
1	A	602	GLY	Peptide
1	A	603	VAL	Peptide
1	A	605	GLY	Peptide
1	A	606	LEU	Peptide
1	A	624	TRP	Peptide

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Mol	Chain	Res	Type	Group
1	A	637	SER	Peptide
1	A	663	PHE	Peptide
1	A	700	GLY	Peptide
1	A	715	TRP	Peptide
1	A	73	PRO	Peptide
1	A	76	MET	Peptide
1	A	80	PHE	Peptide
1	A	81	PRO	Peptide
1	A	84	LEU	Peptide
1	A	85	ALA	Peptide
1	A	856	LYS	Peptide
1	A	86	SER	Peptide
1	A	87	THR	Peptide
1	A	876	GLU	Peptide
1	A	877	ASP	Peptide
1	A	878	ILE	Peptide
1	A	879	TYR	Peptide
1	A	882	GLN	Peptide
1	A	883	ARG	Peptide
1	A	920	SER	Peptide
1	A	93	ASP	Peptide
1	A	935	LEU	Mainchain
1	A	942	ALA	Peptide
1	A	943	GLY	Peptide
1	A	944	ILE	Peptide
1	A	946	ALA	Peptide
1	A	954	ARG	Sidechain
1	A	960	ARG	Peptide
1	A	965	VAL	Peptide
1	A	989	GLY	Peptide

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	10395	0	10078	1110	0
2	B	61	0	52	1	0
3	C	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	39	0	34	0	0
3	E	39	0	34	1	0
3	F	39	0	34	1	0
4	G	28	0	25	0	0
5	A	14	0	13	0	0
All	All	10654	0	10304	1111	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 53.

All (1111) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:878:ILE:HD12	1:A:1323:HIS:CE1	1.53	1.44
1:A:1320:PHE:CE1	1:A:1386:LEU:HD12	1.58	1.39
1:A:1320:PHE:CE1	1:A:1386:LEU:CD1	2.06	1.38
1:A:1180:ILE:HD11	1:A:1213:PHE:CE2	1.66	1.29
1:A:977:GLU:O	1:A:980:PRO:HD2	1.32	1.28
1:A:410:PHE:CE1	1:A:1288:LEU:HD21	1.70	1.27
1:A:1240:TYR:CE2	1:A:1268:ARG:HB2	1.69	1.26
1:A:1330:ILE:CG2	1:A:1335:ASN:HA	1.66	1.25
1:A:197:LEU:HD22	1:A:203:TRP:CH2	1.73	1.24
1:A:401:PHE:HE1	1:A:1406:TYR:OH	1.19	1.23
1:A:1477:MET:SD	1:A:1499:ASP:OD2	1.97	1.23
1:A:528:ILE:HG23	1:A:558:PHE:CE1	1.71	1.22
1:A:878:ILE:CD1	1:A:1323:HIS:HE1	1.53	1.20
1:A:176:TYR:HE2	1:A:233:ARG:HD3	1.04	1.20
1:A:849:CYS:CB	1:A:911:ALA:HB2	1.72	1.20
1:A:1320:PHE:CZ	1:A:1386:LEU:HD12	1.77	1.19
1:A:1305:LEU:HD22	1:A:1309:ILE:HD11	1.23	1.19
1:A:334:ALA:HB2	1:A:389:GLY:HA2	1.20	1.17
1:A:600:LEU:HD22	1:A:609:PHE:CD2	1.77	1.17
1:A:1258:PHE:HB2	1:A:1259:ILE:HG13	1.25	1.16
1:A:1253:VAL:CG1	1:A:1254:ILE:HG13	1.77	1.15
1:A:934:LEU:O	1:A:938:VAL:HG23	1.45	1.15
1:A:974:THR:HG21	1:A:1405:MET:CE	1.77	1.14
1:A:599:GLY:O	1:A:603:VAL:HG23	1.45	1.14
1:A:596:LEU:HD22	1:A:609:PHE:CE1	1.82	1.14
1:A:614:LEU:HD21	1:A:998:ILE:HD11	1.26	1.14
1:A:1000:GLY:O	1:A:1004:PHE:HB2	1.47	1.13
1:A:1180:ILE:CD1	1:A:1213:PHE:CZ	2.30	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:ILE:O	1:A:553:THR:HG22	1.45	1.13
1:A:1180:ILE:HD13	1:A:1213:PHE:HZ	1.14	1.12
1:A:985:VAL:CG2	1:A:1110:ILE:HD11	1.80	1.12
1:A:1180:ILE:CD1	1:A:1213:PHE:CE2	2.31	1.12
1:A:1305:LEU:CD2	1:A:1309:ILE:HD11	1.78	1.12
1:A:985:VAL:HG21	1:A:1110:ILE:HD11	1.19	1.12
1:A:1176:MET:HE1	1:A:1216:GLU:HB2	1.26	1.11
1:A:1181:ILE:HD11	1:A:1275:LEU:HD11	1.32	1.11
1:A:637:SER:OG	1:A:641:PHE:CD2	2.04	1.10
1:A:1180:ILE:HD13	1:A:1213:PHE:CZ	1.88	1.09
1:A:653:PHE:CZ	1:A:657:ILE:HD11	1.86	1.08
1:A:1413:TYR:O	1:A:1417:VAL:HG23	1.53	1.08
1:A:1253:VAL:HG12	1:A:1254:ILE:CG1	1.84	1.08
1:A:1180:ILE:HD11	1:A:1213:PHE:HE2	0.99	1.08
1:A:560:SER:HA	1:A:563:ILE:HD12	1.35	1.08
1:A:653:PHE:CE1	1:A:657:ILE:HD11	1.88	1.07
1:A:1146:ALA:HB3	1:A:1434:PHE:CE2	1.89	1.07
1:A:1152:ILE:HD12	1:A:1152:ILE:H	1.19	1.07
1:A:1304:PHE:O	1:A:1308:VAL:HG23	1.52	1.07
1:A:952:LEU:HD11	1:A:1319:GLU:HG3	1.12	1.06
1:A:374:LEU:HD11	1:A:1351:THR:HG21	1.37	1.06
1:A:968:MET:HG3	1:A:1301:ASN:OD1	1.55	1.06
1:A:603:VAL:O	1:A:604:GLN:HG3	1.55	1.05
1:A:898:THR:HG22	1:A:933:TYR:HB3	1.11	1.05
1:A:1177:MET:SD	1:A:1275:LEU:HD21	1.96	1.05
1:A:1320:PHE:CZ	1:A:1386:LEU:CD1	2.34	1.05
1:A:160:PRO:HG2	1:A:162:THR:HG21	1.35	1.05
1:A:898:THR:CG2	1:A:933:TYR:HB3	1.87	1.04
1:A:265:LEU:HD23	1:A:268:SER:HB3	1.35	1.04
1:A:898:THR:HG22	1:A:933:TYR:CB	1.87	1.04
1:A:1483:LYS:HG2	1:A:1484:ASP:OD1	1.57	1.04
1:A:1119:ARG:HD3	1:A:1412:ASP:OD2	1.58	1.03
1:A:847:ARG:O	1:A:851:LEU:CB	2.06	1.03
1:A:962:LEU:HD21	1:A:968:MET:HE1	1.37	1.03
1:A:985:VAL:HG21	1:A:1110:ILE:CD1	1.88	1.03
1:A:258:LEU:O	1:A:262:VAL:HG23	1.59	1.02
1:A:909:LEU:HD23	1:A:917:TYR:CE2	1.95	1.02
1:A:1457:LEU:CD1	1:A:1474:ILE:HG12	1.88	1.02
1:A:176:TYR:CE2	1:A:233:ARG:HD3	1.93	1.02
1:A:183:LYS:HB2	1:A:196:TYR:OH	1.58	1.02
1:A:873:LEU:HD13	1:A:954:ARG:NH2	1.74	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:967:GLY:HA3	1:A:1301:ASN:ND2	1.75	1.01
1:A:192:HIS:O	1:A:196:TYR:N	1.91	1.01
1:A:1253:VAL:CG1	1:A:1254:ILE:CG1	2.38	1.01
1:A:410:PHE:CE1	1:A:1288:LEU:CD2	2.42	1.00
1:A:401:PHE:CE1	1:A:1406:TYR:OH	2.01	1.00
1:A:528:ILE:CG2	1:A:558:PHE:CE1	2.44	1.00
1:A:157:MET:CE	1:A:230:ARG:HD2	1.91	1.00
1:A:974:THR:HG21	1:A:1405:MET:HE3	1.45	0.99
1:A:1177:MET:CE	1:A:1275:LEU:HD21	1.91	0.99
1:A:1177:MET:HE3	1:A:1275:LEU:HD21	1.45	0.99
1:A:1166:ILE:HG22	1:A:1172:PHE:CD2	1.98	0.98
1:A:265:LEU:HA	1:A:268:SER:HB2	1.42	0.98
1:A:1320:PHE:CE1	1:A:1386:LEU:HD11	1.95	0.98
1:A:64:GLN:CB	1:A:120:LEU:CB	2.41	0.98
1:A:863:THR:HG23	1:A:961:PRO:HG3	1.43	0.97
1:A:909:LEU:CD2	1:A:917:TYR:CE2	2.48	0.97
1:A:704:GLU:HA	1:A:707:TRP:HD1	1.28	0.97
1:A:154:CYS:O	1:A:158:ILE:HG13	1.65	0.96
1:A:265:LEU:HD23	1:A:268:SER:CB	1.96	0.96
1:A:614:LEU:HD21	1:A:998:ILE:CD1	1.95	0.95
1:A:183:LYS:CB	1:A:196:TYR:OH	2.13	0.95
1:A:962:LEU:HD21	1:A:968:MET:CE	1.95	0.95
1:A:1253:VAL:CB	1:A:1254:ILE:HG13	1.96	0.95
1:A:161:ALA:N	1:A:162:THR:HG23	1.82	0.95
1:A:239:THR:HA	1:A:244:TRP:NE1	1.80	0.95
1:A:1209:PHE:O	1:A:1213:PHE:HD1	1.50	0.95
1:A:952:LEU:CD1	1:A:1319:GLU:HG3	1.96	0.95
1:A:971:VAL:O	1:A:974:THR:HG22	1.66	0.94
1:A:977:GLU:O	1:A:980:PRO:CD	2.14	0.94
1:A:1240:TYR:HE2	1:A:1268:ARG:HB2	1.22	0.94
1:A:600:LEU:HD22	1:A:609:PHE:HD2	1.32	0.94
1:A:1253:VAL:HG12	1:A:1254:ILE:HG13	1.45	0.94
1:A:1176:MET:CE	1:A:1216:GLU:HB2	1.97	0.94
1:A:1330:ILE:HG22	1:A:1335:ASN:ND2	1.82	0.93
1:A:952:LEU:HD11	1:A:1319:GLU:CG	1.97	0.93
1:A:962:LEU:CD2	1:A:968:MET:CE	2.46	0.93
1:A:962:LEU:CD2	1:A:968:MET:HE1	1.98	0.93
1:A:1177:MET:SD	1:A:1275:LEU:CD2	2.57	0.93
1:A:600:LEU:CD2	1:A:609:PHE:HD2	1.82	0.93
1:A:288:CYS:SG	1:A:328:CYS:CB	2.56	0.93
1:A:1320:PHE:HE1	1:A:1386:LEU:CD1	1.83	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1206:ASN:HD21	1:A:1268:ARG:HH12	1.17	0.92
1:A:1330:ILE:HG22	1:A:1335:ASN:HD22	1.34	0.92
1:A:940:MET:HE3	1:A:941:CYS:HB2	1.50	0.92
1:A:1330:ILE:O	1:A:1332:ASP:N	2.02	0.92
1:A:528:ILE:HG23	1:A:558:PHE:CD1	2.04	0.92
1:A:1125:LEU:HD12	1:A:1137:ARG:HH22	1.35	0.91
1:A:1263:LEU:HD23	1:A:1266:ILE:HD12	1.50	0.91
1:A:221:GLY:O	1:A:222:HIS:ND1	2.03	0.91
1:A:653:PHE:CZ	1:A:657:ILE:CD1	2.54	0.91
1:A:239:THR:HA	1:A:244:TRP:CD1	2.06	0.91
1:A:197:LEU:CD2	1:A:203:TRP:CH2	2.52	0.91
1:A:940:MET:CE	1:A:941:CYS:HB2	2.01	0.90
1:A:1457:LEU:HD12	1:A:1474:ILE:CD1	2.00	0.90
1:A:161:ALA:H	1:A:162:THR:HG23	1.37	0.90
1:A:600:LEU:CD2	1:A:609:PHE:CD2	2.54	0.90
1:A:872:LEU:CD1	1:A:893:VAL:HG21	2.02	0.90
1:A:1146:ALA:HB3	1:A:1434:PHE:HE2	1.32	0.90
1:A:1253:VAL:HG12	1:A:1254:ILE:HG12	1.52	0.89
1:A:651:LEU:HD21	1:A:727:VAL:HG12	1.54	0.89
1:A:1464:LEU:HD23	1:A:1500:VAL:HG21	1.54	0.89
1:A:872:LEU:HD13	1:A:893:VAL:HG21	1.51	0.89
1:A:197:LEU:HD22	1:A:203:TRP:HH2	1.36	0.89
1:A:927:PHE:O	1:A:931:VAL:HG23	1.72	0.88
1:A:692:MET:HG3	1:A:1089:TYR:CE2	2.09	0.88
1:A:909:LEU:HD22	1:A:917:TYR:CD2	2.07	0.88
1:A:146:ILE:O	1:A:150:ILE:HG13	1.73	0.88
1:A:334:ALA:CB	1:A:389:GLY:HA2	2.03	0.88
1:A:371:LEU:HD13	1:A:399:VAL:HG11	1.55	0.88
1:A:385:LEU:HB2	1:A:1334:TYR:OH	1.73	0.88
1:A:1330:ILE:HG21	1:A:1335:ASN:HA	1.55	0.88
1:A:224:TYR:CD1	1:A:227:ARG:HG3	2.07	0.88
1:A:1481:ILE:HG21	1:A:1485:ASP:HA	1.54	0.87
1:A:334:ALA:HB2	1:A:389:GLY:CA	2.05	0.87
1:A:528:ILE:CG2	1:A:558:PHE:CD1	2.57	0.87
1:A:596:LEU:HD22	1:A:609:PHE:HE1	1.40	0.87
1:A:265:LEU:HA	1:A:268:SER:CB	2.03	0.87
1:A:1305:LEU:HD22	1:A:1309:ILE:CD1	2.03	0.87
1:A:176:TYR:O	1:A:180:VAL:HG23	1.73	0.86
1:A:873:LEU:HD13	1:A:954:ARG:HH21	1.35	0.86
1:A:1151:ARG:HG3	1:A:1438:GLN:CG	2.05	0.86
1:A:224:TYR:HE1	1:A:227:ARG:NH1	1.74	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:867:VAL:O	1:A:871:VAL:HG23	1.76	0.86
1:A:849:CYS:CB	1:A:911:ALA:CB	2.53	0.86
1:A:699:CYS:HB3	1:A:1060:PHE:CE2	2.11	0.86
1:A:371:LEU:CD1	1:A:399:VAL:HG11	2.05	0.86
1:A:224:TYR:CE1	1:A:227:ARG:NH1	2.44	0.85
1:A:288:CYS:SG	1:A:328:CYS:HB3	2.16	0.85
1:A:410:PHE:CD1	1:A:1288:LEU:HD21	2.11	0.85
1:A:528:ILE:HG23	1:A:558:PHE:HE1	1.42	0.85
1:A:1253:VAL:HB	1:A:1254:ILE:HG13	1.56	0.85
1:A:878:ILE:CD1	1:A:1323:HIS:CE1	2.37	0.85
1:A:1436:VAL:HG21	1:A:1460:LEU:HD23	1.58	0.85
1:A:600:LEU:HG	1:A:606:LEU:H	1.40	0.85
1:A:62:PRO:CB	1:A:120:LEU:O	2.25	0.85
1:A:599:GLY:O	1:A:603:VAL:CG2	2.25	0.85
1:A:909:LEU:CD2	1:A:917:TYR:CD2	2.58	0.85
1:A:543:MET:O	1:A:548:GLU:HG3	1.76	0.84
1:A:637:SER:HG	1:A:641:PHE:HD2	1.19	0.84
1:A:1111:LEU:HD21	1:A:1405:MET:N	1.92	0.84
1:A:1177:MET:HE1	1:A:1181:ILE:HG12	1.59	0.84
1:A:905:MET:O	1:A:909:LEU:HB2	1.77	0.84
1:A:1481:ILE:HG12	1:A:1487:ILE:HG12	1.57	0.84
1:A:1457:LEU:HD12	1:A:1474:ILE:CG1	2.08	0.84
1:A:1151:ARG:HG3	1:A:1438:GLN:HG2	1.58	0.84
1:A:1057:VAL:HG12	1:A:1063:TRP:HB2	1.58	0.84
1:A:1324:ILE:O	1:A:1324:ILE:HG22	1.74	0.83
1:A:641:PHE:CD1	1:A:739:LEU:HD21	2.13	0.83
1:A:1166:ILE:HG22	1:A:1172:PHE:HD2	1.39	0.83
1:A:641:PHE:CD1	1:A:739:LEU:CD2	2.61	0.83
1:A:1457:LEU:HD12	1:A:1474:ILE:HG12	1.57	0.83
1:A:521:PHE:O	1:A:525:ILE:HG12	1.79	0.83
1:A:1240:TYR:CE2	1:A:1268:ARG:CB	2.59	0.83
1:A:1240:TYR:OH	1:A:1268:ARG:HD3	1.78	0.83
1:A:1136:TYR:CZ	1:A:1509:GLU:CB	2.61	0.83
1:A:1217:CYS:O	1:A:1221:VAL:HG23	1.78	0.83
1:A:528:ILE:CG2	1:A:558:PHE:HE1	1.93	0.82
1:A:637:SER:OG	1:A:641:PHE:HD2	1.55	0.82
1:A:531:LEU:O	1:A:534:THR:OG1	1.97	0.82
1:A:210:LEU:O	1:A:214:ILE:HG13	1.80	0.82
1:A:62:PRO:O	1:A:120:LEU:N	2.12	0.82
1:A:601:GLU:HG3	1:A:610:ARG:NH2	1.95	0.82
1:A:878:ILE:HG21	1:A:1337:LYS:HG2	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:LEU:CG	1:A:606:LEU:H	1.92	0.81
1:A:704:GLU:HA	1:A:707:TRP:CD1	2.14	0.81
1:A:1488:PHE:CZ	1:A:1489:TYR:CE2	2.68	0.81
1:A:872:LEU:O	1:A:872:LEU:HD23	1.81	0.81
1:A:1330:ILE:CG2	1:A:1335:ASN:CA	2.55	0.81
1:A:944:ILE:O	1:A:945:GLU:HG3	1.81	0.81
1:A:240:ILE:HG23	1:A:241:VAL:HB	1.61	0.81
1:A:245:ARG:O	1:A:249:ASP:HB2	1.80	0.81
1:A:943:GLY:O	1:A:944:ILE:HG13	1.81	0.81
1:A:901:PHE:HE2	1:A:929:VAL:HG11	1.44	0.81
1:A:1176:MET:HE2	1:A:1216:GLU:HG3	1.62	0.81
1:A:1499:ASP:O	1:A:1502:SER:HB2	1.81	0.80
1:A:528:ILE:HD13	1:A:561:ILE:HG21	1.63	0.80
1:A:600:LEU:CD2	1:A:606:LEU:H	1.94	0.80
1:A:1180:ILE:CD1	1:A:1213:PHE:HE2	1.83	0.80
1:A:886:LEU:O	1:A:890:THR:HG22	1.81	0.80
1:A:1131:ARG:HG2	1:A:1131:ARG:HH21	1.47	0.80
1:A:1330:ILE:CG2	1:A:1335:ASN:HD22	1.95	0.80
1:A:909:LEU:HD23	1:A:917:TYR:HE2	1.45	0.79
1:A:1152:ILE:HG12	1:A:1227:HIS:CD2	2.17	0.79
1:A:974:THR:CG2	1:A:1405:MET:CE	2.59	0.79
1:A:550:ILE:O	1:A:553:THR:CG2	2.29	0.79
1:A:600:LEU:HG	1:A:606:LEU:N	1.96	0.79
1:A:863:THR:HG23	1:A:961:PRO:CG	2.12	0.79
1:A:1288:LEU:O	1:A:1291:ALA:HB3	1.81	0.79
1:A:518:SER:HB2	1:A:519:PRO:CD	2.12	0.79
1:A:1151:ARG:CG	1:A:1438:GLN:CG	2.61	0.79
1:A:518:SER:CB	1:A:520:PHE:HD2	1.96	0.79
1:A:55:ASP:O	1:A:59:SER:CB	2.30	0.78
1:A:1136:TYR:OH	1:A:1509:GLU:CB	2.31	0.78
1:A:177:THR:O	1:A:181:VAL:HG23	1.83	0.78
1:A:212:GLY:O	1:A:215:THR:HG22	1.82	0.78
1:A:1330:ILE:HG23	1:A:1335:ASN:HA	1.62	0.78
1:A:570:ILE:HG12	1:A:578:TYR:CE2	2.18	0.78
1:A:247:ILE:HD13	1:A:644:VAL:HG22	1.66	0.78
1:A:922:TRP:HA	1:A:925:LEU:HD12	1.65	0.78
1:A:1245:ILE:O	1:A:1249:MET:HB3	1.84	0.78
1:A:1262:THR:O	1:A:1266:ILE:HG13	1.84	0.78
1:A:591:VAL:HA	1:A:594:ALA:HB3	1.65	0.77
1:A:410:PHE:CD1	1:A:1288:LEU:HD11	2.19	0.77
1:A:1298:THR:HG23	1:A:1409:VAL:HG11	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:GLN:HA	1:A:1334:TYR:OH	1.84	0.77
1:A:651:LEU:HD23	1:A:732:ILE:HD11	1.66	0.77
1:A:1138:ARG:O	1:A:1142:ARG:HG2	1.85	0.77
1:A:372:VAL:HA	1:A:404:THR:HB	1.65	0.77
1:A:556:TYR:CE1	1:A:598:LEU:HD21	2.20	0.76
1:A:974:THR:HG21	1:A:1405:MET:HE1	1.66	0.76
1:A:166:TYR:O	1:A:170:LEU:HG	1.85	0.76
1:A:1429:ASP:O	1:A:1432:MET:HG3	1.84	0.76
1:A:374:LEU:HD12	1:A:400:VAL:HG13	1.67	0.76
1:A:203:TRP:HA	1:A:203:TRP:CE3	2.19	0.76
1:A:962:LEU:HD23	1:A:968:MET:CE	2.16	0.76
1:A:529:ILE:HD11	1:A:619:ARG:HH11	1.51	0.76
1:A:929:VAL:HG21	1:A:957:ARG:HD2	1.67	0.76
1:A:1174:TYR:O	1:A:1178:ILE:HG13	1.86	0.76
1:A:1305:LEU:CD2	1:A:1309:ILE:CD1	2.62	0.75
1:A:593:PHE:CD1	1:A:596:LEU:HD13	2.22	0.75
1:A:1457:LEU:HD12	1:A:1474:ILE:HD11	1.67	0.75
1:A:525:ILE:HG23	1:A:619:ARG:HH12	1.52	0.74
1:A:922:TRP:CZ3	1:A:959:PHE:HB3	2.22	0.74
1:A:1125:LEU:CD1	1:A:1137:ARG:HH22	1.98	0.74
1:A:1180:ILE:CD1	1:A:1213:PHE:HZ	1.81	0.74
1:A:1309:ILE:HA	1:A:1312:VAL:CG2	2.16	0.74
1:A:225:ALA:O	1:A:228:ALA:HB3	1.87	0.74
1:A:1146:ALA:CB	1:A:1434:PHE:CE2	2.69	0.74
1:A:1140:VAL:HG12	1:A:1144:MET:CE	2.17	0.74
1:A:990:ILE:HD13	1:A:1051:TYR:OH	1.87	0.74
1:A:943:GLY:C	1:A:944:ILE:HG13	2.09	0.73
1:A:1173:GLU:HB3	1:A:1278:TYR:OH	1.87	0.73
1:A:593:PHE:HA	1:A:596:LEU:HD12	1.69	0.73
1:A:1457:LEU:CD1	1:A:1474:ILE:CG1	2.63	0.73
1:A:410:PHE:CZ	1:A:1288:LEU:HD21	2.22	0.73
1:A:328:CYS:SG	1:A:329:GLY:N	2.61	0.73
1:A:1184:VAL:HG22	1:A:1272:VAL:HG21	1.69	0.73
1:A:1320:PHE:CZ	1:A:1386:LEU:HD11	2.16	0.73
1:A:1330:ILE:HG23	1:A:1334:TYR:O	1.87	0.73
1:A:1172:PHE:CD1	1:A:1176:MET:HG2	2.23	0.73
1:A:1209:PHE:O	1:A:1213:PHE:CD1	2.40	0.73
1:A:901:PHE:CE2	1:A:929:VAL:HG11	2.24	0.73
1:A:962:LEU:HD21	1:A:968:MET:SD	2.29	0.73
1:A:1446:GLN:NE2	1:A:1489:TYR:CE2	2.57	0.72
1:A:1206:ASN:ND2	1:A:1268:ARG:HH12	1.86	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:GLY:O	1:A:192:HIS:HB3	1.90	0.72
1:A:279:ILE:HG22	1:A:280:TYR:CD1	2.25	0.72
1:A:967:GLY:HA3	1:A:1301:ASN:HD21	1.52	0.72
1:A:123:LEU:O	1:A:189:PHE:CD2	2.41	0.72
1:A:288:CYS:SG	1:A:328:CYS:HB2	2.27	0.72
1:A:1152:ILE:H	1:A:1152:ILE:CD1	1.95	0.72
1:A:539:ASP:OD1	1:A:551:LEU:HD11	1.90	0.72
1:A:1057:VAL:HG23	1:A:1095:PHE:CE2	2.25	0.72
1:A:632:SER:O	1:A:635:THR:OG1	2.07	0.72
1:A:876:GLU:O	1:A:880:LEU:HD23	1.89	0.72
1:A:952:LEU:O	1:A:1316:PHE:HE1	1.72	0.71
1:A:947:LEU:HD22	1:A:950:LEU:HG	1.71	0.71
1:A:959:PHE:O	1:A:962:LEU:HB3	1.90	0.71
1:A:266:LEU:HD12	1:A:266:LEU:O	1.90	0.71
1:A:915:LYS:O	1:A:919:THR:OG1	2.08	0.71
1:A:170:LEU:CD2	1:A:216:LEU:CD2	2.68	0.71
1:A:1323:HIS:O	1:A:1380:ASN:HA	1.90	0.71
1:A:374:LEU:HD21	1:A:1351:THR:HB	1.73	0.71
1:A:929:VAL:HG21	1:A:957:ARG:CD	2.20	0.71
1:A:1468:LYS:HG2	1:A:1469:PRO:HA	1.71	0.71
1:A:898:THR:HG22	1:A:933:TYR:CG	2.25	0.70
1:A:1206:ASN:HD21	1:A:1268:ARG:NH1	1.88	0.70
1:A:1330:ILE:HG22	1:A:1335:ASN:HA	1.69	0.70
1:A:205:ASP:O	1:A:209:THR:HG22	1.91	0.70
1:A:682:TRP:O	1:A:693:ILE:HD12	1.91	0.70
1:A:1184:VAL:CG2	1:A:1272:VAL:HG21	2.21	0.70
1:A:403:GLY:O	1:A:407:PHE:HB2	1.91	0.70
1:A:560:SER:HA	1:A:563:ILE:CD1	2.19	0.70
1:A:861:PHE:O	1:A:865:VAL:HG23	1.92	0.70
1:A:596:LEU:HD22	1:A:609:PHE:CZ	2.27	0.70
1:A:246:THR:O	1:A:250:ALA:HB2	1.91	0.70
1:A:564:VAL:HA	1:A:567:VAL:HG12	1.73	0.70
1:A:397:ILE:O	1:A:401:PHE:HB3	1.91	0.70
1:A:641:PHE:CE1	1:A:739:LEU:HD23	2.27	0.70
1:A:971:VAL:HG13	1:A:1405:MET:HE1	1.73	0.70
1:A:528:ILE:O	1:A:558:PHE:CE1	2.45	0.69
1:A:873:LEU:HD23	1:A:955:VAL:CG2	2.22	0.69
1:A:147:MET:O	1:A:150:ILE:HB	1.92	0.69
1:A:183:LYS:HB2	1:A:196:TYR:HH	1.55	0.69
1:A:641:PHE:CD1	1:A:739:LEU:HD23	2.26	0.69
1:A:1463:PRO:HG2	1:A:1500:VAL:HG11	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:TRP:HA	1:A:203:TRP:HE3	1.56	0.69
1:A:1322:MET:O	1:A:1324:ILE:HG13	1.91	0.69
1:A:157:MET:HE3	1:A:230:ARG:HD2	1.73	0.69
1:A:270:PHE:O	1:A:274:VAL:HG23	1.93	0.69
1:A:276:GLY:O	1:A:280:TYR:HB2	1.93	0.69
1:A:922:TRP:HA	1:A:925:LEU:CD1	2.22	0.69
1:A:605:GLY:CA	1:A:606:LEU:HG	2.23	0.69
1:A:382:GLN:CG	1:A:1348:GLN:HE22	2.06	0.69
1:A:529:ILE:HD11	1:A:619:ARG:NH1	2.07	0.69
1:A:160:PRO:HG2	1:A:162:THR:CG2	2.17	0.69
1:A:525:ILE:CG2	1:A:619:ARG:HH12	2.06	0.69
1:A:663:PHE:O	1:A:666:ASN:HB2	1.91	0.69
1:A:1177:MET:CE	1:A:1181:ILE:HG12	2.22	0.69
1:A:1414:VAL:O	1:A:1418:TYR:HD1	1.75	0.69
1:A:518:SER:HB2	1:A:519:PRO:HD3	1.74	0.68
1:A:1057:VAL:HG23	1:A:1095:PHE:HE2	1.58	0.68
1:A:1125:LEU:HD12	1:A:1137:ARG:NH2	2.05	0.68
1:A:528:ILE:CD1	1:A:561:ILE:HG21	2.24	0.68
1:A:1256:LYS:O	1:A:1258:PHE:N	2.25	0.68
1:A:614:LEU:CD2	1:A:998:ILE:HD11	2.17	0.68
1:A:916:LYS:HA	1:A:919:THR:OG1	1.93	0.68
1:A:924:TRP:O	1:A:928:ILE:HG13	1.93	0.68
1:A:601:GLU:CG	1:A:610:ARG:HH22	2.06	0.68
1:A:1158:HIS:ND1	1:A:1159:PRO:HD3	2.08	0.68
1:A:165:THR:HG21	1:A:168:LEU:CD1	2.23	0.68
1:A:279:ILE:HG22	1:A:280:TYR:HD1	1.58	0.68
1:A:912:VAL:HG13	1:A:913:GLY:N	2.09	0.68
1:A:977:GLU:OE2	1:A:977:GLU:HA	1.94	0.68
1:A:1354:GLY:O	1:A:1358:VAL:HG23	1.93	0.68
1:A:387:SER:OG	1:A:388:ALA:N	2.27	0.67
1:A:889:ILE:O	1:A:893:VAL:HG23	1.93	0.67
1:A:624:TRP:HE3	1:A:625:PRO:HD2	1.58	0.67
1:A:1436:VAL:HG21	1:A:1460:LEU:CD2	2.23	0.67
1:A:1119:ARG:CD	1:A:1412:ASP:OD2	2.40	0.67
1:A:1262:THR:HG22	1:A:1266:ILE:CD1	2.25	0.67
1:A:149:THR:HG23	1:A:176:TYR:OH	1.95	0.67
1:A:260:ASP:OD1	1:A:1285:MET:HB2	1.93	0.67
1:A:601:GLU:CG	1:A:610:ARG:NH2	2.57	0.67
1:A:606:LEU:HB3	1:A:607:SER:HB2	1.76	0.67
1:A:877:ASP:OD2	1:A:1322:MET:HE2	1.94	0.67
1:A:239:THR:HG22	1:A:244:TRP:CZ2	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:876:GLU:O	1:A:880:LEU:CD2	2.43	0.67
1:A:1173:GLU:O	1:A:1177:MET:HB2	1.95	0.67
1:A:1060:PHE:CE1	1:A:1096:ILE:HD11	2.29	0.67
1:A:1351:THR:O	1:A:1352:SER:OG	2.07	0.67
1:A:170:LEU:CD2	1:A:216:LEU:HD21	2.25	0.67
1:A:998:ILE:O	1:A:1002:GLN:HG3	1.95	0.67
1:A:1288:LEU:O	1:A:1288:LEU:HD23	1.94	0.67
1:A:64:GLN:H	1:A:119:SER:HA	1.60	0.66
1:A:265:LEU:HD11	1:A:407:PHE:HB3	1.76	0.66
1:A:410:PHE:HD1	1:A:1288:LEU:HD11	1.59	0.66
1:A:873:LEU:CD1	1:A:954:ARG:HH21	2.08	0.66
1:A:877:ASP:OD2	1:A:1322:MET:CE	2.43	0.66
1:A:1320:PHE:CE1	1:A:1386:LEU:CG	2.76	0.66
1:A:1147:LYS:HB3	1:A:1148:PRO:HD3	1.77	0.66
1:A:658:ILE:O	1:A:662:LEU:HB2	1.96	0.66
1:A:1382:GLY:O	1:A:1383:SER:HB3	1.94	0.66
1:A:223:LEU:HB3	1:A:225:ALA:H	1.60	0.66
1:A:224:TYR:CE1	1:A:227:ARG:HG3	2.30	0.66
1:A:251:LEU:O	1:A:255:ILE:HG13	1.94	0.66
1:A:912:VAL:HG13	1:A:913:GLY:H	1.61	0.66
1:A:971:VAL:HG13	1:A:1405:MET:CE	2.26	0.66
1:A:381:TYR:HD2	1:A:1348:GLN:HE21	1.41	0.66
1:A:985:VAL:CG2	1:A:1110:ILE:CD1	2.59	0.66
1:A:1061:LYS:HE2	1:A:1352:SER:O	1.96	0.66
1:A:1172:PHE:HE1	1:A:1176:MET:SD	2.19	0.66
1:A:1488:PHE:CZ	1:A:1489:TYR:CD2	2.84	0.66
1:A:405:PHE:O	1:A:409:ASN:ND2	2.28	0.66
1:A:711:LEU:HD22	1:A:711:LEU:O	1.96	0.66
1:A:1489:TYR:CE1	1:A:1490:LYS:HB2	2.31	0.66
1:A:150:ILE:CD1	1:A:236:ARG:HD2	2.26	0.66
1:A:603:VAL:C	1:A:604:GLN:HG3	2.14	0.66
1:A:1152:ILE:HD12	1:A:1152:ILE:N	2.03	0.66
1:A:562:TYR:O	1:A:565:GLU:HG3	1.97	0.65
1:A:1261:PRO:O	1:A:1265:ARG:HG3	1.95	0.65
1:A:192:HIS:O	1:A:196:TYR:HB2	1.97	0.65
1:A:856:LYS:HD3	1:A:860:LYS:HE3	1.79	0.65
1:A:192:HIS:HA	1:A:195:ALA:HB3	1.77	0.65
1:A:637:SER:OG	1:A:641:PHE:CE2	2.43	0.65
1:A:269:LEU:HD11	1:A:369:PHE:HD1	1.61	0.65
1:A:1481:ILE:CG2	1:A:1485:ASP:HA	2.27	0.65
1:A:882:GLN:HG3	1:A:882:GLN:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:948:GLN:O	1:A:951:ARG:HG2	1.97	0.65
1:A:653:PHE:CE1	1:A:657:ILE:CD1	2.74	0.64
1:A:849:CYS:O	1:A:853:ALA:HB2	1.96	0.64
1:A:188:GLY:O	1:A:193:PRO:HD3	1.96	0.64
1:A:1000:GLY:O	1:A:1004:PHE:CB	2.35	0.64
1:A:1067:MET:O	1:A:1071:ILE:HG13	1.96	0.64
1:A:234:SER:OG	1:A:654:ILE:CD1	2.45	0.64
1:A:518:SER:HB2	1:A:520:PHE:HD2	1.61	0.64
1:A:876:GLU:C	1:A:880:LEU:HD23	2.18	0.64
1:A:1240:TYR:CD2	1:A:1268:ARG:HB2	2.28	0.64
1:A:55:ASP:O	1:A:59:SER:N	2.31	0.64
1:A:863:THR:O	1:A:867:VAL:HG23	1.98	0.64
1:A:978:ALA:O	1:A:982:ILE:HG12	1.97	0.64
1:A:419:TYR:HD2	1:A:742:ASN:ND2	1.94	0.64
1:A:1111:LEU:HD21	1:A:1405:MET:CA	2.26	0.64
1:A:157:MET:HE2	1:A:230:ARG:HH11	1.61	0.64
1:A:967:GLY:CA	1:A:1301:ASN:ND2	2.57	0.64
1:A:328:CYS:O	1:A:386:ARG:O	2.15	0.64
1:A:1233:TRP:CD1	1:A:1274:ARG:HG3	2.33	0.64
1:A:409:ASN:HD22	1:A:1410:ILE:HD12	1.62	0.64
1:A:1058:ALA:HB1	1:A:1104:LEU:HD11	1.80	0.64
1:A:1172:PHE:CE1	1:A:1176:MET:CG	2.81	0.64
1:A:204:LEU:HD11	1:A:232:LEU:HG	1.79	0.63
1:A:1062:GLY:O	1:A:1065:GLN:HG2	1.97	0.63
1:A:370:ARG:HH11	1:A:380:LEU:HD22	1.63	0.63
1:A:1420:ASP:O	1:A:1424:GLY:HA3	1.99	0.63
1:A:519:PRO:HD2	1:A:520:PHE:N	2.13	0.63
1:A:1423:GLU:O	1:A:1504:ARG:HG3	1.99	0.63
1:A:224:TYR:HD1	1:A:227:ARG:HG3	1.60	0.63
1:A:258:LEU:HD11	1:A:411:ILE:HG23	1.81	0.63
1:A:370:ARG:HH22	1:A:707:TRP:HZ2	1.45	0.63
1:A:400:VAL:HA	1:A:404:THR:HG22	1.79	0.63
1:A:971:VAL:O	1:A:974:THR:CG2	2.46	0.63
1:A:1140:VAL:HG12	1:A:1144:MET:HE1	1.81	0.63
1:A:1147:LYS:HB3	1:A:1148:PRO:CD	2.29	0.63
1:A:247:ILE:HD13	1:A:644:VAL:CG2	2.29	0.63
1:A:1151:ARG:CG	1:A:1438:GLN:HG3	2.29	0.63
1:A:650:LEU:O	1:A:654:ILE:HG12	1.98	0.63
1:A:1295:ALA:O	1:A:1298:THR:HG22	1.99	0.63
1:A:410:PHE:CE1	1:A:1288:LEU:CG	2.82	0.62
1:A:1151:ARG:O	1:A:1153:PRO:HB3	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1345:LEU:O	1:A:1348:GLN:HB2	1.99	0.62
1:A:962:LEU:CD2	1:A:968:MET:SD	2.86	0.62
1:A:1149:VAL:HG12	1:A:1151:ARG:H	1.63	0.62
1:A:1194:GLN:O	1:A:1195:SER:OG	2.09	0.62
1:A:641:PHE:CE1	1:A:739:LEU:CD2	2.83	0.62
1:A:216:LEU:O	1:A:218:VAL:HG23	1.99	0.62
1:A:400:VAL:O	1:A:404:THR:HG22	1.99	0.62
1:A:1324:ILE:O	1:A:1325:ARG:HB2	2.00	0.62
1:A:157:MET:HE1	1:A:230:ARG:HD2	1.79	0.62
1:A:430:LYS:O	1:A:434:ARG:CD	2.48	0.62
1:A:1448:ILE:HD12	1:A:1456:LEU:HD22	1.80	0.62
1:A:1457:LEU:HD11	1:A:1474:ILE:HG12	1.78	0.62
1:A:366:LEU:HD11	1:A:706:MET:CE	2.30	0.62
1:A:1026:ASP:HA	1:A:1078:LYS:HA	1.82	0.62
1:A:1172:PHE:CD1	1:A:1176:MET:CG	2.82	0.62
1:A:1463:PRO:HB2	1:A:1500:VAL:HG13	1.80	0.62
1:A:374:LEU:CD1	1:A:400:VAL:HG13	2.30	0.62
1:A:518:SER:OG	1:A:520:PHE:HB2	2.00	0.62
1:A:560:SER:O	1:A:564:VAL:HG23	2.00	0.61
1:A:985:VAL:O	1:A:988:VAL:HB	1.99	0.61
1:A:1330:ILE:C	1:A:1332:ASP:H	1.99	0.61
1:A:560:SER:CA	1:A:563:ILE:HD12	2.21	0.61
1:A:1176:MET:HE1	1:A:1216:GLU:CB	2.18	0.61
1:A:1262:THR:CG2	1:A:1266:ILE:HD11	2.30	0.61
1:A:1473:LYS:O	1:A:1476:SER:HB3	2.00	0.61
1:A:205:ASP:O	1:A:209:THR:CG2	2.48	0.61
1:A:614:LEU:CD2	1:A:617:VAL:HG21	2.30	0.61
1:A:703:ILE:HG22	1:A:707:TRP:NE1	2.15	0.61
1:A:996:PHE:CE2	1:A:1095:PHE:HA	2.36	0.61
1:A:224:TYR:HE1	1:A:227:ARG:CZ	2.13	0.61
1:A:245:ARG:O	1:A:245:ARG:HD2	2.01	0.61
1:A:884:PRO:HB2	1:A:887:VAL:HB	1.81	0.61
1:A:1132:THR:O	1:A:1136:TYR:CD2	2.53	0.61
1:A:922:TRP:HZ3	1:A:959:PHE:HB3	1.62	0.61
1:A:157:MET:CE	1:A:230:ARG:HH11	2.12	0.61
1:A:567:VAL:O	1:A:571:ILE:HG13	2.00	0.61
1:A:880:LEU:O	1:A:882:GLN:HG2	2.00	0.61
1:A:962:LEU:HD23	1:A:968:MET:HE2	1.82	0.61
1:A:967:GLY:CA	1:A:1301:ASN:HD21	2.12	0.61
1:A:1003:LEU:HD12	1:A:1088:MET:CE	2.30	0.61
1:A:1283:ARG:O	1:A:1287:LEU:HB2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:LYS:HD2	1:A:259:LYS:C	2.22	0.61
1:A:518:SER:HB2	1:A:520:PHE:CD2	2.36	0.61
1:A:1151:ARG:HG2	1:A:1438:GLN:CD	2.20	0.61
1:A:1298:THR:CG2	1:A:1409:VAL:HG11	2.30	0.61
1:A:566:ALA:O	1:A:570:ILE:HD12	2.01	0.60
1:A:269:LEU:HD11	1:A:369:PHE:CD1	2.35	0.60
1:A:878:ILE:HD12	1:A:1323:HIS:NE2	2.12	0.60
1:A:1149:VAL:HG12	1:A:1151:ARG:N	2.16	0.60
1:A:146:ILE:O	1:A:149:THR:HG22	2.01	0.60
1:A:430:LYS:HB3	1:A:434:ARG:NH2	2.16	0.60
1:A:640:ALA:O	1:A:644:VAL:HG23	2.00	0.60
1:A:1317:GLY:O	1:A:1321:PHE:N	2.33	0.60
1:A:154:CYS:O	1:A:158:ILE:CG1	2.45	0.60
1:A:1111:LEU:CD2	1:A:1405:MET:N	2.63	0.60
1:A:1140:VAL:O	1:A:1144:MET:HE2	2.01	0.60
1:A:1140:VAL:CG1	1:A:1144:MET:HE1	2.31	0.60
1:A:1176:MET:HE2	1:A:1216:GLU:CG	2.31	0.60
1:A:620:LEU:HG	1:A:624:TRP:CD1	2.36	0.60
1:A:1139:ALA:O	1:A:1143:THR:HG23	2.02	0.60
1:A:1450:TYR:CD1	1:A:1481:ILE:HD11	2.36	0.60
1:A:419:TYR:CD2	1:A:742:ASN:ND2	2.68	0.60
1:A:243:GLY:O	1:A:245:ARG:N	2.34	0.59
1:A:367:SER:O	1:A:370:ARG:HB3	2.02	0.59
1:A:528:ILE:O	1:A:558:PHE:HE1	1.84	0.59
1:A:1288:LEU:HD23	1:A:1288:LEU:C	2.23	0.59
1:A:165:THR:HB	1:A:168:LEU:HG	1.82	0.59
1:A:1060:PHE:O	1:A:1061:LYS:HD3	2.03	0.59
1:A:165:THR:HB	1:A:168:LEU:H	1.66	0.59
1:A:170:LEU:HD23	1:A:216:LEU:HD21	1.85	0.59
1:A:331:SER:HB2	1:A:388:ALA:O	2.03	0.59
1:A:519:PRO:HD2	1:A:520:PHE:H	1.67	0.59
1:A:934:LEU:O	1:A:938:VAL:CG2	2.35	0.59
1:A:1132:THR:O	1:A:1136:TYR:HD2	1.83	0.59
1:A:1279:PHE:O	1:A:1281:SER:N	2.35	0.59
1:A:1419:GLU:HA	1:A:1419:GLU:OE1	2.03	0.59
1:A:1464:LEU:HD23	1:A:1500:VAL:CG2	2.31	0.59
1:A:370:ARG:HH21	1:A:703:ILE:HG21	1.66	0.59
1:A:883:ARG:O	1:A:883:ARG:HD3	2.03	0.59
1:A:1151:ARG:HG2	1:A:1438:GLN:CG	2.31	0.59
1:A:277:LEU:O	1:A:281:MET:HB2	2.02	0.59
1:A:840:ARG:O	1:A:844:ASN:N	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1330:ILE:HG22	1:A:1335:ASN:CA	2.30	0.59
1:A:371:LEU:HD13	1:A:399:VAL:CG1	2.31	0.58
1:A:1254:ILE:HG21	1:A:1257:TYR:HE2	1.68	0.58
1:A:165:THR:OG1	1:A:168:LEU:HB2	2.03	0.58
1:A:718:ILE:HB	1:A:719:PRO:HD3	1.85	0.58
1:A:974:THR:CG2	1:A:1405:MET:HE1	2.30	0.58
1:A:200:PRO:HD2	1:A:201:TRP:H	1.68	0.58
1:A:149:THR:HG21	1:A:176:TYR:HE1	1.68	0.58
1:A:214:ILE:O	1:A:217:VAL:HB	2.03	0.58
1:A:878:ILE:CG2	1:A:1337:LYS:HG2	2.32	0.58
1:A:1172:PHE:HD1	1:A:1176:MET:HG2	1.65	0.58
1:A:158:ILE:HG23	1:A:687:PHE:CG	2.39	0.58
1:A:703:ILE:HG22	1:A:707:TRP:CE2	2.38	0.58
1:A:880:LEU:O	1:A:882:GLN:N	2.36	0.58
1:A:1450:TYR:CD1	1:A:1481:ILE:CD1	2.86	0.58
1:A:1150:LYS:O	1:A:1151:ARG:HB2	2.04	0.58
1:A:165:THR:HG21	1:A:168:LEU:HD12	1.86	0.58
1:A:183:LYS:HB3	1:A:196:TYR:OH	2.00	0.57
1:A:338:PRO:HD2	1:A:341:TYR:CD2	2.39	0.57
1:A:872:LEU:HD23	1:A:872:LEU:C	2.23	0.57
1:A:1481:ILE:HG23	1:A:1486:HIS:O	2.04	0.57
1:A:550:ILE:C	1:A:553:THR:HG22	2.20	0.57
1:A:977:GLU:C	1:A:980:PRO:HD2	2.20	0.57
1:A:1151:ARG:HG3	1:A:1438:GLN:HG3	1.83	0.57
1:A:1425:LEU:HD12	1:A:1497:VAL:HG13	1.85	0.57
1:A:1454:SER:OG	1:A:1468:LYS:HE2	2.03	0.57
1:A:563:ILE:O	1:A:567:VAL:N	2.27	0.57
1:A:123:LEU:O	1:A:189:PHE:CE2	2.58	0.57
1:A:279:ILE:CG2	1:A:280:TYR:CD1	2.87	0.57
1:A:523:LEU:O	1:A:527:VAL:HG23	2.04	0.57
1:A:1320:PHE:HE1	1:A:1386:LEU:HD11	1.49	0.57
1:A:1420:ASP:O	1:A:1424:GLY:CA	2.53	0.57
1:A:382:GLN:HG3	1:A:1348:GLN:NE2	2.19	0.57
1:A:430:LYS:O	1:A:434:ARG:NE	2.37	0.57
1:A:518:SER:OG	1:A:520:PHE:HD2	1.87	0.57
1:A:925:LEU:O	1:A:929:VAL:HG23	2.05	0.57
1:A:193:PRO:HA	1:A:196:TYR:HB2	1.86	0.57
1:A:614:LEU:HD22	1:A:617:VAL:HG21	1.86	0.57
1:A:1003:LEU:HD12	1:A:1088:MET:HE1	1.87	0.57
1:A:1112:ILE:HD13	1:A:1411:LEU:HD23	1.87	0.57
1:A:1309:ILE:HA	1:A:1312:VAL:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1007:LYS:HB3	1:A:1073:SER:HB2	1.85	0.57
1:A:971:VAL:HG11	1:A:1302:VAL:HG22	1.86	0.57
1:A:1262:THR:HG22	1:A:1266:ILE:HD11	1.84	0.57
1:A:1027:ARG:HE	1:A:1031:LEU:HD12	1.70	0.56
1:A:430:LYS:O	1:A:434:ARG:HD2	2.04	0.56
1:A:273:ALA:HA	1:A:368:VAL:HG21	1.88	0.56
1:A:285:THR:HG22	1:A:350:ASN:HB3	1.86	0.56
1:A:378:GLU:O	1:A:382:GLN:HG3	2.04	0.56
1:A:588:PHE:O	1:A:592:VAL:HG23	2.06	0.56
1:A:600:LEU:HD21	1:A:606:LEU:O	2.05	0.56
1:A:836:SER:O	1:A:840:ARG:N	2.38	0.56
1:A:873:LEU:HD23	1:A:955:VAL:HG22	1.86	0.56
1:A:1060:PHE:HE1	1:A:1096:ILE:HD11	1.68	0.56
1:A:1258:PHE:HB2	1:A:1259:ILE:CG1	2.17	0.56
1:A:1425:LEU:HD21	1:A:1429:ASP:HB3	1.88	0.56
1:A:223:LEU:O	1:A:224:TYR:HB2	2.06	0.56
1:A:366:LEU:HD11	1:A:706:MET:HE1	1.88	0.56
1:A:1150:LYS:O	1:A:1151:ARG:CB	2.52	0.56
1:A:1240:TYR:CZ	1:A:1268:ARG:HD3	2.40	0.56
1:A:603:VAL:O	1:A:604:GLN:CG	2.43	0.56
1:A:1054:LEU:O	1:A:1057:VAL:HG22	2.06	0.56
1:A:1151:ARG:HG2	1:A:1438:GLN:OE1	2.06	0.56
1:A:1490:LYS:O	1:A:1494:GLU:HG3	2.06	0.56
1:A:261:LEU:HD21	1:A:410:PHE:HB3	1.88	0.56
1:A:971:VAL:HA	1:A:1405:MET:HE1	1.86	0.56
1:A:1140:VAL:O	1:A:1143:THR:OG1	2.18	0.56
1:A:1453:LEU:HD23	1:A:1474:ILE:HG21	1.86	0.56
1:A:197:LEU:CD2	1:A:203:TRP:CZ3	2.89	0.56
1:A:922:TRP:HZ3	1:A:959:PHE:CB	2.19	0.56
1:A:600:LEU:HD21	1:A:606:LEU:H	1.70	0.56
1:A:873:LEU:HD13	1:A:954:ARG:HH22	1.67	0.56
1:A:1042:MET:SD	1:A:1053:SER:HB2	2.46	0.56
1:A:1043:ASN:ND2	1:A:1045:ASP:OD2	2.39	0.56
1:A:377:TRP:O	1:A:381:TYR:N	2.26	0.56
1:A:1116:ARG:O	1:A:1120:ARG:HG2	2.06	0.55
1:A:1179:LEU:CD1	1:A:1212:ILE:HG21	2.36	0.55
1:A:1460:LEU:O	1:A:1465:GLN:HB2	2.06	0.55
1:A:258:LEU:HD23	1:A:262:VAL:CG2	2.36	0.55
1:A:267:PHE:HZ	1:A:1272:VAL:HG12	1.70	0.55
1:A:1176:MET:CE	1:A:1216:GLU:CB	2.78	0.55
1:A:1063:TRP:O	1:A:1067:MET:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:SER:OG	1:A:654:ILE:HD11	2.06	0.55
1:A:624:TRP:CD1	1:A:627:LEU:HD23	2.42	0.55
1:A:909:LEU:CD2	1:A:917:TYR:HE2	2.08	0.55
1:A:926:ASP:CG	1:A:957:ARG:HH22	2.10	0.55
1:A:258:LEU:CD1	1:A:411:ILE:HG23	2.37	0.55
1:A:1001:VAL:HG13	1:A:1005:ALA:HB2	1.88	0.55
1:A:518:SER:CB	1:A:519:PRO:CD	2.84	0.55
1:A:880:LEU:O	1:A:882:GLN:CG	2.55	0.55
1:A:193:PRO:O	1:A:197:LEU:HG	2.07	0.55
1:A:600:LEU:CD2	1:A:606:LEU:O	2.55	0.55
1:A:974:THR:CG2	1:A:1405:MET:SD	2.94	0.55
1:A:1149:VAL:HG12	1:A:1150:LYS:N	2.22	0.55
1:A:154:CYS:SG	1:A:158:ILE:HD11	2.47	0.54
1:A:224:TYR:OH	1:A:227:ARG:NH1	2.40	0.54
1:A:382:GLN:CG	1:A:1348:GLN:NE2	2.70	0.54
1:A:162:THR:O	1:A:163:GLN:HG3	2.08	0.54
1:A:1074:ARG:HH11	1:A:1081:ILE:HD11	1.71	0.54
1:A:1158:HIS:HB3	1:A:1159:PRO:CD	2.36	0.54
1:A:652:LEU:HD12	1:A:698:LEU:HD22	1.89	0.54
1:A:1131:ARG:HH21	1:A:1131:ARG:CG	2.18	0.54
1:A:1158:HIS:CG	1:A:1159:PRO:HD3	2.42	0.54
1:A:1253:VAL:HG11	1:A:1254:ILE:CG1	2.34	0.54
1:A:59:SER:O	1:A:60:ALA:HB2	2.07	0.54
1:A:585:VAL:O	1:A:589:ILE:HG13	2.08	0.54
1:A:879:TYR:HB2	1:A:882:GLN:OE1	2.07	0.54
1:A:94:PRO:O	1:A:98:ASN:N	2.35	0.54
1:A:839:GLN:O	1:A:843:SER:N	2.39	0.54
1:A:1349:LEU:HD11	1:A:1358:VAL:HG21	1.89	0.54
1:A:144:TYR:O	1:A:148:ILE:HG13	2.08	0.54
1:A:206:PHE:O	1:A:209:THR:HG22	2.08	0.54
1:A:239:THR:HG22	1:A:244:TRP:CE2	2.43	0.54
1:A:556:TYR:CE1	1:A:598:LEU:CD2	2.91	0.54
1:A:600:LEU:HD21	1:A:609:PHE:HD2	1.72	0.54
1:A:873:LEU:HD22	1:A:954:ARG:HH21	1.73	0.54
1:A:1488:PHE:HZ	1:A:1489:TYR:CE2	2.25	0.54
1:A:394:LEU:O	1:A:398:ILE:HG13	2.08	0.54
1:A:528:ILE:HD13	1:A:561:ILE:CG2	2.36	0.54
1:A:893:VAL:O	1:A:897:LEU:HB2	2.07	0.54
1:A:1220:LYS:HB3	1:A:1228:TYR:HE1	1.72	0.54
1:A:1258:PHE:N	1:A:1258:PHE:CD1	2.75	0.54
1:A:1425:LEU:CD2	1:A:1429:ASP:HB3	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1450:TYR:HD1	1:A:1481:ILE:CD1	2.20	0.54
1:A:681:ARG:NH1	1:A:1068:ASN:HB3	2.22	0.54
1:A:113:ARG:CB	1:A:114:PHE:CB	2.86	0.54
1:A:528:ILE:CG2	1:A:558:PHE:HD1	2.18	0.54
1:A:988:VAL:O	1:A:991:PHE:HB3	2.07	0.54
1:A:1176:MET:CE	1:A:1216:GLU:HG3	2.36	0.54
1:A:1474:ILE:HA	1:A:1477:MET:CE	2.38	0.54
1:A:238:VAL:HG22	1:A:650:LEU:HD23	1.90	0.53
1:A:530:VAL:O	1:A:534:THR:HG23	2.06	0.53
1:A:593:PHE:HD1	1:A:596:LEU:HD13	1.73	0.53
1:A:1228:TYR:CZ	1:A:1234:ASN:HB3	2.43	0.53
1:A:1460:LEU:CD1	1:A:1496:LEU:HD11	2.38	0.53
1:A:1475:LEU:O	1:A:1475:LEU:HG	2.08	0.53
1:A:947:LEU:HD13	1:A:950:LEU:HD11	1.90	0.53
1:A:1172:PHE:CE1	1:A:1176:MET:SD	3.00	0.53
1:A:1415:LEU:O	1:A:1419:GLU:HB2	2.08	0.53
1:A:223:LEU:HD13	1:A:225:ALA:HB2	1.90	0.53
1:A:566:ALA:O	1:A:570:ILE:CD1	2.57	0.53
1:A:866:LEU:HD11	1:A:957:ARG:HE	1.74	0.53
1:A:974:THR:HG23	1:A:1405:MET:SD	2.49	0.53
1:A:1001:VAL:O	1:A:1005:ALA:HB3	2.08	0.53
1:A:568:LEU:O	1:A:572:ALA:N	2.35	0.53
1:A:1184:VAL:CG2	1:A:1272:VAL:CG2	2.87	0.53
1:A:546:GLU:O	1:A:550:ILE:HG13	2.09	0.53
1:A:370:ARG:NH2	1:A:707:TRP:HZ2	2.07	0.53
1:A:1061:LYS:HE2	1:A:1353:ALA:HA	1.91	0.53
1:A:1136:TYR:O	1:A:1140:VAL:HG23	2.09	0.53
1:A:1453:LEU:CD2	1:A:1474:ILE:HG21	2.39	0.53
1:A:660:MET:O	1:A:664:GLY:HA2	2.08	0.53
1:A:1064:LEU:HD23	1:A:1068:ASN:ND2	2.24	0.53
1:A:94:PRO:N	1:A:97:LYS:CB	2.72	0.53
1:A:413:ALA:HA	1:A:1411:LEU:HD13	1.91	0.53
1:A:121:TRP:CB	1:A:122:MET:HA	2.39	0.52
1:A:195:ALA:HA	1:A:198:ARG:HB2	1.91	0.52
1:A:1259:ILE:O	1:A:1260:SER:OG	2.21	0.52
1:A:1266:ILE:O	1:A:1270:LEU:HG	2.09	0.52
1:A:190:ILE:O	1:A:194:PHE:HD2	1.93	0.52
1:A:591:VAL:HA	1:A:594:ALA:CB	2.35	0.52
1:A:1214:PHE:HD1	1:A:1214:PHE:O	1.92	0.52
1:A:1229:PHE:O	1:A:1235:ILE:HD11	2.09	0.52
1:A:1262:THR:HG22	1:A:1266:ILE:HD12	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1466:VAL:HG12	1:A:1470:ASN:HB2	1.91	0.52
1:A:210:LEU:O	1:A:214:ILE:N	2.41	0.52
1:A:833:ALA:O	1:A:837:SER:N	2.39	0.52
1:A:158:ILE:HG23	1:A:687:PHE:CD1	2.45	0.52
1:A:247:ILE:HA	1:A:250:ALA:HB3	1.92	0.52
1:A:264:LEU:HD22	1:A:407:PHE:CE1	2.44	0.52
1:A:140:PRO:HD2	1:A:141:ILE:H	1.73	0.52
1:A:369:PHE:O	1:A:373:THR:HG23	2.09	0.52
1:A:1474:ILE:HA	1:A:1477:MET:HE2	1.92	0.52
1:A:351:PRO:O	1:A:354:GLY:N	2.43	0.52
1:A:528:ILE:HG22	1:A:558:PHE:CD1	2.40	0.52
1:A:858:PHE:O	1:A:861:PHE:HB3	2.09	0.52
1:A:940:MET:HE1	1:A:941:CYS:HB2	1.88	0.52
1:A:382:GLN:HG3	1:A:1348:GLN:HE22	1.75	0.52
1:A:593:PHE:CD1	1:A:596:LEU:CD1	2.91	0.52
1:A:670:ASN:HD22	1:A:712:VAL:HG22	1.74	0.52
1:A:1179:LEU:HD12	1:A:1212:ILE:HG21	1.91	0.52
1:A:224:TYR:CZ	1:A:227:ARG:NH1	2.78	0.52
1:A:1243:LEU:HD12	1:A:1267:LEU:HD12	1.91	0.52
1:A:142:PHE:O	1:A:145:PHE:HB3	2.10	0.52
1:A:878:ILE:O	1:A:878:ILE:HG12	2.10	0.52
1:A:1028:ASN:O	1:A:1032:HIS:N	2.39	0.52
1:A:1065:GLN:HG3	1:A:1066:ILE:N	2.25	0.52
1:A:1320:PHE:CE1	1:A:1386:LEU:HG	2.45	0.52
1:A:374:LEU:CD1	1:A:400:VAL:CG1	2.88	0.51
1:A:557:ILE:O	1:A:561:ILE:HG12	2.11	0.51
1:A:601:GLU:HG2	1:A:610:ARG:HH22	1.75	0.51
1:A:197:LEU:HD23	1:A:203:TRP:CZ3	2.45	0.51
1:A:539:ASP:OD1	1:A:551:LEU:CD1	2.57	0.51
1:A:160:PRO:HD2	1:A:162:THR:OG1	2.09	0.51
1:A:247:ILE:O	1:A:251:LEU:HD12	2.10	0.51
1:A:400:VAL:O	1:A:404:THR:CG2	2.58	0.51
1:A:593:PHE:HA	1:A:596:LEU:CD1	2.38	0.51
1:A:184:VAL:HG22	1:A:196:TYR:CD2	2.45	0.51
1:A:1131:ARG:HG2	1:A:1131:ARG:NH2	2.21	0.51
1:A:1254:ILE:HG21	1:A:1257:TYR:CE2	2.46	0.51
1:A:524:PHE:O	1:A:528:ILE:HG13	2.09	0.51
1:A:971:VAL:C	1:A:974:THR:HG22	2.30	0.51
1:A:1057:VAL:HG12	1:A:1063:TRP:CB	2.33	0.51
1:A:189:PHE:O	1:A:193:PRO:HG2	2.10	0.51
1:A:371:LEU:HB3	1:A:399:VAL:HG12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1046:HIS:HD2	1:A:1049:ASN:ND2	2.08	0.51
1:A:1446:GLN:NE2	1:A:1489:TYR:CD2	2.78	0.51
1:A:625:PRO:HD2	1:A:626:THR:H	1.74	0.51
1:A:884:PRO:CB	1:A:887:VAL:HB	2.41	0.51
1:A:962:LEU:CD1	1:A:1308:VAL:HG21	2.40	0.51
1:A:170:LEU:HD22	1:A:216:LEU:CD2	2.39	0.51
1:A:699:CYS:HB3	1:A:1060:PHE:CZ	2.45	0.51
1:A:1369:ARG:HD3	1:A:1378:PRO:HG2	1.93	0.51
1:A:121:TRP:CB	1:A:122:MET:CA	2.88	0.51
1:A:166:TYR:CE1	1:A:167:ILE:HG13	2.46	0.51
1:A:1363:ALA:HB1	1:A:1384:ARG:HH11	1.76	0.51
1:A:905:MET:HG3	1:A:930:VAL:HG21	1.92	0.51
1:A:191:LEU:O	1:A:194:PHE:HB2	2.11	0.50
1:A:280:TYR:OH	1:A:392:HIS:HB3	2.11	0.50
1:A:957:ARG:C	1:A:959:PHE:H	2.15	0.50
1:A:1489:TYR:O	1:A:1492:VAL:HB	2.12	0.50
1:A:146:ILE:HA	1:A:149:THR:HG22	1.93	0.50
1:A:410:PHE:HE1	1:A:1288:LEU:HG	1.77	0.50
1:A:1177:MET:SD	1:A:1275:LEU:HD23	2.49	0.50
1:A:965:VAL:HG12	1:A:966:ASN:H	1.77	0.50
1:A:250:ALA:O	1:A:254:SER:N	2.44	0.50
1:A:591:VAL:O	1:A:595:ILE:HG13	2.12	0.50
1:A:715:TRP:O	1:A:717:CYS:N	2.44	0.50
1:A:728:GLY:O	1:A:732:ILE:HB	2.12	0.50
1:A:1148:PRO:HG3	1:A:1446:GLN:HG2	1.92	0.50
1:A:172:PHE:HA	1:A:175:ILE:HD12	1.93	0.50
1:A:374:LEU:HD12	1:A:400:VAL:CG1	2.40	0.50
1:A:564:VAL:CA	1:A:567:VAL:HG12	2.39	0.50
1:A:926:ASP:HA	1:A:957:ARG:HH21	1.76	0.50
1:A:953:LEU:HD23	1:A:1316:PHE:HZ	1.77	0.50
1:A:965:VAL:HG12	1:A:966:ASN:N	2.27	0.50
1:A:1396:ILE:HA	1:A:1400:LEU:HD12	1.94	0.50
1:A:1450:TYR:CE1	1:A:1481:ILE:HD11	2.47	0.50
1:A:681:ARG:HH12	1:A:1068:ASN:HB3	1.77	0.50
1:A:913:GLY:O	1:A:917:TYR:CB	2.60	0.50
1:A:1479:ILE:HG23	1:A:1487:ILE:HG21	1.92	0.50
1:A:1483:LYS:CG	1:A:1484:ASP:OD1	2.46	0.50
1:A:355:TYR:HB2	1:A:707:TRP:HZ3	1.76	0.49
1:A:410:PHE:CE1	1:A:1288:LEU:HG	2.47	0.49
1:A:714:ASP:O	1:A:715:TRP:HB3	2.12	0.49
1:A:64:GLN:CA	1:A:120:LEU:CB	2.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:PRO:HG2	1:A:356:THR:HB	1.94	0.49
1:A:519:PRO:CD	1:A:520:PHE:N	2.74	0.49
1:A:563:ILE:CG1	1:A:591:VAL:HG11	2.42	0.49
1:A:1012:VAL:O	1:A:1036:THR:OG1	2.23	0.49
1:A:1140:VAL:HG12	1:A:1144:MET:HE2	1.93	0.49
1:A:77:ARG:O	1:A:79:ILE:N	2.45	0.49
1:A:593:PHE:HA	1:A:596:LEU:HB2	1.93	0.49
1:A:1128:THR:O	1:A:1130:SER:N	2.45	0.49
1:A:1281:SER:OG	1:A:1282:ALA:N	2.45	0.49
1:A:625:PRO:CD	1:A:626:THR:H	2.25	0.49
1:A:374:LEU:HD21	1:A:1351:THR:CG2	2.42	0.49
1:A:605:GLY:O	1:A:606:LEU:HD12	2.12	0.49
1:A:905:MET:O	1:A:905:MET:HE3	2.12	0.49
1:A:374:LEU:HD21	1:A:1351:THR:CB	2.40	0.49
1:A:395:PHE:O	1:A:399:VAL:HG23	2.12	0.49
1:A:846:ARG:O	1:A:850:PHE:CB	2.60	0.49
1:A:1131:ARG:CG	1:A:1131:ARG:NH2	2.76	0.49
1:A:1350:ALA:HA	1:A:1398:THR:HG21	1.92	0.49
1:A:1217:CYS:O	1:A:1221:VAL:N	2.40	0.49
1:A:355:TYR:HB2	1:A:707:TRP:CZ3	2.48	0.49
1:A:531:LEU:HD23	1:A:558:PHE:HZ	1.77	0.49
1:A:1060:PHE:HA	1:A:1063:TRP:CD1	2.48	0.49
1:A:1133:GLN:HE21	1:A:1512:ASP:CB	2.26	0.49
1:A:1488:PHE:O	1:A:1492:VAL:HG23	2.13	0.49
1:A:77:ARG:C	1:A:79:ILE:H	2.15	0.48
1:A:1254:ILE:CG2	1:A:1257:TYR:HE2	2.25	0.48
1:A:627:LEU:HD21	1:A:991:PHE:CE2	2.49	0.48
1:A:876:GLU:HG3	1:A:880:LEU:HD23	1.94	0.48
1:A:1170:ARG:HA	1:A:1170:ARG:HD3	1.64	0.48
1:A:1192:TYR:C	1:A:1192:TYR:CD1	2.86	0.48
1:A:1263:LEU:CD2	1:A:1266:ILE:HD12	2.33	0.48
1:A:265:LEU:CD2	1:A:268:SER:HB3	2.25	0.48
1:A:279:ILE:CG2	1:A:280:TYR:CE1	2.96	0.48
1:A:371:LEU:HD12	1:A:399:VAL:HG11	1.90	0.48
1:A:622:LYS:HG3	1:A:623:PHE:N	2.28	0.48
1:A:878:ILE:O	1:A:878:ILE:HG23	2.12	0.48
1:A:966:ASN:HB3	1:A:1297:ARG:HH22	1.78	0.48
1:A:1007:LYS:O	1:A:1008:PHE:HB2	2.13	0.48
1:A:1039:ASN:HD21	1:A:1043:ASN:HD22	1.61	0.48
1:A:1180:ILE:O	1:A:1184:VAL:HG23	2.13	0.48
1:A:1300:PHE:O	1:A:1303:SER:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:901:PHE:CE2	1:A:929:VAL:CG1	2.96	0.48
1:A:979:VAL:N	1:A:980:PRO:HD2	2.28	0.48
1:A:150:ILE:HD11	1:A:236:ARG:HD2	1.95	0.48
1:A:370:ARG:HD2	1:A:703:ILE:HG13	1.94	0.48
1:A:876:GLU:HG3	1:A:880:LEU:CD2	2.44	0.48
1:A:1346:LEU:O	1:A:1350:ALA:N	2.46	0.48
1:A:563:ILE:O	1:A:567:VAL:HG12	2.13	0.48
1:A:605:GLY:HA2	1:A:606:LEU:HG	1.96	0.48
1:A:684:PHE:CE2	1:A:693:ILE:HD13	2.48	0.48
1:A:909:LEU:HD22	1:A:917:TYR:HD2	1.74	0.48
1:A:1324:ILE:O	1:A:1324:ILE:CG2	2.48	0.48
1:A:967:GLY:HA3	1:A:1301:ASN:HD22	1.71	0.48
1:A:1237:ASP:OD1	1:A:1271:ARG:HD2	2.13	0.48
1:A:1240:TYR:CD1	1:A:1240:TYR:C	2.87	0.48
1:A:1152:ILE:HG12	1:A:1227:HIS:CG	2.49	0.48
1:A:1179:LEU:HD11	1:A:1212:ILE:HD13	1.96	0.48
1:A:1499:ASP:O	1:A:1502:SER:CB	2.59	0.48
1:A:385:LEU:HB2	1:A:1334:TYR:HH	1.75	0.48
1:A:288:CYS:SG	1:A:343:CYS:SG	3.11	0.47
1:A:350:ASN:OD1	1:A:350:ASN:N	2.46	0.47
1:A:1021:HIS:HD2	1:A:1022:GLU:HG3	1.79	0.47
1:A:1466:VAL:HG12	1:A:1470:ASN:CB	2.43	0.47
1:A:581:ASP:O	1:A:585:VAL:HG23	2.14	0.47
1:A:922:TRP:HH2	1:A:959:PHE:HD2	1.62	0.47
1:A:1152:ILE:HB	1:A:1224:LEU:HD22	1.97	0.47
1:A:1217:CYS:SG	1:A:1238:PHE:HD1	2.38	0.47
1:A:221:GLY:O	1:A:222:HIS:CG	2.68	0.47
1:A:366:LEU:HD11	1:A:706:MET:HE3	1.95	0.47
1:A:1308:VAL:O	1:A:1311:PHE:N	2.47	0.47
1:A:121:TRP:N	1:A:122:MET:CB	2.78	0.47
1:A:149:THR:CG2	1:A:176:TYR:HE1	2.27	0.47
1:A:200:PRO:CD	1:A:201:TRP:H	2.27	0.47
1:A:272:PHE:CE1	1:A:398:ILE:CG2	2.98	0.47
1:A:518:SER:OG	1:A:520:PHE:CD2	2.68	0.47
1:A:528:ILE:HG22	1:A:558:PHE:CE1	2.41	0.47
1:A:651:LEU:HD23	1:A:732:ILE:CD1	2.42	0.47
1:A:1093:ILE:HA	1:A:1096:ILE:HG22	1.95	0.47
1:A:1298:THR:CG2	1:A:1409:VAL:CG1	2.92	0.47
1:A:1128:THR:C	1:A:1130:SER:H	2.18	0.47
1:A:1148:PRO:HG2	1:A:1444:ALA:HB1	1.95	0.47
1:A:1400:LEU:O	1:A:1404:ASN:ND2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:MET:HE1	1:A:230:ARG:NH1	2.30	0.47
1:A:944:ILE:C	1:A:945:GLU:HG3	2.33	0.47
1:A:1433:PHE:O	1:A:1436:VAL:HG22	2.14	0.47
3:E:1:NAG:H81	3:F:1:NAG:H83	1.97	0.47
1:A:247:ILE:HA	1:A:250:ALA:CB	2.45	0.47
1:A:290:LYS:HG2	1:A:341:TYR:CE1	2.49	0.47
1:A:384:ALA:O	1:A:387:SER:OG	2.20	0.47
1:A:178:ILE:O	1:A:181:VAL:HB	2.15	0.46
1:A:1064:LEU:CD2	1:A:1068:ASN:HD21	2.28	0.46
1:A:1410:ILE:O	1:A:1414:VAL:HG23	2.15	0.46
1:A:574:SER:O	1:A:578:TYR:N	2.48	0.46
1:A:877:ASP:O	1:A:879:TYR:N	2.47	0.46
1:A:1158:HIS:ND1	1:A:1159:PRO:CD	2.78	0.46
1:A:1234:ASN:O	1:A:1238:PHE:N	2.48	0.46
1:A:519:PRO:CD	1:A:520:PHE:H	2.28	0.46
1:A:251:LEU:HA	1:A:254:SER:OG	2.16	0.46
1:A:1151:ARG:CG	1:A:1438:GLN:HG2	2.32	0.46
1:A:192:HIS:HA	1:A:195:ALA:CB	2.43	0.46
1:A:192:HIS:HA	1:A:195:ALA:H	1.80	0.46
1:A:898:THR:CG2	1:A:933:TYR:CG	2.95	0.46
1:A:1085:ASN:ND2	1:A:1088:MET:SD	2.88	0.46
1:A:1272:VAL:HG12	1:A:1272:VAL:O	2.16	0.46
1:A:165:THR:CB	1:A:168:LEU:HG	2.46	0.46
1:A:401:PHE:O	1:A:405:PHE:HB2	2.14	0.46
1:A:535:PHE:HE2	1:A:558:PHE:CE2	2.34	0.46
1:A:642:VAL:HA	1:A:645:MET:HB2	1.96	0.46
1:A:1314:ALA:HB1	1:A:1342:SER:HB3	1.98	0.46
1:A:254:SER:HG	1:A:255:ILE:HG13	1.81	0.46
1:A:535:PHE:O	1:A:551:LEU:HD21	2.16	0.46
1:A:926:ASP:HA	1:A:957:ARG:NH2	2.31	0.46
1:A:1216:GLU:O	1:A:1220:LYS:HB2	2.16	0.46
1:A:886:LEU:O	1:A:890:THR:CG2	2.60	0.46
1:A:1138:ARG:NH2	1:A:1416:GLU:HG3	2.31	0.46
1:A:1220:LYS:HB3	1:A:1228:TYR:CE1	2.51	0.46
1:A:564:VAL:HA	1:A:567:VAL:CG1	2.42	0.46
1:A:1151:ARG:O	1:A:1153:PRO:CB	2.63	0.46
1:A:515:VAL:CB	1:A:521:PHE:CE1	2.99	0.46
1:A:622:LYS:HE2	1:A:623:PHE:CE1	2.51	0.46
1:A:1355:TRP:O	1:A:1355:TRP:HE3	1.99	0.46
1:A:157:MET:CE	1:A:230:ARG:NH1	2.79	0.45
1:A:687:PHE:O	1:A:691:PHE:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:690:SER:HA	1:A:693:ILE:HG22	1.98	0.45
1:A:1152:ILE:HG21	1:A:1227:HIS:HB2	1.98	0.45
1:A:1336:PHE:CE1	1:A:1345:LEU:HD23	2.50	0.45
1:A:393:ILE:O	1:A:397:ILE:N	2.41	0.45
1:A:913:GLY:O	1:A:917:TYR:HB2	2.17	0.45
1:A:1158:HIS:H	1:A:1160:GLN:HB2	1.82	0.45
1:A:1166:ILE:CG2	1:A:1172:PHE:CD2	2.85	0.45
1:A:373:THR:O	1:A:374:LEU:HB3	2.16	0.45
1:A:377:TRP:CZ3	1:A:381:TYR:CD1	3.04	0.45
1:A:898:THR:CG2	1:A:933:TYR:CB	2.70	0.45
1:A:926:ASP:O	1:A:930:VAL:HG23	2.16	0.45
1:A:965:VAL:O	1:A:967:GLY:N	2.49	0.45
1:A:1318:MET:SD	1:A:1338:THR:O	2.74	0.45
1:A:148:ILE:HG22	1:A:152:ILE:HD11	1.98	0.45
1:A:381:TYR:HD2	1:A:1348:GLN:NE2	2.11	0.45
1:A:381:TYR:CD2	1:A:1348:GLN:NE2	2.82	0.45
1:A:877:ASP:CG	1:A:1322:MET:HE2	2.36	0.45
1:A:1332:ASP:HA	1:A:1335:ASN:HD21	1.81	0.45
1:A:127:THR:HA	1:A:131:ARG:CB	2.46	0.45
1:A:403:GLY:HA2	1:A:407:PHE:HD2	1.81	0.45
1:A:570:ILE:HG12	1:A:578:TYR:CD2	2.52	0.45
1:A:947:LEU:HD13	1:A:950:LEU:CD1	2.46	0.45
1:A:82:ALA:O	1:A:83:GLU:CB	2.64	0.45
1:A:176:TYR:CE2	1:A:233:ARG:CD	2.83	0.45
1:A:916:LYS:HA	1:A:919:THR:HG1	1.80	0.45
1:A:917:TYR:C	1:A:919:THR:H	2.19	0.45
1:A:996:PHE:CZ	1:A:1094:PHE:O	2.70	0.45
1:A:1044:PHE:HD1	1:A:1050:ALA:HB1	1.81	0.45
1:A:1496:LEU:O	1:A:1499:ASP:HB2	2.17	0.45
1:A:1000:GLY:O	1:A:1004:PHE:N	2.44	0.45
1:A:1321:PHE:HA	1:A:1324:ILE:HD11	1.99	0.45
1:A:1220:LYS:HZ1	1:A:1274:ARG:HH12	1.63	0.45
1:A:1287:LEU:HD23	1:A:1287:LEU:O	2.16	0.45
1:A:121:TRP:CB	1:A:122:MET:CB	2.95	0.45
1:A:921:LYS:O	1:A:925:LEU:HG	2.17	0.45
1:A:1243:LEU:CD1	1:A:1267:LEU:HD12	2.46	0.45
1:A:265:LEU:HA	1:A:268:SER:HB3	1.93	0.45
1:A:952:LEU:HD11	1:A:1319:GLU:CB	2.45	0.45
1:A:962:LEU:HG	1:A:968:MET:SD	2.57	0.45
1:A:1046:HIS:HB2	1:A:1049:ASN:HB2	1.99	0.45
1:A:1211:ILE:O	1:A:1215:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ILE:O	1:A:152:ILE:HG13	2.17	0.44
1:A:234:SER:OG	1:A:654:ILE:HD13	2.16	0.44
1:A:279:ILE:HG21	1:A:280:TYR:CE1	2.53	0.44
1:A:616:ARG:O	1:A:619:ARG:HB2	2.17	0.44
1:A:849:CYS:O	1:A:853:ALA:CB	2.64	0.44
1:A:1010:LYS:HG3	1:A:1018:VAL:HG22	1.99	0.44
1:A:1355:TRP:O	1:A:1355:TRP:CE3	2.70	0.44
1:A:359:ASP:OD1	1:A:359:ASP:N	2.51	0.44
1:A:930:VAL:O	1:A:934:LEU:HG	2.17	0.44
1:A:1164:TYR:O	1:A:1164:TYR:CD1	2.71	0.44
1:A:1264:LEU:HD23	1:A:1264:LEU:HA	1.80	0.44
1:A:551:LEU:HD23	1:A:551:LEU:HA	1.84	0.44
1:A:653:PHE:CZ	1:A:657:ILE:HD12	2.49	0.44
1:A:996:PHE:CZ	1:A:1095:PHE:HA	2.52	0.44
1:A:1235:ILE:O	1:A:1239:LEU:HG	2.18	0.44
1:A:1279:PHE:C	1:A:1281:SER:H	2.17	0.44
1:A:154:CYS:SG	1:A:653:PHE:CZ	2.99	0.44
1:A:338:PRO:HD2	1:A:341:TYR:CE2	2.52	0.44
1:A:1350:ALA:O	1:A:1398:THR:HG22	2.17	0.44
1:A:974:THR:HG21	1:A:1405:MET:SD	2.56	0.44
1:A:1095:PHE:O	1:A:1099:GLY:N	2.49	0.44
1:A:1425:LEU:CD2	1:A:1429:ASP:CB	2.95	0.44
1:A:140:PRO:CD	1:A:141:ILE:H	2.30	0.44
1:A:1039:ASN:HD21	1:A:1043:ASN:ND2	2.16	0.44
1:A:1064:LEU:CD2	1:A:1068:ASN:ND2	2.80	0.44
1:A:1186:VAL:O	1:A:1189:ILE:HG12	2.18	0.44
1:A:1322:MET:HB3	1:A:1323:HIS:H	1.72	0.44
1:A:94:PRO:O	1:A:97:LYS:CB	2.66	0.44
1:A:518:SER:HB2	1:A:519:PRO:HD2	1.95	0.44
1:A:878:ILE:O	1:A:879:TYR:CD1	2.71	0.44
1:A:916:LYS:HA	1:A:919:THR:CB	2.48	0.44
1:A:1003:LEU:HD12	1:A:1088:MET:HE3	1.98	0.44
1:A:1328:GLY:O	1:A:1329:ALA:HB2	2.18	0.44
1:A:259:LYS:HG3	1:A:260:ASP:H	1.83	0.44
1:A:1336:PHE:CZ	1:A:1345:LEU:HD23	2.52	0.44
1:A:1401:VAL:HG23	1:A:1402:VAL:HG23	2.00	0.44
1:A:309:TYR:O	1:A:315:HIS:NE2	2.49	0.43
1:A:325:TYR:HA	1:A:326:PRO:HD3	1.84	0.43
1:A:329:GLY:O	1:A:343:CYS:SG	2.76	0.43
1:A:637:SER:O	1:A:641:PHE:HB2	2.18	0.43
1:A:905:MET:HE2	1:A:905:MET:HB3	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:993:TRP:CH2	1:A:1055:LEU:HD13	2.53	0.43
1:A:1024:THR:HB	1:A:1079:GLN:HG3	2.00	0.43
1:A:1253:VAL:HG11	1:A:1254:ILE:HD11	1.98	0.43
1:A:239:THR:HG22	1:A:244:TRP:NE1	2.34	0.43
1:A:372:VAL:CA	1:A:404:THR:HB	2.43	0.43
1:A:876:GLU:HA	1:A:880:LEU:CD2	2.48	0.43
1:A:1228:TYR:HE2	1:A:1238:PHE:HB2	1.84	0.43
1:A:254:SER:OG	1:A:255:ILE:HG13	2.17	0.43
1:A:355:TYR:OH	1:A:711:LEU:HA	2.17	0.43
1:A:366:LEU:CD1	1:A:706:MET:HE3	2.49	0.43
1:A:1055:LEU:HD12	1:A:1058:ALA:HB3	2.00	0.43
1:A:1345:LEU:HD12	1:A:1345:LEU:HA	1.78	0.43
1:A:370:ARG:NH1	1:A:380:LEU:HB2	2.34	0.43
1:A:1158:HIS:CB	1:A:1159:PRO:CD	2.96	0.43
1:A:660:MET:O	1:A:664:GLY:CA	2.66	0.43
1:A:1309:ILE:HA	1:A:1312:VAL:HB	2.01	0.43
1:A:165:THR:OG1	1:A:168:LEU:HD12	2.19	0.43
1:A:237:THR:HG22	1:A:237:THR:O	2.18	0.43
1:A:258:LEU:HD23	1:A:262:VAL:HG22	1.98	0.43
1:A:526:ALA:O	1:A:530:VAL:HG23	2.18	0.43
1:A:1434:PHE:HA	1:A:1437:TRP:HB3	2.01	0.43
1:A:1463:PRO:CG	1:A:1500:VAL:HG11	2.46	0.43
1:A:214:ILE:HA	1:A:217:VAL:CG2	2.48	0.43
1:A:679:LEU:HD23	1:A:683:ASN:HD22	1.83	0.43
1:A:917:TYR:HE1	1:A:923:TYR:HD1	1.66	0.43
1:A:1131:ARG:HD2	1:A:1131:ARG:HA	1.76	0.43
1:A:877:ASP:OD2	1:A:1322:MET:HE3	2.16	0.43
1:A:225:ALA:HA	1:A:228:ALA:HB2	2.00	0.42
1:A:879:TYR:O	1:A:882:GLN:OE1	2.36	0.42
1:A:974:THR:O	1:A:978:ALA:HB2	2.18	0.42
1:A:1152:ILE:CG1	1:A:1227:HIS:CD2	2.98	0.42
1:A:1305:LEU:HD23	1:A:1309:ILE:CD1	2.45	0.42
1:A:1489:TYR:CD1	1:A:1489:TYR:C	2.91	0.42
1:A:322:TRP:O	1:A:324:GLU:N	2.53	0.42
1:A:624:TRP:CB	1:A:627:LEU:HB3	2.49	0.42
1:A:652:LEU:CD1	1:A:698:LEU:HD22	2.49	0.42
1:A:863:THR:CG2	1:A:961:PRO:HG3	2.30	0.42
1:A:1189:ILE:HD11	1:A:1202:LEU:HD13	2.01	0.42
1:A:1283:ARG:O	1:A:1283:ARG:HG2	2.19	0.42
1:A:193:PRO:HA	1:A:196:TYR:CB	2.49	0.42
1:A:368:VAL:O	1:A:371:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1306:LEU:O	1:A:1310:MET:HB2	2.19	0.42
1:A:247:ILE:O	1:A:250:ALA:HB3	2.19	0.42
1:A:979:VAL:N	1:A:980:PRO:CD	2.83	0.42
1:A:146:ILE:O	1:A:149:THR:CG2	2.66	0.42
1:A:336:MET:HA	1:A:337:CYS:CB	2.49	0.42
1:A:395:PHE:O	1:A:398:ILE:HB	2.19	0.42
1:A:645:MET:HE1	1:A:1097:VAL:HG13	2.02	0.42
1:A:305:ARG:O	1:A:309:TYR:N	2.44	0.42
1:A:374:LEU:CD1	1:A:1351:THR:HG21	2.28	0.42
1:A:921:LYS:O	1:A:924:TRP:HB2	2.19	0.42
1:A:203:TRP:CE3	1:A:203:TRP:CA	2.97	0.42
1:A:274:VAL:O	1:A:277:LEU:HB3	2.19	0.42
1:A:375:ASP:C	1:A:377:TRP:N	2.73	0.42
1:A:1072:ASP:OD2	1:A:1082:ARG:HA	2.20	0.42
1:A:1177:MET:HE1	1:A:1177:MET:O	2.19	0.42
1:A:1182:LEU:HD12	1:A:1182:LEU:HA	1.80	0.42
1:A:62:PRO:O	1:A:119:SER:CB	2.68	0.42
1:A:897:LEU:CD1	1:A:901:PHE:CE1	3.03	0.42
1:A:144:TYR:HD1	1:A:144:TYR:HA	1.75	0.42
1:A:1240:TYR:CE2	1:A:1268:ARG:HD3	2.54	0.42
1:A:173:LEU:HD13	1:A:216:LEU:HD11	2.02	0.42
1:A:205:ASP:OD1	1:A:236:ARG:NH2	2.52	0.42
1:A:269:LEU:HD23	1:A:269:LEU:HA	1.92	0.41
1:A:286:GLN:HE21	1:A:345:GLN:HG2	1.85	0.41
1:A:1492:VAL:O	1:A:1496:LEU:HB2	2.20	0.41
1:A:343:CYS:O	2:B:1:NAG:H61	2.19	0.41
1:A:645:MET:HE3	1:A:1097:VAL:HG11	2.03	0.41
1:A:929:VAL:HG21	1:A:957:ARG:CG	2.50	0.41
1:A:1003:LEU:CD1	1:A:1088:MET:HE3	2.50	0.41
1:A:1151:ARG:O	1:A:1153:PRO:CA	2.69	0.41
1:A:1039:ASN:OD1	1:A:1040:SER:N	2.54	0.41
1:A:1177:MET:HE3	1:A:1275:LEU:CD2	2.33	0.41
1:A:1309:ILE:HA	1:A:1312:VAL:CB	2.50	0.41
1:A:375:ASP:C	1:A:377:TRP:H	2.24	0.41
1:A:395:PHE:CE2	1:A:399:VAL:HG21	2.55	0.41
1:A:400:VAL:HA	1:A:404:THR:CG2	2.49	0.41
1:A:977:GLU:O	1:A:980:PRO:CG	2.66	0.41
1:A:1179:LEU:HD23	1:A:1179:LEU:HA	1.81	0.41
1:A:1414:VAL:CG1	1:A:1418:TYR:HE1	2.33	0.41
1:A:1466:VAL:CG1	1:A:1470:ASN:HB2	2.50	0.41
1:A:1479:ILE:CG2	1:A:1487:ILE:HG21	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ILE:CG2	1:A:241:VAL:HB	2.42	0.41
1:A:966:ASN:HD22	1:A:966:ASN:HA	1.73	0.41
1:A:1254:ILE:CG2	1:A:1257:TYR:CE2	3.03	0.41
1:A:1460:LEU:HB2	1:A:1465:GLN:HA	2.03	0.41
1:A:1483:LYS:HA	1:A:1484:ASP:HA	1.68	0.41
1:A:176:TYR:N	1:A:176:TYR:CD1	2.88	0.41
1:A:259:LYS:CD	1:A:260:ASP:N	2.84	0.41
1:A:410:PHE:CZ	1:A:1288:LEU:CD2	2.94	0.41
1:A:706:MET:O	1:A:706:MET:HG2	2.19	0.41
1:A:397:ILE:O	1:A:401:PHE:N	2.49	0.41
1:A:580:LYS:HD2	1:A:580:LYS:HA	1.69	0.41
1:A:884:PRO:HB3	1:A:887:VAL:HG21	2.01	0.41
1:A:912:VAL:CG1	1:A:913:GLY:N	2.79	0.41
1:A:148:ILE:HG22	1:A:152:ILE:CD1	2.51	0.41
1:A:682:TRP:HH2	1:A:1067:MET:HE1	1.85	0.41
1:A:866:LEU:C	1:A:869:THR:HG22	2.41	0.41
1:A:873:LEU:CD2	1:A:954:ARG:HH21	2.34	0.41
1:A:900:PHE:O	1:A:904:GLU:HB2	2.21	0.41
1:A:1351:THR:C	1:A:1352:SER:HG	2.09	0.41
1:A:1468:LYS:HA	1:A:1469:PRO:C	2.41	0.41
1:A:170:LEU:HD22	1:A:216:LEU:HD22	2.01	0.41
1:A:211:ILE:HA	1:A:214:ILE:CG1	2.51	0.41
1:A:223:LEU:HB3	1:A:225:ALA:N	2.34	0.41
1:A:223:LEU:HD13	1:A:225:ALA:CB	2.49	0.41
1:A:259:LYS:CG	1:A:260:ASP:N	2.84	0.41
1:A:398:ILE:O	1:A:402:TYR:CB	2.69	0.41
1:A:645:MET:HE3	1:A:1097:VAL:CG1	2.50	0.41
1:A:896:VAL:HG12	1:A:896:VAL:O	2.21	0.41
1:A:996:PHE:HZ	1:A:1094:PHE:O	2.04	0.41
1:A:1192:TYR:C	1:A:1192:TYR:HD1	2.23	0.41
1:A:247:ILE:CD1	1:A:644:VAL:CG2	2.98	0.41
1:A:271:VAL:O	1:A:274:VAL:HB	2.21	0.41
1:A:293:PRO:HB2	1:A:296:GLY:HA3	2.03	0.41
1:A:614:LEU:HD11	1:A:998:ILE:HG13	2.03	0.41
1:A:633:VAL:O	1:A:636:LYS:HB3	2.21	0.41
1:A:996:PHE:CE2	1:A:1095:PHE:CA	3.03	0.41
1:A:1060:PHE:HE1	1:A:1096:ILE:CD1	2.34	0.41
1:A:94:PRO:O	1:A:97:LYS:N	2.54	0.40
1:A:211:ILE:HA	1:A:214:ILE:HG13	2.03	0.40
1:A:238:VAL:HG11	1:A:248:VAL:CG2	2.51	0.40
1:A:243:GLY:C	1:A:245:ARG:N	2.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:TYR:HD1	1:A:347:TYR:HA	1.76	0.40
1:A:1177:MET:CE	1:A:1275:LEU:CD2	2.81	0.40
1:A:1341:GLN:HE21	1:A:1341:GLN:HB2	1.58	0.40
1:A:885:VAL:HG13	1:A:886:LEU:N	2.36	0.40
1:A:1214:PHE:O	1:A:1214:PHE:CD1	2.74	0.40
1:A:1312:VAL:HG12	1:A:1313:TYR:CD1	2.56	0.40
1:A:1100:SER:HA	1:A:1104:LEU:HD12	2.03	0.40
1:A:64:GLN:N	1:A:118:LYS:O	2.54	0.40
1:A:192:HIS:CA	1:A:195:ALA:H	2.34	0.40
1:A:213:TYR:O	1:A:217:VAL:HG23	2.22	0.40
1:A:561:ILE:HG12	1:A:561:ILE:H	1.67	0.40
1:A:955:VAL:O	1:A:955:VAL:HG12	2.20	0.40
1:A:1480:PRO:HG2	1:A:1491:ASP:OD2	2.20	0.40
1:A:600:LEU:HG	1:A:605:GLY:C	2.39	0.40
1:A:662:LEU:O	1:A:662:LEU:HD23	2.21	0.40
1:A:1489:TYR:CD1	1:A:1490:LYS:N	2.89	0.40
1:A:1502:SER:O	1:A:1505:GLY:N	2.49	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1317/1596 (82%)	1078 (82%)	170 (13%)	69 (5%)	1	17

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ALA
1	A	87	THR
1	A	88	PRO
1	A	94	PRO

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Mol	Chain	Res	Type
1	A	111	ILE
1	A	124	ASP
1	A	125	PRO
1	A	128	PRO
1	A	159	MET
1	A	163	GLN
1	A	220	LEU
1	A	222	HIS
1	A	604	GLN
1	A	878	ILE
1	A	882	GLN
1	A	1158	HIS
1	A	1256	LYS
1	A	1322	MET
1	A	1331	ASP
1	A	1383	SER
1	A	81	PRO
1	A	83	GLU
1	A	625	PRO
1	A	904	GLU
1	A	1253	VAL
1	A	1329	ALA
1	A	1384	ARG
1	A	1426	THR
1	A	1507	PRO
1	A	62	PRO
1	A	113	ARG
1	A	121	TRP
1	A	160	PRO
1	A	351	PRO
1	A	360	THR
1	A	387	SER
1	A	607	SER
1	A	876	GLU
1	A	1151	ARG
1	A	1153	PRO
1	A	1312	VAL
1	A	1506	SER
1	A	86	SER
1	A	319	PRO
1	A	323	ILE
1	A	330	ASN

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Mol	Chain	Res	Type
1	A	337	CYS
1	A	374	LEU
1	A	714	ASP
1	A	1019	LEU
1	A	1154	LYS
1	A	1251	SER
1	A	1280	GLN
1	A	1502	SER
1	A	58	GLY
1	A	82	ALA
1	A	93	ASP
1	A	242	PRO
1	A	606	LEU
1	A	947	LEU
1	A	944	ILE
1	A	1160	GLN
1	A	1366	GLU
1	A	574	SER
1	A	218	VAL
1	A	883	ARG
1	A	1152	ILE
1	A	967	GLY
1	A	140	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	1054/1411 (75%)	925 (88%)	129 (12%)	4 19

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	TYR
1	A	153	HIS
1	A	157	MET

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Mol	Chain	Res	Type
1	A	166	TYR
1	A	187	ARG
1	A	189	PHE
1	A	196	TYR
1	A	203	TRP
1	A	210	LEU
1	A	213	TYR
1	A	219	ASP
1	A	222	HIS
1	A	224	TYR
1	A	226	LEU
1	A	249	ASP
1	A	257	SER
1	A	258	LEU
1	A	259	LYS
1	A	336	MET
1	A	343	CYS
1	A	378	GLU
1	A	379	ASP
1	A	383	LEU
1	A	402	TYR
1	A	420	THR
1	A	425	ARG
1	A	521	PHE
1	A	524	PHE
1	A	546	GLU
1	A	547	PHE
1	A	551	LEU
1	A	563	ILE
1	A	573	LEU
1	A	577	PHE
1	A	598	LEU
1	A	601	GLU
1	A	619	ARG
1	A	704	GLU
1	A	854	LYS
1	A	857	TYR
1	A	877	ASP
1	A	879	TYR
1	A	880	LEU
1	A	883	ARG
1	A	894	ASP

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Mol	Chain	Res	Type
1	A	897	LEU
1	A	904	GLU
1	A	905	MET
1	A	909	LEU
1	A	915	LYS
1	A	916	LYS
1	A	925	LEU
1	A	933	TYR
1	A	937	PHE
1	A	940	MET
1	A	947	LEU
1	A	953	LEU
1	A	956	PHE
1	A	958	LEU
1	A	962	LEU
1	A	966	ASN
1	A	969	GLN
1	A	975	LEU
1	A	1003	LEU
1	A	1010	LYS
1	A	1027	ARG
1	A	1042	MET
1	A	1074	ARG
1	A	1125	LEU
1	A	1126	SER
1	A	1131	ARG
1	A	1133	GLN
1	A	1141	MET
1	A	1145	SER
1	A	1150	LYS
1	A	1151	ARG
1	A	1152	ILE
1	A	1156	THR
1	A	1160	GLN
1	A	1161	SER
1	A	1162	LEU
1	A	1170	ARG
1	A	1171	LYS
1	A	1172	PHE
1	A	1177	MET
1	A	1183	ASN
1	A	1190	ASP

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Mol	Chain	Res	Type
1	A	1192	TYR
1	A	1197	GLU
1	A	1202	LEU
1	A	1214	PHE
1	A	1216	GLU
1	A	1226	HIS
1	A	1230	LYS
1	A	1231	ASP
1	A	1250	LEU
1	A	1255	GLU
1	A	1258	PHE
1	A	1264	LEU
1	A	1276	LEU
1	A	1277	ARG
1	A	1279	PHE
1	A	1283	ARG
1	A	1294	LYS
1	A	1301	ASN
1	A	1304	PHE
1	A	1305	LEU
1	A	1310	MET
1	A	1316	PHE
1	A	1320	PHE
1	A	1325	ARG
1	A	1326	ASP
1	A	1331	ASP
1	A	1341	GLN
1	A	1345	LEU
1	A	1368	CYS
1	A	1405	MET
1	A	1406	TYR
1	A	1420	ASP
1	A	1425	LEU
1	A	1429	ASP
1	A	1432	MET
1	A	1438	GLN
1	A	1468	LYS
1	A	1473	LYS
1	A	1483	LYS
1	A	1496	LEU
1	A	1503	ARG
1	A	1504	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	HIS
1	A	291	HIS
1	A	382	GLN
1	A	409	ASN
1	A	661	GLN
1	A	670	ASN
1	A	859	GLN
1	A	966	ASN
1	A	1002	GLN
1	A	1021	HIS
1	A	1046	HIS
1	A	1068	ASN
1	A	1118	GLN
1	A	1133	GLN
1	A	1183	ASN
1	A	1194	GLN
1	A	1206	ASN
1	A	1226	HIS
1	A	1227	HIS
1	A	1301	ASN
1	A	1323	HIS
1	A	1335	ASN
1	A	1341	GLN
1	A	1348	GLN
1	A	1439	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

19 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	B	1	1,2	14,14,15	0.50	0	17,19,21	0.55	0
2	NAG	B	2	2	14,14,15	0.43	0	17,19,21	0.79	1 (5%)
2	BMA	B	3	2	11,11,12	0.91	0	15,15,17	1.85	5 (33%)
2	BMA	B	4	2	11,11,12	0.79	0	15,15,17	1.25	1 (6%)
2	BMA	B	5	2	11,11,12	0.87	0	15,15,17	1.94	4 (26%)
3	NAG	C	1	3,1	14,14,15	0.44	0	17,19,21	0.62	0
3	NAG	C	2	3	14,14,15	0.23	0	17,19,21	0.65	1 (5%)
3	BMA	C	3	3	11,11,12	0.96	1 (9%)	15,15,17	0.83	0
3	NAG	D	1	3,1	14,14,15	0.64	0	17,19,21	1.31	3 (17%)
3	NAG	D	2	3	14,14,15	0.54	0	17,19,21	0.80	1 (5%)
3	BMA	D	3	3	11,11,12	0.88	0	15,15,17	0.81	0
3	NAG	E	1	3,1	14,14,15	0.40	0	17,19,21	0.74	1 (5%)
3	NAG	E	2	3	14,14,15	0.35	0	17,19,21	0.46	0
3	BMA	E	3	3	11,11,12	1.00	1 (9%)	15,15,17	0.86	0
3	NAG	F	1	3,1	14,14,15	0.43	0	17,19,21	0.61	0
3	NAG	F	2	3	14,14,15	0.91	1 (7%)	17,19,21	1.02	2 (11%)
3	BMA	F	3	3	11,11,12	0.57	0	15,15,17	0.99	1 (6%)
4	NAG	G	1	1,4	14,14,15	0.22	0	17,19,21	0.89	1 (5%)
4	NAG	G	2	4	14,14,15	0.29	0	17,19,21	0.66	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	BMA	B	3	2	-	1/2/19/22	0/1/1/1
2	BMA	B	4	2	-	0/2/19/22	0/1/1/1
2	BMA	B	5	2	-	2/2/19/22	0/1/1/1
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	C	3	3	-	1/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	2/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	NAG	O5-C1	-3.05	1.38	1.43
3	C	3	BMA	C1-C2	2.30	1.57	1.52
3	E	3	BMA	C4-C3	2.15	1.57	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	BMA	C1-O5-C5	5.05	119.03	112.19
2	B	5	BMA	C1-C2-C3	3.77	114.31	109.67
2	B	5	BMA	C1-O5-C5	3.74	117.26	112.19
3	D	1	NAG	C1-O5-C5	3.12	116.42	112.19
4	G	1	NAG	C1-O5-C5	3.04	116.31	112.19
2	B	5	BMA	O2-C2-C3	-3.00	104.13	110.14
3	D	1	NAG	C3-C4-C5	2.86	115.34	110.24
2	B	5	BMA	O5-C1-C2	2.83	115.14	110.77
3	F	3	BMA	C1-O5-C5	2.76	115.93	112.19
2	B	3	BMA	O5-C1-C2	2.68	114.90	110.77
3	E	1	NAG	C1-O5-C5	2.60	115.71	112.19
3	D	1	NAG	C4-C3-C2	2.48	114.66	111.02
2	B	4	BMA	C1-O5-C5	2.42	115.47	112.19
2	B	2	NAG	C1-O5-C5	2.39	115.43	112.19
2	B	3	BMA	O2-C2-C3	-2.37	105.40	110.14
4	G	2	NAG	C1-O5-C5	2.33	115.35	112.19
3	F	2	NAG	O4-C4-C5	-2.32	103.55	109.30
3	D	2	NAG	C1-O5-C5	2.17	115.13	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	NAG	O3-C3-C2	-2.13	105.05	109.47
2	B	3	BMA	C3-C4-C5	-2.08	106.53	110.24
3	C	2	NAG	C1-O5-C5	2.08	115.01	112.19
2	B	3	BMA	O5-C5-C4	-2.02	105.91	110.83

There are no chirality outliers.

All (17) torsion outliers are listed below:

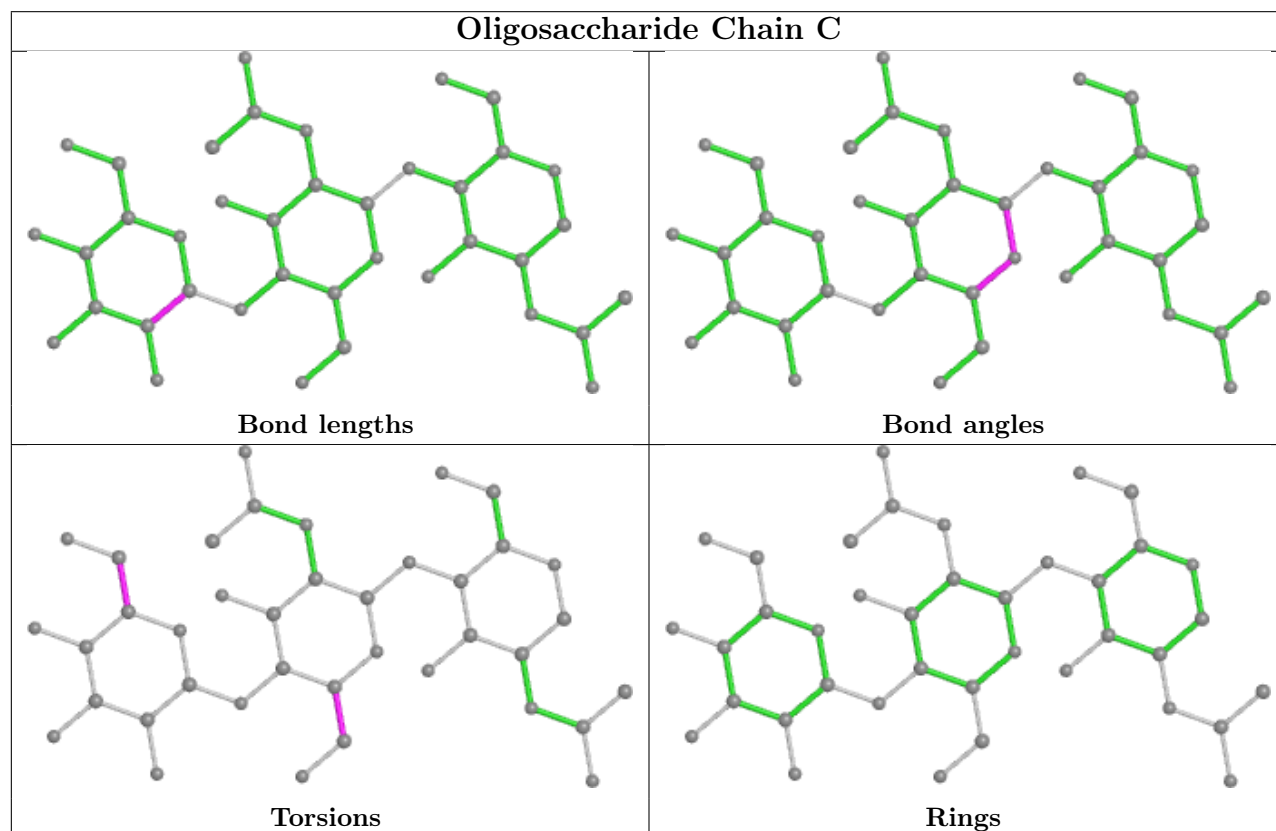
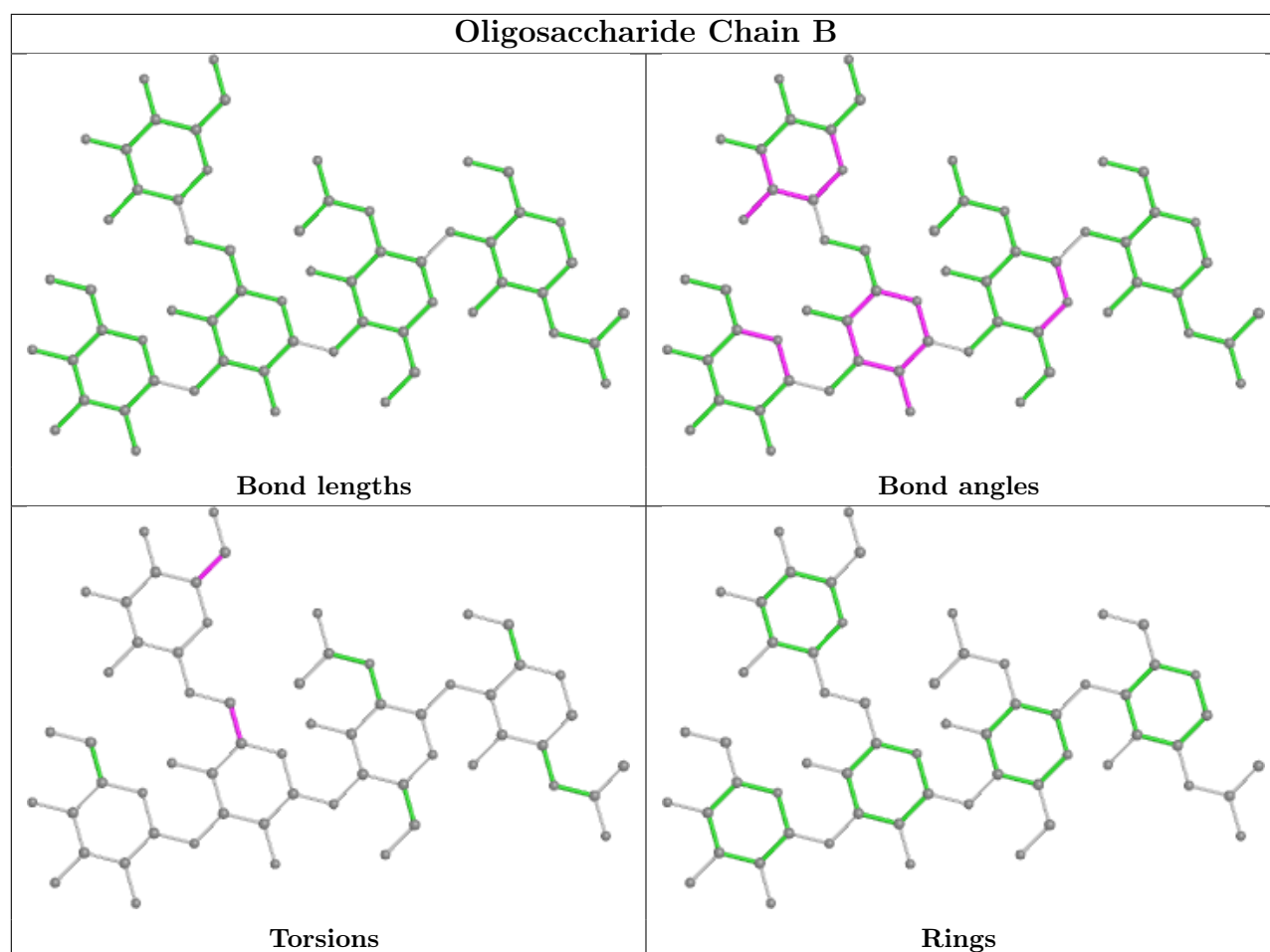
Mol	Chain	Res	Type	Atoms
2	B	5	BMA	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
2	B	5	BMA	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
2	B	3	BMA	O5-C5-C6-O6
3	F	3	BMA	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
3	F	3	BMA	C4-C5-C6-O6
3	C	3	BMA	C4-C5-C6-O6

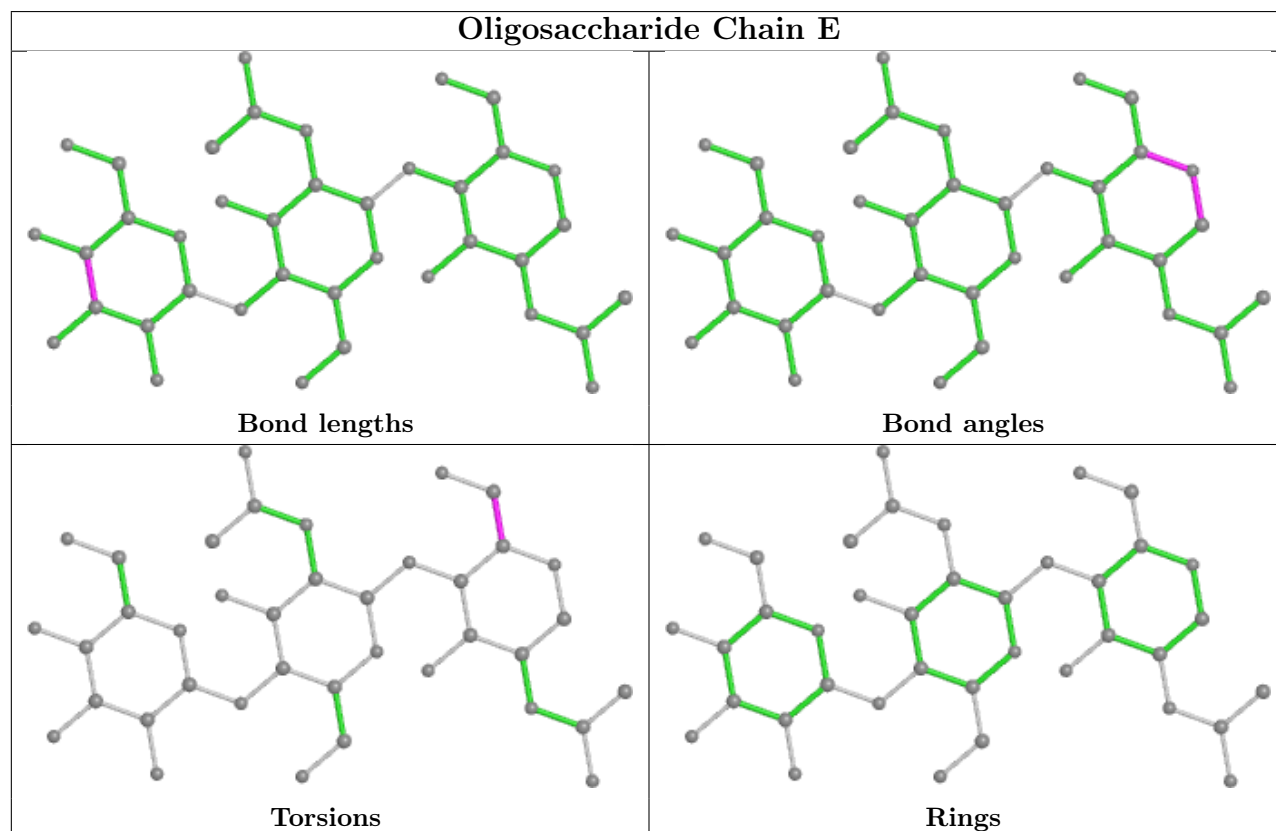
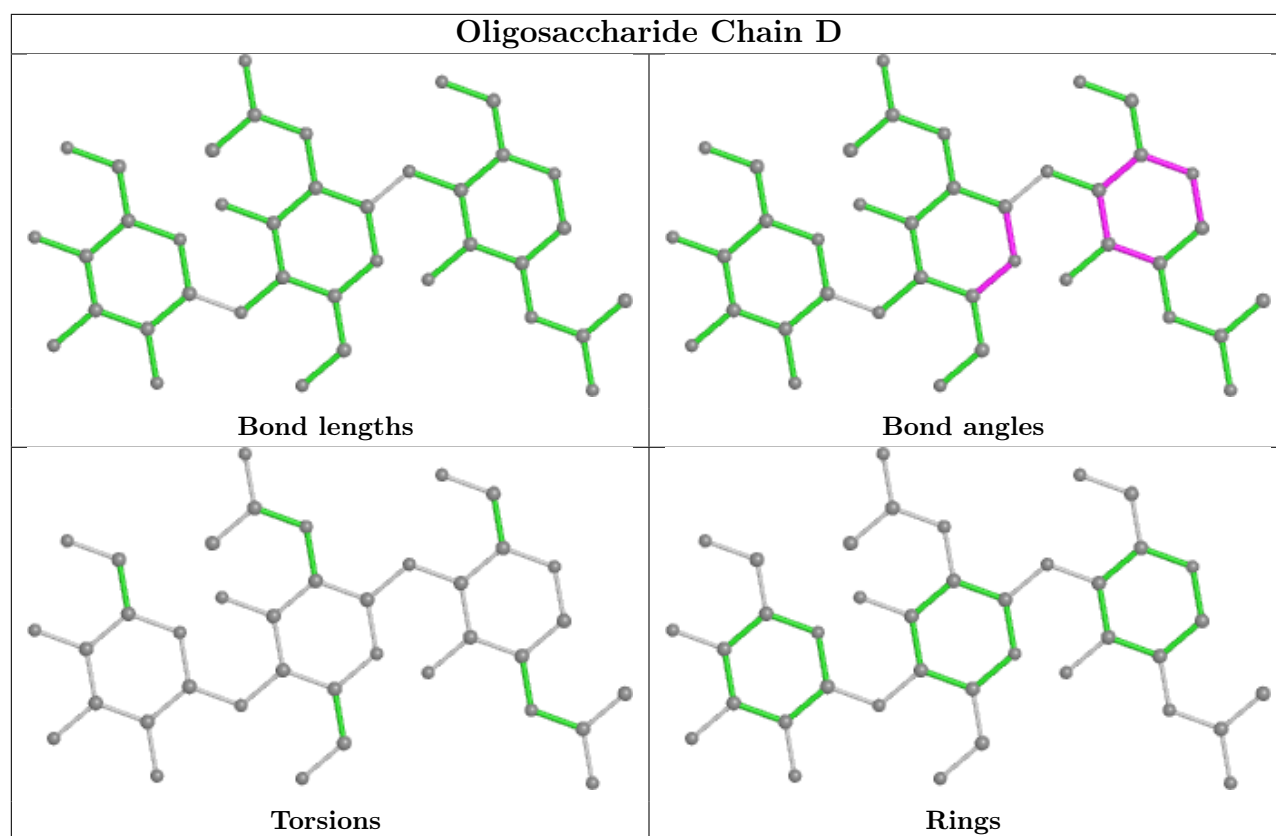
There are no ring outliers.

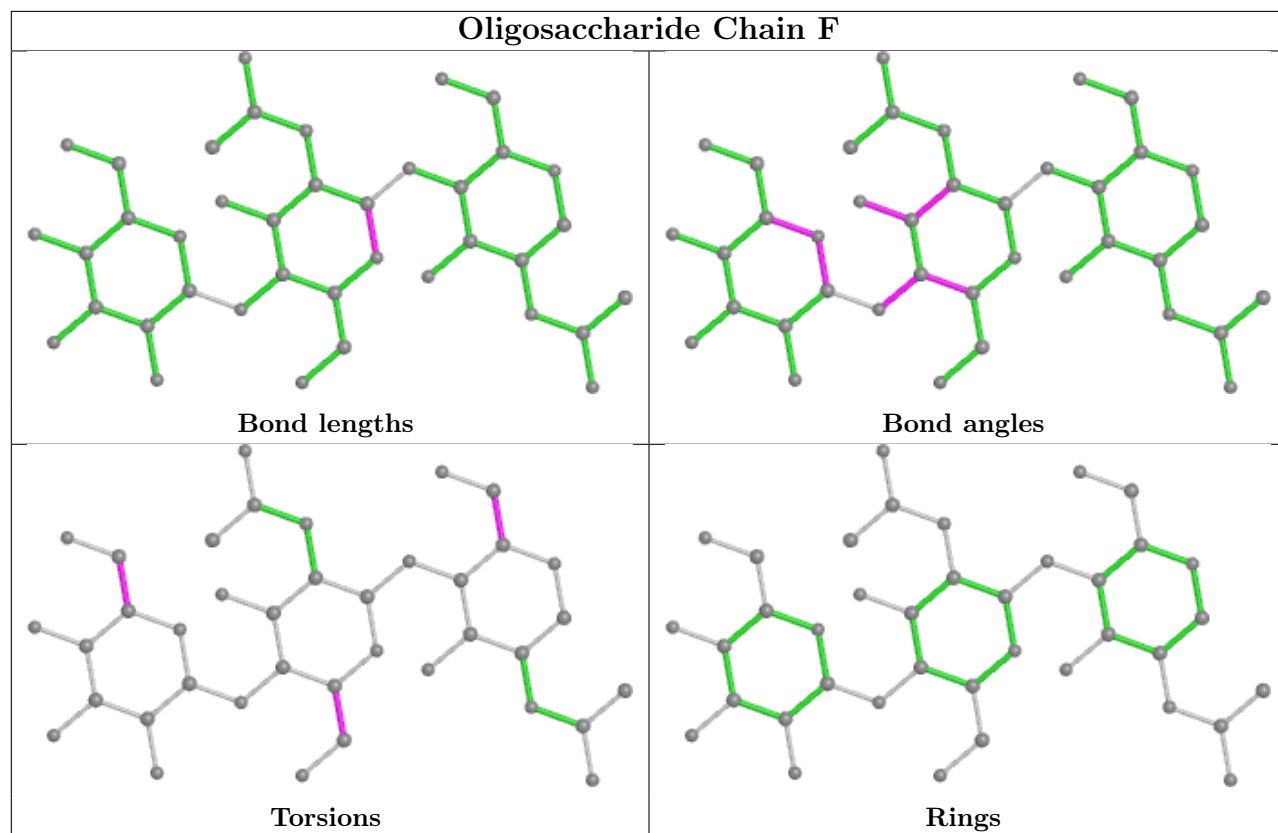
3 monomers are involved in 2 short contacts:

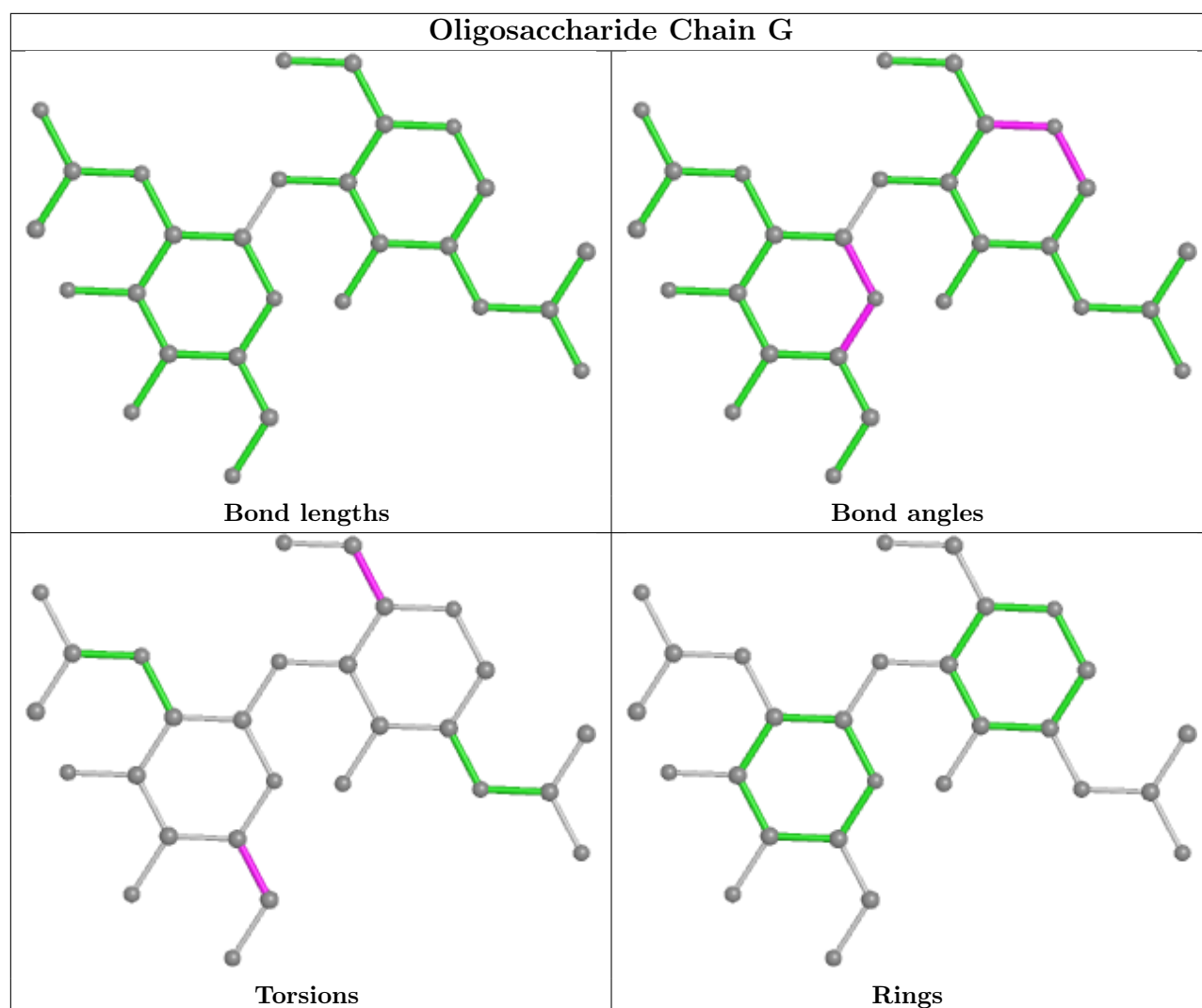
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1	NAG	1	0
2	B	1	NAG	1	0
3	F	1	NAG	1	0

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









5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
5	NAG	A	1606	1	14,14,15	0.49	0	17,19,21	0.64	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1606	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1606	NAG	C1-O5-C5	2.17	115.13	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1606	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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.

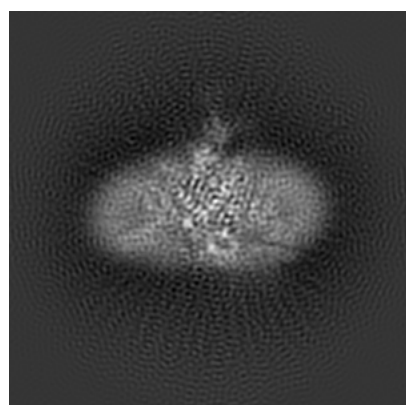
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6698. These allow visual inspection of the internal detail of the map and identification of artifacts.

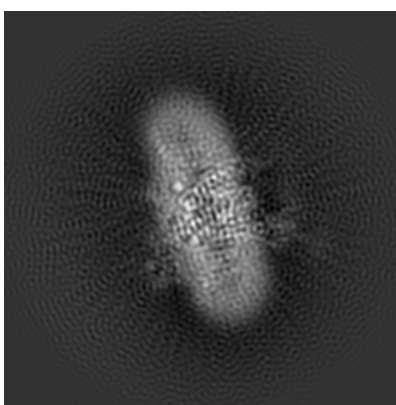
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

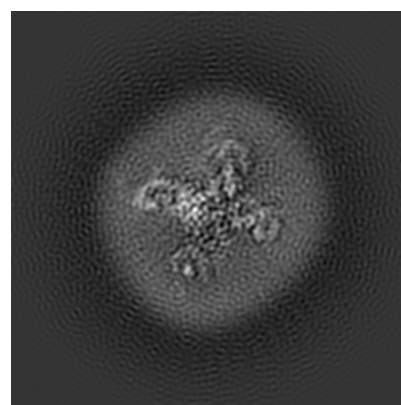
6.1.1 Primary map



X



Y

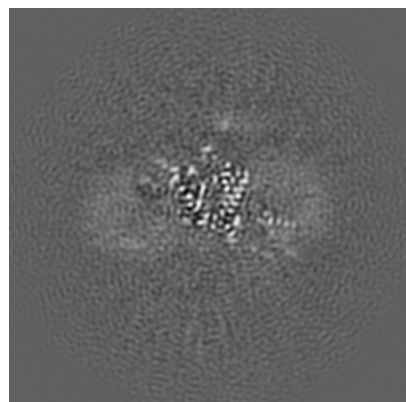


Z

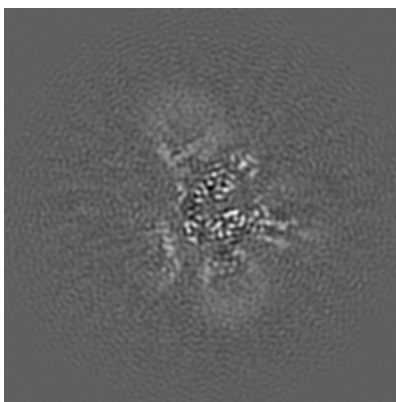
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

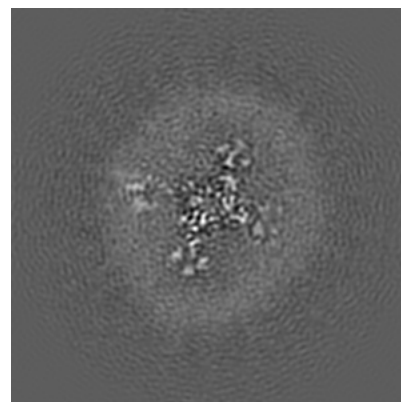
6.2.1 Primary map



X Index: 100



Y Index: 100

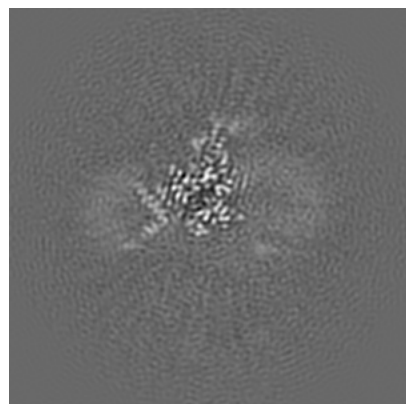


Z Index: 100

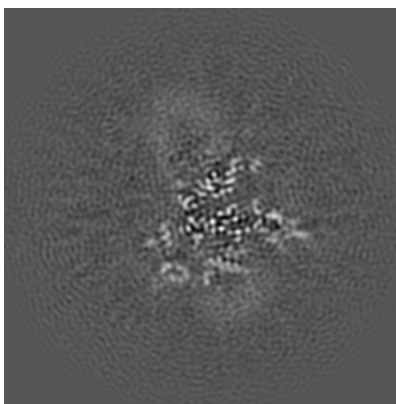
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

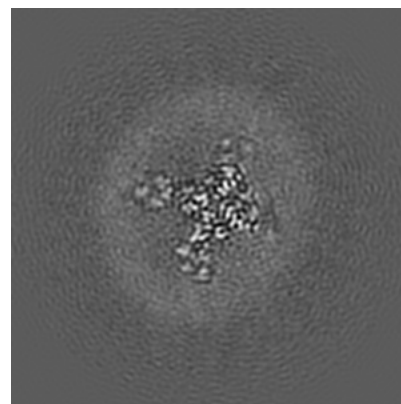
6.3.1 Primary map



X Index: 94



Y Index: 102

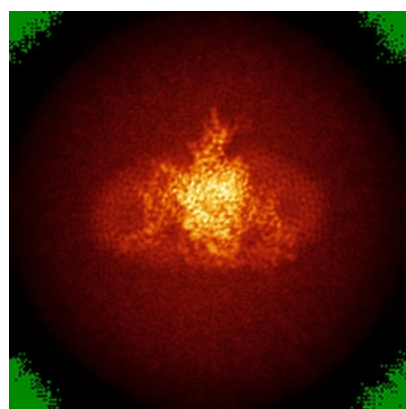


Z Index: 107

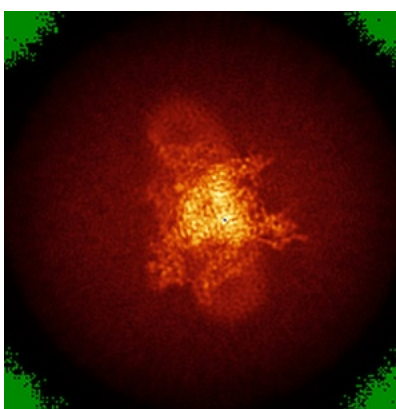
The images above show the largest variance slices of the map in three orthogonal directions.

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

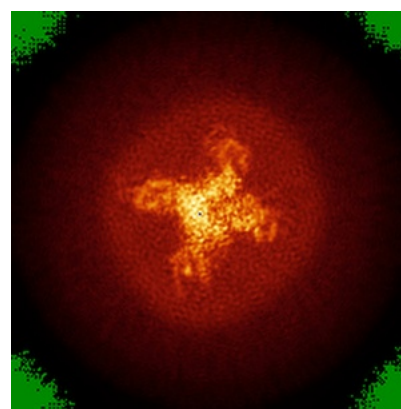
6.4.1 Primary map



X



Y



Z

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 0.0465. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

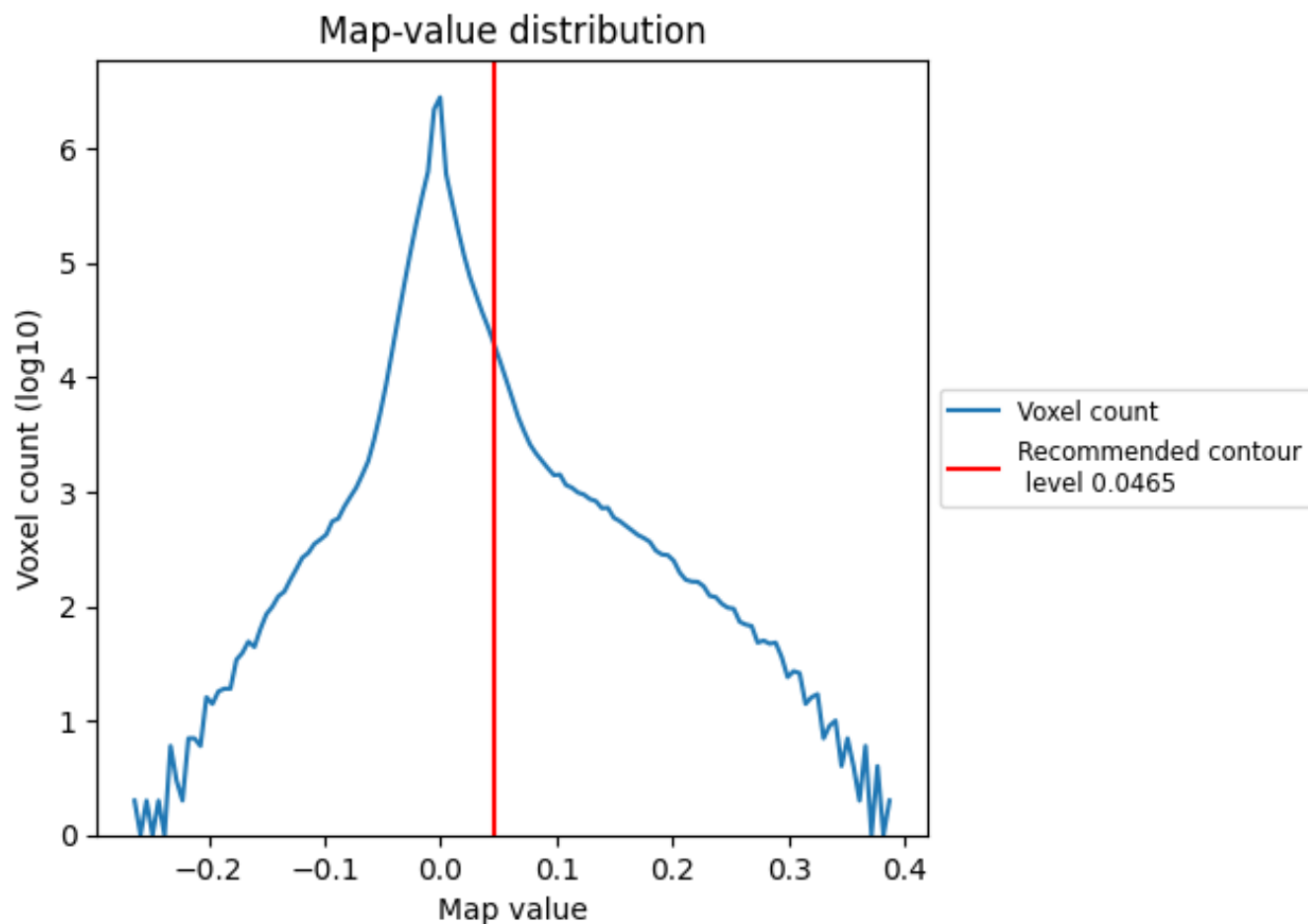
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

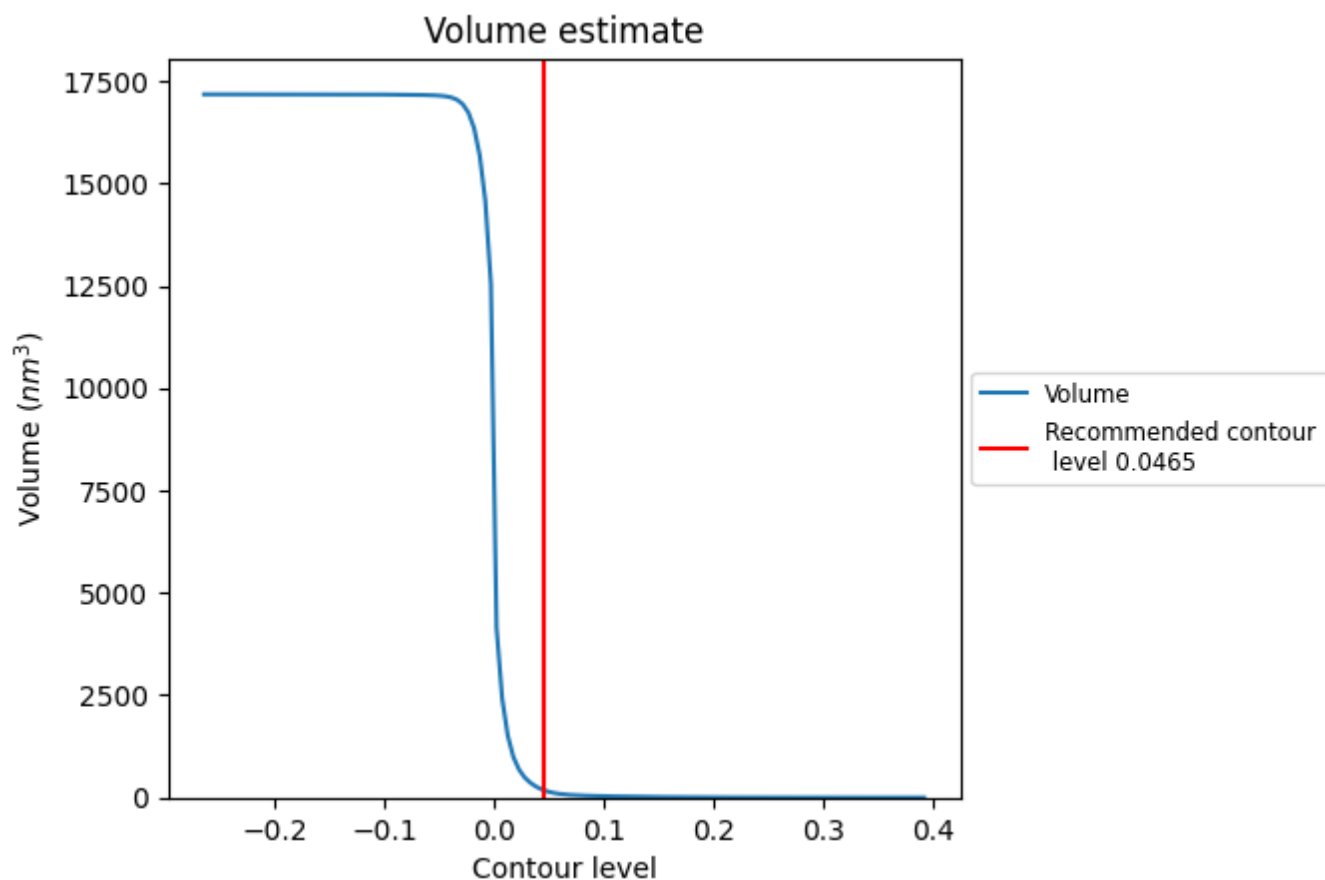
This section contains the results of statistical analysis of the map.

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.

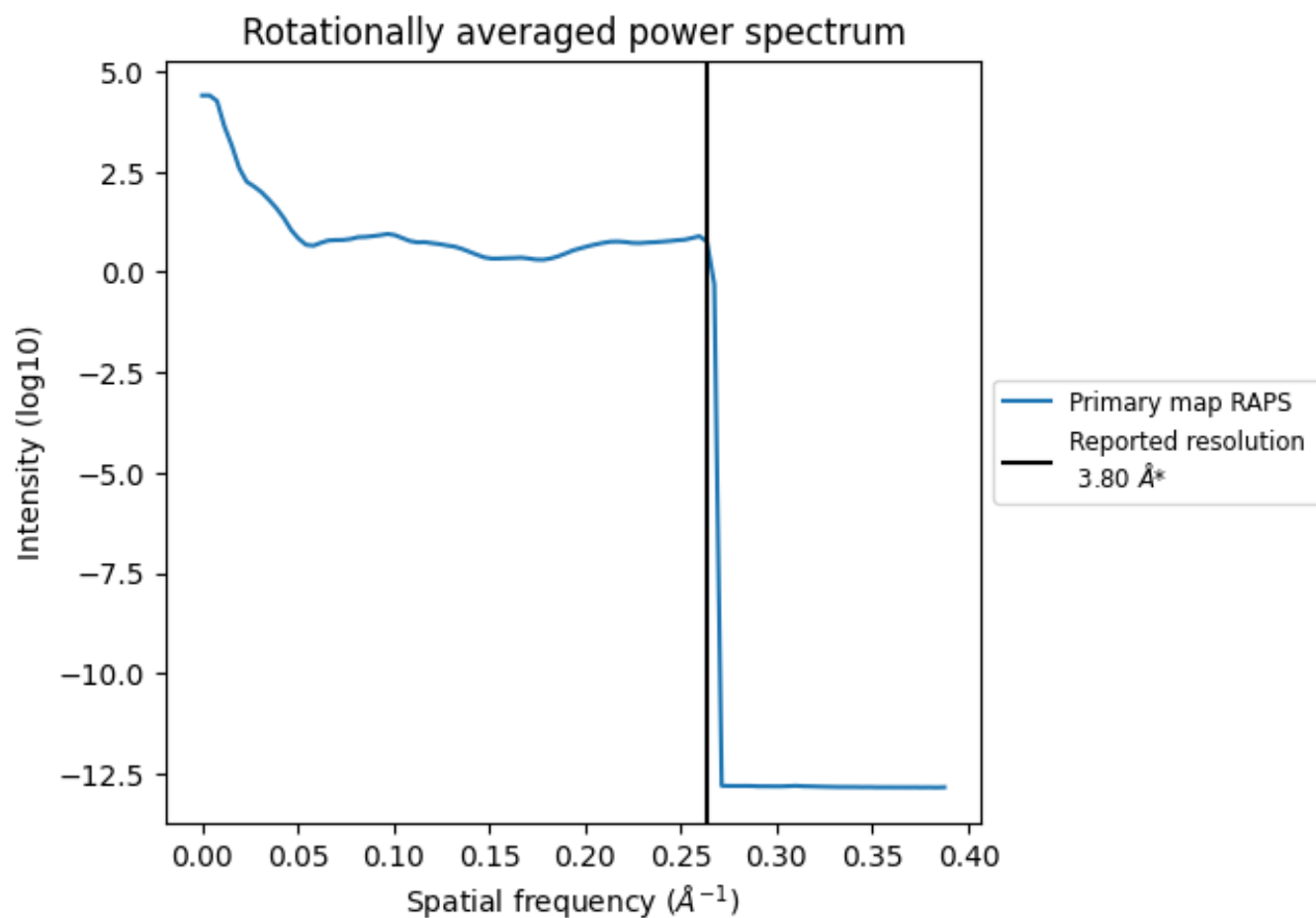
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 174 nm³; this corresponds to an approximate mass of 157 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 0.263 Å⁻¹

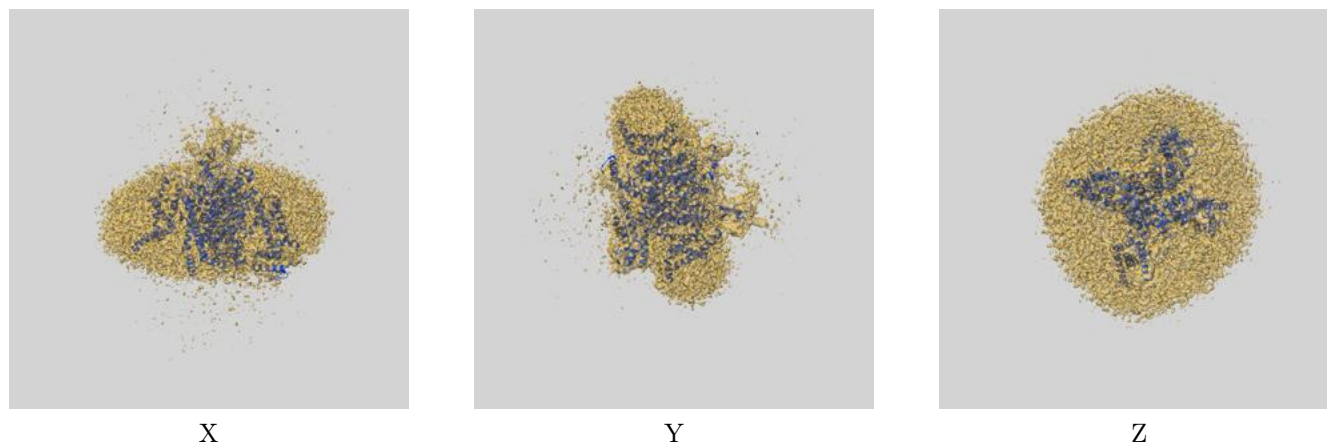
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

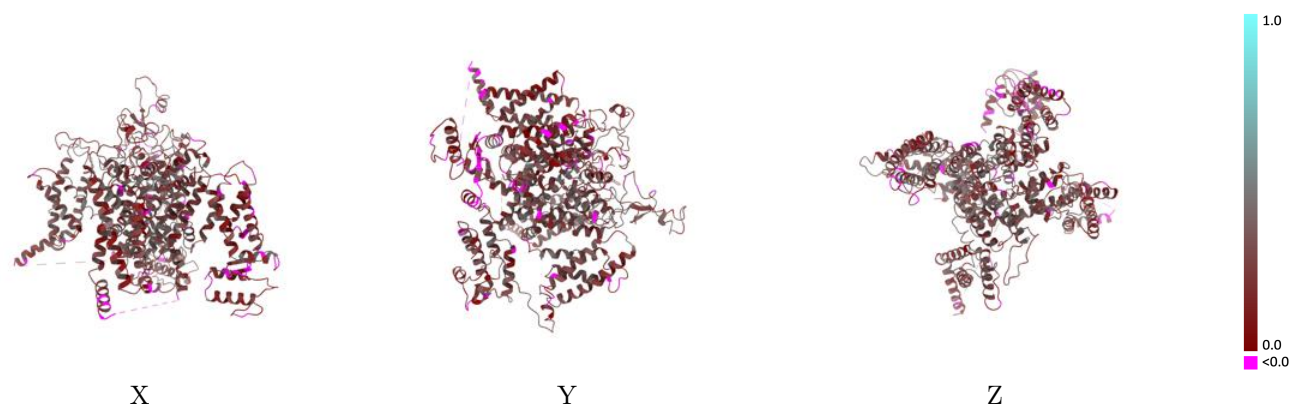
This section contains information regarding the fit between EMDB map EMD-6698 and PDB model 5X0M. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



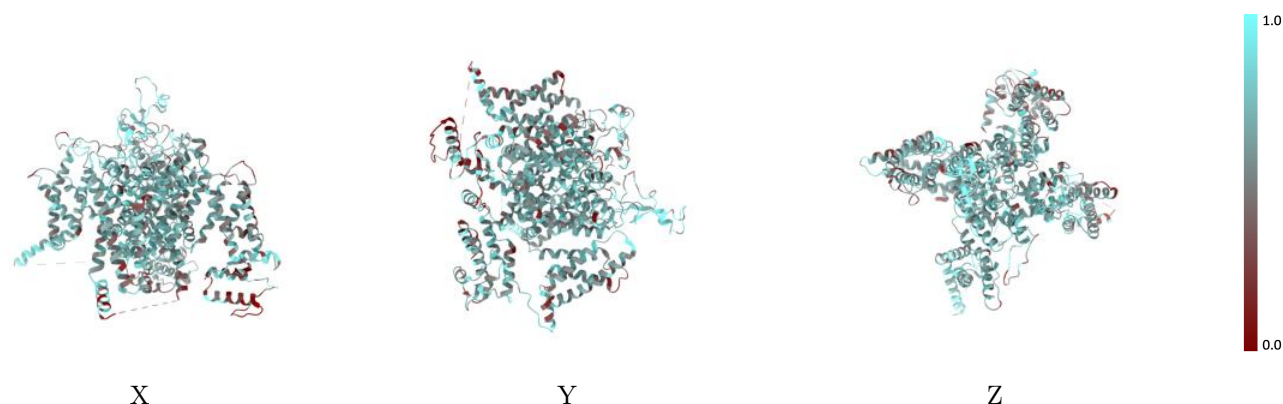
The images above show the 3D surface view of the map at the recommended contour level 0.0465 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



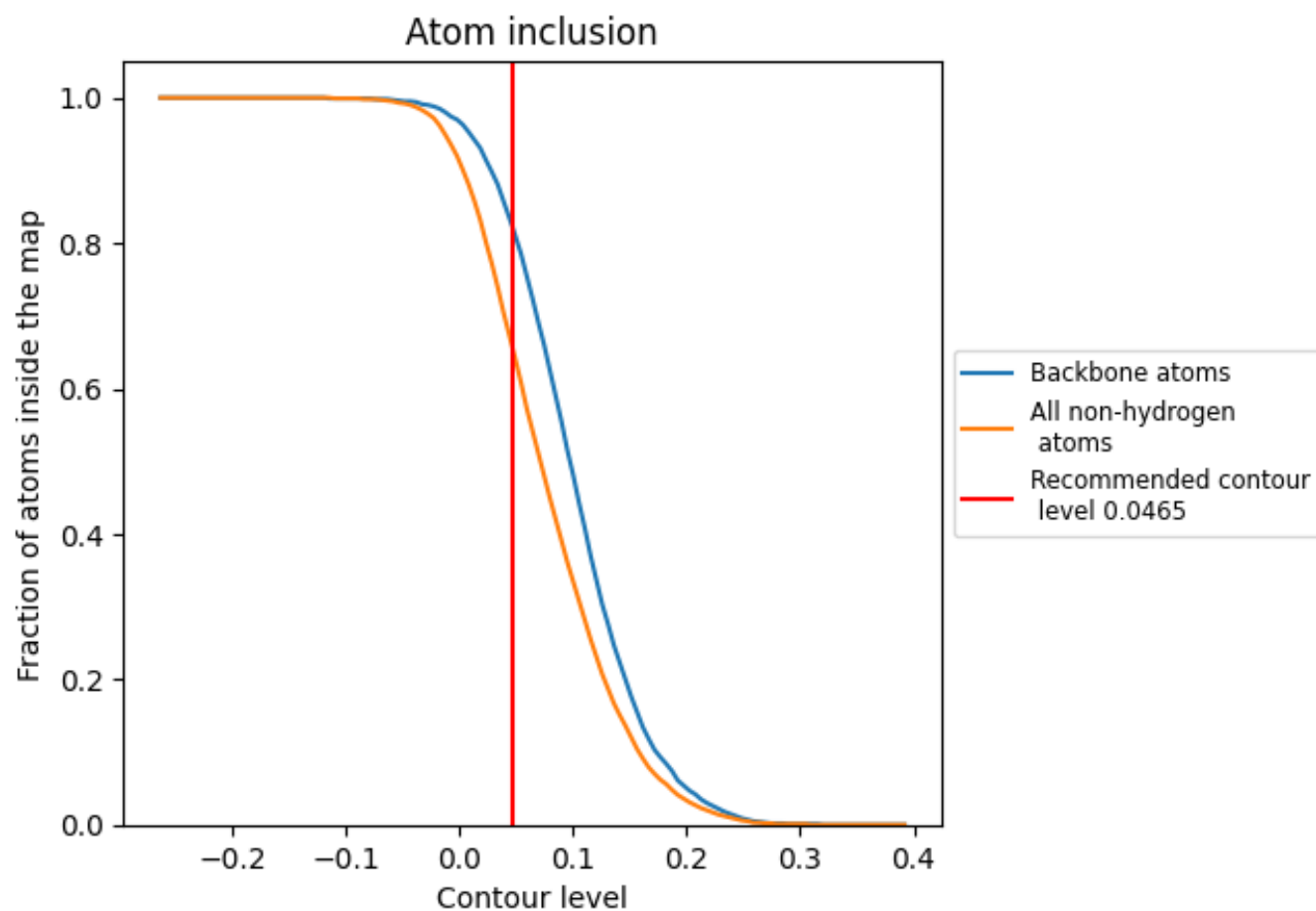
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0465).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 66% 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 (0.0465) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6560	<div></div> 0.2620
A	<div></div> 0.6600	<div></div> 0.2630
B	<div></div> 0.8530	<div></div> 0.3360
C	<div></div> 0.3850	<div></div> 0.1580
D	<div></div> 0.2310	<div></div> 0.0900
E	<div></div> 0.4360	<div></div> 0.1330
F	<div></div> 0.4870	<div></div> 0.1530
G	<div></div> 0.4640	<div></div> 0.2130

1.0

0.0

<0.0