



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 03:46 AM UTC

PDB ID : 8I03 / pdb_00008i03
EMDB ID : EMD-35093
Title : Cryo-EM structure of the SIN3L complex from *S. pombe*
Authors : Wang, C.; Guo, Z.; Zhan, X.
Deposited on : 2023-01-10
Resolution : 3.20 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

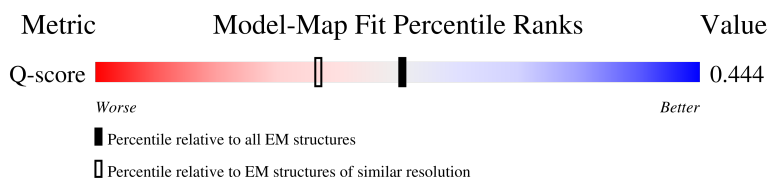
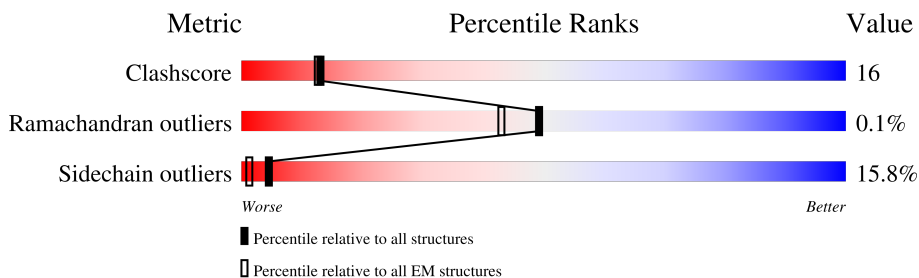
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	1522	
2	B	1154	
3	C	405	
3	D	405	

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Mol	Chain	Length	Quality of chain
4	E	491	25%9%66%
5	F	240	66%25%5%
6	G	267	9%46%15%38%
7	H	305	27%12%59%
8	I	351	34%16%47%
9	J	431	30%43%17%10%
9	K	431	90%30%43%17%10%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 29430 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 Paired amphipathic helix protein pst1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	616	Total	C	N	O	S	0	0
			5072	3237	869	941	25		

- Molecule 2 is a protein called Paired amphipathic helix protein pst3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	639	Total	C	N	O	S	0	0
			5305	3399	909	975	22		

- Molecule 3 is a protein called Histone deacetylase clr6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	370	Total	C	N	O	S	0	0
			2962	1881	505	557	19		
3	D	363	Total	C	N	O	S	0	0
			2911	1847	496	549	19		

- Molecule 4 is a protein called Transcriptional regulatory protein dep1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	169	Total	C	N	O	S	0	0
			1328	829	242	249	8		

- Molecule 5 is a protein called Transcriptional regulatory protein rxt2.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	F	228	Total	C	N	O	P	S	0	0
			1831	1137	314	368	4	8		

- Molecule 6 is a protein called Transcriptional regulatory protein sds3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	166	Total	C	N	O	S	0	0
			1306	805	235	261	5		

- Molecule 7 is a protein called Chromatin modification-related protein png2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	126	Total	C	N	O	S	0	0
			994	621	167	200	6		

- Molecule 8 is a protein called Transcriptional regulatory protein rxt3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	185	Total	C	N	O	S	0	0
			1505	972	256	273	4		

- Molecule 9 is a protein called RbAp48-related WD40 repeat-containing protein prw1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	388	Total	C	N	O	S	0	0
			3105	1957	533	599	16		
9	K	388	Total	C	N	O	S	0	0
			3105	1957	533	599	16		

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
10	C	1	Total	Zn	0
			1	1	
10	D	1	Total	Zn	0
			1	1	

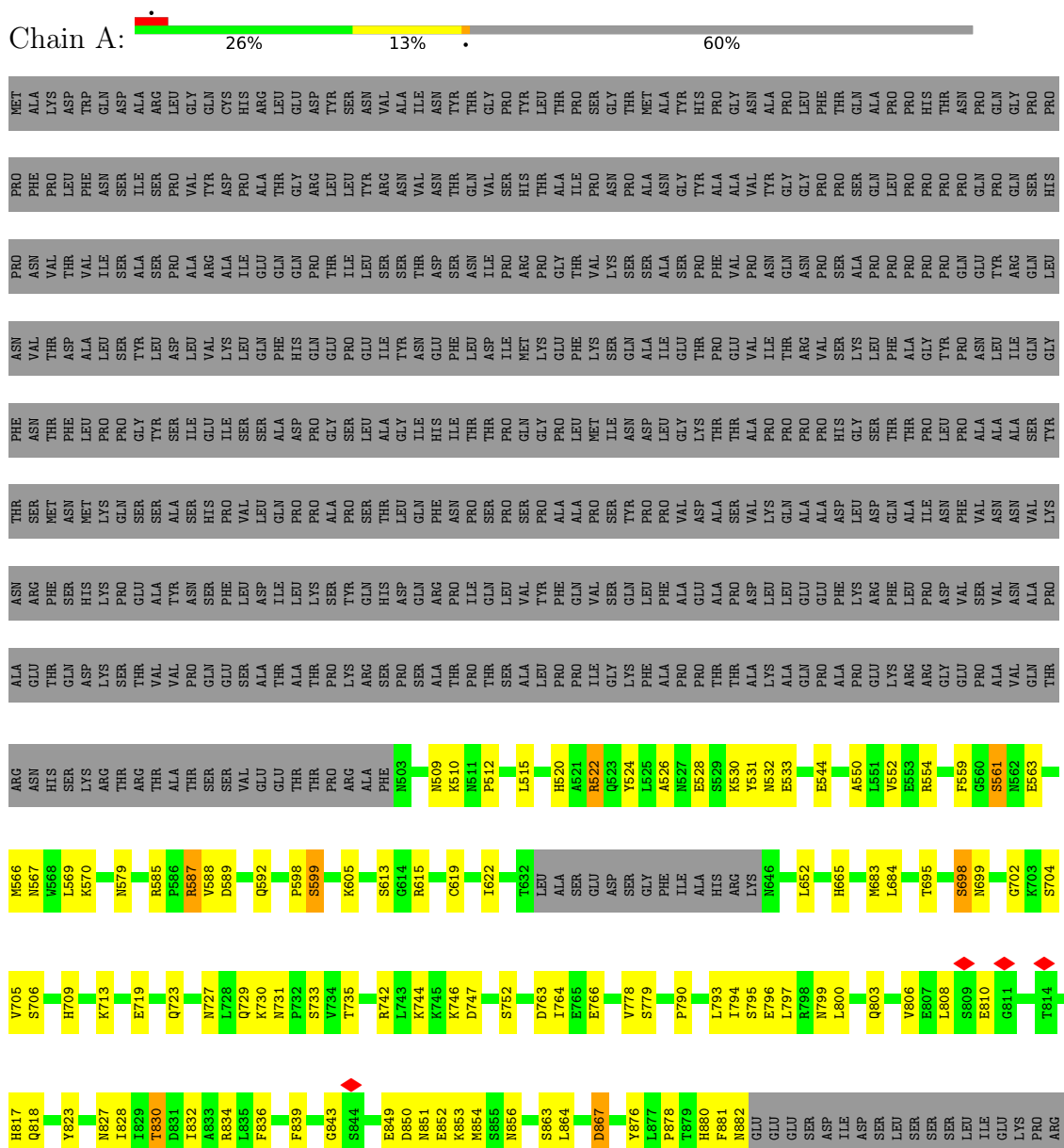
- Molecule 11 is POTASSIUM ION (CCD ID: K) (formula: K).

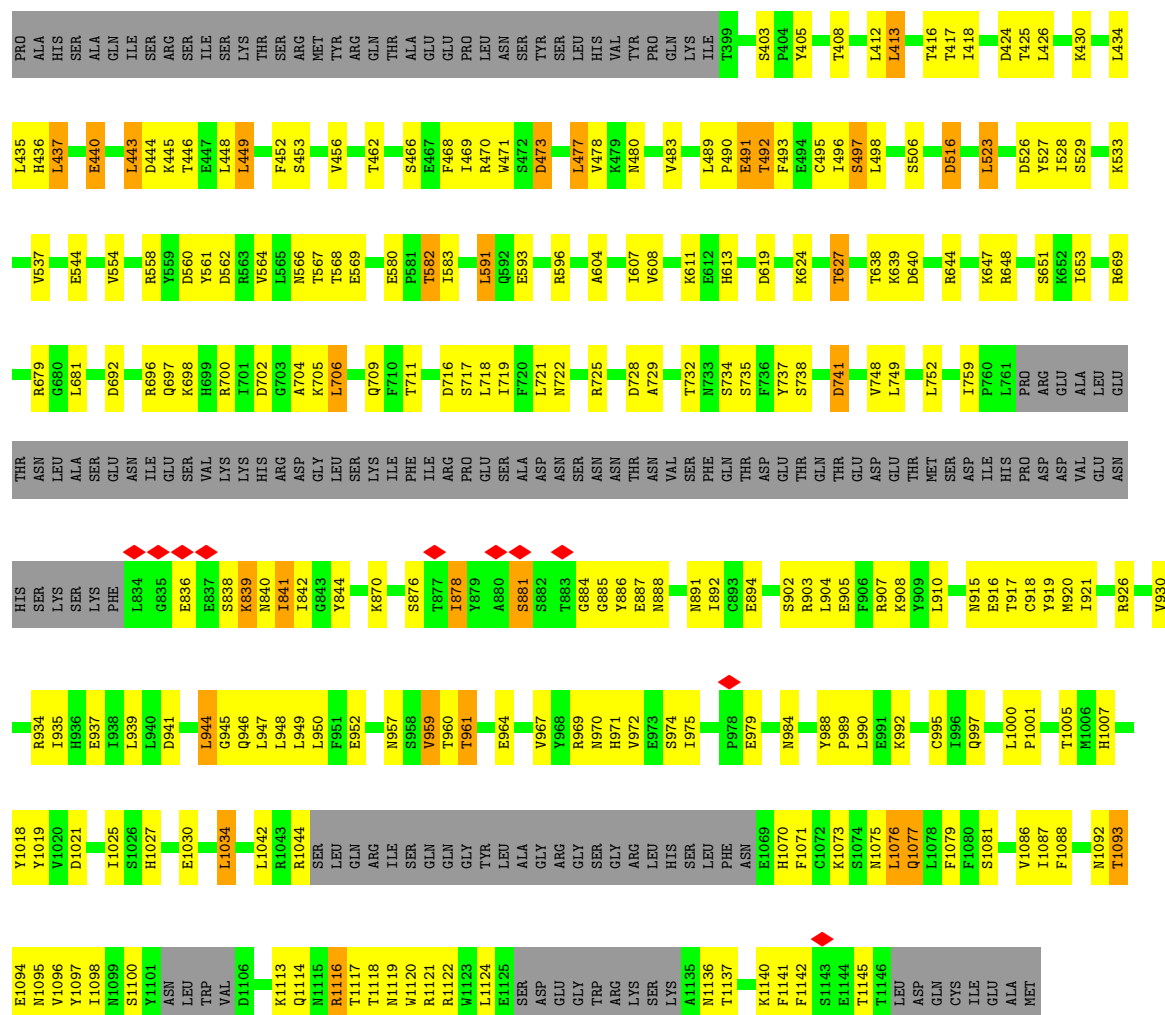
Mol	Chain	Residues	Atoms		AltConf
11	C	2	Total	K	0
			2	2	
11	D	2	Total	K	0
			2	2	

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.

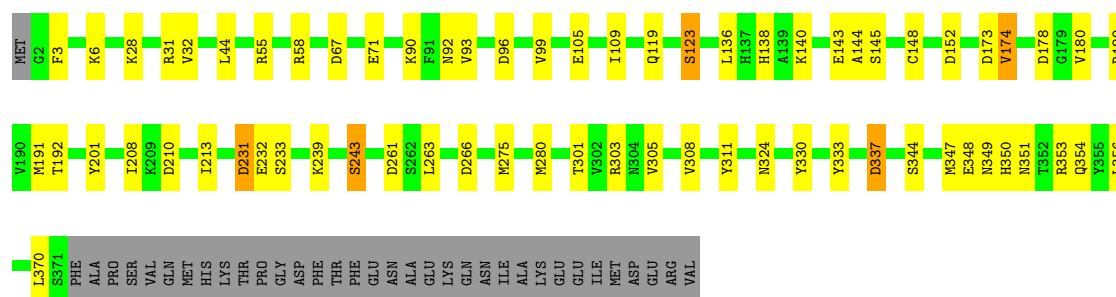
- Molecule 1: Paired amphipathic helix protein pst1





• Molecule 3: Histone deacetylase clr6

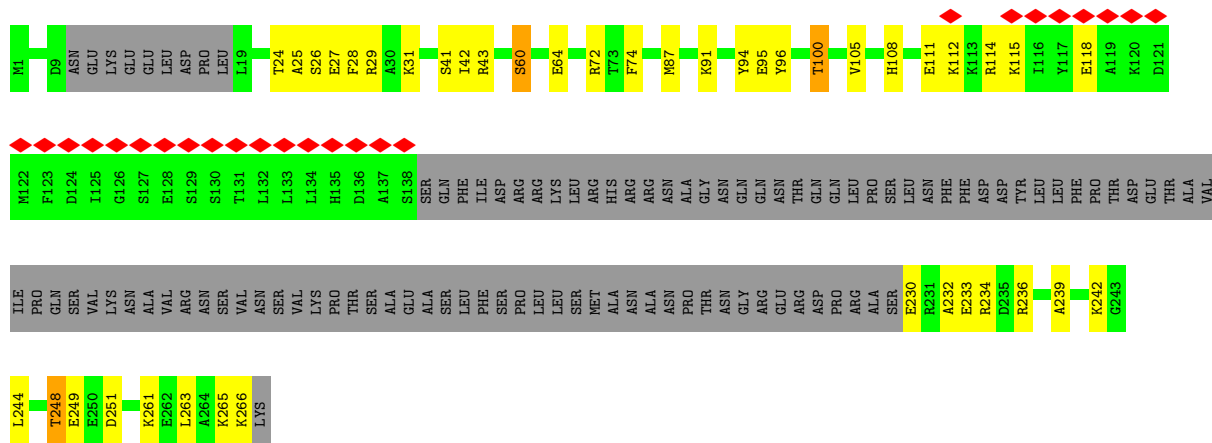
Chain C: 75% 15% 9%



• Molecule 3: Histone deacetylase clr6

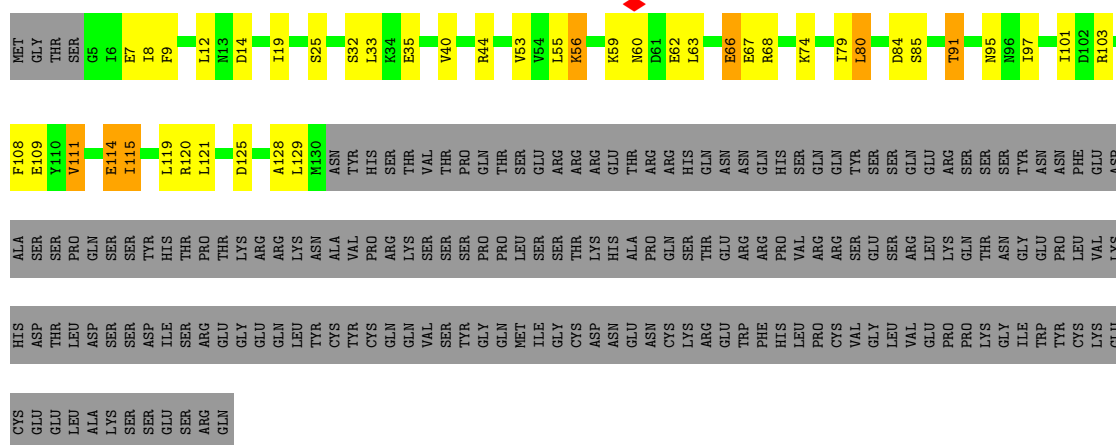
Chain D: 71% 16% 10%





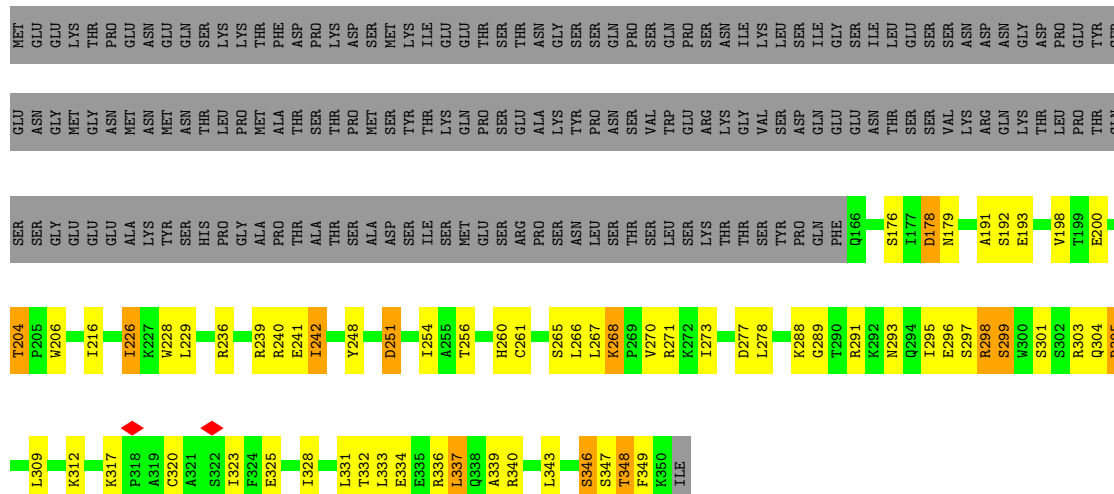
• Molecule 7: Chromatin modification-related protein png2

Chain H: 27% 12% 59%

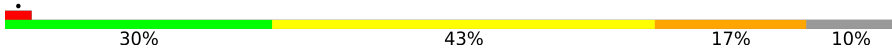


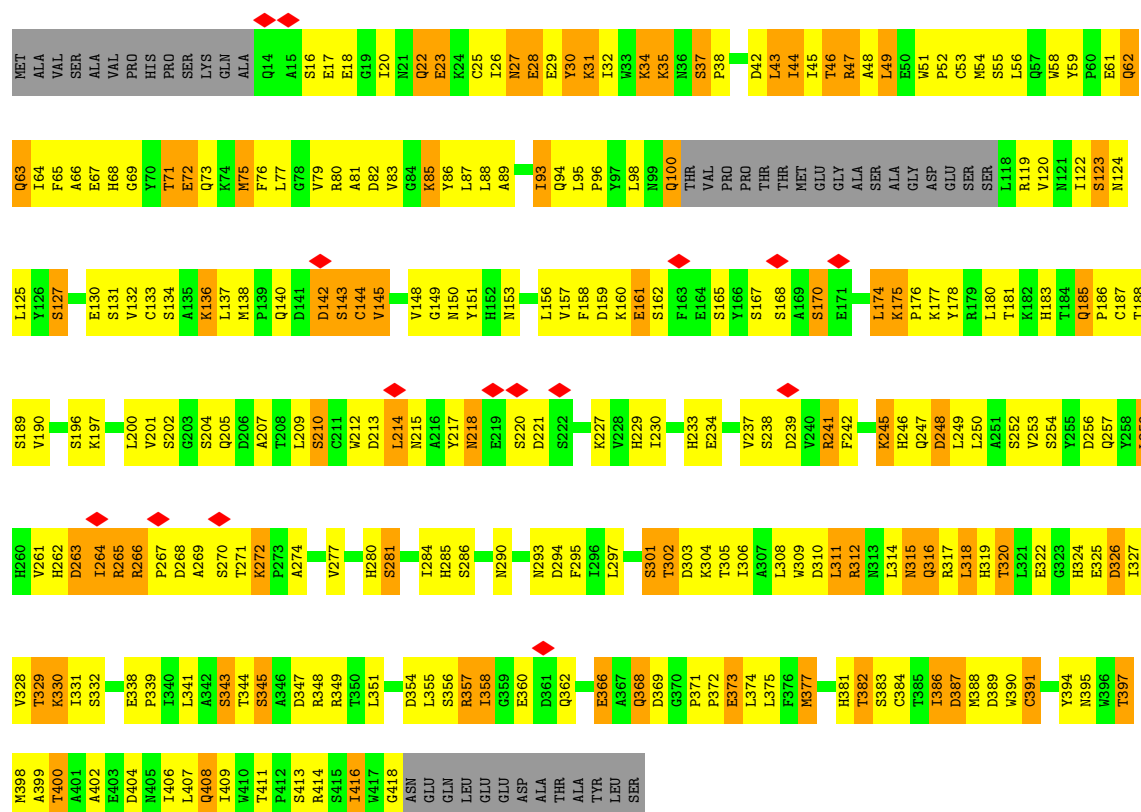
• Molecule 8: Transcriptional regulatory protein rxt3

Chain I: 34% 16% 47%

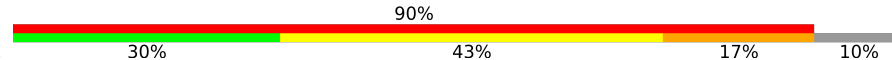


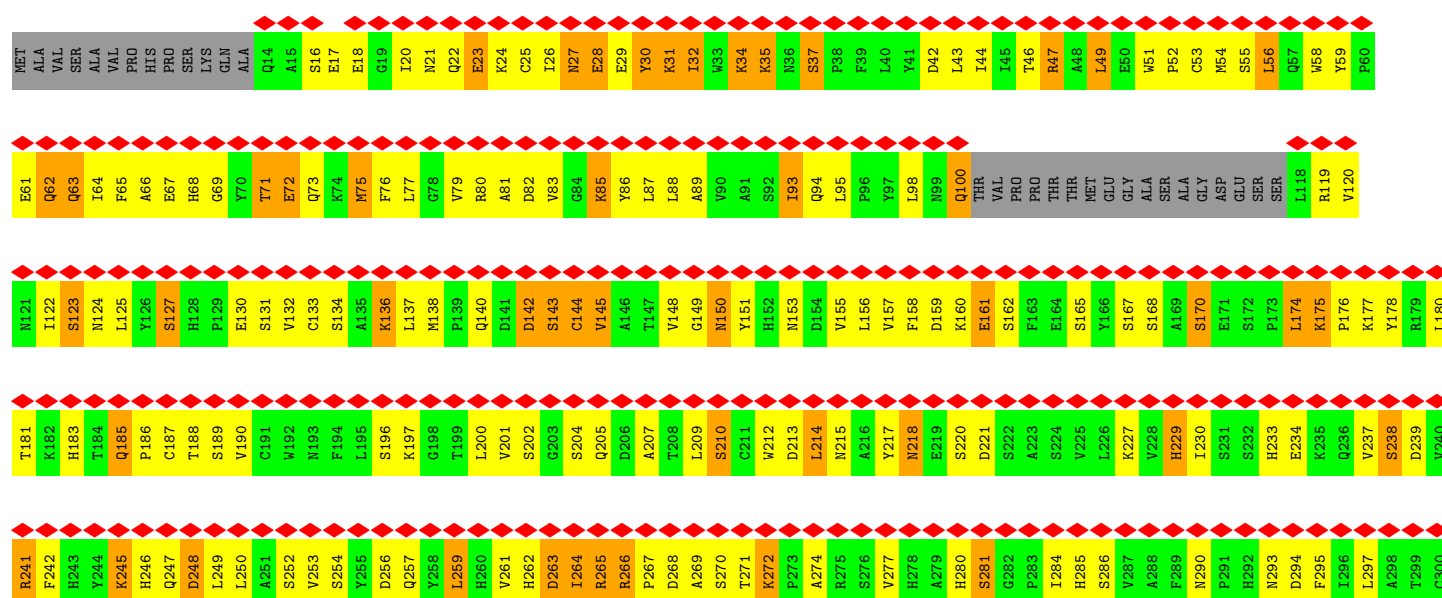
• Molecule 9: RbAp48-related WD40 repeat-containing protein prw1

Chain J:  30% 43% 17% 10%



• Molecule 9: RbAp48-related WD40 repeat-containing protein prw1

Chain K:  30% 43% 17% 10%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	389222	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.00	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.124	Depositor
Minimum map value	-0.065	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	Depositor
Map size ($\text{\AA}$)	391.32, 391.32, 391.32	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.087, 1.087, 1.087	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, SEP, ZN

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	0.40	0/5194	0.49	0/7023
2	B	0.40	0/5421	0.49	0/7321
3	C	0.62	0/3040	0.49	0/4121
3	D	0.59	0/2988	0.48	0/4054
4	E	0.41	0/1342	0.52	0/1804
5	F	0.56	0/1823	0.66	0/2458
6	G	0.37	0/1314	0.41	0/1755
7	H	0.45	0/1004	0.54	0/1353
8	I	0.47	0/1543	0.49	0/2099
9	J	0.25	0/3190	0.61	3/4345 (0.1%)
9	K	0.25	0/3190	0.61	3/4345 (0.1%)
All	All	0.44	0/30049	0.53	6/40678 (0.0%)

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	3
5	F	0	1
All	All	0	4

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	31	LYS	N-CA-CB	5.48	119.62	110.41
9	J	31	LYS	N-CA-CB	5.48	119.61	110.41
9	K	30	TYR	CA-C-N	-5.04	111.75	121.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	30	TYR	C-N-CA	-5.04	111.75	121.58
9	J	30	TYR	CA-C-N	-5.03	111.78	121.58
9	J	30	TYR	C-N-CA	-5.03	111.78	121.58

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1204	TYR	Peptide
1	A	977	TRP	Peptide
1	A	978	VAL	Peptide
5	F	49	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	5072	0	4988	188	0
2	B	5305	0	5285	220	0
3	C	2962	0	2818	38	0
3	D	2911	0	2761	42	0
4	E	1328	0	1304	34	0
5	F	1831	0	1769	70	0
6	G	1306	0	1267	29	0
7	H	994	0	997	26	0
8	I	1505	0	1524	54	0
9	J	3105	0	2960	197	0
9	K	3105	0	2960	207	0
10	C	1	0	0	0	0
10	D	1	0	0	0	0
11	C	2	0	0	0	0
11	D	2	0	0	0	0
All	All	29430	0	28633	951	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 16.

All (951) 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)
2:B:435:LEU:HD11	5:F:11:PHE:CD1	1.64	1.30
2:B:1076:LEU:HD13	2:B:1095:ASN:ND2	1.55	1.21
2:B:1093:THR:OG1	9:J:48:ALA:HB3	1.44	1.16
2:B:1076:LEU:HD22	2:B:1095:ASN:OD1	1.46	1.15
2:B:1093:THR:HG1	9:J:48:ALA:HB3	1.08	1.09
1:A:1204:TYR:HD2	9:K:17:GLU:HB3	1.16	1.08
2:B:1093:THR:OG1	9:J:48:ALA:CB	2.07	1.01
2:B:435:LEU:CD1	5:F:11:PHE:CD1	2.43	1.01
5:F:27:SEP:O3P	5:F:57:SER:OG	1.84	0.96
2:B:1076:LEU:HD13	2:B:1095:ASN:HD21	1.18	0.96
1:A:1201:TRP:O	1:A:1205:ILE:HB	1.65	0.95
2:B:412:LEU:HD21	5:F:5:GLU:HG2	1.49	0.94
2:B:1097:TYR:HB3	9:J:44:ILE:HG13	1.48	0.93
9:K:266:ARG:HH11	9:K:266:ARG:HG3	1.34	0.93
2:B:435:LEU:HD11	5:F:11:PHE:HD1	1.22	0.92
2:B:405:TYR:CE1	5:F:13:GLN:HB2	2.04	0.91
8:I:273:ILE:HB	8:I:317:LYS:HD2	1.51	0.90
9:J:266:ARG:HG3	9:J:266:ARG:HH11	1.34	0.90
2:B:1098:ILE:HD13	9:J:43:LEU:CD1	2.03	0.89
1:A:1204:TYR:CD2	9:K:17:GLU:HB3	2.06	0.89
2:B:1075:ASN:O	2:B:1093:THR:HG22	1.74	0.88
1:A:977:TRP:CD2	9:K:28:GLU:HB3	2.08	0.88
2:B:1098:ILE:HD13	9:J:43:LEU:HD11	1.58	0.86
2:B:435:LEU:HD21	5:F:11:PHE:HB2	1.56	0.86
2:B:1098:ILE:CD1	9:J:43:LEU:CD1	2.54	0.86
9:K:263:ASP:OD1	9:K:265:ARG:NH2	2.09	0.86
1:A:978:VAL:N	9:K:28:GLU:OE1	2.10	0.85
2:B:405:TYR:CZ	5:F:13:GLN:HG3	2.11	0.85
9:J:263:ASP:OD1	9:J:265:ARG:NH2	2.09	0.85
1:A:977:TRP:HB2	9:K:28:GLU:O	1.77	0.84
2:B:1076:LEU:CD1	2:B:1095:ASN:HD21	1.91	0.84
1:A:977:TRP:O	9:K:31:LYS:HG2	1.79	0.83
9:J:345:SER:OG	9:J:347:ASP:OD2	1.97	0.82
2:B:405:TYR:OH	5:F:13:GLN:CD	2.22	0.81
9:K:345:SER:OG	9:K:347:ASP:OD2	1.97	0.81
3:D:329:ASP:OD1	3:D:329:ASP:N	2.13	0.80
1:A:978:VAL:HG21	9:K:27:ASN:HB3	1.65	0.79
9:K:148:VAL:HG11	9:K:187:CYS:HB2	1.66	0.78
1:A:1206:GLY:HA2	9:K:24:LYS:HZ2	1.49	0.78
8:I:178:ASP:OD1	8:I:178:ASP:N	2.17	0.78
1:A:1202:CYS:O	1:A:1205:ILE:HG22	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:148:VAL:HG11	9:J:187:CYS:HB2	1.65	0.77
2:B:839:LYS:NZ	2:B:957:ASN:O	2.16	0.77
1:A:563:GLU:OE1	1:A:567:ASN:ND2	2.18	0.77
1:A:978:VAL:HA	9:K:31:LYS:CD	2.15	0.76
2:B:1095:ASN:HB2	9:J:46:THR:OG1	1.84	0.76
9:K:27:ASN:H	9:K:27:ASN:HD22	1.34	0.76
9:J:27:ASN:HD22	9:J:27:ASN:H	1.34	0.76
1:A:544:GLU:O	1:A:585:ARG:NH1	2.19	0.76
9:J:66:ALA:O	9:J:100:GLN:NE2	2.19	0.75
1:A:978:VAL:HA	9:K:31:LYS:HD3	1.67	0.75
9:K:66:ALA:O	9:K:100:GLN:NE2	2.19	0.74
1:A:980:CYS:N	1:A:992:ASP:OD1	2.16	0.74
9:K:23:GLU:O	9:K:27:ASN:ND2	2.19	0.74
9:K:144:CYS:HA	9:K:158:PHE:O	1.88	0.74
1:A:1210:MET:HE1	1:A:1215:GLU:HG2	1.69	0.74
9:J:23:GLU:O	9:J:27:ASN:ND2	2.19	0.74
1:A:1173:ASN:ND2	1:A:1176:THR:OG1	2.21	0.74
8:I:240:ARG:O	8:I:298:ARG:NH1	2.21	0.73
8:I:273:ILE:CB	8:I:317:LYS:HD2	2.19	0.73
2:B:1098:ILE:HD13	9:J:96:PRO:HG2	1.70	0.73
9:J:144:CYS:HA	9:J:158:PHE:O	1.88	0.73
1:A:1169:CYS:SG	1:A:1182:ARG:NH1	2.61	0.72
5:F:2:LYS:HD2	5:F:2:LYS:N	2.04	0.72
9:J:280:HIS:HB2	9:J:284:ILE:HD11	1.71	0.72
2:B:1098:ILE:CD1	9:J:96:PRO:HG2	2.19	0.72
3:C:58:ARG:NH1	3:C:71:GLU:OE1	2.22	0.72
2:B:405:TYR:CE1	5:F:13:GLN:CB	2.73	0.72
2:B:1073:LYS:HB3	2:B:1094:GLU:OE2	1.90	0.71
2:B:1098:ILE:HD12	9:J:43:LEU:HD12	1.72	0.71
9:K:280:HIS:HB2	9:K:284:ILE:HD11	1.71	0.71
3:C:239:LYS:O	3:C:243:SER:OG	2.07	0.71
3:D:169:TYR:OH	3:D:171:ASP:OD1	2.08	0.71
2:B:1098:ILE:CD1	9:J:43:LEU:HD12	2.20	0.71
1:A:1050:LEU:HD21	4:E:373:LYS:HD2	1.73	0.70
1:A:999:ARG:NH2	1:A:1139:ASP:O	2.24	0.70
2:B:523:LEU:HD11	3:D:158:LEU:HD11	1.71	0.70
2:B:1094:GLU:HB3	9:J:47:ARG:NH1	2.06	0.70
9:J:233:HIS:NE2	9:J:252:SER:OG	2.22	0.70
1:A:1173:ASN:O	1:A:1177:ARG:N	2.23	0.70
4:E:340:MET:HB3	4:E:345:THR:HA	1.71	0.70
9:J:190:VAL:HB	9:J:200:LEU:HD11	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:ASN:ND2	7:H:109:GLU:OE2	2.25	0.70
2:B:1076:LEU:HD23	2:B:1076:LEU:N	2.05	0.70
9:J:375:LEU:HG	9:J:416:ILE:HD11	1.74	0.70
2:B:640:ASP:OD2	2:B:644:ARG:NH1	2.24	0.69
7:H:63:LEU:HD22	7:H:68:ARG:HG2	1.72	0.69
8:I:242:ILE:HG12	8:I:297:SER:HB2	1.74	0.69
8:I:337:LEU:HB3	9:J:80:ARG:NH2	2.07	0.69
9:J:254:SER:OG	9:J:256:ASP:OD2	2.08	0.69
1:A:977:TRP:HB3	9:K:32:ILE:HB	1.73	0.69
4:E:464:THR:O	5:F:71:ARG:NH2	2.26	0.69
9:K:375:LEU:HG	9:K:416:ILE:HD11	1.74	0.69
9:K:233:HIS:NE2	9:K:252:SER:OG	2.21	0.69
9:K:315:ASN:OD1	9:K:315:ASN:N	2.23	0.69
1:A:1205:ILE:HG13	9:K:20:ILE:O	1.93	0.69
8:I:323:ILE:HG13	9:J:22:GLN:HE21	1.58	0.69
2:B:1076:LEU:HD23	2:B:1076:LEU:H	1.58	0.69
5:F:15:LEU:HD23	5:F:15:LEU:C	2.18	0.69
9:J:157:VAL:O	9:J:177:LYS:N	2.26	0.69
9:K:157:VAL:O	9:K:177:LYS:N	2.26	0.69
2:B:444:ASP:OD1	2:B:445:LYS:N	2.26	0.68
9:J:123:SER:OG	9:J:124:ASN:OD1	2.12	0.68
9:K:123:SER:OG	9:K:124:ASN:OD1	2.12	0.68
1:A:793:LEU:HD23	1:A:1015:ARG:HH21	1.57	0.68
9:K:29:GLU:OE2	9:K:349:ARG:NH2	2.26	0.68
9:J:381:HIS:HE2	9:J:400:THR:HG1	1.41	0.68
1:A:1136:TYR:OH	1:A:1140:ARG:NH1	2.27	0.68
9:J:201:VAL:HB	9:J:242:PHE:HE2	1.58	0.68
9:K:190:VAL:HB	9:K:200:LEU:HD11	1.74	0.68
1:A:978:VAL:HG13	9:K:27:ASN:O	1.93	0.68
1:A:1205:ILE:HG12	9:K:24:LYS:HD2	1.74	0.68
2:B:1042:LEU:HD22	9:J:369:ASP:HB3	1.75	0.68
9:K:284:ILE:HD13	9:K:301:SER:HB2	1.76	0.68
7:H:56:LYS:HG3	7:H:59:LYS:HD3	1.76	0.67
2:B:405:TYR:CZ	5:F:13:GLN:CG	2.76	0.67
8:I:331:LEU:O	8:I:336:ARG:NH1	2.27	0.67
5:F:191:GLU:OE2	5:F:194:ARG:NH2	2.24	0.67
9:J:29:GLU:OE2	9:J:349:ARG:NH2	2.26	0.67
1:A:587:ARG:NH2	3:C:143:GLU:OE1	2.27	0.67
6:G:248:THR:HG23	6:G:251:ASP:HB2	1.77	0.67
1:A:1196:SER:O	1:A:1200:LYS:N	2.17	0.67
9:J:284:ILE:HD13	9:J:301:SER:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:568:THR:OG1	2:B:640:ASP:OD1	2.10	0.67
1:A:790:PRO:HA	1:A:793:LEU:HD12	1.76	0.66
9:J:382:THR:OG1	9:J:404:ASP:OD1	2.09	0.66
2:B:412:LEU:CD2	5:F:5:GLU:HG2	2.24	0.66
9:K:201:VAL:HB	9:K:242:PHE:HE2	1.59	0.66
2:B:497:SER:OG	2:B:498:LEU:N	2.26	0.66
5:F:121:GLU:HG2	5:F:228:VAL:HG11	1.77	0.65
9:J:81:ALA:HB3	9:J:85:LYS:HB3	1.78	0.65
9:K:266:ARG:HB3	9:K:269:ALA:HB2	1.79	0.65
8:I:239:ARG:NH1	8:I:241:GLU:OE1	2.29	0.65
9:K:382:THR:OG1	9:K:404:ASP:OD1	2.09	0.65
1:A:998:ASP:HA	1:A:1144:ARG:HG2	1.77	0.65
7:H:91:THR:O	7:H:95:ASN:ND2	2.29	0.65
9:K:81:ALA:HB3	9:K:85:LYS:HB3	1.78	0.65
9:K:254:SER:OG	9:K:256:ASP:OD2	2.08	0.65
1:A:834:ARG:HA	1:A:876:TYR:HB3	1.79	0.64
1:A:982:PHE:HE2	1:A:992:ASP:HA	1.61	0.64
3:D:232:GLU:N	3:D:232:GLU:OE1	2.28	0.64
7:H:53:VAL:HG23	7:H:60:ASN:HB3	1.79	0.64
2:B:435:LEU:CD1	5:F:11:PHE:CE1	2.80	0.64
1:A:818:GLN:HE22	1:A:1183:LEU:H	1.45	0.64
1:A:1206:GLY:HA2	9:K:24:LYS:NZ	2.12	0.64
2:B:473:ASP:OD1	2:B:473:ASP:N	2.27	0.64
2:B:718:LEU:HA	2:B:721:LEU:HD12	1.79	0.64
2:B:1076:LEU:HA	2:B:1093:THR:HG22	1.79	0.64
2:B:1044:ARG:NH1	9:J:366:GLU:OE1	2.30	0.64
1:A:550:ALA:O	1:A:554:ARG:NH1	2.30	0.63
3:D:188:ASP:OD1	3:D:188:ASP:N	2.26	0.63
2:B:1070:HIS:CE1	2:B:1100:SER:OG	2.52	0.63
8:I:291:ARG:HB2	8:I:296:GLU:HG3	1.80	0.63
9:J:266:ARG:HB3	9:J:269:ALA:HB2	1.79	0.63
1:A:723:GLN:O	1:A:727:ASN:ND2	2.29	0.63
2:B:916:GLU:HA	2:B:919:TYR:HB2	1.79	0.63
4:E:406:THR:O	4:E:410:THR:HG23	1.98	0.63
9:J:187:CYS:HA	9:J:204:SER:HA	1.80	0.63
1:A:779:SER:O	1:A:779:SER:OG	2.17	0.63
9:J:207:ALA:HA	9:J:237:VAL:HG23	1.81	0.63
1:A:852:GLU:O	1:A:856:ASN:ND2	2.32	0.62
1:A:977:TRP:CE3	9:K:28:GLU:HB3	2.34	0.62
1:A:977:TRP:HB2	9:K:28:GLU:C	2.22	0.62
9:K:187:CYS:HA	9:K:204:SER:HA	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:827:ASN:O	1:A:830:THR:OG1	2.14	0.62
1:A:1166:ASN:HD21	1:A:1183:LEU:HD21	1.64	0.62
2:B:934:ARG:HH21	5:F:83:PRO:HG3	1.65	0.62
9:J:315:ASN:OD1	9:J:315:ASN:N	2.23	0.62
1:A:992:ASP:HB3	1:A:994:THR:HG23	1.81	0.62
3:C:231:ASP:OD1	3:C:231:ASP:N	2.32	0.62
9:J:159:ASP:HB3	9:J:177:LYS:HD3	1.81	0.62
2:B:480:ASN:ND2	8:I:179:ASN:OD1	2.33	0.62
3:C:261:ASP:OD1	3:C:261:ASP:N	2.27	0.61
1:A:1031:GLU:OE1	1:A:1070:VAL:N	2.29	0.61
2:B:544:GLU:OE1	2:B:679:ARG:NH1	2.33	0.61
5:F:19:SEP:O3P	8:I:299:SER:CB	2.47	0.61
8:I:337:LEU:HB3	9:J:80:ARG:HH22	1.66	0.61
1:A:849:GLU:H	1:A:849:GLU:CD	2.09	0.61
9:J:311:LEU:HA	9:J:314:LEU:HD21	1.82	0.61
9:J:338:GLU:HG2	9:J:339:PRO:HD3	1.82	0.61
2:B:947:LEU:HD21	2:B:975:ILE:HG21	1.82	0.61
9:K:159:ASP:HB3	9:K:177:LYS:HD3	1.81	0.61
3:D:349:ASN:OD1	3:D:350:HIS:N	2.34	0.61
9:K:207:ALA:HA	9:K:237:VAL:HG23	1.81	0.61
1:A:1201:TRP:HA	9:K:20:ILE:HG21	1.81	0.61
2:B:430:LYS:O	2:B:434:LEU:HG	2.00	0.61
2:B:1121:ARG:HA	2:B:1124:LEU:HD12	1.81	0.61
9:K:311:LEU:HA	9:K:314:LEU:HD21	1.82	0.61
8:I:334:GLU:OE2	9:J:80:ARG:NH1	2.33	0.61
1:A:977:TRP:NE1	1:A:1209:ILE:O	2.33	0.61
2:B:884:GLY:O	2:B:888:ASN:N	2.27	0.61
5:F:15:LEU:HD23	5:F:15:LEU:O	2.01	0.61
2:B:1093:THR:OG1	9:J:48:ALA:HB2	2.00	0.60
9:J:156:LEU:HB3	9:J:176:PRO:HG3	1.83	0.60
1:A:853:LYS:HD2	1:A:1124:THR:HB	1.82	0.60
1:A:1202:CYS:SG	1:A:1203:TYR:N	2.73	0.60
2:B:436:HIS:NE2	2:B:440:GLU:OE1	2.34	0.60
2:B:737:TYR:HB3	2:B:741:ASP:HB2	1.83	0.60
1:A:1131:GLN:HA	1:A:1134:MET:HG2	1.83	0.60
2:B:435:LEU:HD21	5:F:11:PHE:CB	2.30	0.60
9:K:156:LEU:HB3	9:K:176:PRO:HG3	1.83	0.60
9:J:94:GLN:HG3	9:J:119:ARG:H	1.67	0.60
3:C:263:LEU:HD11	3:C:308:VAL:HG21	1.83	0.59
1:A:1205:ILE:HG12	9:K:24:LYS:HB2	1.84	0.59
9:K:338:GLU:HG2	9:K:339:PRO:HD3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:241:ARG:HH11	9:K:241:ARG:HG2	1.67	0.59
3:C:140:LYS:NZ	3:C:178:ASP:OD2	2.36	0.59
5:F:143:THR:OG1	5:F:189:SER:OG	2.20	0.59
1:A:796:GLU:O	1:A:800:LEU:HG	2.02	0.59
8:I:323:ILE:HG13	9:J:22:GLN:NE2	2.16	0.59
9:J:241:ARG:HG2	9:J:241:ARG:HH11	1.68	0.59
9:K:94:GLN:HG3	9:K:119:ARG:H	1.68	0.59
3:D:261:ASP:N	3:D:261:ASP:OD1	2.33	0.59
9:K:266:ARG:HG3	9:K:266:ARG:NH1	2.12	0.59
9:K:217:TYR:HD2	9:K:218:ASN:H	1.51	0.59
2:B:944:LEU:O	2:B:947:LEU:HB2	2.03	0.59
3:D:178:ASP:OD1	3:D:178:ASP:N	2.25	0.59
9:K:143:SER:HB2	9:K:160:LYS:HD2	1.85	0.59
1:A:977:TRP:CG	9:K:28:GLU:HB3	2.38	0.59
2:B:1070:HIS:HE1	2:B:1100:SER:H	1.49	0.59
9:K:25:CYS:HA	9:K:28:GLU:HB2	1.85	0.59
1:A:1205:ILE:HG23	9:K:24:LYS:HD2	1.83	0.58
2:B:887:GLU:OE1	2:B:891:ASN:ND2	2.36	0.58
7:H:108:PHE:HA	7:H:111:VAL:HG13	1.84	0.58
9:J:217:TYR:HD2	9:J:218:ASN:H	1.51	0.58
9:J:25:CYS:HA	9:J:28:GLU:HB2	1.85	0.58
2:B:405:TYR:CE1	5:F:13:GLN:CG	2.87	0.58
2:B:413:LEU:O	2:B:417:THR:HG23	2.04	0.58
9:J:143:SER:HB2	9:J:160:LYS:HD2	1.85	0.58
1:A:599:SER:OG	3:C:210:ASP:OD2	2.21	0.58
2:B:1093:THR:HG1	9:J:48:ALA:CB	1.94	0.58
5:F:2:LYS:HD2	5:F:2:LYS:H	1.68	0.58
2:B:1076:LEU:HA	2:B:1093:THR:CG2	2.33	0.58
2:B:1095:ASN:O	9:J:45:ILE:HA	2.03	0.58
9:K:319:HIS:CD2	9:K:320:THR:H	2.22	0.58
2:B:516:ASP:OD1	2:B:516:ASP:N	2.25	0.58
2:B:941:ASP:OD1	2:B:944:LEU:N	2.37	0.58
2:B:1113:LYS:HD3	9:J:338:GLU:CD	2.29	0.57
3:C:119:GLN:O	3:C:123:SER:OG	2.21	0.57
1:A:1148:ARG:O	1:A:1152:MET:HG3	2.04	0.57
2:B:944:LEU:HD11	2:B:948:LEU:HD22	1.86	0.57
9:J:209:LEU:HB2	9:J:230:ILE:HB	1.86	0.57
9:K:209:LEU:HB2	9:K:230:ILE:HB	1.86	0.57
3:D:322:ASP:OD1	3:D:323:GLU:N	2.34	0.57
1:A:1004:LEU:HD12	1:A:1005:PHE:H	1.69	0.57
2:B:905:GLU:OE1	2:B:905:GLU:N	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:10:ARG:O	5:F:10:ARG:HD3	2.05	0.57
9:J:319:HIS:CD2	9:J:320:THR:H	2.22	0.57
1:A:1154:ARG:HH11	1:A:1190:THR:HG22	1.69	0.57
3:D:213:ILE:HG22	3:D:214:GLY:H	1.70	0.57
8:I:191:ALA:O	8:I:192:SER:OG	2.22	0.57
9:K:59:TYR:HB3	9:K:61:GLU:OE2	2.05	0.57
1:A:742:ARG:NH1	6:G:251:ASP:OD2	2.37	0.57
1:A:795:SER:O	1:A:799:ASN:ND2	2.38	0.57
1:A:1151:ILE:HD13	1:A:1207:SER:HA	1.86	0.57
2:B:969:ARG:NH1	2:B:1005:THR:OG1	2.38	0.57
2:B:1075:ASN:O	2:B:1093:THR:CG2	2.51	0.57
9:J:59:TYR:HB3	9:J:61:GLU:OE2	2.05	0.56
1:A:550:ALA:HB1	1:A:554:ARG:HH12	1.70	0.56
1:A:977:TRP:HB3	9:K:32:ILE:HD12	1.86	0.56
1:A:1151:ILE:O	1:A:1155:ILE:HG12	2.05	0.56
2:B:533:LYS:HE3	5:F:48:TYR:CD2	2.41	0.56
2:B:1070:HIS:HE1	2:B:1100:SER:CB	2.19	0.56
2:B:1141:PHE:CE1	9:J:312:ARG:HB3	2.41	0.56
4:E:340:MET:HA	4:E:343:ASN:HB2	1.88	0.56
9:J:187:CYS:SG	9:J:202:SER:OG	2.55	0.56
1:A:799:ASN:C	1:A:803:GLN:HE21	2.13	0.56
3:C:138:HIS:O	3:C:145:SER:HB3	2.06	0.56
3:D:123:SER:OG	3:D:125:ASN:ND2	2.39	0.56
3:D:235:GLU:HG3	3:D:239:LYS:HE3	1.87	0.56
1:A:979:ASN:H	9:K:31:LYS:NZ	2.04	0.56
2:B:1075:ASN:HB2	2:B:1094:GLU:H	1.69	0.56
3:D:67:ASP:OD2	3:D:67:ASP:N	2.33	0.56
9:K:178:TYR:HE2	9:K:214:LEU:HB3	1.71	0.56
2:B:405:TYR:CD2	5:F:16:PHE:CD1	2.94	0.56
3:D:239:LYS:O	3:D:243:SER:OG	2.19	0.55
9:J:65:PHE:O	9:J:69:GLY:N	2.34	0.55
9:J:177:LYS:HE3	9:J:178:TYR:CZ	2.41	0.55
9:K:330:LYS:NZ	9:K:387:ASP:OD1	2.39	0.55
2:B:470:ARG:HH11	5:F:15:LEU:HD21	1.71	0.55
2:B:1113:LYS:HD3	9:J:338:GLU:OE2	2.07	0.55
3:D:231:ASP:OD1	3:D:231:ASP:N	2.39	0.55
1:A:699:ASN:ND2	1:A:702:GLY:O	2.39	0.55
4:E:443:LYS:HE2	7:H:8:ILE:HD12	1.88	0.55
6:G:233:GLU:HA	6:G:236:ARG:HG2	1.88	0.55
1:A:1208:TYR:HB2	9:K:21:ASN:HB3	1.89	0.55
2:B:1070:HIS:CE1	2:B:1100:SER:H	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:359:ARG:HA	4:E:362:ASP:OD1	2.06	0.55
8:I:192:SER:OG	8:I:193:GLU:OE1	2.25	0.55
9:J:178:TYR:HE2	9:J:214:LEU:HB3	1.71	0.55
9:J:330:LYS:NZ	9:J:387:ASP:OD1	2.39	0.55
9:K:395:ASN:OD1	9:K:395:ASN:N	2.30	0.55
2:B:582:THR:O	2:B:582:THR:OG1	2.23	0.55
1:A:598:PRO:HD2	3:C:210:ASP:OD1	2.07	0.55
2:B:984:ASN:ND2	2:B:997:GLN:OE1	2.28	0.55
9:J:183:HIS:NE2	9:J:210:SER:OG	2.39	0.55
1:A:1149:GLN:HA	1:A:1152:MET:HE2	1.88	0.55
2:B:1073:LYS:CB	2:B:1094:GLU:OE2	2.55	0.55
6:G:24:THR:OG1	6:G:25:ALA:N	2.38	0.55
9:K:167:SER:OG	9:K:170:SER:OG	2.19	0.55
4:E:382:MET:HG3	6:G:72:ARG:HB2	1.89	0.55
3:D:8:VAL:HG13	3:D:128:ILE:HB	1.89	0.55
9:J:167:SER:OG	9:J:170:SER:OG	2.19	0.55
9:K:177:LYS:HE3	9:K:178:TYR:CZ	2.41	0.55
9:K:183:HIS:NE2	9:K:210:SER:OG	2.39	0.55
1:A:1128:ARG:O	1:A:1132:VAL:HG23	2.07	0.54
1:A:1136:TYR:CZ	1:A:1140:ARG:HD2	2.41	0.54
2:B:468:PHE:HE1	5:F:11:PHE:HE2	1.54	0.54
2:B:734:SER:OG	2:B:735:SER:N	2.38	0.54
2:B:1042:LEU:HB3	9:J:369:ASP:OD2	2.07	0.54
1:A:1145:THR:O	1:A:1150:GLN:NE2	2.41	0.54
2:B:453:SER:HA	2:B:456:VAL:HG12	1.89	0.54
2:B:838:SER:HB2	2:B:959:VAL:HG21	1.87	0.54
9:J:27:ASN:HD22	9:J:27:ASN:N	2.04	0.54
9:J:53:CYS:HA	9:J:79:VAL:HG12	1.89	0.54
1:A:880:HIS:CE1	1:A:882:ASN:HB2	2.43	0.54
9:K:58:TRP:CE2	9:K:75:MET:HE1	2.43	0.54
1:A:763:ASP:O	1:A:766:GLU:HG3	2.08	0.54
9:K:27:ASN:HD22	9:K:27:ASN:N	2.04	0.54
9:K:153:ASN:HA	9:K:186:PRO:HA	1.90	0.54
2:B:716:ASP:OD1	2:B:717:SER:N	2.40	0.54
4:E:402:GLN:O	4:E:406:THR:HG23	2.07	0.54
9:K:400:THR:HG23	9:K:408:GLN:HB3	1.90	0.54
2:B:1094:GLU:HB3	9:J:47:ARG:HH11	1.73	0.54
9:K:53:CYS:HA	9:K:79:VAL:HG12	1.89	0.54
1:A:978:VAL:HA	9:K:31:LYS:HE2	1.90	0.54
2:B:669:ARG:NE	3:D:348:GLU:HB2	2.23	0.54
2:B:1076:LEU:HB3	2:B:1095:ASN:HD21	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:185:GLN:HB3	9:K:205:GLN:HB2	1.89	0.54
2:B:1073:LYS:CG	2:B:1094:GLU:OE2	2.56	0.54
8:I:289:GLY:N	8:I:299:SER:OG	2.41	0.54
9:J:326:ASP:CG	9:J:327:ILE:H	2.14	0.54
9:K:65:PHE:O	9:K:69:GLY:N	2.34	0.54
9:K:326:ASP:CG	9:K:327:ILE:H	2.14	0.54
1:A:588:VAL:HB	7:H:128:ALA:HB3	1.90	0.53
3:D:57:THR:OG1	3:D:58:ARG:N	2.39	0.53
1:A:977:TRP:HB3	9:K:32:ILE:CD1	2.37	0.53
9:J:31:LYS:HA	9:J:34:LYS:HB3	1.90	0.53
9:J:58:TRP:CE2	9:J:75:MET:HE1	2.43	0.53
9:J:400:THR:HG23	9:J:408:GLN:HB3	1.90	0.53
1:A:683:MET:SD	1:A:733:SER:HA	2.48	0.53
3:C:105:GLU:O	3:C:109:ILE:HG13	2.08	0.53
8:I:267:LEU:HB3	9:J:368:GLN:NE2	2.24	0.53
1:A:1204:TYR:O	9:K:21:ASN:ND2	2.41	0.53
2:B:997:GLN:HE22	2:B:1007:HIS:CE1	2.27	0.53
9:K:381:HIS:HE2	9:K:400:THR:HG1	1.50	0.53
2:B:435:LEU:HD13	5:F:11:PHE:CE1	2.44	0.53
2:B:902:SER:OG	2:B:903:ARG:N	2.42	0.53
3:D:128:ILE:HG21	3:D:316:LEU:HD22	1.91	0.53
4:E:394:LEU:HD13	5:F:158:PRO:HA	1.91	0.53
8:I:337:LEU:HD22	9:J:80:ARG:HH21	1.73	0.53
9:K:31:LYS:HA	9:K:34:LYS:HB3	1.90	0.53
2:B:904:LEU:HD23	2:B:904:LEU:H	1.74	0.53
3:D:96:ASP:OD1	5:F:47:TYR:OH	2.26	0.53
9:J:302:THR:HA	9:J:327:ILE:HG23	1.91	0.53
1:A:1132:VAL:HG13	1:A:1157:THR:HG22	1.91	0.52
2:B:1070:HIS:CE1	2:B:1100:SER:CB	2.92	0.52
2:B:1142:PHE:HA	2:B:1145:THR:HG22	1.91	0.52
3:C:3:PHE:CE1	3:C:6:LYS:HE3	2.44	0.52
5:F:2:LYS:H	5:F:2:LYS:CD	2.22	0.52
9:K:167:SER:O	9:K:170:SER:OG	2.21	0.52
2:B:424:ASP:OD1	2:B:425:THR:N	2.42	0.52
2:B:1096:VAL:HA	9:J:44:ILE:O	2.09	0.52
4:E:341:ILE:HD11	6:G:105:VAL:HG12	1.89	0.52
1:A:978:VAL:HG21	9:K:27:ASN:CB	2.37	0.52
1:A:978:VAL:HA	9:K:31:LYS:CE	2.38	0.52
9:J:257:GLN:HG2	9:J:281:SER:C	2.34	0.52
2:B:748:VAL:HG21	2:B:939:LEU:HD21	1.89	0.52
8:I:229:LEU:HD12	8:I:270:VAL:HG11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:273:ILE:HB	8:I:317:LYS:CD	2.34	0.52
1:A:817:HIS:HA	1:A:1182:ARG:HB2	1.90	0.52
1:A:864:LEU:HG	1:A:1140:ARG:HD3	1.92	0.52
4:E:340:MET:O	4:E:345:THR:N	2.42	0.52
5:F:163:PRO:HG2	5:F:166:GLU:HB2	1.92	0.52
6:G:261:LYS:HG2	6:G:265:LYS:HZ3	1.74	0.52
9:K:257:GLN:HG2	9:K:281:SER:C	2.34	0.52
3:D:164:HIS:H	3:D:164:HIS:CD2	2.26	0.52
4:E:457:ASN:HA	4:E:461:GLY:O	2.10	0.52
7:H:115:ILE:HG22	7:H:120:ARG:HE	1.75	0.52
9:J:185:GLN:HB3	9:J:205:GLN:HB2	1.89	0.52
2:B:1076:LEU:N	2:B:1076:LEU:CD2	2.73	0.52
5:F:82:ASP:OD1	5:F:83:PRO:HD2	2.09	0.52
9:J:153:ASN:HA	9:J:186:PRO:HA	1.90	0.52
2:B:1018:TYR:OH	2:B:1030:GLU:OE2	2.28	0.52
3:C:178:ASP:OD1	3:C:178:ASP:N	2.31	0.52
3:C:191:MET:HE1	3:C:370:LEU:HD11	1.91	0.52
9:J:62:GLN:HB2	9:J:73:GLN:OE1	2.10	0.52
9:K:187:CYS:SG	9:K:202:SER:OG	2.55	0.52
9:K:302:THR:HA	9:K:327:ILE:HG23	1.91	0.52
2:B:697:GLN:HE21	2:B:709:GLN:HE21	1.58	0.52
2:B:1076:LEU:CD1	2:B:1095:ASN:ND2	2.48	0.52
5:F:19:SEP:O3P	8:I:299:SER:HB2	2.09	0.52
5:F:170:ILE:HG22	7:H:66:GLU:HA	1.90	0.52
9:J:49:LEU:HD23	9:J:53:CYS:SG	2.49	0.52
9:J:136:LYS:HG3	9:J:190:VAL:HG23	1.92	0.52
9:K:326:ASP:CG	9:K:327:ILE:N	2.68	0.52
2:B:564:VAL:HG22	2:B:607:ILE:HD13	1.92	0.52
9:J:30:TYR:C	9:J:30:TYR:CD1	2.88	0.52
9:J:326:ASP:CG	9:J:327:ILE:N	2.68	0.52
9:K:136:LYS:HG3	9:K:190:VAL:HG23	1.92	0.52
1:A:1208:TYR:CD1	9:K:25:CYS:HB2	2.45	0.51
2:B:840:ASN:HB3	2:B:990:LEU:HB2	1.91	0.51
5:F:150:MET:HE2	5:F:183:GLN:HG2	1.91	0.51
9:J:167:SER:O	9:J:170:SER:OG	2.21	0.51
9:K:261:VAL:O	9:K:274:ALA:N	2.43	0.51
1:A:1072:GLU:O	1:A:1076:GLN:HG3	2.09	0.51
1:A:1110:GLU:OE2	1:A:1111:LYS:N	2.42	0.51
3:C:92:ASN:ND2	3:C:144:ALA:O	2.44	0.51
7:H:14:ASP:CG	7:H:103:ARG:HH12	2.18	0.51
1:A:977:TRP:C	9:K:31:LYS:HG2	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:186:THR:O	3:D:186:THR:OG1	2.27	0.51
9:K:49:LEU:HD23	9:K:53:CYS:SG	2.49	0.51
1:A:983:THR:HB	1:A:987:GLY:HA2	1.91	0.51
2:B:717:SER:OG	2:B:759:ILE:HD12	2.10	0.51
1:A:1194:LEU:O	1:A:1195:LYS:HE2	2.10	0.51
4:E:419:GLN:HG3	6:G:28:PHE:CD1	2.45	0.51
9:K:30:TYR:CD1	9:K:30:TYR:C	2.88	0.51
1:A:790:PRO:O	1:A:794:ILE:HG12	2.10	0.51
2:B:1098:ILE:HD12	9:J:43:LEU:CD1	2.32	0.51
1:A:520:HIS:O	1:A:520:HIS:ND1	2.36	0.51
1:A:1151:ILE:CD1	1:A:1207:SER:HA	2.40	0.51
9:J:257:GLN:HB3	9:J:280:HIS:O	2.10	0.51
2:B:915:ASN:O	2:B:919:TYR:N	2.44	0.51
2:B:405:TYR:OH	5:F:13:GLN:HG3	2.11	0.51
2:B:580:GLU:HG3	2:B:583:ILE:HB	1.93	0.51
2:B:722:ASN:ND2	2:B:886:TYR:OH	2.43	0.51
6:G:96:TYR:O	6:G:100:THR:OG1	2.22	0.51
8:I:339:ALA:O	8:I:343:LEU:HG	2.11	0.51
9:J:261:VAL:O	9:J:274:ALA:N	2.43	0.51
9:J:371:PRO:HB2	9:J:373:GLU:OE1	2.11	0.51
9:K:371:PRO:HB2	9:K:373:GLU:OE1	2.11	0.51
2:B:405:TYR:OH	5:F:13:GLN:CG	2.58	0.51
2:B:1070:HIS:HE1	2:B:1100:SER:OG	1.93	0.51
9:K:326:ASP:OD2	9:K:327:ILE:N	2.34	0.51
3:D:166:ARG:NH2	3:D:250:ARG:O	2.31	0.50
4:E:344:GLU:O	4:E:350:ASN:ND2	2.44	0.50
1:A:1205:ILE:HG13	9:K:20:ILE:C	2.35	0.50
3:C:351:ASN:HB3	3:C:356:LEU:HD21	1.93	0.50
9:K:62:GLN:HB2	9:K:73:GLN:OE1	2.10	0.50
2:B:1021:ASP:O	2:B:1025:ILE:HG22	2.12	0.50
8:I:254:ILE:HD13	8:I:278:LEU:HD11	1.93	0.50
9:K:58:TRP:HD1	9:K:389:ASP:CG	2.20	0.50
2:B:979:GLU:N	2:B:979:GLU:OE2	2.45	0.50
9:K:257:GLN:HB3	9:K:280:HIS:O	2.10	0.50
1:A:867:ASP:OD1	1:A:867:ASP:N	2.45	0.50
5:F:37:LEU:HB2	5:F:40:LYS:HG3	1.94	0.50
1:A:852:GLU:HG3	1:A:881:PHE:CD2	2.46	0.50
2:B:916:GLU:H	2:B:916:GLU:CD	2.20	0.50
2:B:1073:LYS:HG2	2:B:1094:GLU:OE2	2.11	0.50
9:J:326:ASP:OD2	9:J:327:ILE:N	2.34	0.50
9:K:71:THR:OG1	9:K:73:GLN:NE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:967:VAL:HG22	2:B:971:HIS:CE1	2.47	0.50
4:E:469:GLU:OE2	4:E:469:GLU:N	2.43	0.50
9:J:414:ARG:O	9:J:418:GLY:N	2.33	0.50
9:K:217:TYR:HD2	9:K:218:ASN:N	2.09	0.50
1:A:559:PHE:HB2	1:A:566:MET:HE2	1.93	0.50
1:A:977:TRP:CD1	1:A:977:TRP:N	2.79	0.50
2:B:437:LEU:HB3	2:B:443:LEU:HD12	1.94	0.50
4:E:432:THR:OG1	4:E:433:MET:N	2.44	0.50
2:B:903:ARG:HE	2:B:907:ARG:NH2	2.09	0.50
2:B:1097:TYR:CZ	9:J:38:PRO:HA	2.46	0.50
7:H:62:GLU:O	7:H:68:ARG:NH1	2.45	0.50
9:K:47:ARG:HG2	9:K:120:VAL:HB	1.94	0.50
2:B:624:LYS:HG2	2:B:627:THR:HG23	1.94	0.49
2:B:728:ASP:O	2:B:732:THR:HG23	2.12	0.49
2:B:926:ARG:NH2	5:F:89:ASP:OD2	2.45	0.49
8:I:325:GLU:HA	8:I:328:ILE:HG12	1.94	0.49
9:K:133:CYS:H	9:K:149:GLY:HA2	1.77	0.49
6:G:248:THR:OG1	6:G:249:GLU:N	2.43	0.49
9:K:51:TRP:HB3	9:K:80:ARG:O	2.13	0.49
9:K:58:TRP:HZ3	9:K:73:GLN:HB2	1.78	0.49
9:J:47:ARG:HG2	9:J:120:VAL:HB	1.94	0.49
2:B:970:ASN:HD21	2:B:1027:HIS:HB2	1.75	0.49
5:F:225:ASN:ND2	5:F:227:GLN:H	2.10	0.49
8:I:325:GLU:OE2	9:J:348:ARG:NH1	2.36	0.49
9:K:354:ASP:HB2	9:K:375:LEU:HD13	1.94	0.49
1:A:1013:PHE:HB2	1:A:1119:GLN:HB3	1.93	0.49
3:C:173:ASP:OD1	3:C:174:VAL:N	2.46	0.49
9:J:58:TRP:HD1	9:J:389:ASP:CG	2.20	0.49
9:J:177:LYS:HG2	9:J:178:TYR:CE1	2.47	0.49
1:A:605:LYS:NZ	5:F:219:GLY:O	2.40	0.49
2:B:988:TYR:O	2:B:992:LYS:N	2.45	0.49
2:B:1071:PHE:CD1	2:B:1071:PHE:C	2.91	0.49
5:F:2:LYS:N	5:F:2:LYS:CD	2.73	0.49
6:G:114:ARG:O	6:G:118:GLU:HG3	2.13	0.49
9:J:133:CYS:H	9:J:149:GLY:HA2	1.77	0.49
9:J:217:TYR:HD2	9:J:218:ASN:N	2.09	0.49
1:A:982:PHE:HE1	9:K:27:ASN:OD1	1.95	0.49
9:J:51:TRP:HB3	9:J:80:ARG:O	2.13	0.49
9:K:87:LEU:HG	9:K:127:SER:HA	1.95	0.49
9:K:177:LYS:HG2	9:K:178:TYR:CE1	2.47	0.49
2:B:752:LEU:HD21	2:B:948:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:233:GLU:OE1	6:G:234:ARG:HG2	2.12	0.49
9:J:241:ARG:HH11	9:J:241:ARG:CG	2.26	0.49
9:K:241:ARG:HH11	9:K:241:ARG:CG	2.26	0.49
1:A:832:ILE:HG22	1:A:836:PHE:CE2	2.48	0.49
9:J:58:TRP:HZ3	9:J:73:GLN:HB2	1.78	0.49
9:J:71:THR:OG1	9:J:73:GLN:NE2	2.45	0.49
9:K:27:ASN:O	9:K:30:TYR:HB3	2.13	0.49
1:A:589:ASP:OD1	1:A:589:ASP:N	2.38	0.48
1:A:665:HIS:CD2	6:G:244:LEU:HG	2.48	0.48
2:B:490:PRO:HA	2:B:493:PHE:CE2	2.47	0.48
2:B:608:VAL:HG13	2:B:639:LYS:HG3	1.94	0.48
2:B:838:SER:O	2:B:841:ILE:HG22	2.13	0.48
2:B:984:ASN:HB3	2:B:997:GLN:HG2	1.94	0.48
6:G:24:THR:HG23	6:G:27:GLU:H	1.77	0.48
9:J:140:GLN:CD	9:J:140:GLN:H	2.21	0.48
9:K:290:ASN:HB3	9:K:293:ASN:O	2.13	0.48
9:K:414:ARG:O	9:K:418:GLY:N	2.33	0.48
1:A:977:TRP:CZ3	9:K:29:GLU:HG2	2.47	0.48
9:K:140:GLN:CD	9:K:140:GLN:H	2.21	0.48
1:A:589:ASP:OD1	7:H:128:ALA:HB1	2.13	0.48
1:A:981:LYS:HB2	1:A:989:LEU:HD22	1.95	0.48
3:D:191:MET:HE2	3:D:219:TYR:HA	1.94	0.48
8:I:337:LEU:O	8:I:340:ARG:HB3	2.14	0.48
9:J:290:ASN:HB3	9:J:293:ASN:O	2.13	0.48
9:K:266:ARG:HD3	9:K:268:ASP:HB3	1.94	0.48
1:A:1065:PRO:HG3	1:A:1080:ARG:CZ	2.43	0.48
5:F:15:LEU:C	5:F:15:LEU:CD2	2.85	0.48
7:H:9:PHE:HB3	7:H:12:LEU:HB3	1.94	0.48
8:I:236:ARG:HG3	8:I:239:ARG:NH1	2.29	0.48
9:J:27:ASN:O	9:J:30:TYR:HB3	2.13	0.48
3:C:337:ASP:OD2	3:C:337:ASP:N	2.29	0.48
5:F:87:ASP:HB3	5:F:93:ASN:HD21	1.79	0.48
9:J:133:CYS:N	9:J:149:GLY:HA2	2.29	0.48
9:J:354:ASP:HB2	9:J:375:LEU:HD13	1.94	0.48
1:A:704:SER:O	1:A:704:SER:OG	2.32	0.48
1:A:991:ASP:HB3	1:A:1202:CYS:HB2	1.95	0.48
3:C:275:MET:HG3	3:C:308:VAL:HG22	1.96	0.48
9:J:180:LEU:HD23	9:J:212:TRP:CE3	2.49	0.48
9:J:266:ARG:HG2	9:J:267:PRO:HD2	1.96	0.48
9:J:386:ILE:HG22	9:J:387:ASP:OD1	2.14	0.48
9:K:55:SER:HA	9:K:387:ASP:OD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:449:LEU:HD21	2:B:466:SER:OG	2.14	0.48
2:B:1141:PHE:CE2	9:J:311:LEU:HB2	2.49	0.48
9:J:63:GLN:OE1	9:J:63:GLN:HA	2.13	0.48
9:J:266:ARG:HD3	9:J:268:ASP:HB3	1.94	0.48
9:K:180:LEU:HD23	9:K:212:TRP:CE3	2.49	0.48
2:B:405:TYR:HD2	5:F:16:PHE:CD1	2.32	0.48
5:F:38:LYS:NZ	8:I:251:ASP:OD2	2.38	0.48
9:J:30:TYR:C	9:J:30:TYR:HD1	2.22	0.48
9:K:63:GLN:HA	9:K:63:GLN:OE1	2.13	0.48
9:K:75:MET:HE3	9:K:75:MET:HB2	1.77	0.48
9:K:386:ILE:HG22	9:K:387:ASP:OD1	2.14	0.48
2:B:711:THR:HG22	2:B:995:CYS:SG	2.54	0.47
9:K:133:CYS:N	9:K:149:GLY:HA2	2.29	0.47
9:K:331:ILE:HG22	9:K:343:SER:HB3	1.95	0.47
2:B:569:GLU:OE1	2:B:644:ARG:NH1	2.37	0.47
2:B:1076:LEU:CB	2:B:1095:ASN:HD21	2.27	0.47
2:B:1077:GLN:NE2	2:B:1077:GLN:N	2.62	0.47
9:J:87:LEU:HG	9:J:127:SER:HA	1.95	0.47
2:B:613:HIS:HD2	4:E:480:LEU:HD11	1.79	0.47
3:C:349:ASN:OD1	3:C:350:HIS:N	2.48	0.47
9:J:55:SER:HA	9:J:387:ASP:OD2	2.14	0.47
9:J:295:PHE:HB3	9:J:310:ASP:OD2	2.15	0.47
9:K:397:THR:HG23	9:K:411:THR:HB	1.97	0.47
1:A:1020:LEU:HD13	1:A:1112:LEU:HD23	1.96	0.47
2:B:453:SER:OG	2:B:462:THR:OG1	2.18	0.47
2:B:604:ALA:O	2:B:608:VAL:HG23	2.14	0.47
2:B:1114:GLN:O	2:B:1118:THR:HG23	2.13	0.47
2:B:1141:PHE:CZ	9:J:312:ARG:HB3	2.49	0.47
6:G:60:SER:O	6:G:64:GLU:HG3	2.15	0.47
9:J:248:ASP:OD1	9:J:264:ILE:HG23	2.15	0.47
1:A:744:LYS:HE2	6:G:74:PHE:HE2	1.78	0.47
1:A:977:TRP:C	9:K:28:GLU:HA	2.38	0.47
2:B:1118:THR:C	2:B:1122:ARG:HE	2.23	0.47
9:J:331:ILE:HG22	9:J:343:SER:HB3	1.95	0.47
9:K:248:ASP:OD1	9:K:264:ILE:HG23	2.15	0.47
1:A:522:ARG:C	1:A:524:TYR:H	2.22	0.47
1:A:982:PHE:CE2	9:K:24:LYS:HE3	2.49	0.47
8:I:268:LYS:HZ1	8:I:270:VAL:HA	1.79	0.47
9:J:72:GLU:OE1	9:J:94:GLN:NE2	2.48	0.47
9:J:397:THR:HG23	9:J:411:THR:HB	1.97	0.47
9:K:295:PHE:HB3	9:K:310:ASP:OD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:806:VAL:HG12	1:A:810:GLU:OE1	2.15	0.47
2:B:564:VAL:O	2:B:568:THR:HG23	2.14	0.47
4:E:382:MET:HB3	6:G:72:ARG:HH11	1.80	0.47
5:F:193:ILE:O	5:F:197:THR:OG1	2.30	0.47
9:K:178:TYR:CD1	9:K:217:TYR:HE1	2.33	0.47
1:A:977:TRP:CZ2	1:A:1211:SER:HA	2.49	0.47
2:B:870:LYS:HB2	2:B:886:TYR:CE2	2.49	0.47
2:B:1000:LEU:HB3	2:B:1001:PRO:HD2	1.96	0.47
3:C:3:PHE:HE1	3:C:6:LYS:HE3	1.80	0.47
3:D:165:GLN:HG3	3:D:166:ARG:HG3	1.96	0.47
9:K:72:GLU:OE1	9:K:94:GLN:NE2	2.48	0.47
1:A:579:ASN:O	1:A:579:ASN:ND2	2.48	0.47
1:A:797:LEU:HD21	1:A:1183:LEU:HD13	1.96	0.47
1:A:1194:LEU:C	1:A:1195:LYS:HE2	2.40	0.47
5:F:77:PHE:HB3	5:F:90:ASN:OD1	2.15	0.47
9:K:30:TYR:C	9:K:30:TYR:HD1	2.22	0.47
1:A:719:GLU:OE2	1:A:719:GLU:N	2.48	0.47
1:A:1206:GLY:CA	9:K:24:LYS:HZ2	2.23	0.47
3:D:33:ARG:HD3	3:D:330:TYR:OH	2.15	0.47
5:F:23:ASP:OD1	5:F:23:ASP:N	2.43	0.47
9:K:266:ARG:HG2	9:K:267:PRO:HD2	1.96	0.47
1:A:1127:ARG:NH1	1:A:1127:ARG:HA	2.30	0.46
1:A:1208:TYR:CG	9:K:25:CYS:SG	3.06	0.46
9:J:138:MET:HG2	9:J:140:GLN:NE2	2.30	0.46
8:I:347:SER:O	8:I:349:PHE:N	2.48	0.46
2:B:725:ARG:NE	2:B:894:GLU:OE2	2.48	0.46
2:B:878:ILE:O	2:B:881:SER:OG	2.32	0.46
1:A:1089:ASN:OD1	1:A:1090:GLY:N	2.47	0.46
2:B:426:LEU:HD23	2:B:426:LEU:HA	1.80	0.46
2:B:445:LYS:HD3	2:B:471:TRP:HD1	1.80	0.46
2:B:741:ASP:OD1	2:B:741:ASP:N	2.48	0.46
1:A:850:ASP:HA	1:A:853:LYS:HE2	1.96	0.46
1:A:1201:TRP:O	9:K:20:ILE:HD12	2.15	0.46
2:B:491:GLU:H	2:B:491:GLU:HG2	1.37	0.46
2:B:700:ARG:HG3	2:B:704:ALA:O	2.16	0.46
2:B:1076:LEU:HD22	2:B:1095:ASN:CG	2.32	0.46
3:D:136:LEU:O	3:D:151:ASN:ND2	2.46	0.46
7:H:74:LYS:HA	7:H:74:LYS:HD3	1.76	0.46
9:K:86:TYR:C	9:K:87:LEU:HD12	2.41	0.46
9:K:136:LYS:HB3	9:K:136:LYS:HE3	1.58	0.46
9:K:406:ILE:HD12	9:K:406:ILE:HA	1.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:GLU:O	1:A:567:ASN:ND2	2.48	0.46
2:B:885:GLY:HA2	2:B:888:ASN:HD22	1.81	0.46
2:B:1098:ILE:HD11	9:J:96:PRO:HG2	1.94	0.46
9:K:150:ASN:OD1	9:K:150:ASN:N	2.44	0.46
3:D:44:LEU:HD11	3:D:321:LEU:HD21	1.98	0.46
5:F:177:GLU:O	5:F:181:THR:HG23	2.16	0.46
9:J:175:LYS:HE2	9:J:175:LYS:HB3	1.48	0.46
9:J:178:TYR:CD1	9:J:217:TYR:HE1	2.33	0.46
9:J:301:SER:OG	9:J:302:THR:N	2.49	0.46
9:K:399:ALA:HA	9:K:408:GLN:O	2.16	0.46
1:A:1036:SER:O	1:A:1040:ASP:HB3	2.16	0.46
2:B:1113:LYS:O	2:B:1117:THR:HG23	2.16	0.46
5:F:10:ARG:C	5:F:10:ARG:CD	2.89	0.46
6:G:244:LEU:H	6:G:244:LEU:HD22	1.81	0.46
9:J:86:TYR:C	9:J:87:LEU:HD12	2.41	0.46
2:B:971:HIS:O	2:B:974:SER:OG	2.28	0.46
3:C:301:THR:O	3:C:305:VAL:HG23	2.16	0.46
4:E:475:ASP:OD1	4:E:475:ASP:N	2.47	0.46
6:G:108:HIS:NE2	6:G:112:LYS:HE3	2.31	0.46
6:G:111:GLU:O	6:G:115:LYS:HG3	2.15	0.46
9:K:86:TYR:CD2	9:K:131:SER:HA	2.51	0.46
1:A:709:HIS:O	1:A:713:LYS:HG3	2.15	0.46
8:I:251:ASP:OD1	8:I:251:ASP:N	2.47	0.46
8:I:266:LEU:HD12	8:I:266:LEU:H	1.80	0.46
9:J:399:ALA:HA	9:J:408:GLN:O	2.16	0.46
9:K:324:HIS:CE1	9:K:351:LEU:HD12	2.51	0.46
1:A:510:LYS:HD3	1:A:510:LYS:HA	1.59	0.45
9:J:86:TYR:CD2	9:J:131:SER:HA	2.51	0.45
9:J:27:ASN:H	9:J:27:ASN:ND2	2.09	0.45
9:J:142:ASP:OD2	9:J:142:ASP:N	2.49	0.45
9:K:54:MET:HG2	9:K:132:VAL:O	2.16	0.45
9:K:138:MET:HG2	9:K:140:GLN:NE2	2.30	0.45
9:K:263:ASP:OD2	9:K:266:ARG:HB2	2.16	0.45
1:A:1072:GLU:HG3	1:A:1076:GLN:HE21	1.81	0.45
4:E:339:GLU:O	4:E:343:ASN:N	2.48	0.45
4:E:364:VAL:HG13	6:G:87:MET:HE2	1.98	0.45
9:J:54:MET:HG2	9:J:132:VAL:O	2.16	0.45
9:J:263:ASP:OD2	9:J:266:ARG:HB2	2.16	0.45
9:J:391:CYS:SG	9:J:394:TYR:HB2	2.57	0.45
1:A:1056:PRO:C	1:A:1058:GLU:H	2.24	0.45
2:B:1120:TRP:HZ2	9:J:318:LEU:HD11	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:26:SER:HA	6:G:29:ARG:NH1	2.31	0.45
7:H:14:ASP:OD1	7:H:103:ARG:NH1	2.38	0.45
9:J:253:VAL:HG12	9:J:259:LEU:HG	1.99	0.45
9:J:285:HIS:HD2	9:J:329:THR:HA	1.81	0.45
9:K:301:SER:OG	9:K:302:THR:N	2.49	0.45
2:B:916:GLU:OE2	2:B:916:GLU:N	2.38	0.45
3:D:213:ILE:O	3:D:216:GLY:N	2.49	0.45
4:E:329:LYS:HA	4:E:329:LYS:HD3	1.60	0.45
4:E:345:THR:O	4:E:347:GLU:HB2	2.16	0.45
9:K:386:ILE:H	9:K:402:ALA:HA	1.82	0.45
9:K:391:CYS:SG	9:K:394:TYR:HB2	2.57	0.45
1:A:978:VAL:HB	1:A:979:ASN:C	2.42	0.45
1:A:1117:ILE:HD12	1:A:1117:ILE:HA	1.77	0.45
2:B:926:ARG:O	2:B:930:VAL:HG23	2.16	0.45
4:E:366:LEU:HD12	4:E:366:LEU:HA	1.81	0.45
9:J:245:LYS:HB2	9:J:294:ASP:OD1	2.17	0.45
1:A:1131:GLN:HB3	1:A:1135:TYR:CZ	2.52	0.45
2:B:470:ARG:HH11	5:F:15:LEU:CD2	2.29	0.45
2:B:918:CYS:O	2:B:921:ILE:HG22	2.17	0.45
3:C:275:MET:HE3	3:C:311:TYR:CD1	2.51	0.45
8:I:242:ILE:HD11	8:I:248:TYR:CE1	2.51	0.45
9:J:324:HIS:CE1	9:J:351:LEU:HD12	2.51	0.45
1:A:512:PRO:HA	1:A:515:LEU:HD12	1.99	0.45
2:B:405:TYR:HE1	5:F:13:GLN:HB2	1.72	0.45
9:J:157:VAL:O	9:J:176:PRO:HB2	2.17	0.45
9:K:245:LYS:HB2	9:K:294:ASP:OD1	2.17	0.45
9:K:328:VAL:HA	9:K:345:SER:HB2	1.99	0.45
1:A:852:GLU:HG3	1:A:881:PHE:HD2	1.80	0.45
2:B:478:VAL:HG22	8:I:288:LYS:HG2	1.98	0.45
2:B:491:GLU:OE2	2:B:533:LYS:NZ	2.46	0.45
2:B:562:ASP:OD1	2:B:647:LYS:NZ	2.50	0.45
3:D:137:HIS:HA	3:D:151:ASN:HD21	1.81	0.45
9:J:328:VAL:HA	9:J:345:SER:HB2	1.99	0.45
9:K:142:ASP:OD2	9:K:142:ASP:N	2.49	0.45
9:K:253:VAL:HG12	9:K:259:LEU:HG	1.98	0.45
1:A:615:ARG:HB3	1:A:619:CYS:HB2	1.99	0.44
1:A:1132:VAL:HA	1:A:1135:TYR:CD2	2.52	0.44
1:A:1194:LEU:HB3	1:A:1199:GLU:OE2	2.17	0.44
3:C:347:MET:HE2	3:C:347:MET:HB3	1.69	0.44
3:D:47:LYS:HE2	3:D:319:GLU:OE2	2.17	0.44
9:K:175:LYS:HB3	9:K:175:LYS:HE2	1.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:210:SER:HB2	9:K:212:TRP:CE2	2.52	0.44
1:A:828:ILE:O	1:A:832:ILE:HG13	2.17	0.44
1:A:977:TRP:HE1	1:A:1210:MET:C	2.25	0.44
1:A:1208:TYR:CZ	1:A:1214:THR:HB	2.52	0.44
4:E:360:ARG:HD3	6:G:94:TYR:CD1	2.52	0.44
6:G:263:LEU:HD23	6:G:263:LEU:HA	1.84	0.44
9:K:407:LEU:HD12	9:K:408:GLN:H	1.82	0.44
3:C:67:ASP:O	3:C:71:GLU:HB2	2.18	0.44
3:C:136:LEU:HB3	3:C:148:CYS:HB3	1.97	0.44
7:H:84:ASP:N	7:H:84:ASP:OD1	2.50	0.44
2:B:526:ASP:O	2:B:527:TYR:CG	2.70	0.44
1:A:528:GLU:HA	1:A:531:TYR:HB3	1.99	0.44
8:I:333:LEU:O	8:I:337:LEU:HB2	2.15	0.44
7:H:114:GLU:O	7:H:114:GLU:HG2	2.18	0.44
9:J:210:SER:HB2	9:J:212:TRP:CE2	2.52	0.44
9:J:217:TYR:CD2	9:J:218:ASN:N	2.86	0.44
9:K:157:VAL:O	9:K:176:PRO:HB2	2.17	0.44
2:B:838:SER:HB2	2:B:959:VAL:CG2	2.46	0.44
4:E:340:MET:O	4:E:344:GLU:N	2.50	0.44
1:A:698:SER:HA	1:A:729:GLN:NE2	2.32	0.44
1:A:744:LYS:HE2	6:G:74:PHE:CE2	2.52	0.44
2:B:1076:LEU:CG	2:B:1095:ASN:HD21	2.30	0.44
3:D:14:GLU:CD	3:D:14:GLU:H	2.26	0.44
3:D:132:TRP:CE3	3:D:132:TRP:HA	2.53	0.44
6:G:230:GLU:HG3	6:G:232:ALA:H	1.82	0.44
7:H:80:LEU:HD13	7:H:80:LEU:HA	1.77	0.44
9:J:316:GLN:O	9:J:316:GLN:HG3	2.18	0.44
9:J:369:ASP:N	9:J:369:ASP:OD1	2.50	0.44
9:K:238:SER:OG	9:K:284:ILE:O	2.33	0.44
1:A:1205:ILE:HG23	9:K:24:LYS:CD	2.48	0.44
2:B:1019:TYR:CD2	2:B:1019:TYR:C	2.96	0.44
3:C:28:LYS:O	3:C:31:ARG:HD3	2.18	0.44
8:I:260:HIS:HB2	8:I:295:ILE:HG21	1.99	0.44
9:J:386:ILE:H	9:J:402:ALA:HA	1.82	0.44
1:A:876:TYR:O	1:A:878:PRO:HD3	2.18	0.43
2:B:452:PHE:HE1	2:B:462:THR:HA	1.82	0.43
2:B:591:LEU:HD22	2:B:591:LEU:HA	1.78	0.43
7:H:7:GLU:OE2	7:H:7:GLU:N	2.51	0.43
8:I:236:ARG:HG3	8:I:239:ARG:HH12	1.82	0.43
9:J:407:LEU:HD12	9:J:408:GLN:H	1.82	0.43
9:K:285:HIS:HD2	9:K:329:THR:HA	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:854:MET:SD	1:A:1120:LEU:HD23	2.58	0.43
2:B:424:ASP:OD2	2:B:426:LEU:HB2	2.17	0.43
1:A:1186:ARG:HD2	1:A:1186:ARG:N	2.34	0.43
2:B:405:TYR:CZ	5:F:13:GLN:CD	2.95	0.43
2:B:916:GLU:O	2:B:920:MET:HG2	2.18	0.43
2:B:1116:ARG:O	2:B:1120:TRP:HB3	2.19	0.43
9:K:233:HIS:CD2	9:K:237:VAL:HG22	2.53	0.43
1:A:1057:SER:HB3	1:A:1097:CYS:HB3	2.01	0.43
4:E:433:MET:HG3	4:E:433:MET:O	2.19	0.43
9:K:123:SER:OG	9:K:124:ASN:N	2.52	0.43
2:B:728:ASP:OD1	2:B:729:ALA:N	2.51	0.43
2:B:1087:ILE:HG13	9:J:27:ASN:OD1	2.18	0.43
3:C:330:TYR:HB3	3:C:333:TYR:CD2	2.53	0.43
5:F:142:TYR:HB2	7:H:44:ARG:HD2	2.00	0.43
8:I:303:ARG:H	8:I:303:ARG:HG2	1.60	0.43
1:A:524:TYR:C	1:A:526:ALA:H	2.26	0.43
1:A:763:ASP:OD2	1:A:764:ILE:N	2.51	0.43
2:B:842:ILE:HB	2:B:959:VAL:HG22	2.00	0.43
3:C:31:ARG:HG2	3:C:32:VAL:N	2.32	0.43
5:F:110:LEU:HD22	5:F:217:CYS:SG	2.59	0.43
8:I:200:GLU:N	8:I:200:GLU:OE2	2.51	0.43
9:J:156:LEU:HD23	9:J:176:PRO:HG3	2.00	0.43
1:A:746:LYS:HA	1:A:746:LYS:HD2	1.80	0.43
1:A:1104:PHE:HA	1:A:1107:TYR:CZ	2.54	0.43
1:A:1204:TYR:O	9:K:20:ILE:HG13	2.19	0.43
5:F:31:ALA:O	5:F:33:THR:N	2.52	0.43
9:K:131:SER:OG	9:K:151:TYR:HB2	2.18	0.43
9:K:217:TYR:CD2	9:K:218:ASN:N	2.86	0.43
2:B:961:THR:HG1	2:B:964:GLU:CD	2.26	0.43
3:C:232:GLU:CD	3:C:232:GLU:H	2.27	0.43
8:I:293:ASN:OD1	8:I:293:ASN:N	2.51	0.43
9:J:127:SER:O	9:J:174:LEU:HD12	2.19	0.43
9:J:266:ARG:HG3	9:J:266:ARG:NH1	2.11	0.43
9:K:316:GLN:O	9:K:316:GLN:HG3	2.18	0.43
1:A:1143:ARG:HB3	1:A:1143:ARG:NH1	2.34	0.43
2:B:1034:LEU:HD23	2:B:1034:LEU:HA	1.75	0.43
3:D:301:THR:O	3:D:305:VAL:HG23	2.19	0.43
5:F:35:ARG:O	5:F:37:LEU:HD23	2.19	0.43
9:J:362:GLN:OE1	9:J:372:PRO:HD3	2.19	0.43
9:J:374:LEU:HD12	9:J:375:LEU:H	1.84	0.43
9:K:23:GLU:HA	9:K:26:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:156:LEU:HD23	9:K:176:PRO:HG3	2.00	0.43
9:K:358:ILE:H	9:K:358:ILE:HG12	1.41	0.43
1:A:730:LYS:HB2	1:A:730:LYS:HE3	1.70	0.43
1:A:978:VAL:CA	9:K:31:LYS:HE2	2.49	0.43
2:B:941:ASP:O	2:B:944:LEU:HB3	2.19	0.43
3:D:136:LEU:HB3	3:D:148:CYS:SG	2.59	0.43
4:E:440:LEU:HA	4:E:440:LEU:HD23	1.71	0.43
8:I:204:THR:C	8:I:206:TRP:H	2.27	0.43
8:I:305:ASP:OD1	8:I:305:ASP:N	2.52	0.43
9:J:123:SER:OG	9:J:124:ASN:N	2.52	0.43
9:J:136:LYS:HE3	9:J:136:LYS:HB3	1.58	0.43
9:K:161:GLU:O	9:K:165:SER:N	2.42	0.43
9:K:230:ILE:HG21	9:K:262:HIS:CD2	2.54	0.43
2:B:840:ASN:OD1	2:B:989:PRO:HB2	2.18	0.42
9:J:65:PHE:HB3	9:J:68:HIS:HB2	2.01	0.42
9:J:131:SER:OG	9:J:151:TYR:HB2	2.18	0.42
9:J:230:ILE:HG21	9:J:262:HIS:CD2	2.54	0.42
9:J:316:GLN:HE21	9:J:316:GLN:HB2	1.69	0.42
9:K:389:ASP:OD2	9:K:390:TRP:N	2.52	0.42
2:B:561:TYR:CD1	2:B:647:LYS:HB2	2.54	0.42
9:K:17:GLU:HA	9:K:20:ILE:HD11	2.01	0.42
9:K:145:VAL:HG23	9:K:158:PHE:HB2	2.00	0.42
1:A:1110:GLU:O	1:A:1113:VAL:HG12	2.19	0.42
1:A:1134:MET:O	1:A:1138:LYS:HG3	2.19	0.42
2:B:1079:PHE:HB3	2:B:1088:PHE:HB2	2.01	0.42
5:F:104:LEU:O	5:F:105:THR:OG1	2.29	0.42
8:I:228:TRP:HA	8:I:228:TRP:CE3	2.55	0.42
9:J:233:HIS:CD2	9:J:237:VAL:HG22	2.53	0.42
9:K:16:SER:O	9:K:20:ILE:HG12	2.20	0.42
9:K:362:GLN:OE1	9:K:372:PRO:HD3	2.19	0.42
2:B:593:GLU:OE1	2:B:596:ARG:NH1	2.52	0.42
2:B:839:LYS:HG3	2:B:844:TYR:OH	2.19	0.42
5:F:106:LYS:HE2	5:F:108:GLN:HG3	2.02	0.42
9:J:23:GLU:HA	9:J:26:ILE:HD12	2.01	0.42
9:J:145:VAL:HG23	9:J:158:PHE:HB2	2.01	0.42
1:A:880:HIS:NE2	1:A:882:ASN:HB2	2.34	0.42
2:B:905:GLU:O	2:B:908:LYS:HG3	2.20	0.42
3:C:280:MET:HE3	3:C:280:MET:HB3	1.90	0.42
5:F:23:ASP:OD2	8:I:298:ARG:NH2	2.53	0.42
9:K:72:GLU:HA	9:K:93:ILE:O	2.19	0.42
2:B:698:LYS:HB3	2:B:698:LYS:HE2	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:91:LYS:O	6:G:95:GLU:HG2	2.19	0.42
9:J:338:GLU:HG2	9:J:339:PRO:CD	2.50	0.42
9:K:374:LEU:HD12	9:K:375:LEU:H	1.84	0.42
3:D:252:GLU:O	3:D:291:PRO:HD2	2.20	0.42
8:I:346:SER:C	8:I:348:THR:H	2.28	0.42
9:J:17:GLU:HA	9:J:20:ILE:HD11	2.01	0.42
9:J:72:GLU:HA	9:J:93:ILE:O	2.19	0.42
9:J:308:LEU:HD12	9:J:319:HIS:HB3	2.01	0.42
9:J:358:ILE:H	9:J:358:ILE:HG12	1.41	0.42
1:A:1111:LYS:O	1:A:1114:THR:HB	2.20	0.42
1:A:1201:TRP:HA	9:K:20:ILE:HD13	2.01	0.42
2:B:491:GLU:OE1	2:B:533:LYS:HD2	2.20	0.42
2:B:1075:ASN:O	2:B:1093:THR:CB	2.68	0.42
2:B:1092:ASN:OD1	9:J:47:ARG:NH2	2.53	0.42
3:D:135:GLY:HA2	3:D:153:ILE:HD11	2.02	0.42
4:E:347:GLU:HG2	4:E:348:ARG:HD3	2.00	0.42
9:J:16:SER:O	9:J:20:ILE:HG12	2.19	0.42
9:K:127:SER:O	9:K:174:LEU:HD12	2.19	0.42
1:A:1044:ASN:OD1	3:C:324:ASN:HB3	2.19	0.42
1:A:1086:ILE:HG22	1:A:1087:ASP:O	2.19	0.42
1:A:1132:VAL:HG21	1:A:1161:PHE:CZ	2.54	0.42
2:B:972:VAL:O	2:B:975:ILE:HG22	2.20	0.42
4:E:352:CYS:HA	4:E:355:LEU:HG	2.01	0.42
7:H:55:LEU:HD23	7:H:55:LEU:HA	1.92	0.42
8:I:271:ARG:HG3	8:I:271:ARG:HH11	1.84	0.42
9:J:389:ASP:OD2	9:J:390:TRP:N	2.52	0.42
2:B:1097:TYR:OH	9:J:38:PRO:HB3	2.20	0.41
3:C:347:MET:HG2	3:C:348:GLU:N	2.34	0.41
9:K:185:GLN:O	9:K:204:SER:OG	2.38	0.41
5:F:48:TYR:CE2	8:I:305:ASP:HB2	2.55	0.41
9:K:161:GLU:O	9:K:165:SER:OG	2.29	0.41
9:K:269:ALA:HA	9:K:272:LYS:O	2.20	0.41
1:A:509:ASN:O	1:A:510:LYS:HB2	2.21	0.41
2:B:477:LEU:HD23	8:I:176:SER:OG	2.20	0.41
7:H:56:LYS:HA	7:H:56:LYS:HD3	1.70	0.41
9:J:161:GLU:O	9:J:165:SER:N	2.42	0.41
9:J:269:ALA:HA	9:J:272:LYS:O	2.20	0.41
9:K:65:PHE:HB3	9:K:68:HIS:HB2	2.01	0.41
9:K:308:LEU:HD12	9:K:319:HIS:HB3	2.01	0.41
9:K:309:TRP:CZ2	9:K:317:ARG:HG2	2.56	0.41
9:K:310:ASP:HB2	9:K:318:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:357:ARG:HA	9:K:360:GLU:HG3	2.02	0.41
1:A:977:TRP:CD1	1:A:1209:ILE:O	2.73	0.41
4:E:421:SER:O	4:E:424:ASP:HB3	2.20	0.41
7:H:63:LEU:HB3	7:H:68:ARG:NH1	2.35	0.41
9:J:310:ASP:HB2	9:J:318:LEU:HD11	2.03	0.41
9:K:89:ALA:HA	9:K:124:ASN:O	2.21	0.41
1:A:999:ARG:NH1	1:A:1139:ASP:OD1	2.53	0.41
1:A:1129:LEU:HD12	1:A:1132:VAL:HB	2.01	0.41
2:B:1124:LEU:HD13	9:J:312:ARG:HH21	1.86	0.41
5:F:223:ASN:O	5:F:225:ASN:N	2.53	0.41
6:G:239:ALA:O	6:G:242:LYS:HE3	2.21	0.41
9:J:59:TYR:CE2	9:J:76:PHE:HB2	2.55	0.41
9:K:250:LEU:HG	9:K:262:HIS:HB2	2.02	0.41
9:K:351:LEU:HD22	9:K:377:MET:HB2	2.01	0.41
9:K:369:ASP:OD1	9:K:369:ASP:N	2.50	0.41
3:C:354:GLN:CD	3:C:354:GLN:H	2.28	0.41
3:D:58:ARG:O	3:D:62:THR:HG23	2.21	0.41
9:K:31:LYS:O	9:K:35:LYS:HB2	2.21	0.41
9:K:56:LEU:HD21	9:K:401:ALA:HB2	2.03	0.41
1:A:530:LYS:HA	1:A:533:GLU:HG3	2.01	0.41
1:A:566:MET:O	1:A:570:LYS:HG3	2.21	0.41
2:B:446:THR:HG22	2:B:471:TRP:CZ2	2.55	0.41
2:B:489:LEU:N	2:B:490:PRO:HD2	2.36	0.41
2:B:1070:HIS:HE1	2:B:1100:SER:N	2.17	0.41
9:J:27:ASN:ND2	9:J:27:ASN:N	2.68	0.41
9:J:75:MET:HE3	9:J:75:MET:HB2	1.77	0.41
9:J:351:LEU:HD22	9:J:377:MET:HB2	2.01	0.41
1:A:561:SER:O	1:A:563:GLU:N	2.54	0.41
1:A:587:ARG:HE	1:A:587:ARG:HB2	1.49	0.41
1:A:991:ASP:CG	1:A:993:GLY:H	2.28	0.41
2:B:692:ASP:O	2:B:696:ARG:HG3	2.21	0.41
3:C:261:ASP:HA	3:C:266:ASP:OD1	2.21	0.41
9:J:31:LYS:O	9:J:35:LYS:HB2	2.21	0.41
9:J:309:TRP:CZ2	9:J:317:ARG:HG2	2.56	0.41
9:K:59:TYR:CE2	9:K:76:PHE:HB2	2.56	0.41
9:K:201:VAL:HB	9:K:242:PHE:CE2	2.48	0.41
1:A:839:PHE:O	1:A:843:GLY:N	2.54	0.41
2:B:435:LEU:HD21	5:F:11:PHE:CG	2.55	0.41
2:B:749:LEU:HD13	2:B:935:ILE:HD11	2.03	0.41
2:B:752:LEU:HD21	2:B:948:LEU:CD2	2.51	0.41
2:B:944:LEU:HG	2:B:945:GLY:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:949:LEU:HA	2:B:952:GLU:HG3	2.03	0.41
3:D:191:MET:HB2	3:D:191:MET:HE3	1.83	0.41
9:J:253:VAL:HB	9:J:284:ILE:HG21	2.03	0.41
9:K:27:ASN:ND2	9:K:27:ASN:N	2.68	0.41
9:K:52:PRO:HD2	9:K:80:ARG:O	2.21	0.41
9:K:253:VAL:HB	9:K:284:ILE:HG21	2.03	0.41
3:C:55:ARG:H	3:C:55:ARG:HG2	1.67	0.41
8:I:277:ASP:O	8:I:312:LYS:N	2.44	0.41
9:J:34:LYS:O	9:J:37:SER:OG	2.39	0.41
9:K:155:VAL:HB	9:K:180:LEU:HB2	2.03	0.41
9:K:158:PHE:CE2	9:K:176:PRO:HB3	2.56	0.41
1:A:818:GLN:HE22	1:A:1183:LEU:N	2.14	0.40
1:A:1070:VAL:HA	1:A:1073:GLN:HG3	2.02	0.40
1:A:1127:ARG:HA	1:A:1127:ARG:CZ	2.50	0.40
4:E:345:THR:O	4:E:346:HIS:C	2.64	0.40
9:K:34:LYS:O	9:K:37:SER:OG	2.39	0.40
1:A:978:VAL:CG1	9:K:27:ASN:O	2.65	0.40
1:A:995:LYS:HE2	1:A:995:LYS:HB3	1.89	0.40
1:A:1218:LEU:HD13	1:A:1218:LEU:HA	1.89	0.40
2:B:558:ARG:HH11	2:B:558:ARG:HD2	1.77	0.40
5:F:106:LYS:HD3	5:F:109:ASP:OD1	2.21	0.40
5:F:183:GLN:HG3	6:G:43:ARG:HD3	2.03	0.40
9:J:89:ALA:HA	9:J:124:ASN:O	2.20	0.40
9:J:158:PHE:CE2	9:J:176:PRO:HB3	2.56	0.40
2:B:489:LEU:O	2:B:492:THR:HG23	2.20	0.40
2:B:554:VAL:O	2:B:558:ARG:HG2	2.22	0.40
2:B:702:ASP:OD1	2:B:702:ASP:N	2.53	0.40
2:B:705:LYS:HG2	2:B:706:LEU:H	1.86	0.40
2:B:1140:LYS:HE2	9:J:263:ASP:HB2	2.02	0.40
7:H:120:ARG:O	7:H:121:LEU:HD23	2.21	0.40
8:I:226:ILE:HD11	8:I:320:CYS:HB2	2.04	0.40
9:K:214:LEU:H	9:K:214:LEU:HG	1.56	0.40
2:B:725:ARG:HA	2:B:728:ASP:OD2	2.21	0.40
2:B:946:GLN:O	2:B:950:LEU:N	2.27	0.40
3:D:40:VAL:HG21	7:H:35:GLU:HG2	2.04	0.40
4:E:453:LEU:HD23	4:E:453:LEU:HA	1.77	0.40
9:J:52:PRO:HD2	9:J:80:ARG:O	2.21	0.40
9:J:250:LEU:HG	9:J:262:HIS:HB2	2.02	0.40
9:K:229:HIS:ND1	9:K:229:HIS:C	2.79	0.40
1:A:977:TRP:HZ3	9:K:29:GLU:HG2	1.85	0.40
2:B:648:ARG:O	2:B:651:SER:OG	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:353:ARG:HA	3:C:353:ARG:HD2	1.89	0.40
3:D:213:ILE:HG22	3:D:214:GLY:N	2.36	0.40
3:D:275:MET:HE2	3:D:275:MET:HB3	1.86	0.40
8:I:273:ILE:CG2	8:I:317:LYS:HD2	2.51	0.40
8:I:337:LEU:O	8:I:337:LEU:HD23	2.22	0.40
9:J:157:VAL:HG13	9:J:178:TYR:H	1.86	0.40
9:J:357:ARG:HA	9:J:360:GLU:HG3	2.02	0.40
9:K:157:VAL:HG13	9:K:178:TYR:H	1.86	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	610/1522 (40%)	555 (91%)	55 (9%)	0	100	100
2	B	629/1154 (54%)	585 (93%)	44 (7%)	0	100	100
3	C	368/405 (91%)	341 (93%)	27 (7%)	0	100	100
3	D	361/405 (89%)	330 (91%)	31 (9%)	0	100	100
4	E	165/491 (34%)	158 (96%)	7 (4%)	0	100	100
5	F	222/240 (92%)	190 (86%)	30 (14%)	2 (1%)	14	47
6	G	160/267 (60%)	155 (97%)	5 (3%)	0	100	100
7	H	124/305 (41%)	113 (91%)	11 (9%)	0	100	100
8	I	183/351 (52%)	167 (91%)	16 (9%)	0	100	100
9	J	384/431 (89%)	368 (96%)	16 (4%)	0	100	100
9	K	384/431 (89%)	368 (96%)	16 (4%)	0	100	100
All	All	3590/6002 (60%)	3330 (93%)	258 (7%)	2 (0%)	49	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	F	32	LEU
5	F	31	ALA

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	567/1364 (42%)	515 (91%)	52 (9%)	8	33
2	B	590/1060 (56%)	526 (89%)	64 (11%)	6	27
3	C	320/351 (91%)	300 (94%)	20 (6%)	16	48
3	D	315/351 (90%)	284 (90%)	31 (10%)	7	31
4	E	137/448 (31%)	125 (91%)	12 (9%)	9	35
5	F	198/209 (95%)	179 (90%)	19 (10%)	8	32
6	G	130/238 (55%)	123 (95%)	7 (5%)	20	53
7	H	112/280 (40%)	92 (82%)	20 (18%)	2	9
8	I	170/322 (53%)	149 (88%)	21 (12%)	4	21
9	J	348/382 (91%)	215 (62%)	133 (38%)	0	0
9	K	348/382 (91%)	215 (62%)	133 (38%)	0	0
All	All	3235/5387 (60%)	2723 (84%)	512 (16%)	4	13

All (512) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	522	ARG
1	A	552	VAL
1	A	561	SER
1	A	569	LEU
1	A	587	ARG
1	A	592	GLN
1	A	599	SER
1	A	613	SER
1	A	622	ILE
1	A	652	LEU

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Mol	Chain	Res	Type
1	A	684	LEU
1	A	695	THR
1	A	698	SER
1	A	705	VAL
1	A	706	SER
1	A	731	ASN
1	A	735	THR
1	A	747	ASP
1	A	752	SER
1	A	778	VAL
1	A	808	LEU
1	A	823	TYR
1	A	830	THR
1	A	851	ASN
1	A	863	SER
1	A	867	ASP
1	A	973	THR
1	A	977	TRP
1	A	978	VAL
1	A	983	THR
1	A	1019	THR
1	A	1022	SER
1	A	1033	MET
1	A	1041	VAL
1	A	1043	SER
1	A	1055	HIS
1	A	1060	LEU
1	A	1079	GLU
1	A	1085	GLU
1	A	1102	HIS
1	A	1113	VAL
1	A	1116	ILE
1	A	1117	ILE
1	A	1125	THR
1	A	1164	ASP
1	A	1176	THR
1	A	1182	ARG
1	A	1193	THR
1	A	1196	SER
1	A	1208	TYR
1	A	1210	MET
1	A	1214	THR

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Mol	Chain	Res	Type
2	B	403	SER
2	B	408	THR
2	B	413	LEU
2	B	416	THR
2	B	418	ILE
2	B	437	LEU
2	B	440	GLU
2	B	443	LEU
2	B	448	LEU
2	B	449	LEU
2	B	469	ILE
2	B	473	ASP
2	B	477	LEU
2	B	483	VAL
2	B	491	GLU
2	B	492	THR
2	B	495	CYS
2	B	496	ILE
2	B	497	SER
2	B	506	SER
2	B	516	ASP
2	B	523	LEU
2	B	528	ILE
2	B	529	SER
2	B	537	VAL
2	B	560	ASP
2	B	566	ASN
2	B	567	THR
2	B	582	THR
2	B	591	LEU
2	B	611	LYS
2	B	619	ASP
2	B	627	THR
2	B	638	THR
2	B	653	ILE
2	B	681	LEU
2	B	706	LEU
2	B	719	ILE
2	B	738	SER
2	B	741	ASP
2	B	836	GLU
2	B	839	LYS

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Mol	Chain	Res	Type
2	B	841	ILE
2	B	876	SER
2	B	878	ILE
2	B	881	SER
2	B	892	ILE
2	B	910	LEU
2	B	917	THR
2	B	937	GLU
2	B	944	LEU
2	B	959	VAL
2	B	960	THR
2	B	961	THR
2	B	1034	LEU
2	B	1076	LEU
2	B	1077	GLN
2	B	1081	SER
2	B	1086	VAL
2	B	1093	THR
2	B	1116	ARG
2	B	1119	ASN
2	B	1136	ASN
2	B	1137	THR
3	C	44	LEU
3	C	90	LYS
3	C	93	VAL
3	C	96	ASP
3	C	99	VAL
3	C	123	SER
3	C	152	ASP
3	C	174	VAL
3	C	180	VAL
3	C	189	ARG
3	C	192	THR
3	C	201	TYR
3	C	208	ILE
3	C	213	ILE
3	C	231	ASP
3	C	233	SER
3	C	243	SER
3	C	303	ARG
3	C	337	ASP
3	C	344	SER

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Mol	Chain	Res	Type
3	D	8	VAL
3	D	16	VAL
3	D	42	TYR
3	D	46	GLU
3	D	57	THR
3	D	60	ASP
3	D	71	GLU
3	D	89	LEU
3	D	127	GLU
3	D	132	TRP
3	D	174	VAL
3	D	178	ASP
3	D	180	VAL
3	D	186	THR
3	D	188	ASP
3	D	191	MET
3	D	192	THR
3	D	194	SER
3	D	213	ILE
3	D	215	THR
3	D	227	ASP
3	D	229	ILE
3	D	231	ASP
3	D	233	SER
3	D	236	SER
3	D	260	THR
3	D	315	LEU
3	D	329	ASP
3	D	348	GLU
3	D	361	SER
3	D	369	ASN
4	E	353	ILE
4	E	366	LEU
4	E	401	ARG
4	E	406	THR
4	E	412	CYS
4	E	415	LEU
4	E	416	LEU
4	E	422	VAL
4	E	424	ASP
4	E	438	SER
4	E	459	PHE

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Mol	Chain	Res	Type
4	E	468	ILE
5	F	23	ASP
5	F	37	LEU
5	F	54	SER
5	F	59	ILE
5	F	61	ILE
5	F	75	SER
5	F	82	ASP
5	F	84	GLU
5	F	108	GLN
5	F	116	ILE
5	F	151	VAL
5	F	154	LEU
5	F	156	ASP
5	F	167	VAL
5	F	168	PHE
5	F	183	GLN
5	F	213	VAL
5	F	225	ASN
5	F	228	VAL
6	G	31	LYS
6	G	41	SER
6	G	42	ILE
6	G	60	SER
6	G	100	THR
6	G	248	THR
6	G	266	LYS
7	H	19	ILE
7	H	25	SER
7	H	32	SER
7	H	33	LEU
7	H	40	VAL
7	H	56	LYS
7	H	66	GLU
7	H	67	GLU
7	H	79	ILE
7	H	80	LEU
7	H	85	SER
7	H	91	THR
7	H	97	ILE
7	H	101	ILE
7	H	111	VAL

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Mol	Chain	Res	Type
7	H	114	GLU
7	H	115	ILE
7	H	119	LEU
7	H	125	ASP
7	H	129	LEU
8	I	178	ASP
8	I	198	VAL
8	I	204	THR
8	I	216	ILE
8	I	226	ILE
8	I	242	ILE
8	I	251	ASP
8	I	256	THR
8	I	261	CYS
8	I	265	SER
8	I	268	LYS
8	I	298	ARG
8	I	299	SER
8	I	301	SER
8	I	304	GLN
8	I	305	ASP
8	I	309	LEU
8	I	332	THR
8	I	337	LEU
8	I	346	SER
8	I	348	THR
9	J	18	GLU
9	J	22	GLN
9	J	23	GLU
9	J	27	ASN
9	J	28	GLU
9	J	32	ILE
9	J	34	LYS
9	J	35	LYS
9	J	37	SER
9	J	42	ASP
9	J	43	LEU
9	J	44	ILE
9	J	46	THR
9	J	47	ARG
9	J	49	LEU
9	J	56	LEU

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Mol	Chain	Res	Type
9	J	62	GLN
9	J	63	GLN
9	J	64	ILE
9	J	67	GLU
9	J	71	THR
9	J	72	GLU
9	J	75	MET
9	J	77	LEU
9	J	82	ASP
9	J	83	VAL
9	J	85	LYS
9	J	88	LEU
9	J	93	ILE
9	J	95	LEU
9	J	98	LEU
9	J	100	GLN
9	J	122	ILE
9	J	123	SER
9	J	125	LEU
9	J	127	SER
9	J	130	GLU
9	J	134	SER
9	J	136	LYS
9	J	137	LEU
9	J	142	ASP
9	J	143	SER
9	J	144	CYS
9	J	145	VAL
9	J	150	ASN
9	J	161	GLU
9	J	162	SER
9	J	168	SER
9	J	170	SER
9	J	174	LEU
9	J	175	LYS
9	J	181	THR
9	J	185	GLN
9	J	188	THR
9	J	189	SER
9	J	196	SER
9	J	197	LYS
9	J	210	SER

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Mol	Chain	Res	Type
9	J	213	ASP
9	J	214	LEU
9	J	215	ASN
9	J	218	ASN
9	J	220	SER
9	J	221	ASP
9	J	227	LYS
9	J	229	HIS
9	J	234	GLU
9	J	238	SER
9	J	239	ASP
9	J	241	ARG
9	J	245	LYS
9	J	246	HIS
9	J	247	GLN
9	J	248	ASP
9	J	249	LEU
9	J	259	LEU
9	J	263	ASP
9	J	264	ILE
9	J	265	ARG
9	J	266	ARG
9	J	270	SER
9	J	271	THR
9	J	272	LYS
9	J	277	VAL
9	J	281	SER
9	J	286	SER
9	J	297	LEU
9	J	301	SER
9	J	302	THR
9	J	303	ASP
9	J	304	LYS
9	J	305	THR
9	J	306	ILE
9	J	311	LEU
9	J	312	ARG
9	J	315	ASN
9	J	316	GLN
9	J	318	LEU
9	J	320	THR
9	J	322	GLU

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Mol	Chain	Res	Type
9	J	325	GLU
9	J	326	ASP
9	J	329	THR
9	J	330	LYS
9	J	332	SER
9	J	341	LEU
9	J	343	SER
9	J	344	THR
9	J	345	SER
9	J	355	LEU
9	J	356	SER
9	J	357	ARG
9	J	358	ILE
9	J	366	GLU
9	J	368	GLN
9	J	373	GLU
9	J	377	MET
9	J	382	THR
9	J	383	SER
9	J	384	CYS
9	J	386	ILE
9	J	387	ASP
9	J	388	MET
9	J	391	CYS
9	J	395	ASN
9	J	397	THR
9	J	398	MET
9	J	400	THR
9	J	406	ILE
9	J	408	GLN
9	J	409	ILE
9	J	413	SER
9	J	416	ILE
9	K	18	GLU
9	K	22	GLN
9	K	23	GLU
9	K	27	ASN
9	K	28	GLU
9	K	32	ILE
9	K	34	LYS
9	K	35	LYS
9	K	37	SER

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Mol	Chain	Res	Type
9	K	42	ASP
9	K	43	LEU
9	K	44	ILE
9	K	46	THR
9	K	47	ARG
9	K	49	LEU
9	K	56	LEU
9	K	62	GLN
9	K	63	GLN
9	K	64	ILE
9	K	67	GLU
9	K	71	THR
9	K	72	GLU
9	K	75	MET
9	K	77	LEU
9	K	82	ASP
9	K	83	VAL
9	K	85	LYS
9	K	88	LEU
9	K	93	ILE
9	K	95	LEU
9	K	98	LEU
9	K	100	GLN
9	K	122	ILE
9	K	123	SER
9	K	125	LEU
9	K	127	SER
9	K	130	GLU
9	K	134	SER
9	K	136	LYS
9	K	137	LEU
9	K	142	ASP
9	K	143	SER
9	K	144	CYS
9	K	145	VAL
9	K	150	ASN
9	K	161	GLU
9	K	162	SER
9	K	168	SER
9	K	170	SER
9	K	174	LEU
9	K	175	LYS

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Mol	Chain	Res	Type
9	K	181	THR
9	K	185	GLN
9	K	188	THR
9	K	189	SER
9	K	196	SER
9	K	197	LYS
9	K	210	SER
9	K	213	ASP
9	K	214	LEU
9	K	215	ASN
9	K	218	ASN
9	K	220	SER
9	K	221	ASP
9	K	227	LYS
9	K	229	HIS
9	K	234	GLU
9	K	238	SER
9	K	239	ASP
9	K	241	ARG
9	K	245	LYS
9	K	246	HIS
9	K	247	GLN
9	K	248	ASP
9	K	249	LEU
9	K	259	LEU
9	K	263	ASP
9	K	264	ILE
9	K	265	ARG
9	K	266	ARG
9	K	270	SER
9	K	271	THR
9	K	272	LYS
9	K	277	VAL
9	K	281	SER
9	K	286	SER
9	K	297	LEU
9	K	301	SER
9	K	302	THR
9	K	303	ASP
9	K	304	LYS
9	K	305	THR
9	K	306	ILE

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Mol	Chain	Res	Type
9	K	311	LEU
9	K	312	ARG
9	K	315	ASN
9	K	316	GLN
9	K	318	LEU
9	K	320	THR
9	K	322	GLU
9	K	325	GLU
9	K	326	ASP
9	K	329	THR
9	K	330	LYS
9	K	332	SER
9	K	341	LEU
9	K	343	SER
9	K	344	THR
9	K	345	SER
9	K	355	LEU
9	K	356	SER
9	K	357	ARG
9	K	358	ILE
9	K	366	GLU
9	K	368	GLN
9	K	373	GLU
9	K	377	MET
9	K	382	THR
9	K	383	SER
9	K	384	CYS
9	K	386	ILE
9	K	387	ASP
9	K	388	MET
9	K	391	CYS
9	K	395	ASN
9	K	397	THR
9	K	398	MET
9	K	400	THR
9	K	406	ILE
9	K	408	GLN
9	K	409	ILE
9	K	413	SER
9	K	416	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	511	ASN
1	A	549	ASN
1	A	579	ASN
1	A	665	HIS
1	A	720	HIS
1	A	729	GLN
1	A	799	ASN
1	A	803	GLN
1	A	827	ASN
1	A	846	HIS
1	A	856	ASN
1	A	882	ASN
1	A	979	ASN
1	A	1088	GLN
1	A	1119	GLN
1	A	1178	GLN
2	B	421	HIS
2	B	474	ASN
2	B	549	GLN
2	B	584	HIS
2	B	697	GLN
2	B	722	ASN
2	B	888	ASN
2	B	970	ASN
2	B	984	ASN
2	B	997	GLN
2	B	1036	GLN
2	B	1070	HIS
2	B	1075	ASN
2	B	1077	GLN
2	B	1095	ASN
2	B	1110	GLN
2	B	1114	GLN
2	B	1115	ASN
2	B	1119	ASN
3	C	88	GLN
3	C	164	HIS
3	C	222	ASN
3	C	324	ASN
3	C	350	HIS
3	D	20	HIS
3	D	85	GLN
3	D	125	ASN

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Mol	Chain	Res	Type
3	D	151	ASN
3	D	164	HIS
3	D	218	ASN
3	D	222	ASN
3	D	324	ASN
4	E	335	ASN
4	E	392	GLN
4	E	417	ASN
4	E	437	GLN
4	E	442	GLN
5	F	108	GLN
5	F	122	GLN
5	F	165	HIS
5	F	174	GLN
5	F	225	ASN
7	H	95	ASN
8	I	166	GLN
9	J	21	ASN
9	J	22	GLN
9	J	27	ASN
9	J	94	GLN
9	J	99	ASN
9	J	152	HIS
9	J	205	GLN
9	J	246	HIS
9	J	260	HIS
9	J	285	HIS
9	J	316	GLN
9	J	319	HIS
9	J	324	HIS
9	K	21	ASN
9	K	27	ASN
9	K	152	HIS
9	K	205	GLN
9	K	260	HIS
9	K	285	HIS
9	K	316	GLN
9	K	319	HIS
9	K	324	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
5	SEP	F	24	5	8,9,10	0.66	0	7,12,14	0.64	0
5	SEP	F	19	5	8,9,10	0.65	0	7,12,14	0.74	0
5	SEP	F	27	5	8,9,10	0.66	0	7,12,14	0.63	0
5	SEP	F	22	5	8,9,10	0.67	0	7,12,14	0.62	0

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	SEP	F	24	5	-	1/6/8/10	-
5	SEP	F	19	5	-	2/6/8/10	-
5	SEP	F	27	5	-	1/6/8/10	-
5	SEP	F	22	5	-	3/6/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	19	SEP	N-CA-CB-OG
5	F	19	SEP	C-CA-CB-OG

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Mol	Chain	Res	Type	Atoms
5	F	22	SEP	CB-OG-P-O1P
5	F	22	SEP	CB-OG-P-O3P
5	F	27	SEP	C-CA-CB-OG
5	F	24	SEP	N-CA-CB-OG
5	F	22	SEP	CB-OG-P-O2P

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	19	SEP	2	0
5	F	27	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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.

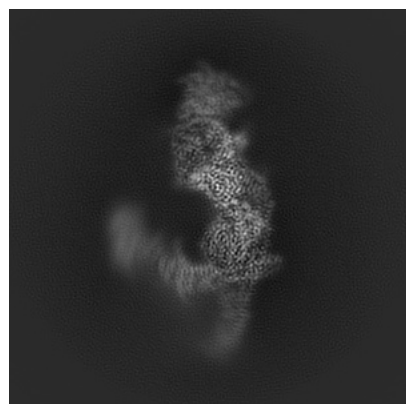
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35093. These allow visual inspection of the internal detail of the map and identification of artifacts.

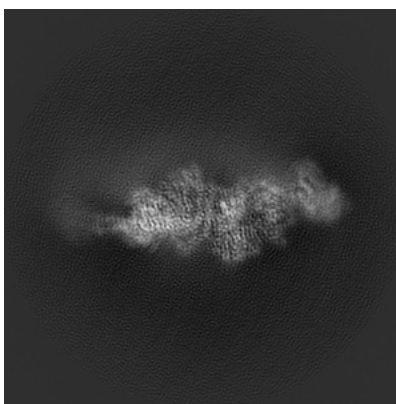
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

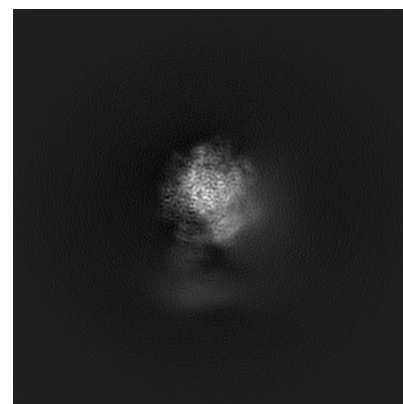
6.1.1 Primary map



X

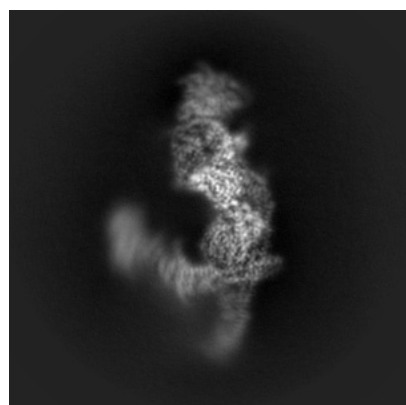


Y

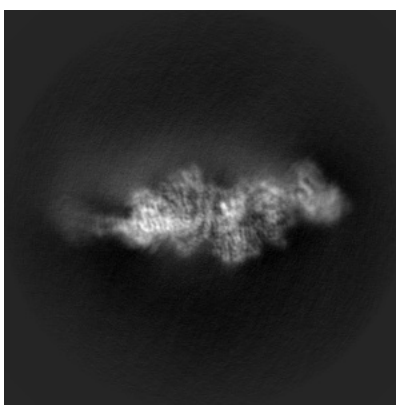


Z

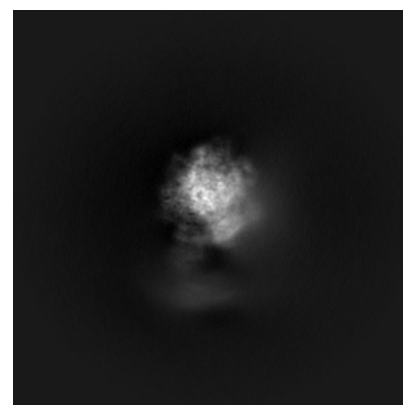
6.1.2 Raw map



X



Y

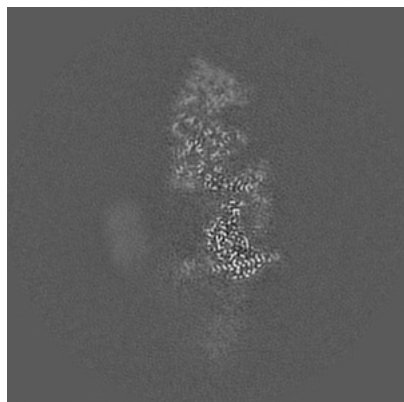


Z

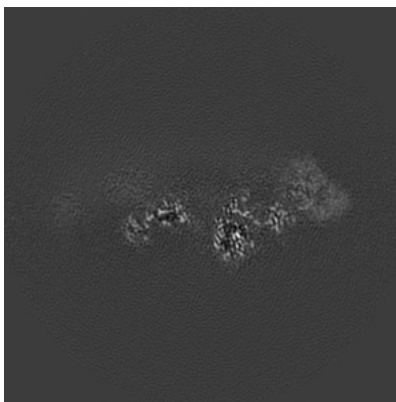
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

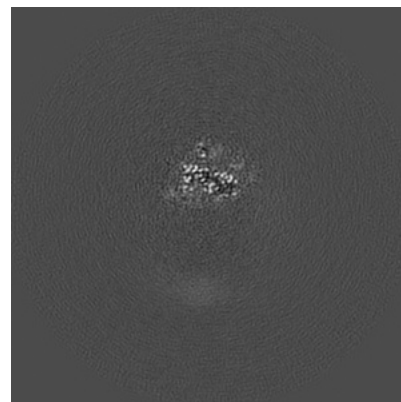
6.2.1 Primary map



X Index: 180

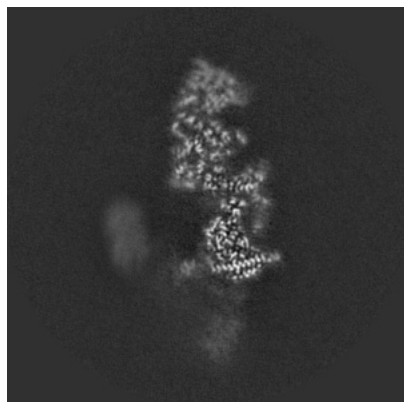


Y Index: 180

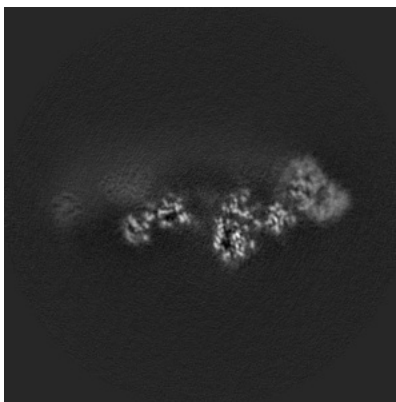


Z Index: 180

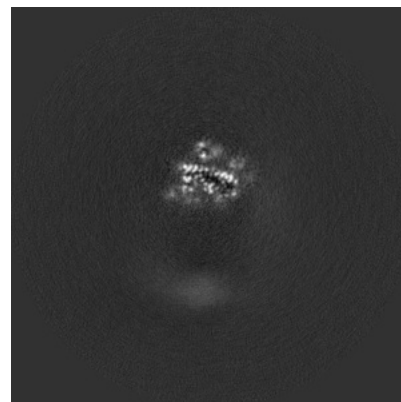
6.2.2 Raw map



X Index: 180



Y Index: 180

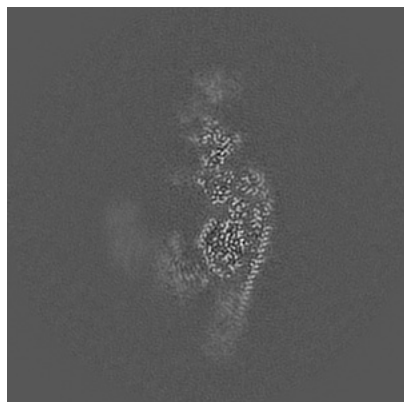


Z Index: 180

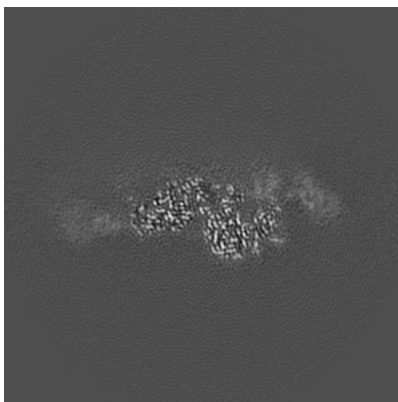
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

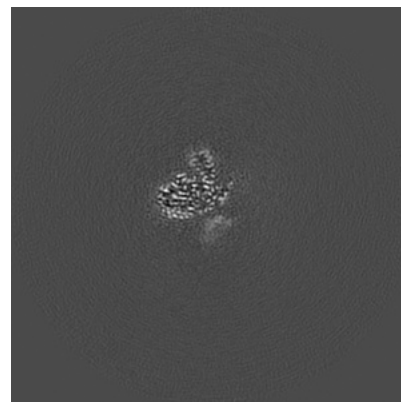
6.3.1 Primary map



X Index: 170

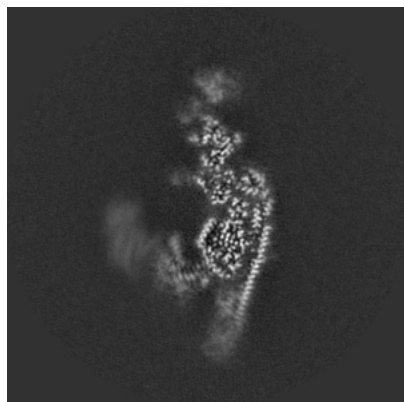


Y Index: 197

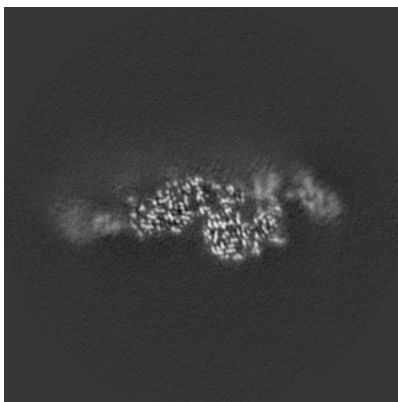


Z Index: 200

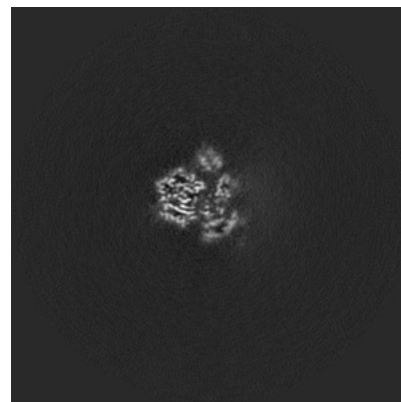
6.3.2 Raw map



X Index: 170



Y Index: 197

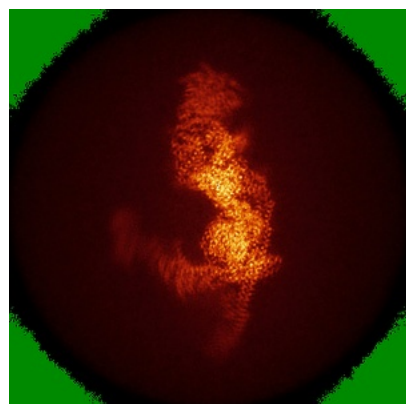


Z Index: 210

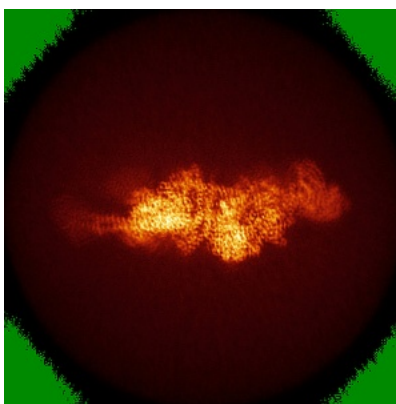
The images above show the largest variance slices of the map in three orthogonal directions.

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

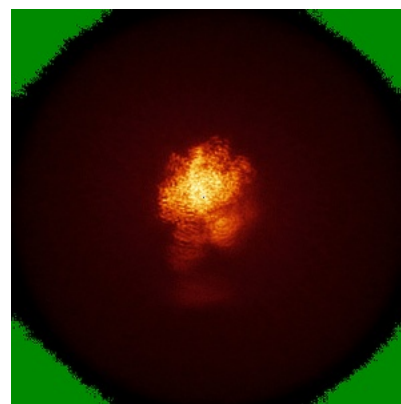
6.4.1 Primary map



X

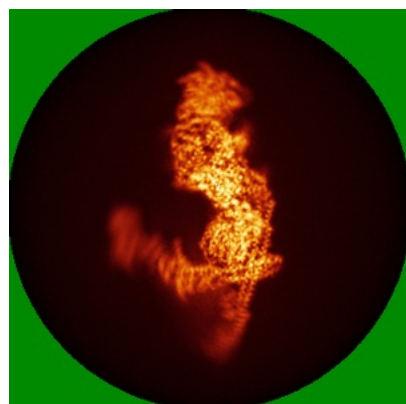


Y



Z

6.4.2 Raw map



X



Y

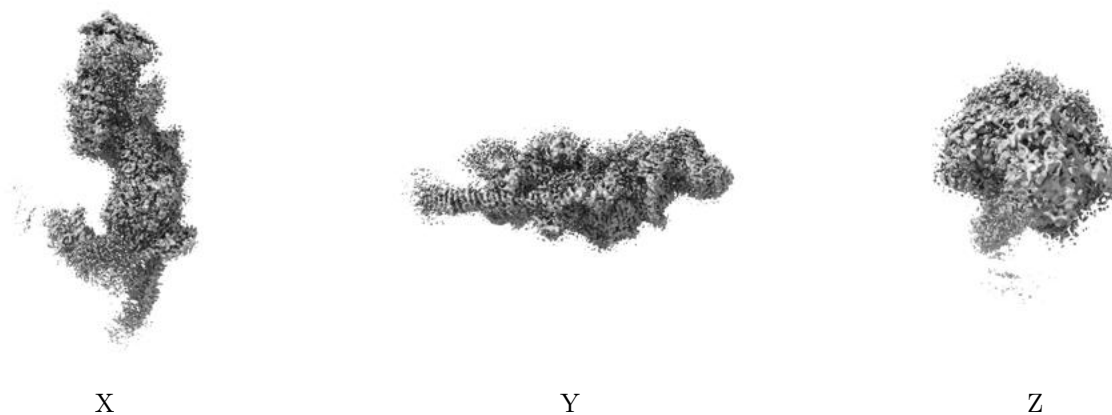


Z

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 0.012. 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.

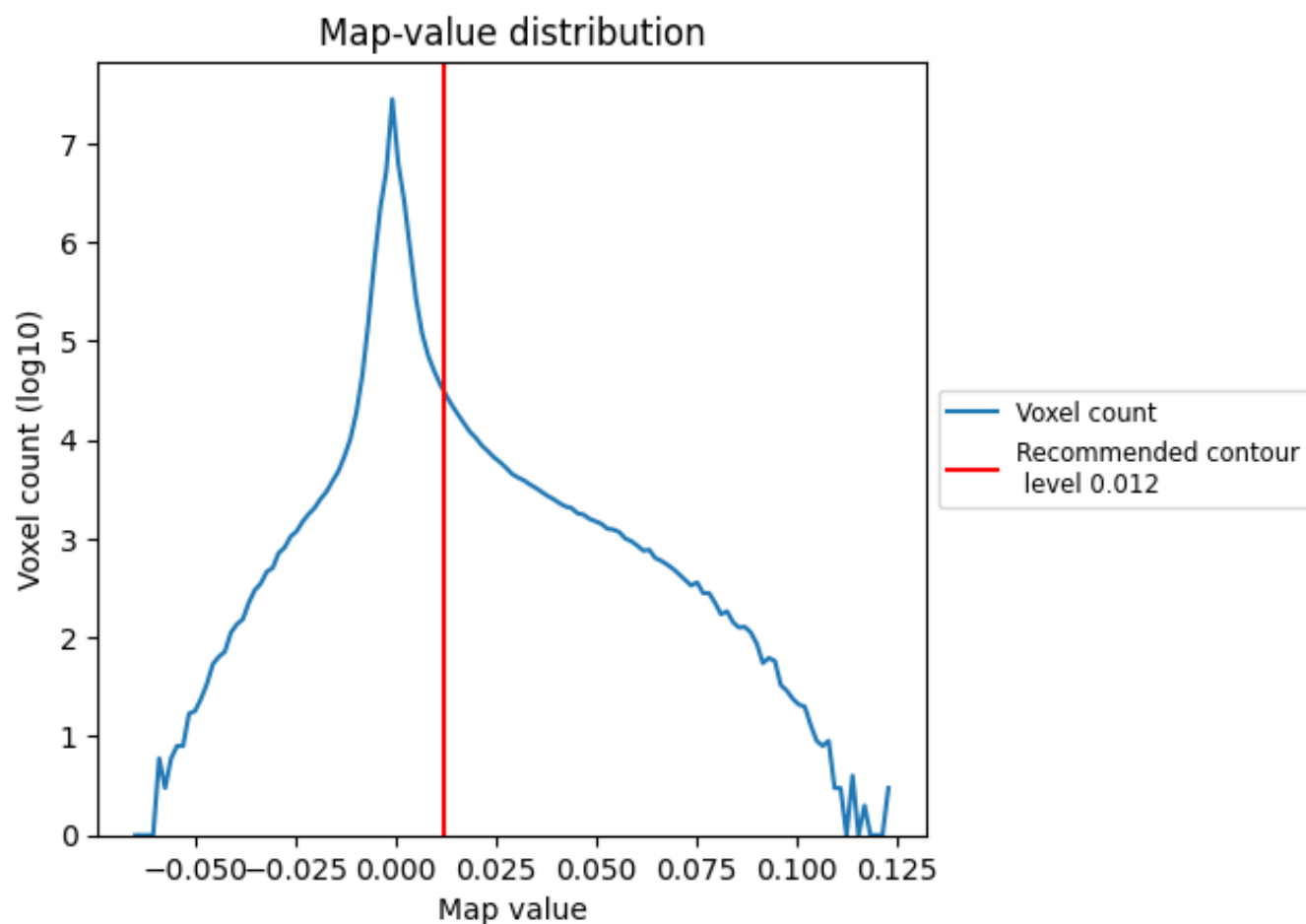
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

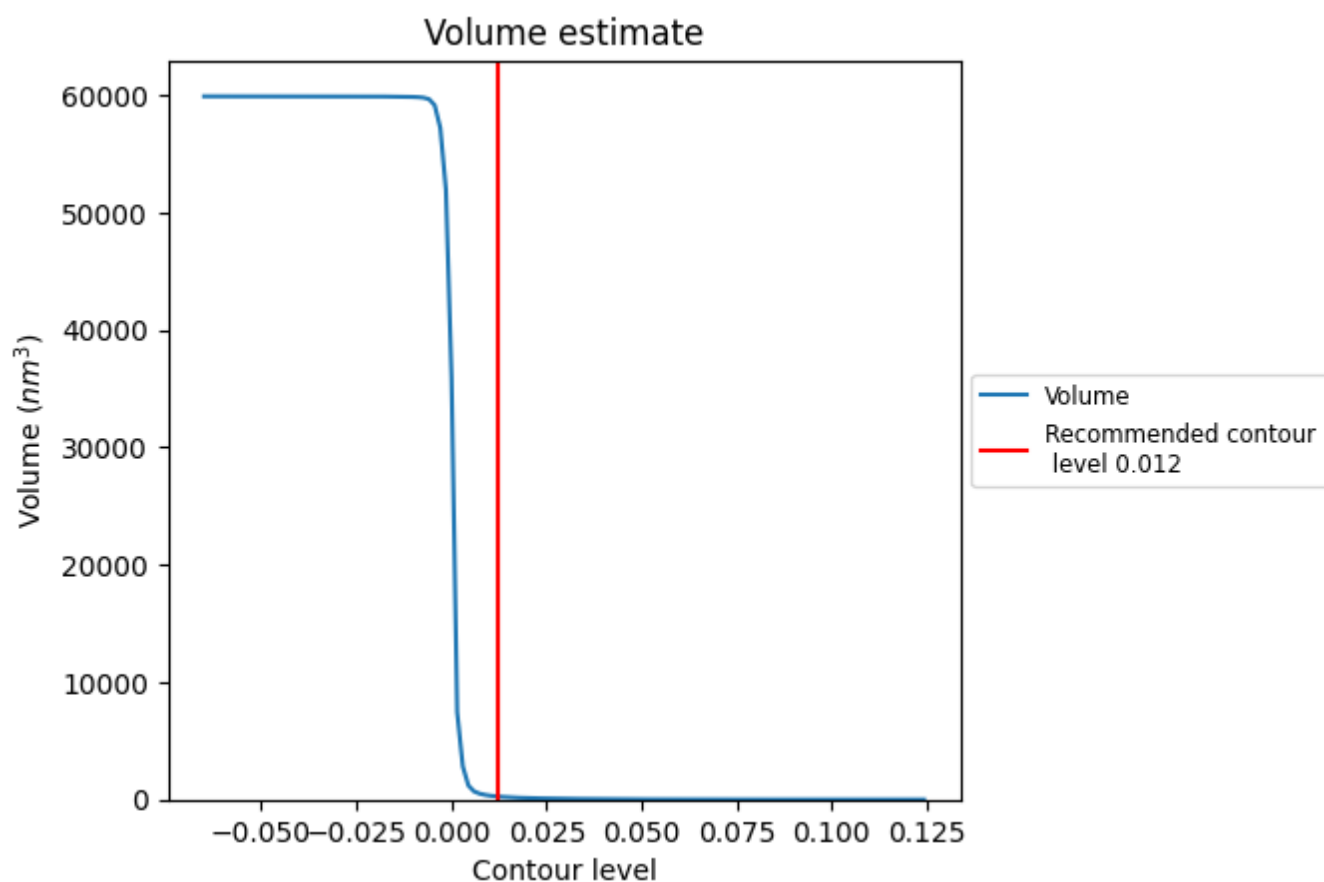
This section contains the results of statistical analysis of the map.

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.

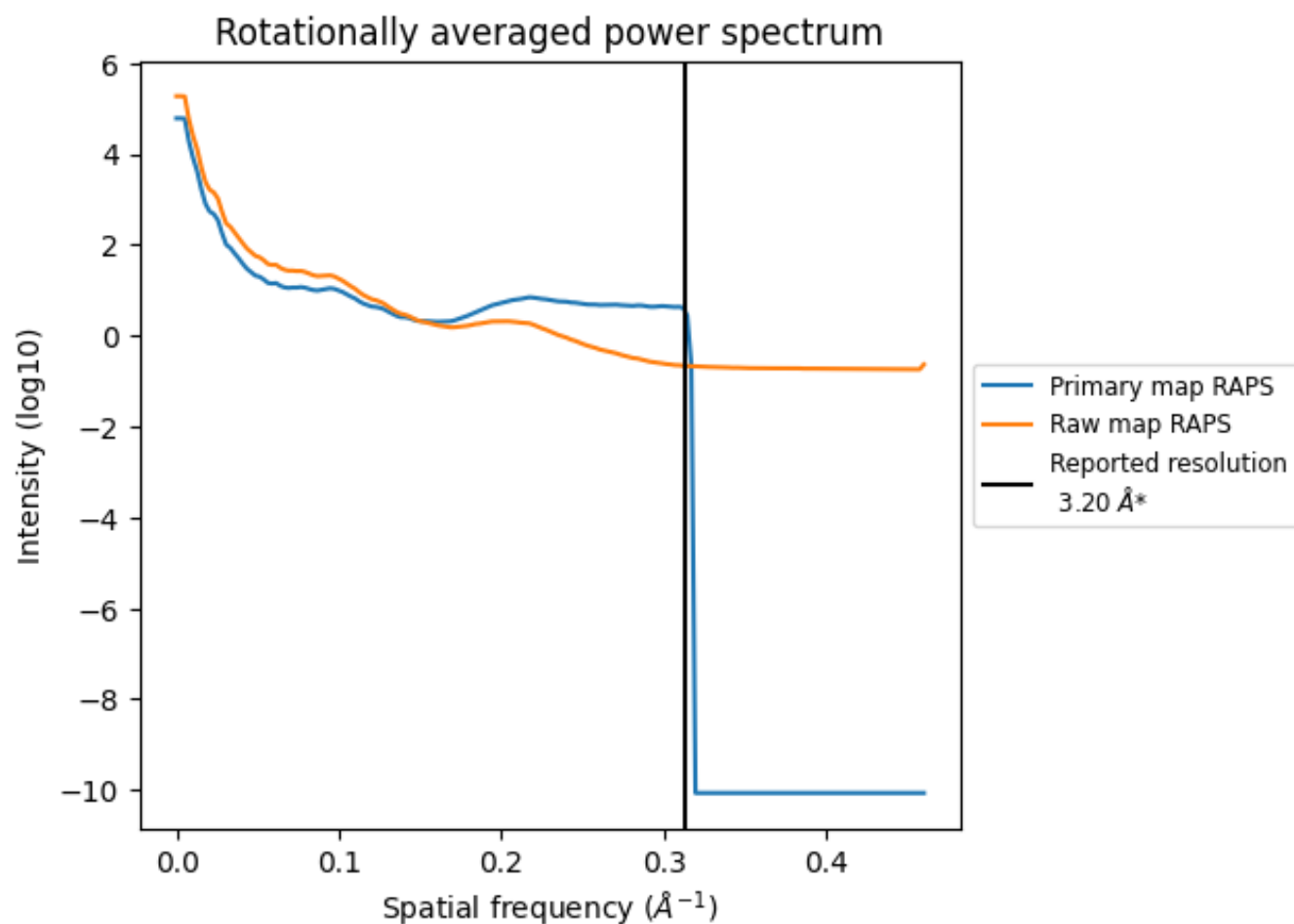
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 265 nm^3 ; this corresponds to an approximate mass of 240 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 ⓘ

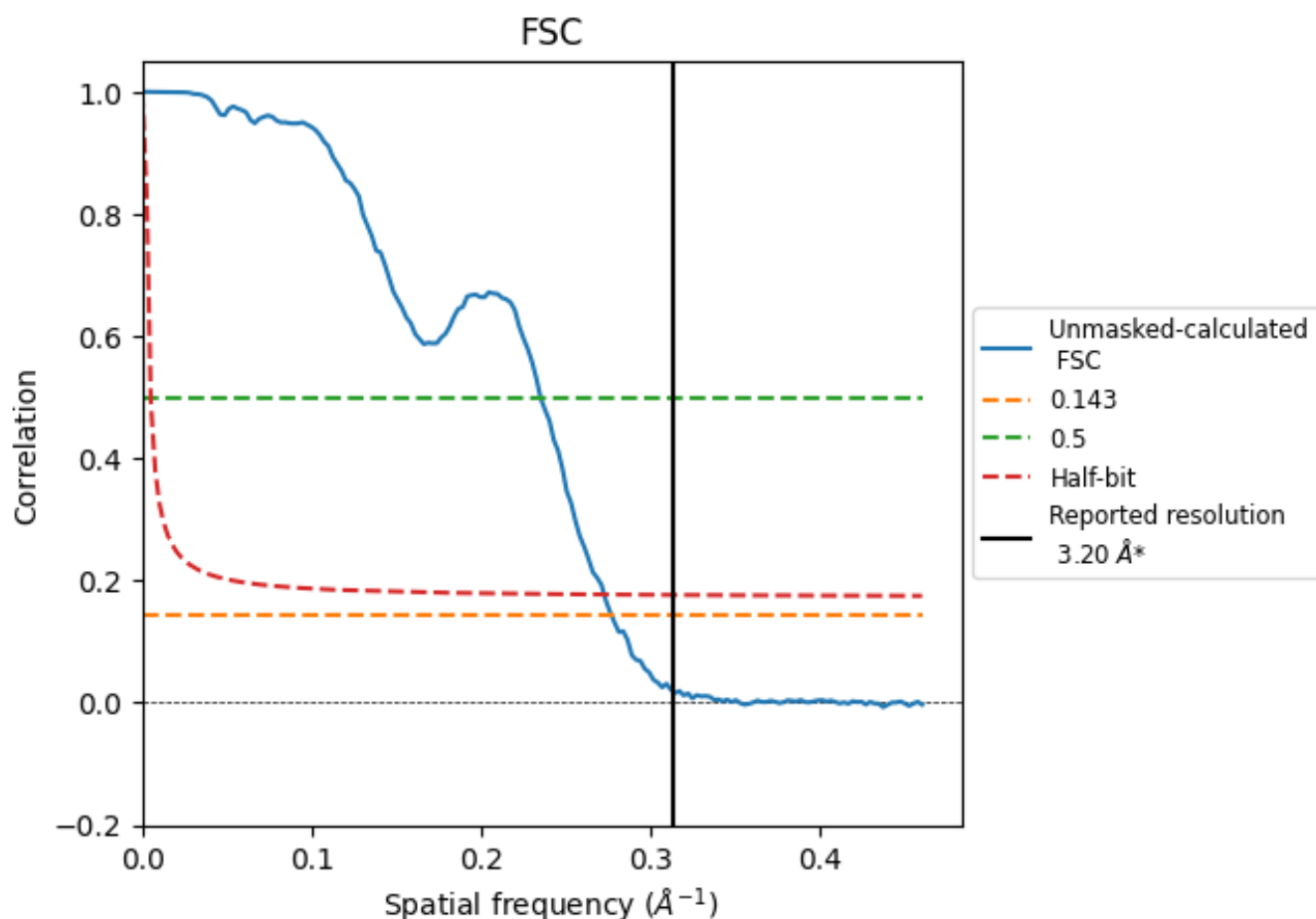


*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

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 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

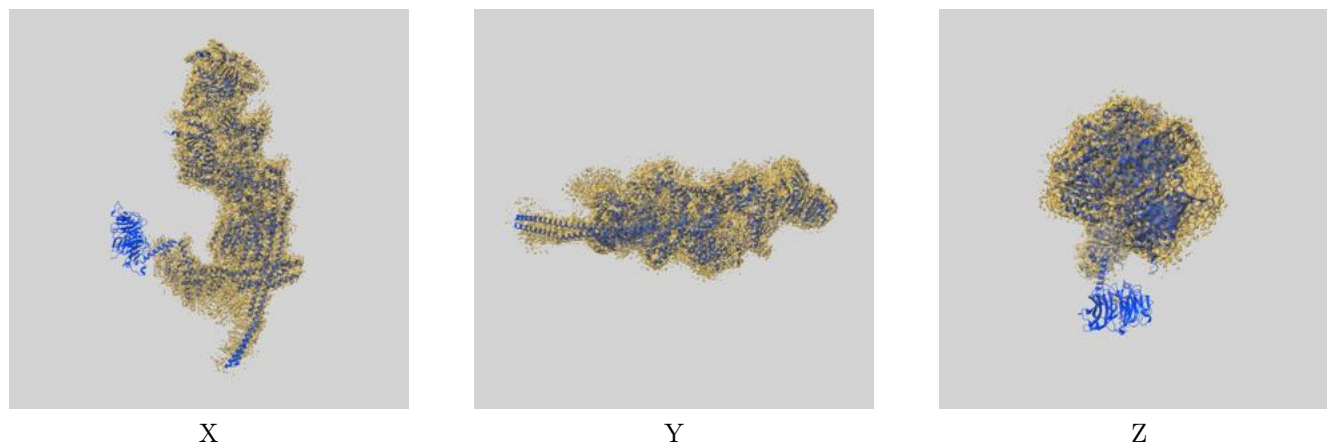
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.61	4.26	3.67

*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 3.61 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

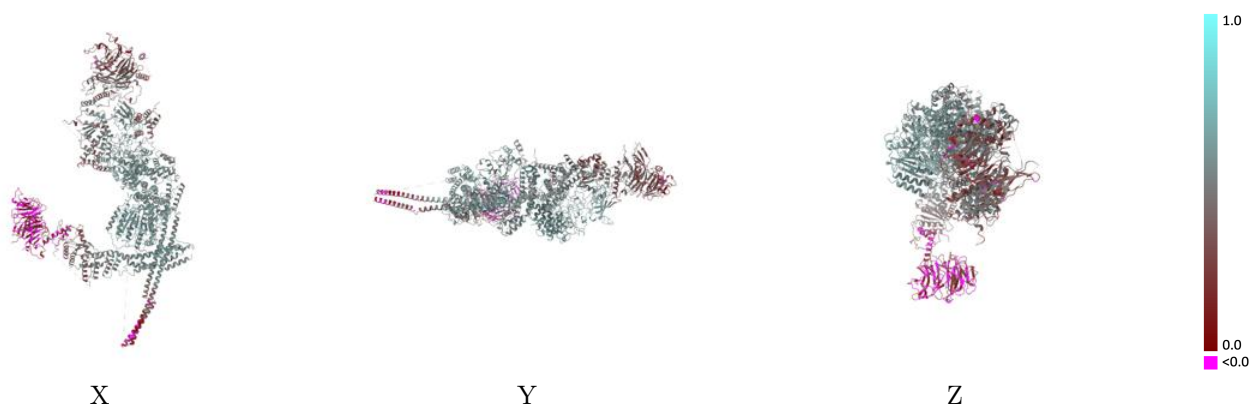
This section contains information regarding the fit between EMDB map EMD-35093 and PDB model 8I03. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



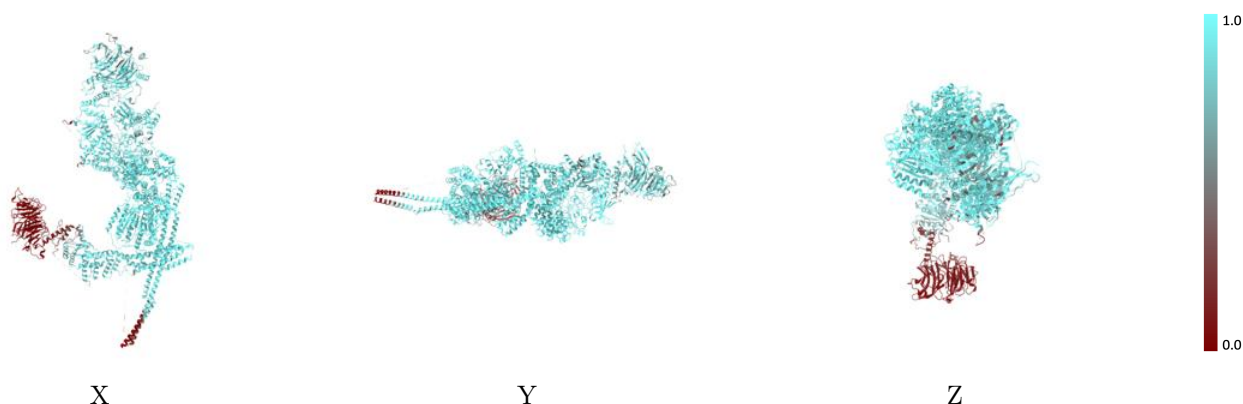
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



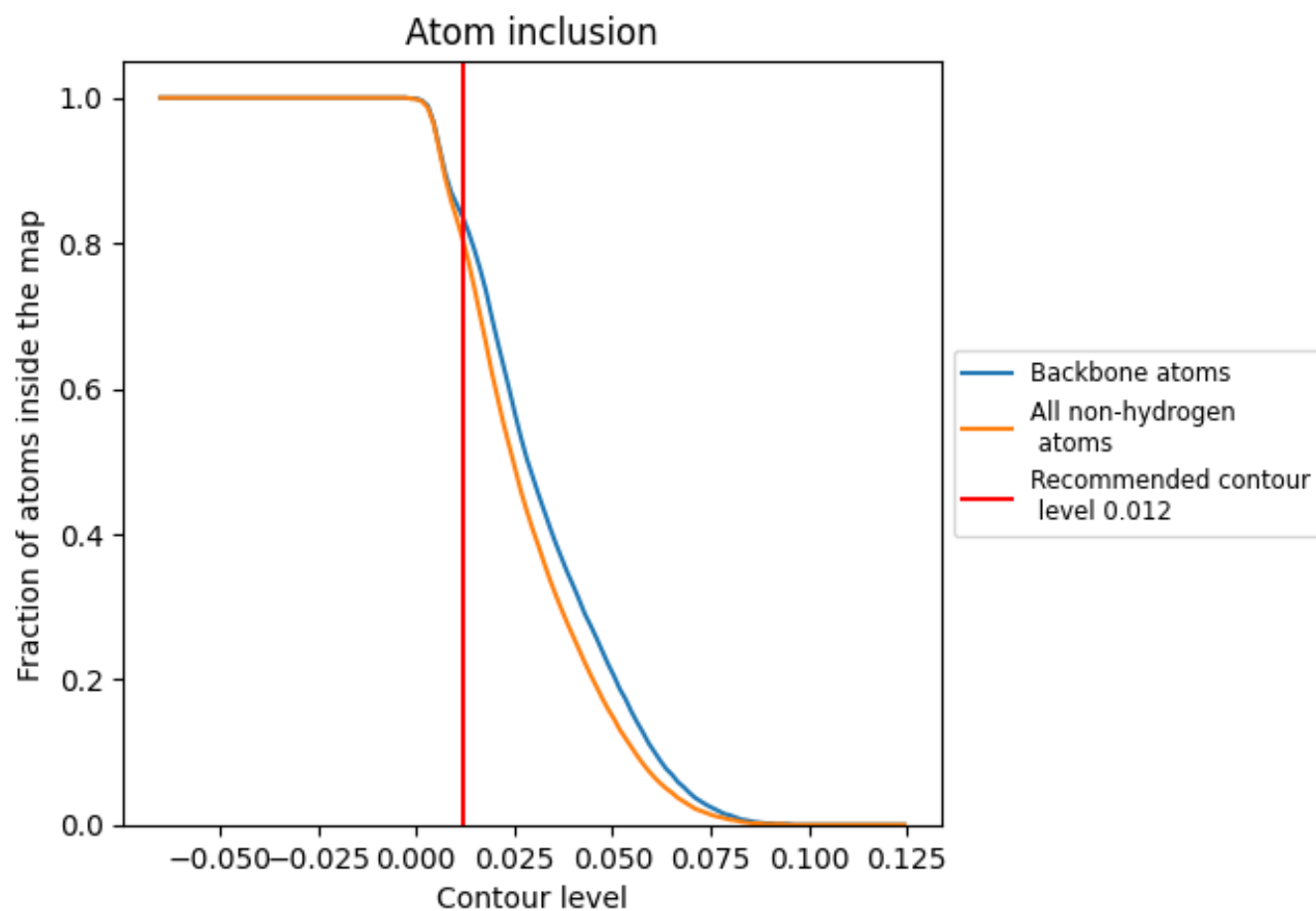
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8020	0.4440
A	0.8470	0.4620
B	0.9070	0.4810
C	0.9780	0.5940
D	0.9780	0.5890
E	0.8730	0.4760
F	0.9310	0.5430
G	0.8140	0.4590
H	0.9380	0.5430
I	0.9300	0.5300
J	0.8000	0.3300
K	0.0070	0.0360

1.0

0.0

<0.0