



## Full wwPDB EM Validation Report ⓘ

Apr 24, 2023 – 02:26 PM JST

PDB ID : 8I03  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev50  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.32.2

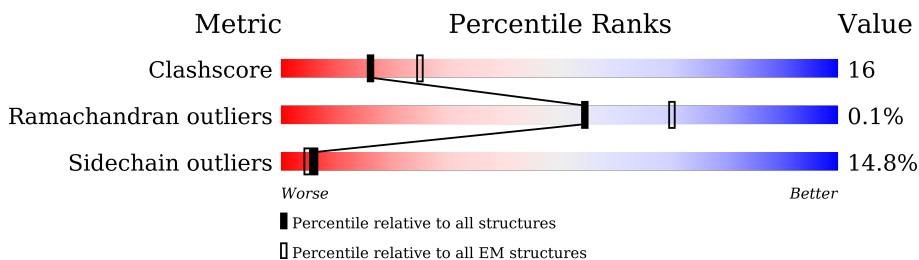
# 1 Overall quality at a glance

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.




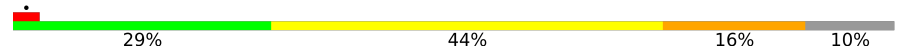
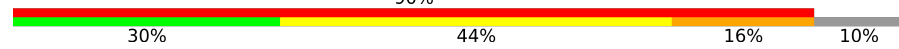
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1522	26% 13% 60%
2	B	1154	36% 18% 45%
3	C	405	75% 15% 9%
3	D	405	70% 17% 10%
4	E	491	26% 8% 66%
5	F	240	69% 21% 5% 5%
6	G	267	9% 46% 14% 38%
7	H	305	28% 11% 59%

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Mol	Chain	Length	Quality of chain
8	I	351	 <p>35% 16% 47%</p>
9	J	431	 <p>29% 44% 16% 10%</p>
9	K	431	 <p>30% 44% 16% 10%</p>

## 2 Entry composition i

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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
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
			Total	C	N	O	P	S		
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 (three-letter code: ZN) (formula: Zn).

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

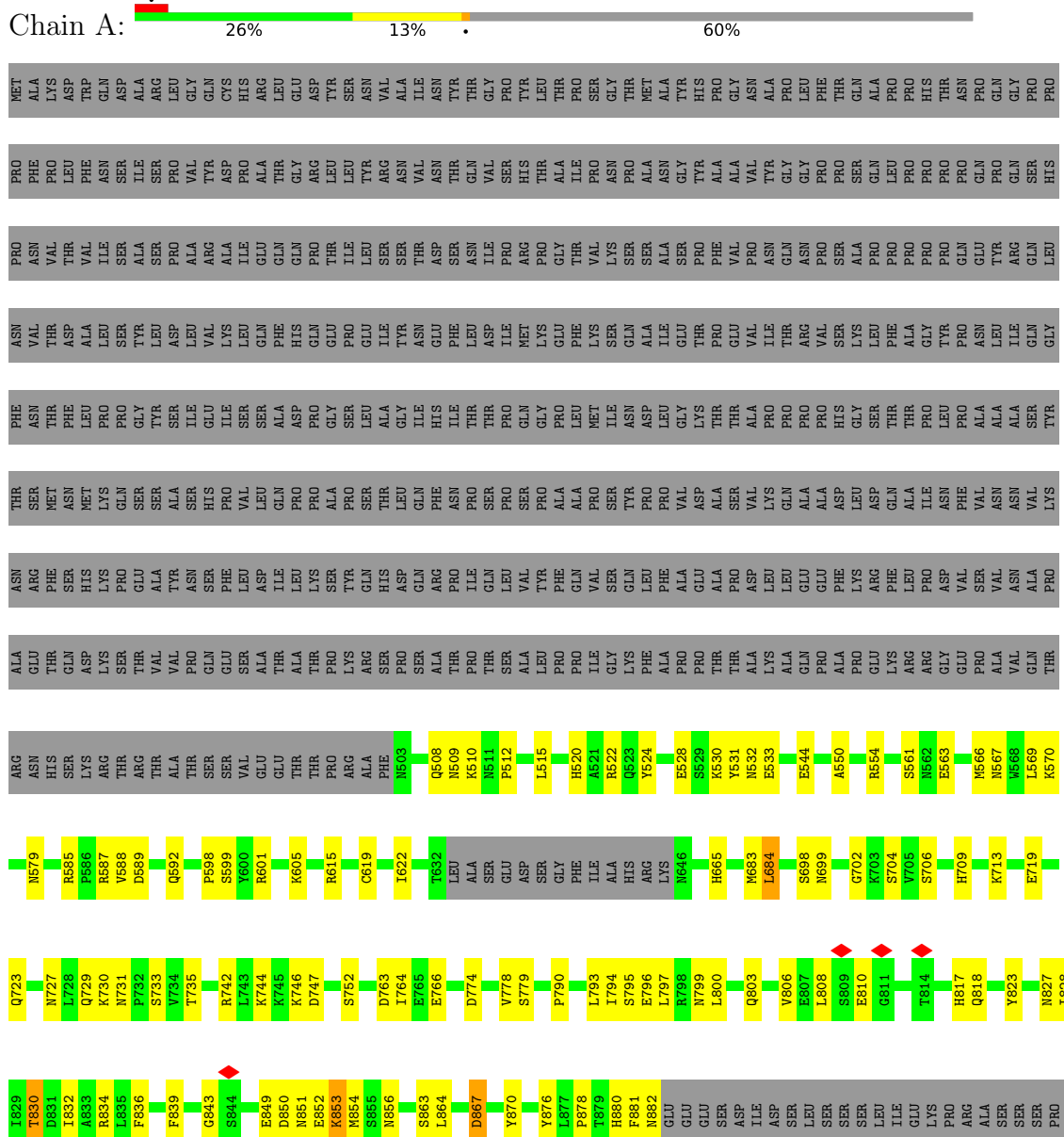
- Molecule 11 is POTASSIUM ION (three-letter code: K) (formula: K).

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

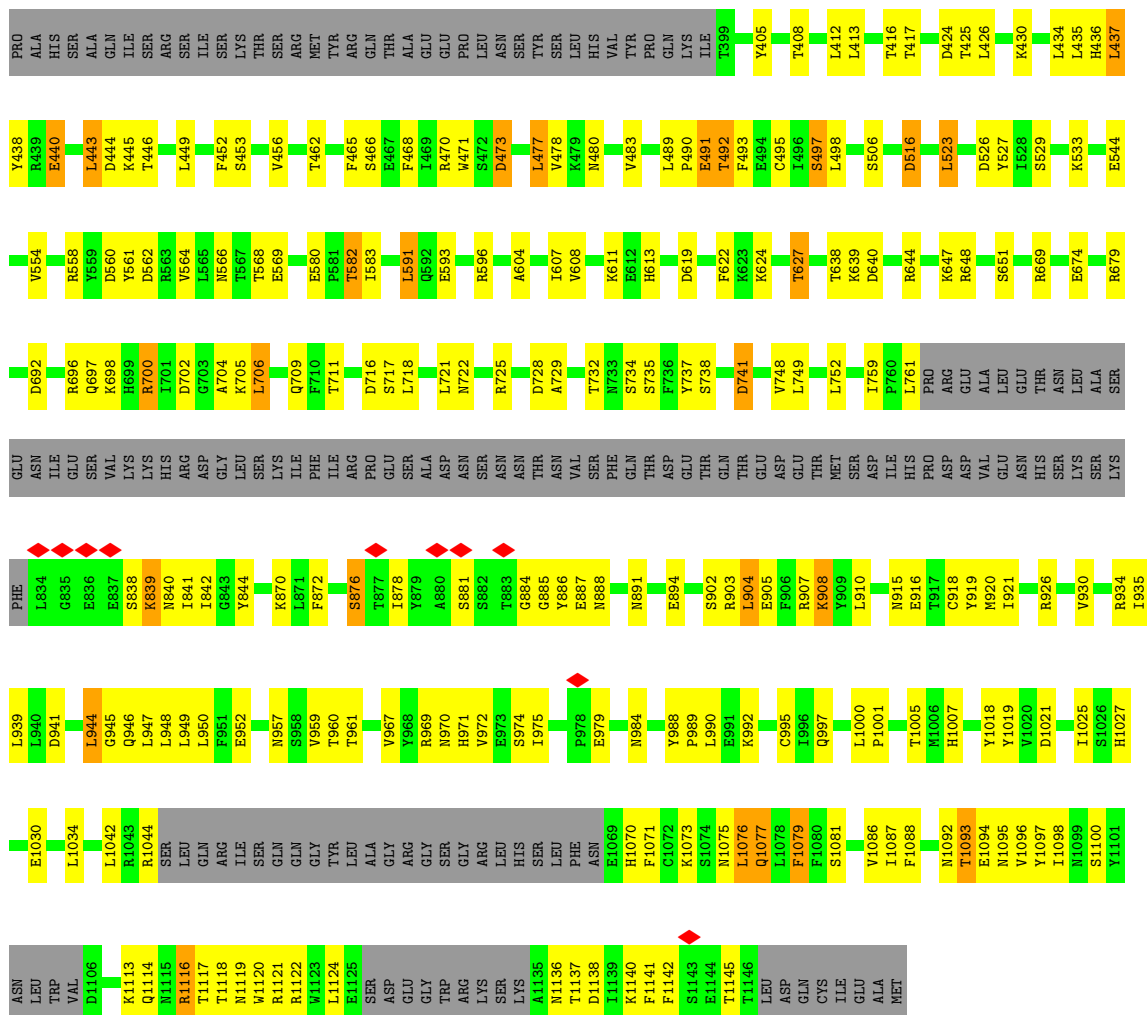
### 3 Residue-property plots

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.

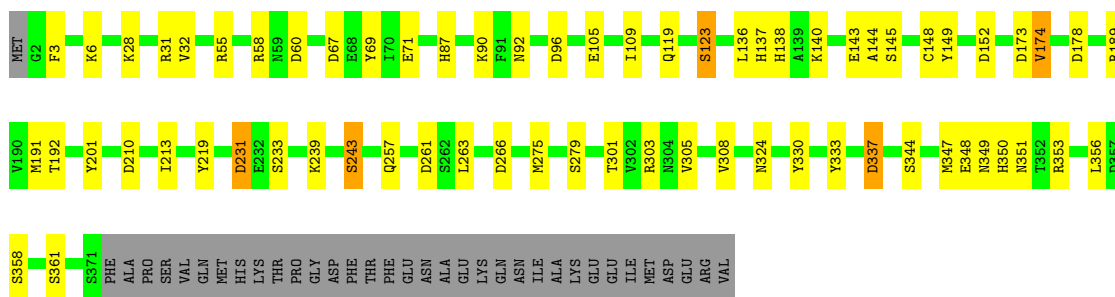
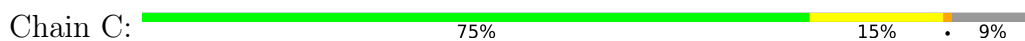
- Molecule 1: Paired amphipathic helix protein pst1







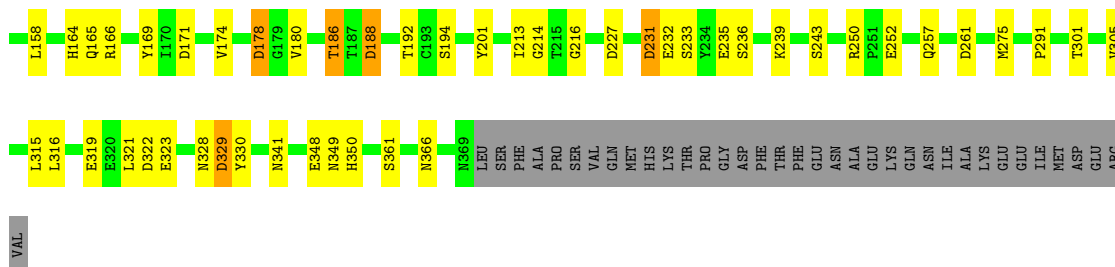
• Molecule 3: Histone deacetylase clr6



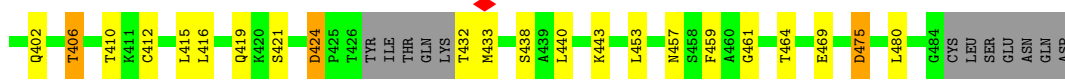
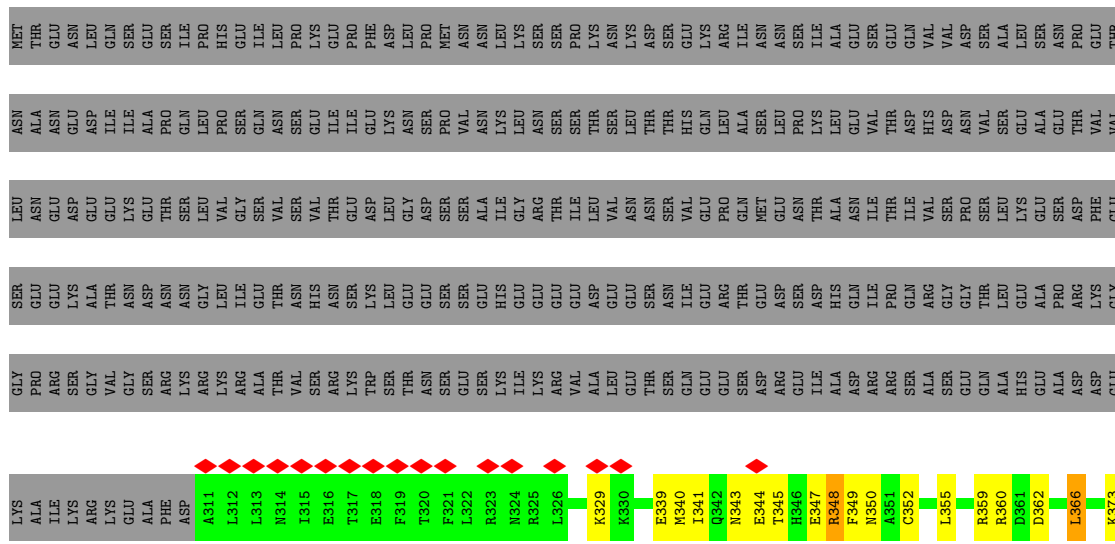
• Molecule 3: Histone deacetylase clr6



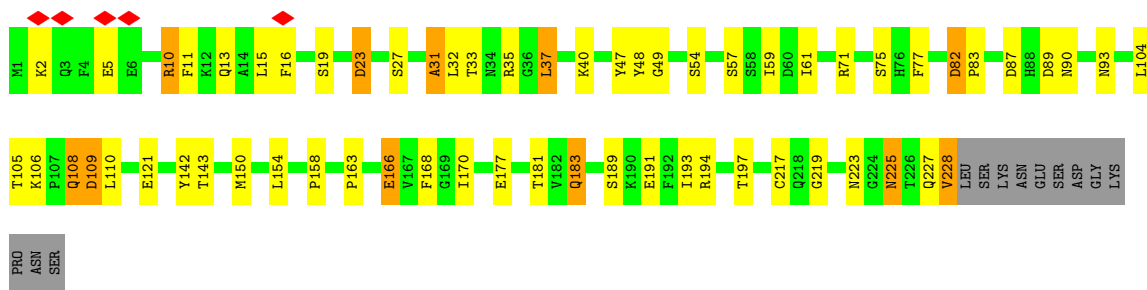




• Molecule 4: Transcriptional regulatory protein dep1



• Molecule 5: Transcriptional regulatory protein rxt2

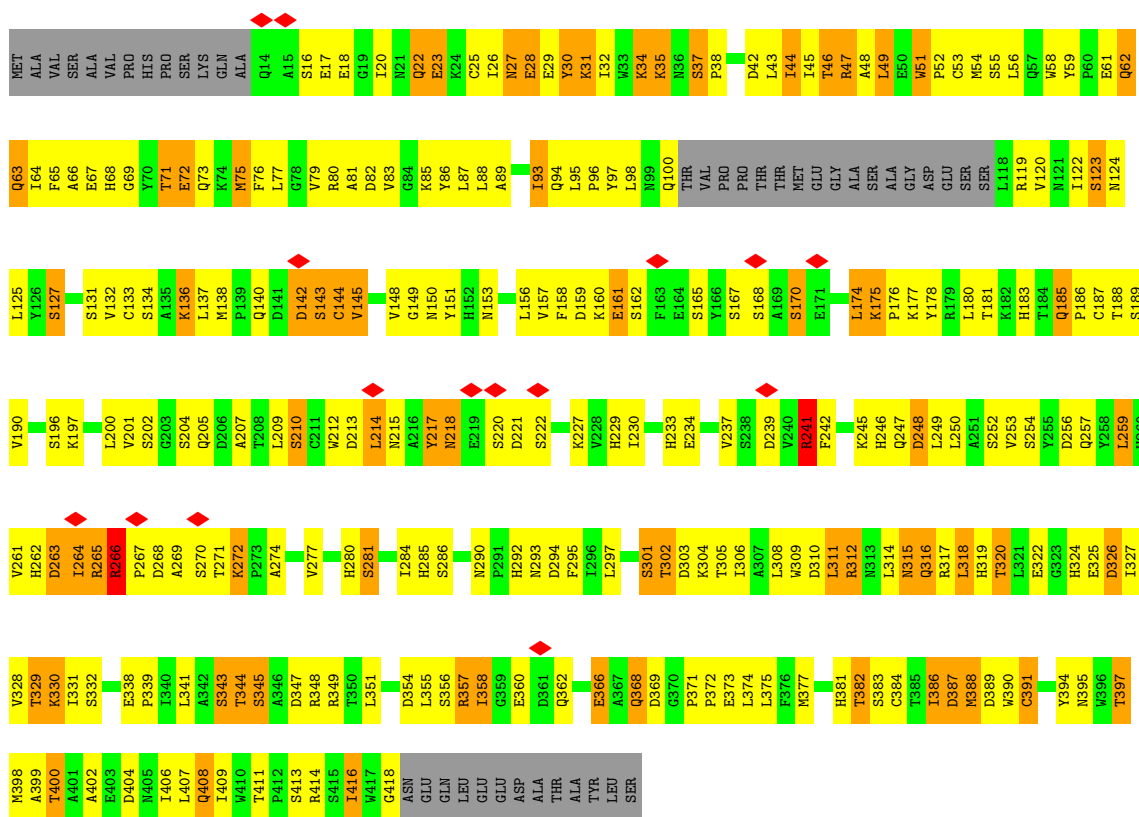


• Molecule 6: Transcriptional regulatory protein sds3

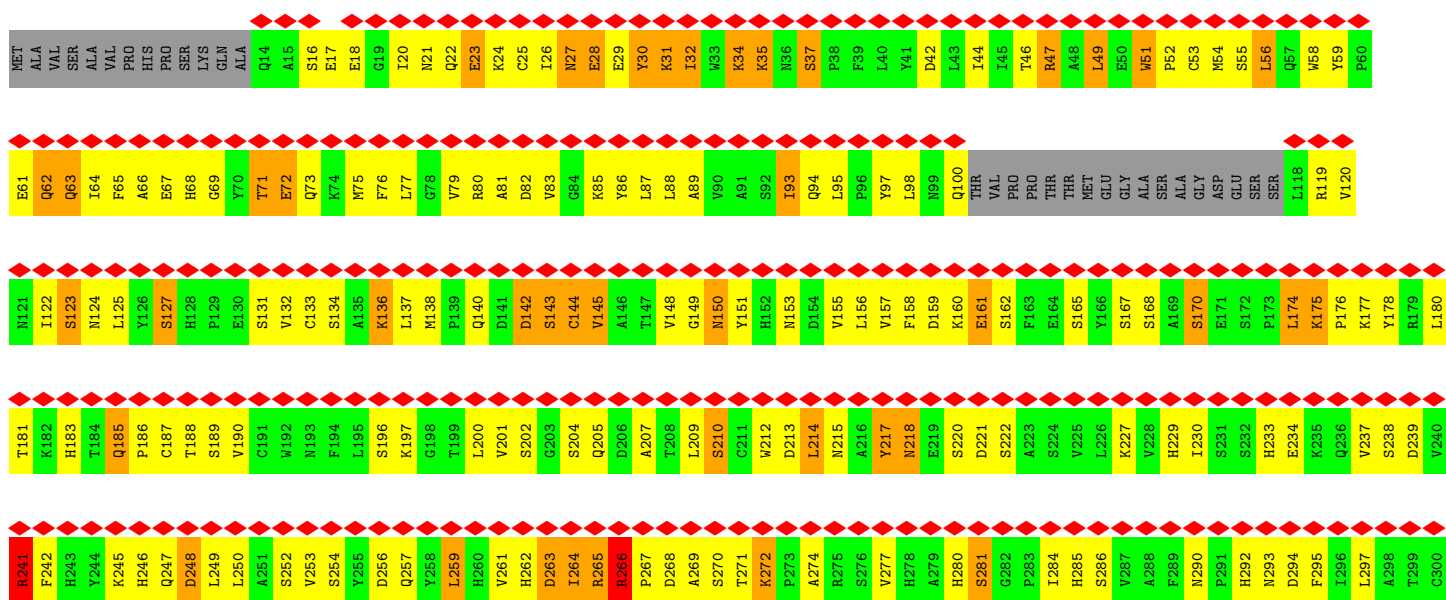




• Molecule 9: RbAp48-related WD40 repeat-containing protein prw1



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



S301	D361	GEN
T302	Q362	LEU
D303	P363	GLU
K304	A364	ASP
T305	E365	ALA
I306	E366	THR
A307	A367	ALA
L308	Q368	TYR
W309	D369	LEU
D310	G370	SER
L311	P371	
R312	P372	
N313	E373	
L314	L374	
N315	L375	
Q316	F376	
R317	M377	
L318	H378	
H319	G379	
T320	G380	
L321	H381	
E322	T382	
G323	S383	
H324	C384	
E325	T385	
D326	I386	
I327	D387	
V328	M388	
T329	D389	
K330	W390	
I331	C391	
S332	P392	
F333	N393	
S334	Y394	
P335	N395	
H336	W396	
E337	T397	
E338	M398	
P339	A399	
I340	T400	
L341	A401	
A342	A402	
S343	E403	
T344	D404	
S345	N405	
A346	I406	
D347	L407	
R348	Q408	
R349	I409	
T350	W410	
L351	T411	
V352	P412	
W353	S413	
D354	R414	
L355	S415	
S356	I416	
R357	W417	
I358	G418	
G359	ASN	
E360	GLU	

## 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: SEP, ZN, K

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	0.47	0/5194	0.52	1/7023 (0.0%)
2	B	0.46	0/5421	0.49	0/7321
3	C	0.72	0/3040	0.54	0/4121
3	D	0.70	0/2988	0.54	0/4054
4	E	0.47	0/1342	0.49	0/1804
5	F	0.59	0/1823	0.55	0/2458
6	G	0.43	0/1314	0.45	0/1755
7	H	0.50	0/1004	0.58	0/1353
8	I	0.54	0/1543	0.49	0/2099
9	J	0.32	0/3190	0.63	4/4345 (0.1%)
9	K	0.32	0/3190	0.63	4/4345 (0.1%)
All	All	0.51	0/30049	0.54	9/40678 (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 (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	684	LEU	CA-CB-CG	6.20	129.56	115.30
9	K	266	ARG	NE-CZ-NH1	5.93	123.27	120.30
9	J	266	ARG	NE-CZ-NH1	5.82	123.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	241	ARG	NE-CZ-NH1	5.53	123.07	120.30
9	J	241	ARG	NE-CZ-NH1	5.53	123.06	120.30
9	K	266	ARG	NE-CZ-NH2	-5.08	117.76	120.30
9	J	266	ARG	NE-CZ-NH2	-5.06	117.77	120.30
9	K	31	LYS	N-CA-CB	5.01	119.62	110.60
9	J	31	LYS	N-CA-CB	5.01	119.61	110.60

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5072	0	4988	182	0
2	B	5305	0	5285	216	0
3	C	2962	0	2818	35	0
3	D	2911	0	2761	39	0
4	E	1328	0	1304	32	0
5	F	1831	0	1768	68	0
6	G	1306	0	1267	28	0
7	H	994	0	997	26	0
8	I	1505	0	1524	52	0
9	J	3105	0	2960	197	0
9	K	3105	0	2960	206	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	28632	930	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 (930) 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
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
2:B:405:TYR:OH	5:F:13:GLN:CD	2.22	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
5:F:15:LEU:HD23	5:F:15:LEU:C	2.18	0.64
9:K:382:THR:OG1	9:K:404:ASP:OD1	2.09	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:OG	1:A:779:SER:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:977:TRP:CE3	9:K:28:GLU:HB3	2.34	0.62
9:K:187:CYS:HA	9:K:204:SER:HA	1.80	0.62
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
3:C:231:ASP:OD1	3:C:231:ASP:N	2.32	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:338:GLU:HG2	9:K:339:PRO:HD3	1.83	0.59
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
3:D:67:ASP:OD2	3:D:67:ASP:N	2.33	0.58
1:A:977:TRP:HB2	9:K:28:GLU:C	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:905:GLU:OE1	2:B:905:GLU:N	2.34	0.57
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
3:C:119:GLN:O	3:C:123:SER:OG	2.21	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
3:C:138:HIS:O	3:C:145:SER:HB3	2.06	0.56
3:D:57:THR:OG1	3:D:58:ARG:N	2.39	0.56
3:D:123:SER:OG	3:D:125:ASN:ND2	2.39	0.56
1:A:849:GLU:H	1:A:849:GLU:CD	2.09	0.56
6:G:24:THR:OG1	6:G:25:ALA:N	2.38	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:1073:LYS:CB	2:B:1094:GLU:OE2	2.55	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
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
9:K:185:GLN:HB3	9:K:205:GLN:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:65:PHE:O	9:K:69:GLY:N	2.34	0.54
9:K:381:HIS:HE2	9:K:400:THR:HG1	1.49	0.54
1:A:588:VAL:HB	7:H:128:ALA:HB3	1.90	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: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
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
2:B:1113:LYS:HD3	9:J:338:GLU:CD	2.29	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
2:B:748:VAL:HG21	2:B:939:LEU:HD21	1.89	0.52
6:G:261:LYS:HG2	6:G:265:LYS:HZ3	1.74	0.52
8:I:229:LEU:HD12	8:I:270:VAL:HG11	1.92	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:163:PRO:HG2	5:F:166:GLU:HB2	1.92	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
8:I:268:LYS:HZ1	8:I:270:VAL:HA	1.74	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
2:B:564:VAL:HG22	2:B:607:ILE:HD13	1.92	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:405:TYR:OH	5:F:13:GLN:CG	2.58	0.51
2:B:840:ASN:HB3	2:B:990:LEU:HB2	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:799:ASN:C	1:A:803:GLN:HE21	2.13	0.50
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
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
4:E:432:THR:OG1	4:E:433:MET:N	2.44	0.50
8:I:254:ILE:HD13	8:I:278:LEU:HD11	1.93	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: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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:J:326:ASP:CG	9:J:327:ILE:H	2.14	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
9:K:326:ASP:CG	9:K:327:ILE:H	2.14	0.49
2:B:752:LEU:HD21	2:B:948:LEU:HD21	1.94	0.49
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
5:F:150:MET:HE1	5:F:183:GLN:HG2	1.94	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:K:290:ASN:HB3	9:K:293:ASN:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
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
9:K:63:GLN:HA	9:K:63:GLN:OE1	2.13	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:J:257:GLN:HG2	9:J:281:SER:C	2.34	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
9:K:257:GLN:HG2	9:K:281:SER:C	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:982:PHE:CE2	9:K:24:LYS:HE3	2.49	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
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
8:I:251:ASP:OD1	8:I:251:ASP:N	2.47	0.47
9:J:30:TYR:C	9:J:30:TYR:CD1	2.88	0.47
9:K:178:TYR:CD1	9:K:217:TYR:HE1	2.33	0.47
9:K:326:ASP:CG	9:K:327:ILE:N	2.68	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:J:326:ASP:CG	9:J:327:ILE:N	2.68	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
5:F:77:PHE:HB3	5:F:90:ASN:OD1	2.15	0.47
7:H:14:ASP:CG	7:H:103:ARG:HH12	2.18	0.47
1:A:719:GLU:OE2	1:A:719:GLU:N	2.48	0.47
1:A:977:TRP:C	9:K:31:LYS:HG2	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:K:30:TYR:CD1	9:K:30:TYR:C	2.88	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
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: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
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:C:191:MET:HE2	3:C:219:TYR:HA	1.96	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
6:G:244:LEU:H	6:G:244:LEU:HD22	1.81	0.46
1:A:1205:ILE:HG13	9:K:20:ILE:C	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:HIS:O	1:A:713:LYS:HG3	2.15	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
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
2:B:1120:TRP:HZ2	9:J:318:LEU:HD11	1.82	0.45
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
8:I:268:LYS:NZ	8:I:269:PRO:O	2.31	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: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
3:D:239:LYS:O	3:D:243:SER:OG	2.19	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:58:TRP:HD1	9:K:389:ASP:CG	2.20	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
9:K:369:ASP:OD1	9:K:369:ASP:N	2.50	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:D:47:LYS:HE2	3:D:319:GLU:OE2	2.17	0.44
9:J:58:TRP:HD1	9:J:389:ASP:CG	2.20	0.44
9:K:175:LYS:HB3	9:K:175:LYS:HE2	1.48	0.44
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: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
2:B:1071:PHE:CD1	2:B:1071:PHE:C	2.91	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
9:K:161:GLU:O	9:K:165:SER:OG	2.29	0.44
5:F:15:LEU:C	5:F:15:LEU:CD2	2.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1076:LEU:CG	2:B:1095:ASN:HD21	2.30	0.44
3:D:132:TRP:CE3	3:D:132:TRP:HA	2.53	0.44
3:D:275:MET:HE2	3:D:341:ASN:HA	1.99	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
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:140:GLN:H	9:J:140:GLN:CD	2.21	0.44
9:J:386:ILE:H	9:J:402:ALA:HA	1.82	0.44
9:K:140:GLN:H	9:K:140:GLN:CD	2.21	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
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
9:K:30:TYR:C	9:K:30:TYR:HD1	2.22	0.43
1:A:1186:ARG:HD2	1:A:1186:ARG:N	2.34	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:156:LEU:HD23	9:J:176:PRO:HG3	2.00	0.43
1:A:522:ARG:C	1:A:524:TYR:H	2.22	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
8:I:293:ASN:OD1	8:I:293:ASN:N	2.51	0.43
9:J:123:SER:OG	9:J:124:ASN:N	2.52	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:30:TYR:C	9:J:30:TYR:HD1	2.22	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
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:305:ASP:OD1	8:I:305:ASP: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
1:A:977:TRP:C	9:K:28:GLU:HA	2.38	0.42
2:B:840:ASN:OD1	2:B:989:PRO:HB2	2.18	0.42
3:C:358:SER:O	3:C:361:SER:OG	2.35	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:27:ASN:H	9:K:27:ASN:ND2	2.09	0.42
9:K:389:ASP:OD2	9:K:390:TRP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:561:TYR:CD1	2:B:647:LYS:HB2	2.54	0.42
2:B:1118:THR:C	2:B:1122:ARG:HE	2.23	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
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
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
1:A:1194:LEU:C	1:A:1195:LYS:HE2	2.40	0.42
3:D:252:GLU:O	3:D:291:PRO:HD2	2.20	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
9:K:344:THR:HB	9:K:388:MET:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:69:TYR:OH	3:C:149:TYR:O	2.30	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:J:58:TRP:CE2	9:J:75:MET:HE1	2.55	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: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
2:B:1076:LEU:HD22	2:B:1095:ASN:CG	2.32	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
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:J:344:THR:HB	9:J:388:MET:HE2	2.01	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
3:D:58:ARG:O	3:D:62:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:86:TYR:C	9:J:87:LEU:HD12	2.41	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: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
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
2:B:949:LEU:HA	2:B:952:GLU:HG3	2.03	0.41
5:F:10:ARG:C	5:F:10:ARG:CD	2.89	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:86:TYR:C	9:K:87:LEU:HD12	2.41	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
2:B:872:PHE:O	2:B:876:SER:OG	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:1056:PRO:C	1:A:1058:GLU:H	2.24	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
1:A:977:TRP:HZ3	9:K:29:GLU:HG2	1.85	0.40
1:A:978:VAL:HB	1:A:979:ASN:C	2.42	0.40
2:B:648:ARG:O	2:B:651:SER:OG	2.33	0.40
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
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%)	17	56
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%)	54	83

All (2) Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	567/1364 (42%)	521 (92%)	46 (8%)	11	42
2	B	590/1060 (56%)	537 (91%)	53 (9%)	9	34
3	C	320/351 (91%)	300 (94%)	20 (6%)	18	52
3	D	315/351 (90%)	284 (90%)	31 (10%)	8	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	137/448 (31%)	125 (91%)	12 (9%)	10	36
5	F	198/209 (95%)	182 (92%)	16 (8%)	11	42
6	G	130/238 (55%)	120 (92%)	10 (8%)	13	44
7	H	112/280 (40%)	95 (85%)	17 (15%)	3	13
8	I	170/322 (53%)	158 (93%)	12 (7%)	14	47
9	J	348/382 (91%)	217 (62%)	131 (38%)	0	0
9	K	348/382 (91%)	217 (62%)	131 (38%)	0	0
All	All	3235/5387 (60%)	2756 (85%)	479 (15%)	6	14

All (479) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	508	GLN
1	A	569	LEU
1	A	592	GLN
1	A	601	ARG
1	A	622	ILE
1	A	684	LEU
1	A	706	SER
1	A	731	ASN
1	A	735	THR
1	A	747	ASP
1	A	752	SER
1	A	774	ASP
1	A	778	VAL
1	A	808	LEU
1	A	823	TYR
1	A	830	THR
1	A	851	ASN
1	A	853	LYS
1	A	863	SER
1	A	867	ASP
1	A	870	TYR
1	A	973	THR
1	A	977	TRP
1	A	978	VAL
1	A	981	LYS
1	A	1014	PHE
1	A	1022	SER
1	A	1033	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1039	HIS
1	A	1041	VAL
1	A	1043	SER
1	A	1055	HIS
1	A	1059	ARG
1	A	1060	LEU
1	A	1110	GLU
1	A	1113	VAL
1	A	1117	ILE
1	A	1125	THR
1	A	1158	GLU
1	A	1176	THR
1	A	1193	THR
1	A	1196	SER
1	A	1202	CYS
1	A	1208	TYR
1	A	1210	MET
1	A	1214	THR
2	B	408	THR
2	B	416	THR
2	B	437	LEU
2	B	438	TYR
2	B	440	GLU
2	B	443	LEU
2	B	465	PHE
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	497	SER
2	B	506	SER
2	B	516	ASP
2	B	523	LEU
2	B	529	SER
2	B	560	ASP
2	B	566	ASN
2	B	582	THR
2	B	591	LEU
2	B	611	LYS
2	B	619	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	622	PHE
2	B	627	THR
2	B	638	THR
2	B	674	GLU
2	B	700	ARG
2	B	706	LEU
2	B	738	SER
2	B	741	ASP
2	B	761	LEU
2	B	839	LYS
2	B	876	SER
2	B	904	LEU
2	B	908	LYS
2	B	910	LEU
2	B	944	LEU
2	B	960	THR
2	B	961	THR
2	B	1019	TYR
2	B	1076	LEU
2	B	1077	GLN
2	B	1079	PHE
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
2	B	1138	ASP
3	C	60	ASP
3	C	87	HIS
3	C	90	LYS
3	C	96	ASP
3	C	123	SER
3	C	137	HIS
3	C	152	ASP
3	C	174	VAL
3	C	189	ARG
3	C	192	THR
3	C	201	TYR
3	C	213	ILE
3	C	231	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	C	233	SER
3	C	243	SER
3	C	257	GLN
3	C	279	SER
3	C	303	ARG
3	C	337	ASP
3	C	344	SER
3	D	15	ASP
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	87	HIS
3	D	89	LEU
3	D	127	GLU
3	D	132	TRP
3	D	137	HIS
3	D	145	SER
3	D	174	VAL
3	D	178	ASP
3	D	180	VAL
3	D	186	THR
3	D	188	ASP
3	D	192	THR
3	D	194	SER
3	D	201	TYR
3	D	227	ASP
3	D	231	ASP
3	D	233	SER
3	D	236	SER
3	D	257	GLN
3	D	315	LEU
3	D	328	ASN
3	D	329	ASP
3	D	361	SER
3	D	366	ASN
4	E	348	ARG
4	E	349	PHE
4	E	366	LEU
4	E	393	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	E	406	THR
4	E	412	CYS
4	E	415	LEU
4	E	416	LEU
4	E	424	ASP
4	E	438	SER
4	E	459	PHE
4	E	475	ASP
5	F	10	ARG
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	108	GLN
5	F	109	ASP
5	F	154	LEU
5	F	166	GLU
5	F	168	PHE
5	F	183	GLN
5	F	225	ASN
5	F	228	VAL
6	G	41	SER
6	G	58	ARG
6	G	83	TYR
6	G	94	TYR
6	G	99	LYS
6	G	100	THR
6	G	242	LYS
6	G	248	THR
6	G	251	ASP
6	G	266	LYS
7	H	32	SER
7	H	33	LEU
7	H	37	ASP
7	H	40	VAL
7	H	42	ASP
7	H	59	LYS
7	H	66	GLU
7	H	80	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	H	85	SER
7	H	97	ILE
7	H	101	ILE
7	H	103	ARG
7	H	114	GLU
7	H	115	ILE
7	H	118	GLN
7	H	119	LEU
7	H	125	ASP
8	I	178	ASP
8	I	198	VAL
8	I	204	THR
8	I	251	ASP
8	I	256	THR
8	I	261	CYS
8	I	265	SER
8	I	268	LYS
8	I	299	SER
8	I	305	ASP
8	I	332	THR
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	30	TYR
9	J	32	ILE
9	J	34	LYS
9	J	35	LYS
9	J	37	SER
9	J	42	ASP
9	J	44	ILE
9	J	46	THR
9	J	47	ARG
9	J	49	LEU
9	J	51	TRP
9	J	56	LEU
9	J	62	GLN
9	J	63	GLN
9	J	64	ILE
9	J	67	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	88	LEU
9	J	93	ILE
9	J	95	LEU
9	J	97	TYR
9	J	98	LEU
9	J	122	ILE
9	J	123	SER
9	J	125	LEU
9	J	127	SER
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
9	J	213	ASP
9	J	214	LEU
9	J	215	ASN
9	J	217	TYR
9	J	218	ASN
9	J	220	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	J	221	ASP
9	J	222	SER
9	J	227	LYS
9	J	229	HIS
9	J	234	GLU
9	J	239	ASP
9	J	241	ARG
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	292	HIS
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
9	J	325	GLU
9	J	326	ASP
9	J	329	THR
9	J	330	LYS
9	J	332	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	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	30	TYR
9	K	32	ILE
9	K	34	LYS
9	K	35	LYS
9	K	37	SER
9	K	42	ASP
9	K	44	ILE
9	K	46	THR
9	K	47	ARG
9	K	49	LEU
9	K	51	TRP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	88	LEU
9	K	93	ILE
9	K	95	LEU
9	K	97	TYR
9	K	98	LEU
9	K	122	ILE
9	K	123	SER
9	K	125	LEU
9	K	127	SER
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
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

*Continued on next page...*

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	K	214	LEU
9	K	215	ASN
9	K	217	TYR
9	K	218	ASN
9	K	220	SER
9	K	221	ASP
9	K	222	SER
9	K	227	LYS
9	K	229	HIS
9	K	234	GLU
9	K	239	ASP
9	K	241	ARG
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	292	HIS
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
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

*Continued on next page...*

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Mol	Chain	Res	Type
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	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 (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	511	ASN
1	A	665	HIS
1	A	720	HIS
1	A	729	GLN
1	A	762	HIS
1	A	799	ASN
1	A	803	GLN

*Continued on next page...*

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	827	ASN
1	A	846	HIS
1	A	856	ASN
1	A	882	ASN
1	A	1119	GLN
2	B	421	HIS
2	B	474	ASN
2	B	584	HIS
2	B	697	GLN
2	B	722	ASN
2	B	888	ASN
2	B	970	ASN
2	B	1036	GLN
2	B	1070	HIS
2	B	1075	ASN
2	B	1077	GLN
2	B	1095	ASN
2	B	1114	GLN
2	B	1115	ASN
3	C	37	ASN
3	C	88	GLN
3	C	164	HIS
3	C	350	HIS
3	D	20	HIS
3	D	85	GLN
3	D	125	ASN
3	D	164	HIS
3	D	222	ASN
3	D	324	ASN
4	E	335	ASN
4	E	392	GLN
4	E	417	ASN
4	E	437	GLN
5	F	108	GLN
5	F	122	GLN
5	F	165	HIS
5	F	174	GLN
5	F	225	ASN
7	H	13	ASN
7	H	95	ASN
8	I	166	GLN
8	I	187	ASN

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Mol	Chain	Res	Type
9	J	21	ASN
9	J	22	GLN
9	J	27	ASN
9	J	94	GLN
9	J	152	HIS
9	J	193	ASN
9	J	218	ASN
9	J	260	HIS
9	J	285	HIS
9	J	316	GLN
9	J	319	HIS
9	K	21	ASN
9	K	27	ASN
9	K	152	HIS
9	K	193	ASN
9	K	218	ASN
9	K	260	HIS
9	K	285	HIS
9	K	316	GLN
9	K	319	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	0.64	0	8,12,14	0.62	0
5	SEP	F	27	5	8,9,10	0.64	0	8,12,14	0.61	0
5	SEP	F	19	5	8,9,10	0.63	0	8,12,14	0.71	0
5	SEP	F	22	5	8,9,10	0.64	0	8,12,14	0.61	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	-	1/5/8/10	-
5	SEP	F	27	5	-	0/5/8/10	-
5	SEP	F	19	5	-	1/5/8/10	-
5	SEP	F	22	5	-	3/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	19	SEP	N-CA-CB-OG
5	F	22	SEP	CB-OG-P-O1P
5	F	22	SEP	CB-OG-P-O3P
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	27	SEP	1	0
5	F	19	SEP	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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.

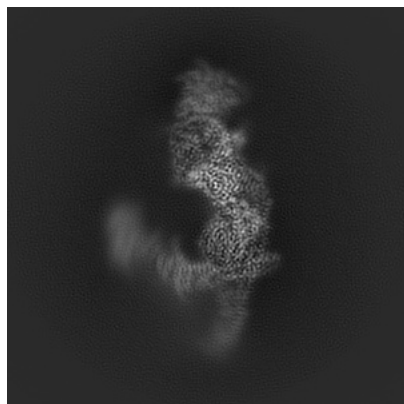
## 6 Map visualisation [i](#)

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.

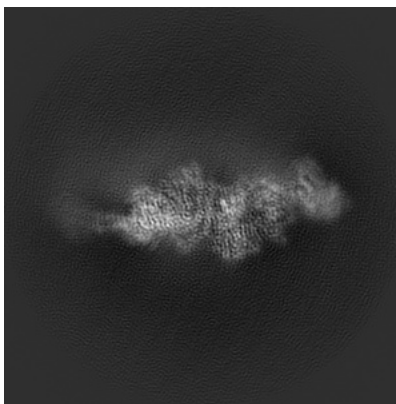
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

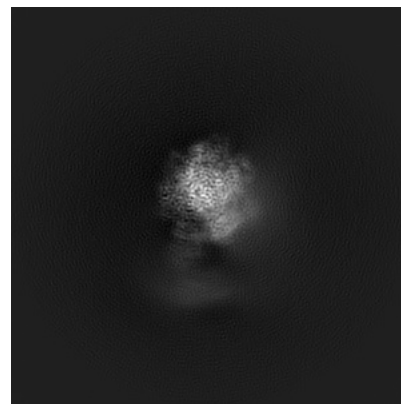
#### 6.1.1 Primary map



X

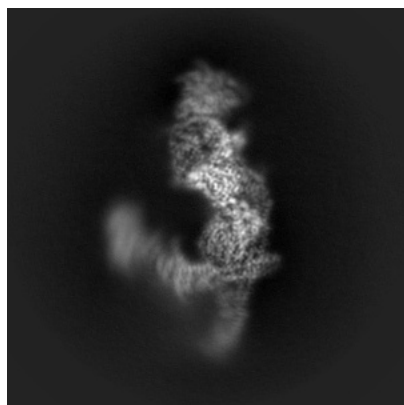


Y

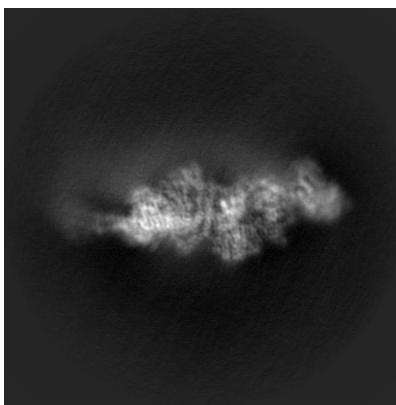


Z

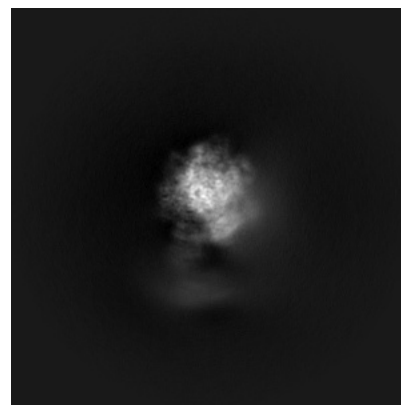
#### 6.1.2 Raw map



X



Y



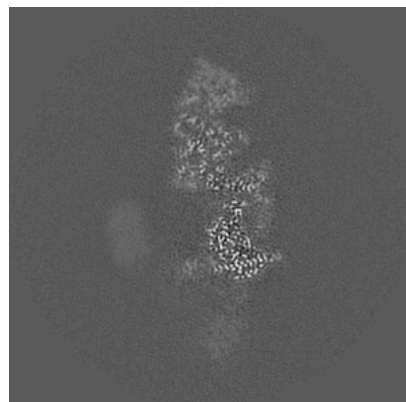
Z

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

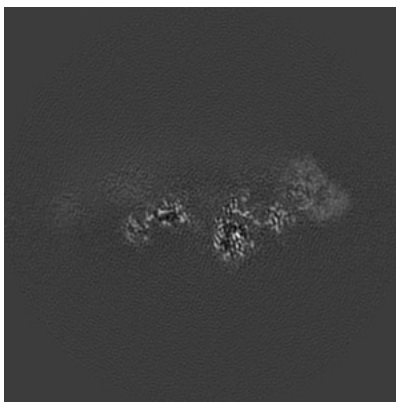


## 6.2 Central slices [i](#)

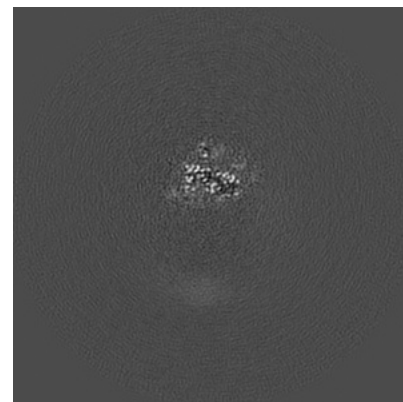
### 6.2.1 Primary map



X Index: 180

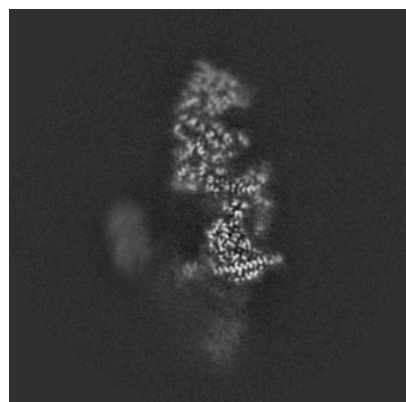


Y Index: 180

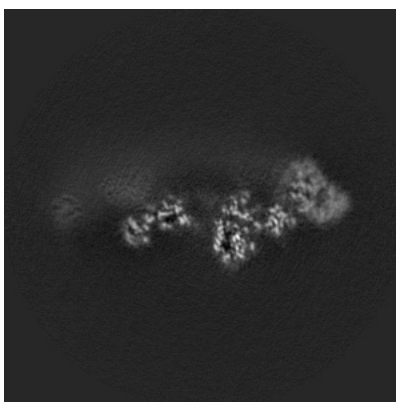


Z Index: 180

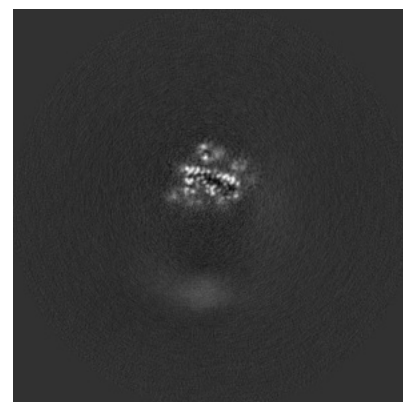
### 6.2.2 Raw map



X Index: 180



Y Index: 180

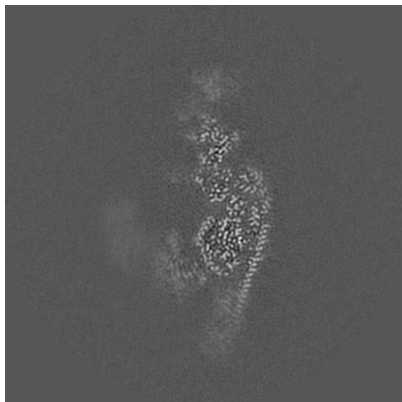


Z Index: 180

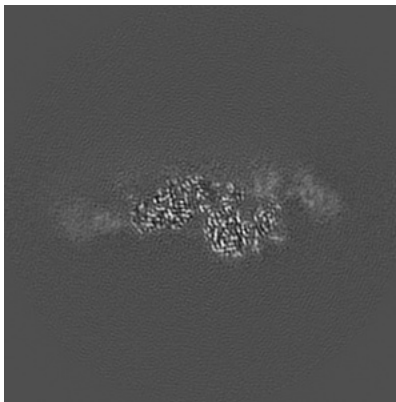
The images above show central slices of the map in three orthogonal directions.

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

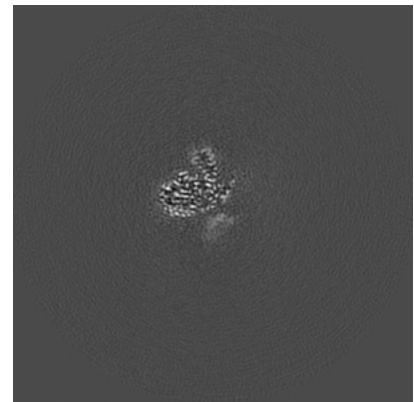
### 6.3.1 Primary map



X Index: 170

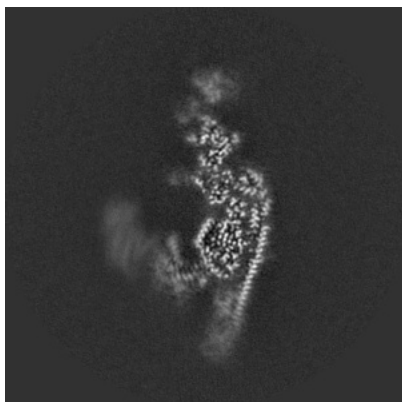


Y Index: 197

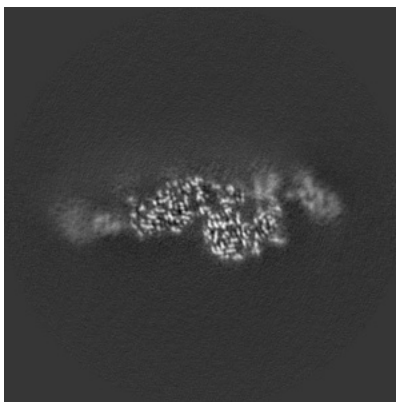


Z Index: 200

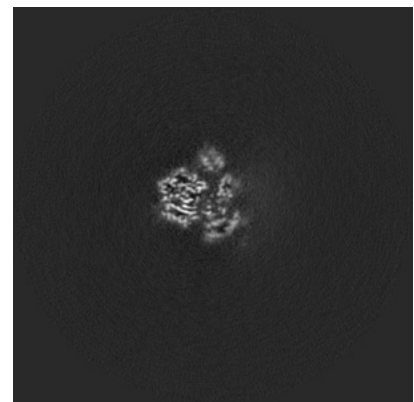
### 6.3.2 Raw map



X Index: 170



Y Index: 197

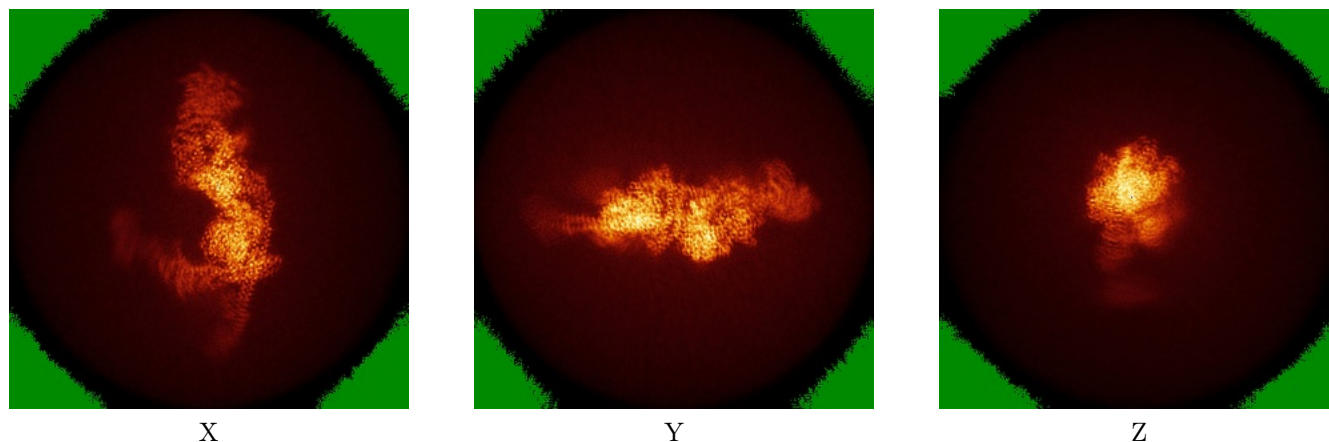


Z Index: 210

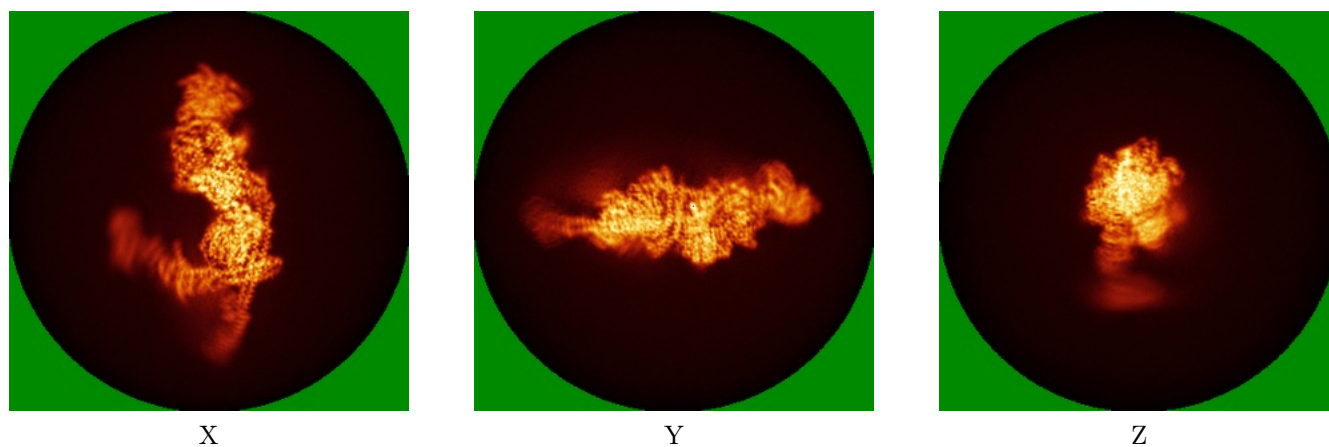
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



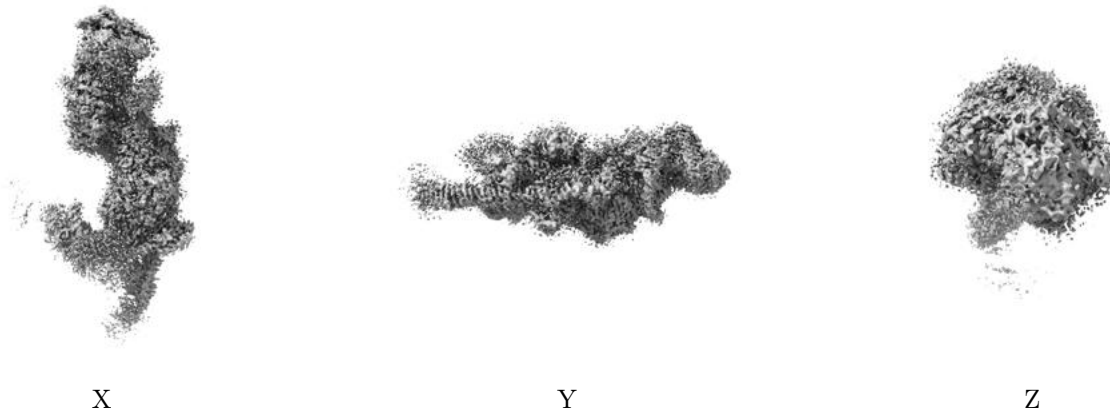
### 6.4.2 Raw map



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.

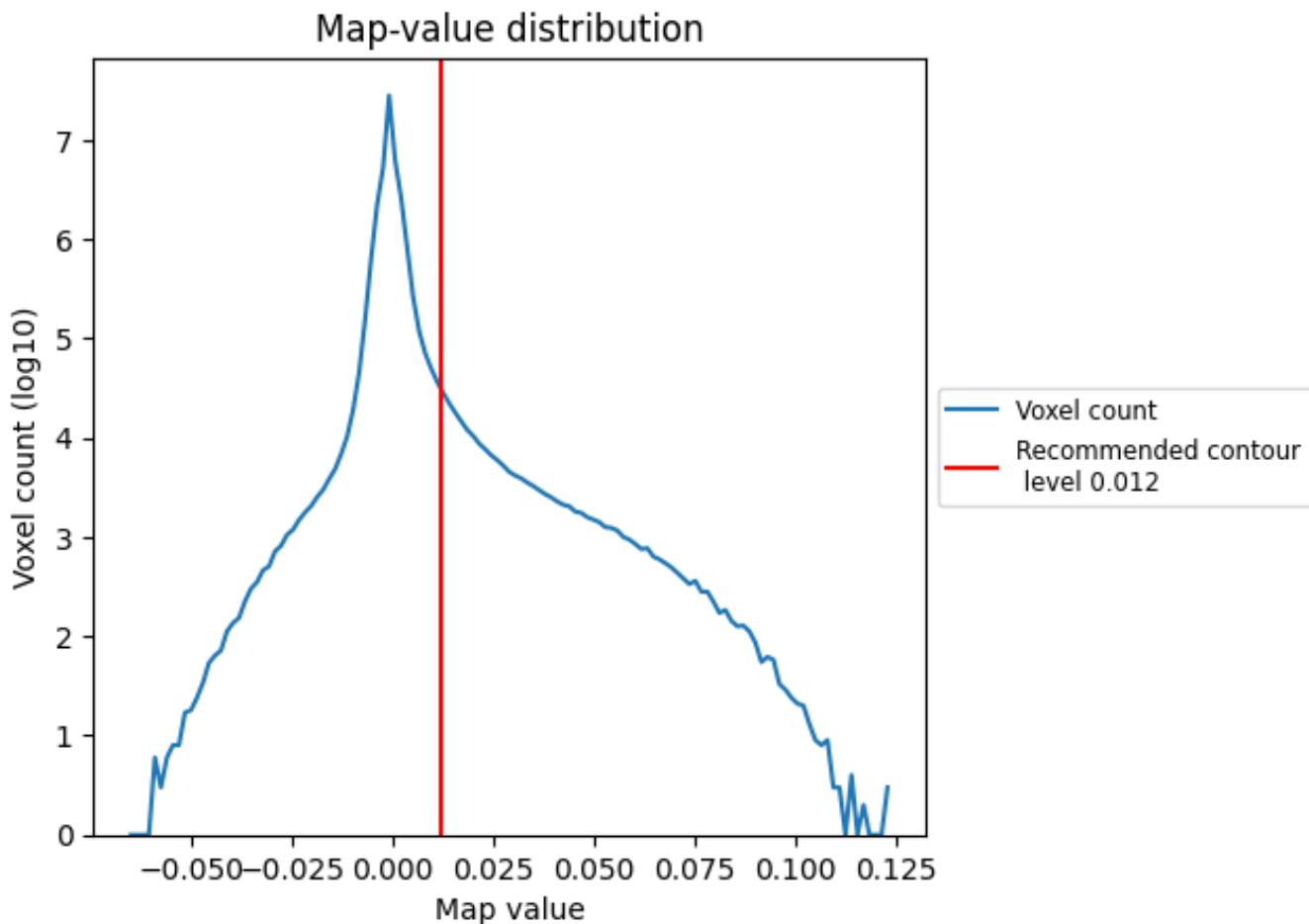
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

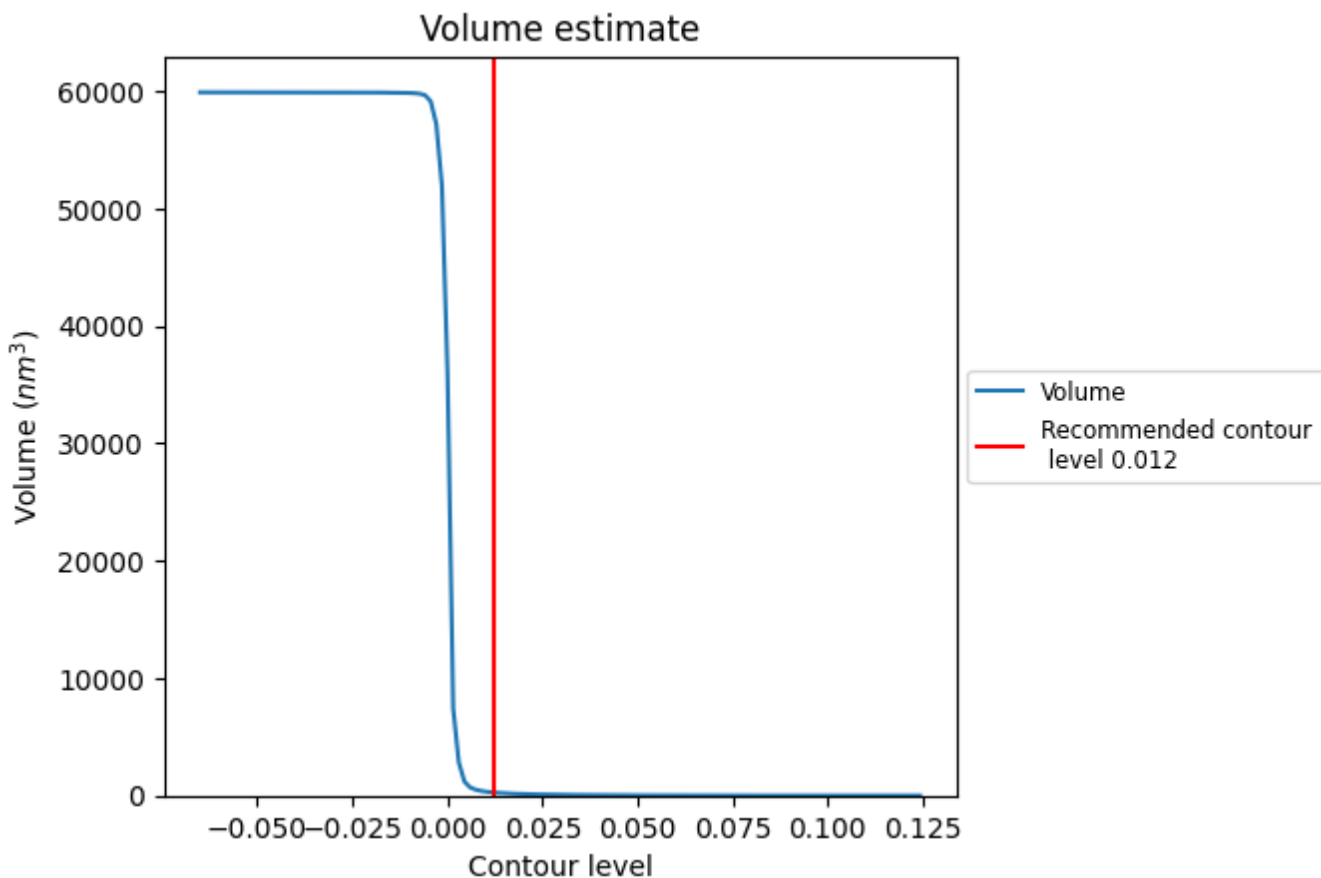
This section contains the results of statistical analysis of the map.

### 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.

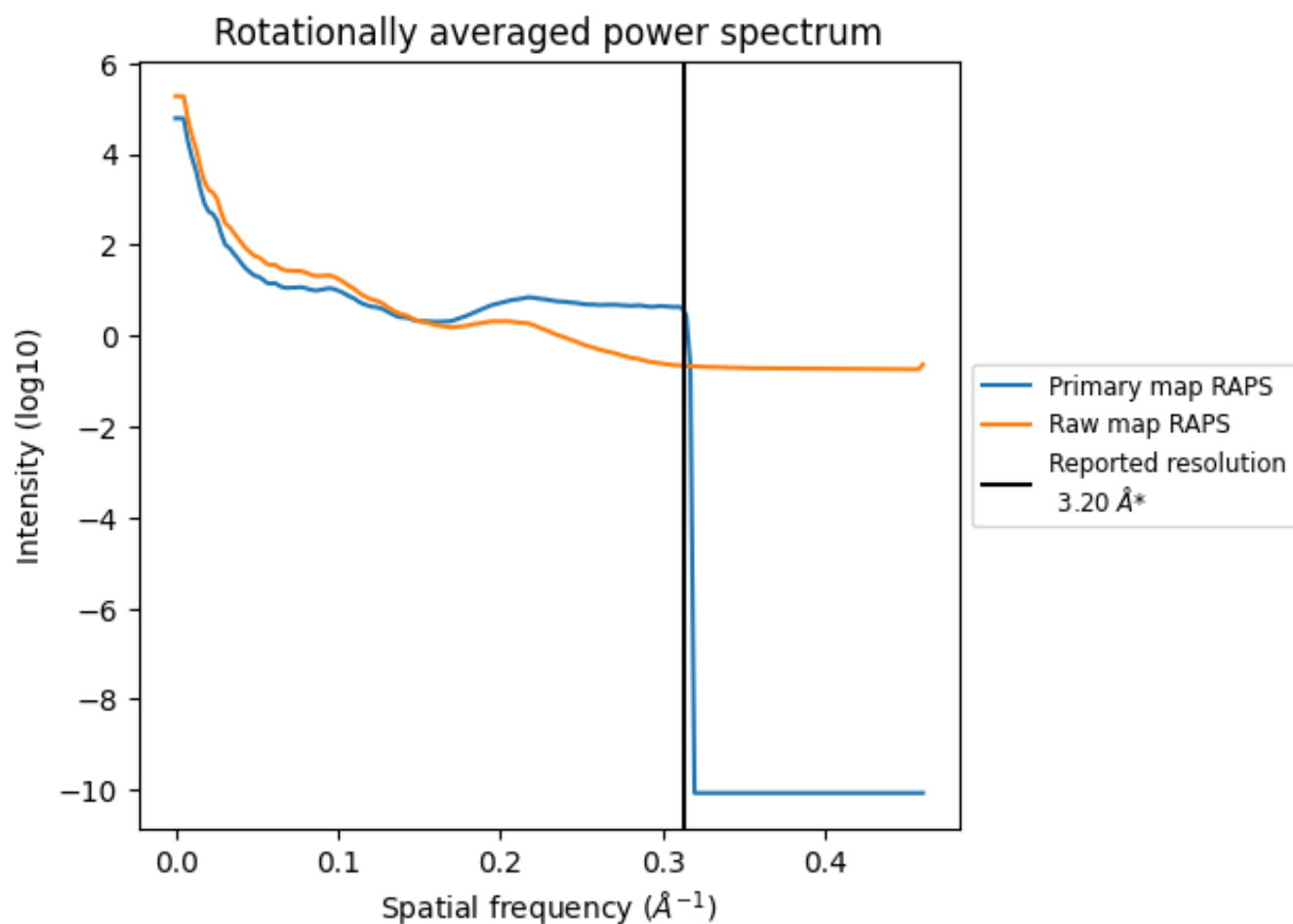
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 265 nm<sup>3</sup>; 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 [i](#)

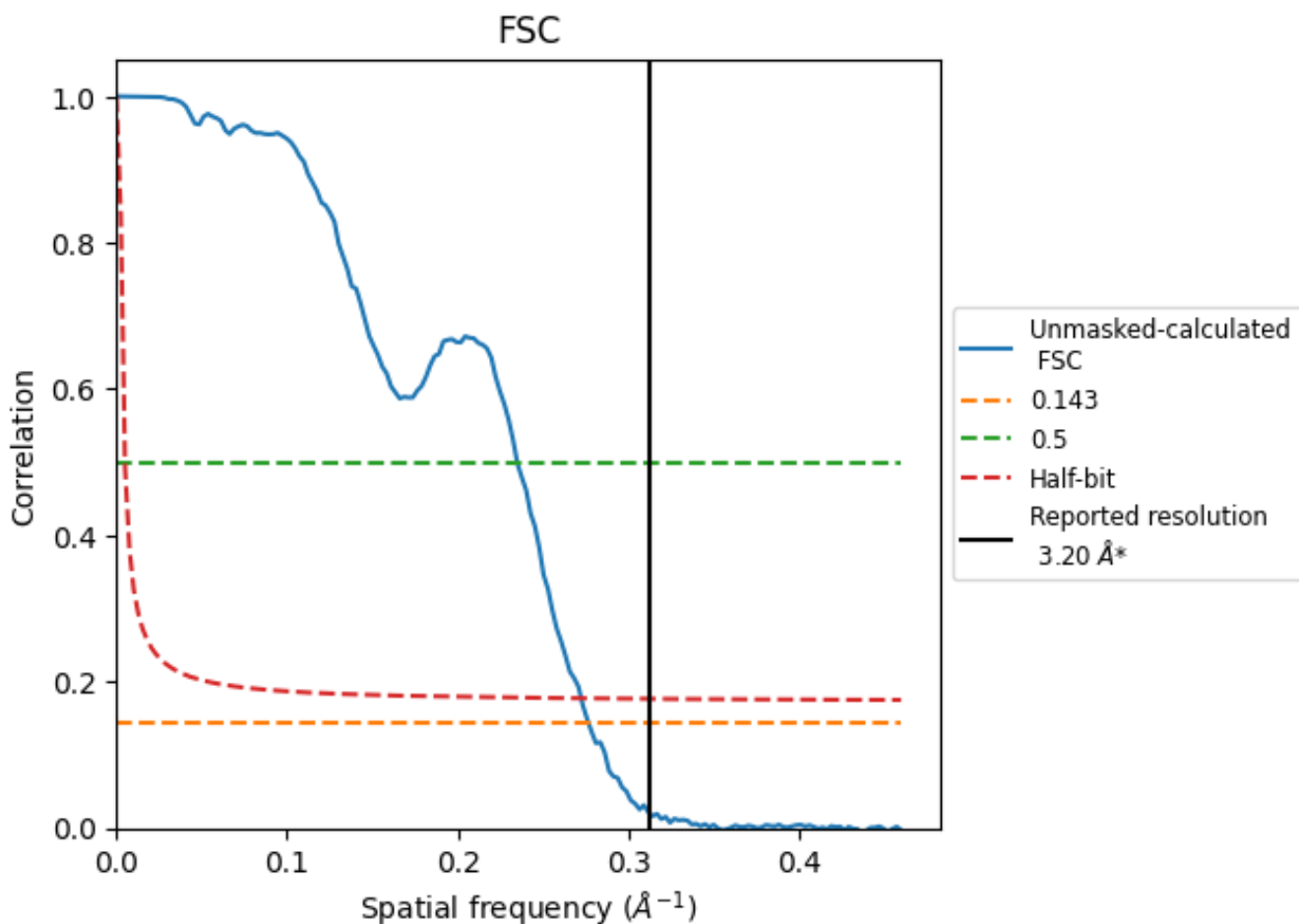


\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

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

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

### 8.1 FSC [\(i\)](#)



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



## 8.2 Resolution estimates [i](#)

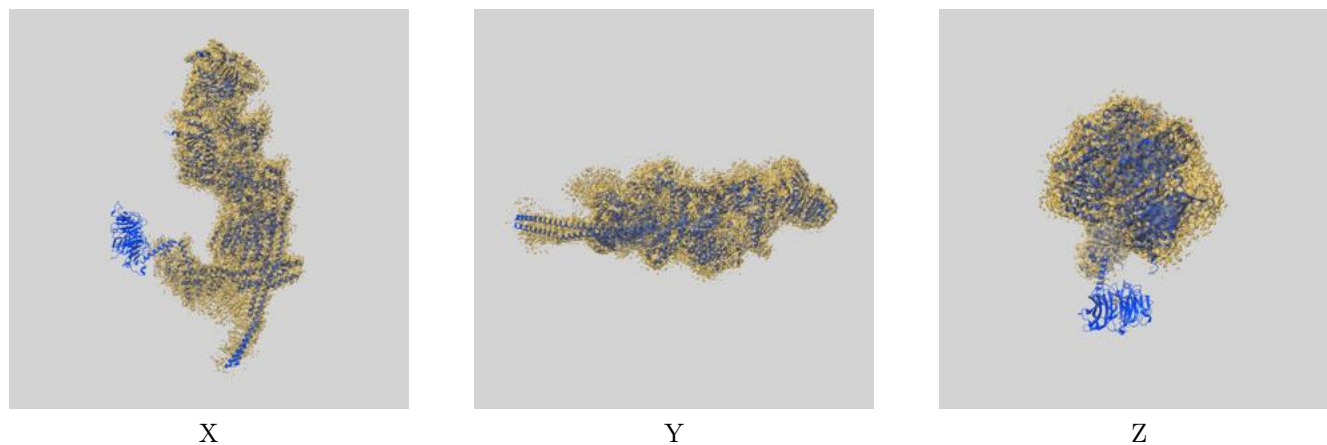
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.61	4.26	3.67

\*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](#)

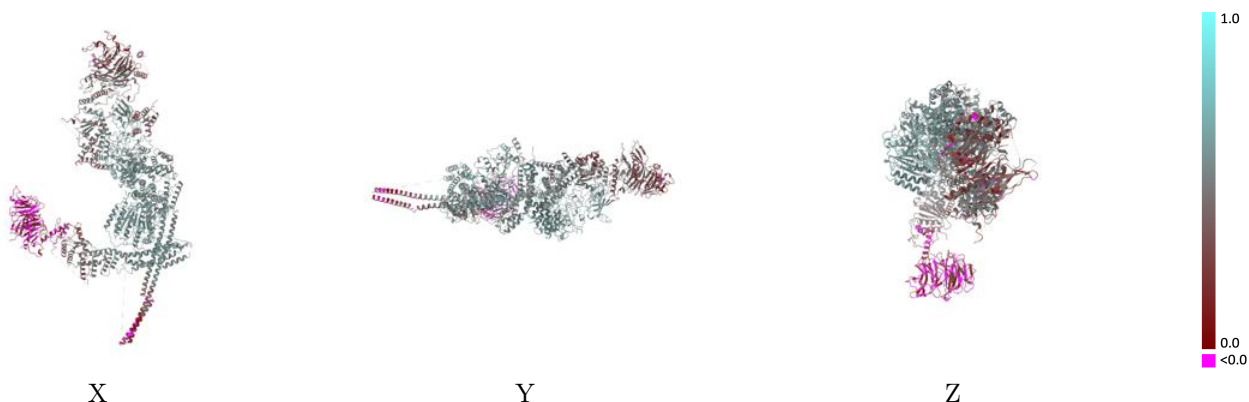
This section contains information regarding the fit between EMDB map EMD-35093 and PDB model 8I03. Per-residue inclusion information can be found in section [3](#) on page [6](#).

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



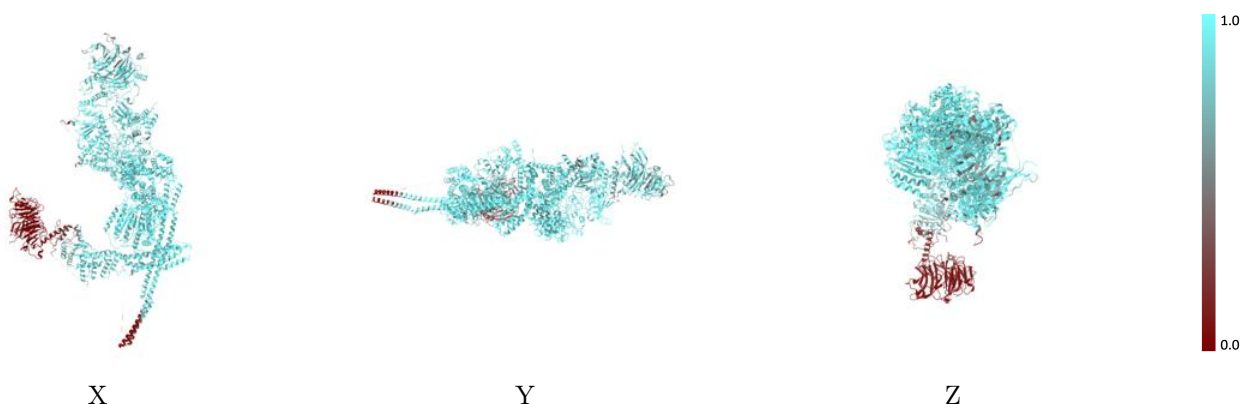
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



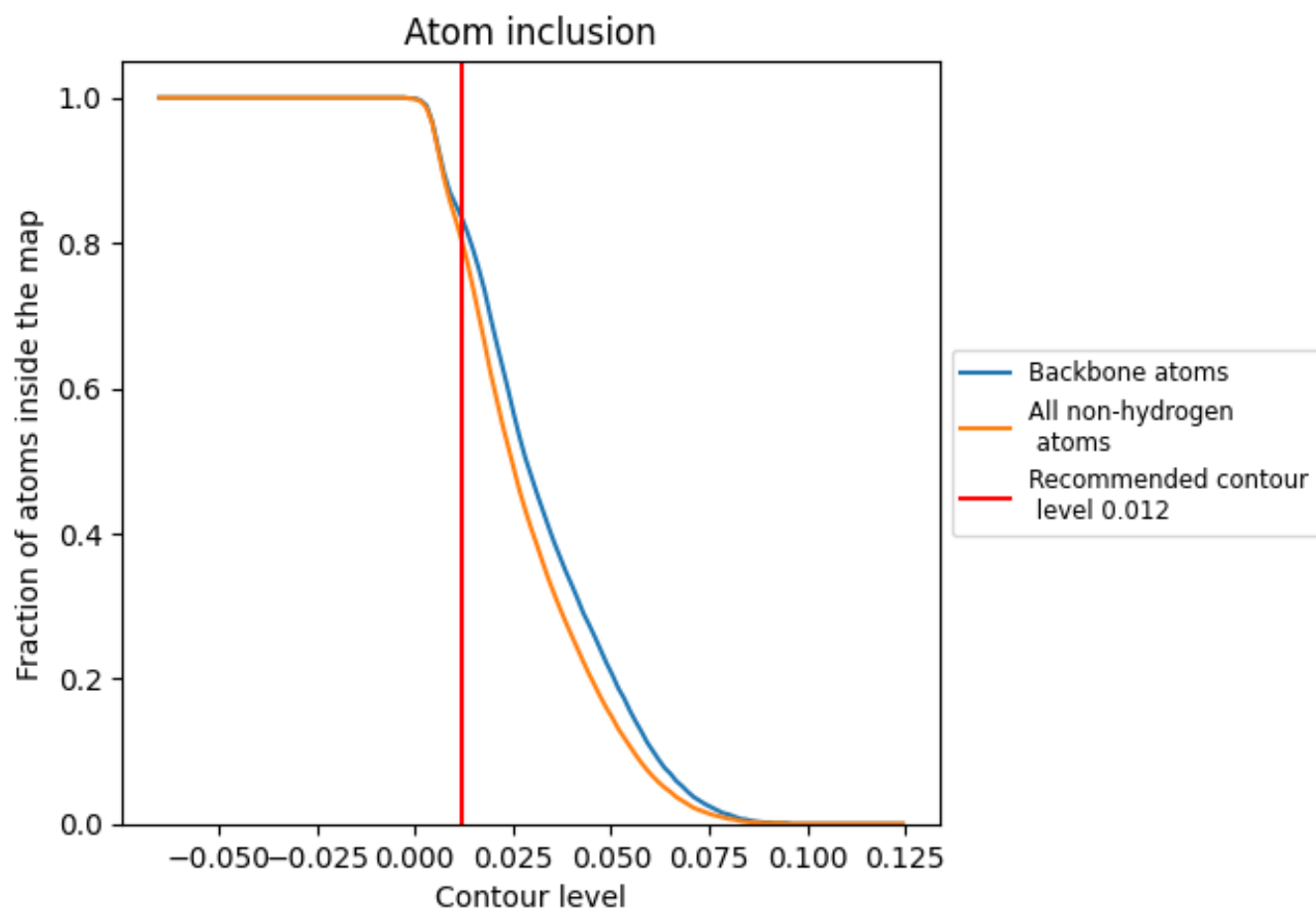
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

