Full wwPDB EM Validation Report (i)

Aug 27, 2026 – 05:42 am BST

PDB ID	:	7ARC / pdb_00007arc
EMDB ID	:	EMD-11879
Title	:	Cryo-EM structure of Polytomella Complex-I (peripheral arm)
Authors	:	Klusch, N.; Kuehlbrandt, W.; Yildiz, O.
Deposited on	:	2020-10-23
Resolution	:	2.88 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 (i) 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 (i)) were used in the production of this report:

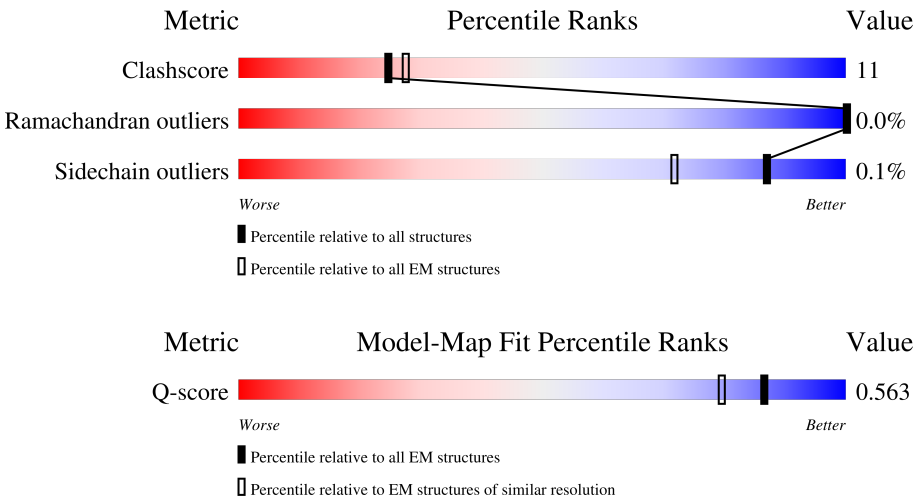
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.88 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	12111 (2.38 - 3.38)

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 <=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	B	164	18% 73% 21% 6%
2	C	217	6% 71% 28%
3	D	395	8% 66% 34%
4	E	276	14% 63% 22% 15%

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Mol	Chain	Length	Quality of chain
5	F	469	8% 70% 22% 8%
6	G	720	5% 74% 21% 5%
7	I	229	27% 68% 19% 13%
8	P	370	12% 73% 21% 6%
9	Q	185	7% 64% 23% 12%
10	R	132	20% 69% 13% 18%
11	S	98	10% 64% 33%
12	U	122	46% 41% 28% 31%
13	V	159	16% 71% 13% 16%
14	W	137	26% 65% 28% 7%
15	q	155	15% 82%
16	r	121	31% 38% 12% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	SF4	F	501	-	-	X	-

2 Entry composition (i)

There are 23 unique types of molecules in this entry. The entry contains 27699 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 PSST.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	154	1206	774	208	211	13	0	0

- Molecule 2 is a protein called ND9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	216	1808	1169	302	332	5	0	0

- Molecule 3 is a protein called ND7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	395	3178	2029	557	569	23	0	0

- Molecule 4 is a protein called 24 kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	235	1806	1135	306	350	15	0	0

- Molecule 5 is a protein called 51 kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	430	3322	2088	594	617	23	0	0

- Molecule 6 is a protein called 75 kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	682	5166	3243	919	980	24	0	0

- Molecule 7 is a protein called TYKY.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	I	199	1602	1000	274	317	11	0	0

- Molecule 8 is a protein called 39 kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	P	347	2701	1713	464	514	10	0	0

- Molecule 9 is a protein called 18 kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	Q	162	1276	812	227	233	4	0	0

- Molecule 10 is a protein called 13 kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	R	108	812	510	138	159	5	0	0

- Molecule 11 is a protein called B8.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	S	95	716	450	124	142	0	0

- Molecule 12 is a protein called SDAP2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	U	84	655	414	103	138	0	0

- Molecule 13 is a protein called B13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	V	134	1052	671	170	209	2	0	0

- Molecule 14 is a protein called B14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	W	127	1074	695	185	188	6	0	0

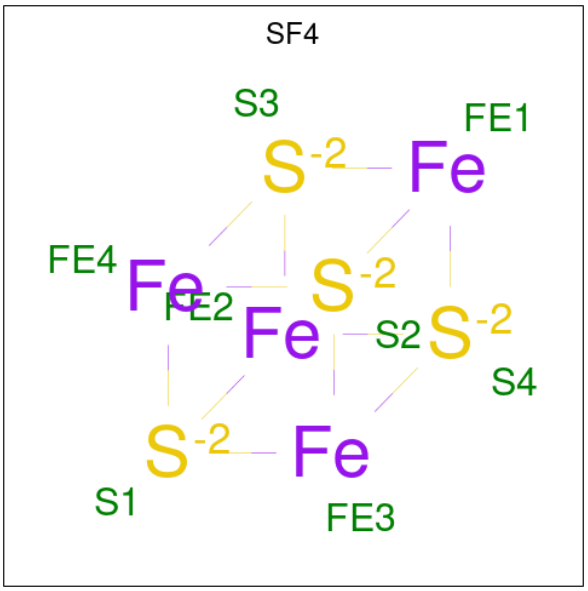
- Molecule 15 is a protein called B17.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	q	28	243	160	43	39	1	0	0

- Molecule 16 is a protein called B14.5a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	r	60	493	317	88	87	1	0	0

- Molecule 17 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
17	B	1	8	4	4	0
17	F	1	8	4	4	0
17	G	1	8	4	4	0
17	G	1	8	4	4	0

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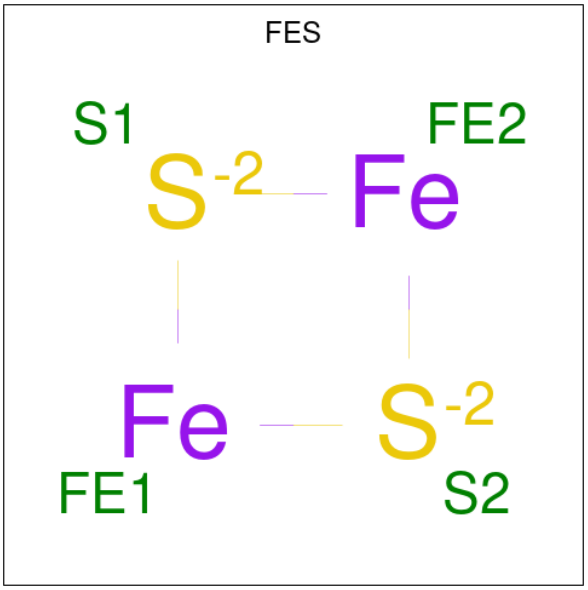
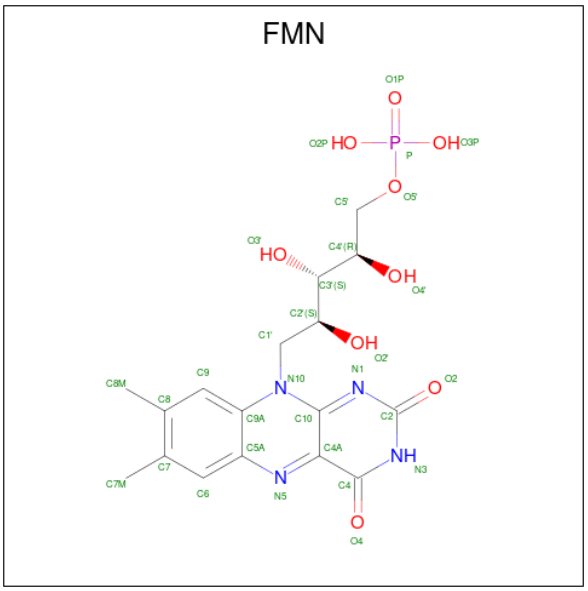
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
17	I	1	8	4	4	0
17	I	1	8	4	4	0

- Molecule 18 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



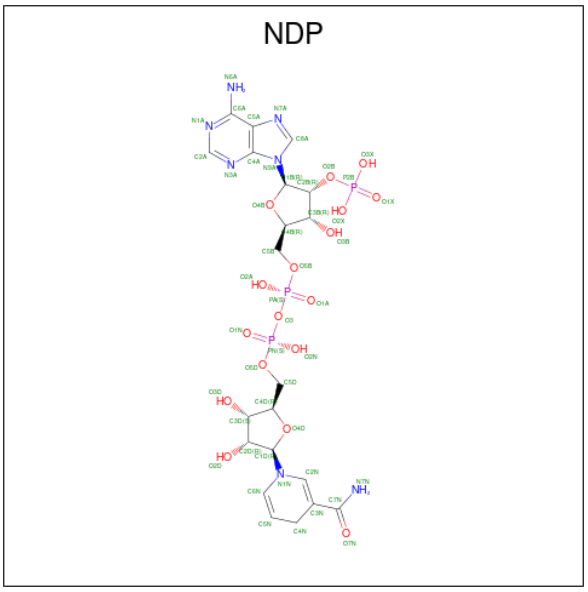
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
18	E	1	4	2	2	0
18	G	1	4	2	2	0

- Molecule 19 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
19	F	1	31	17	4	9	1	0

- Molecule 20 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

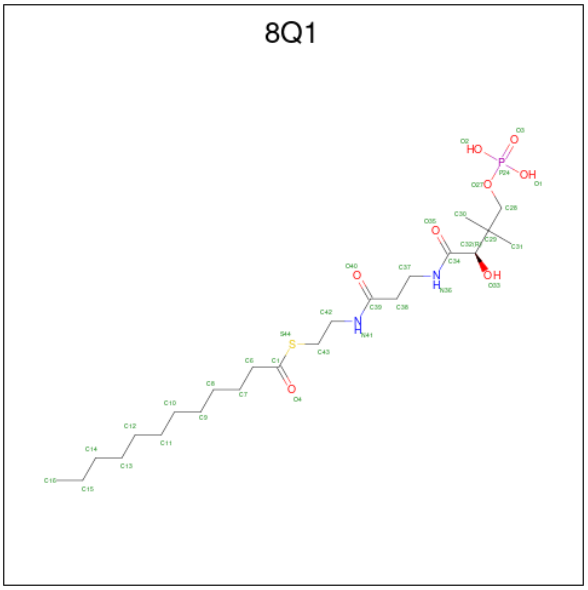


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
20	P	1	48	21	7	17	3	0

- Molecule 21 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
21	R	1	1	1	0

- Molecule 22 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
22	W	1	35	23	2	8	1	1	0

- Molecule 23 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
23	B	14	14	14	0
23	C	36	36	36	0
23	D	44	44	44	0
23	E	12	12	12	0
23	F	17	17	17	0
23	G	113	113	113	0
23	I	36	36	36	0

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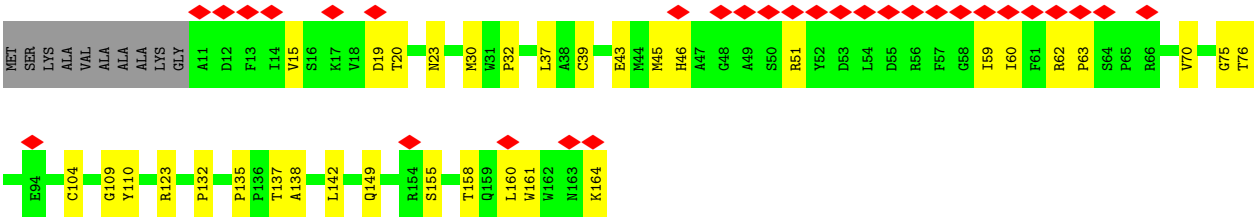
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
23	P	56	56	56	0
			Total	O	
23	Q	36	36	36	0
			Total	O	
23	R	9	9	9	0
			Total	O	
23	S	8	8	8	0
			Total	O	
23	V	10	10	10	0
			Total	O	
23	W	12	12	12	0
			Total	O	
23	q	8	8	8	0
			Total	O	
23	r	7	7	7	0

3 Residue-property plots (i)

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.

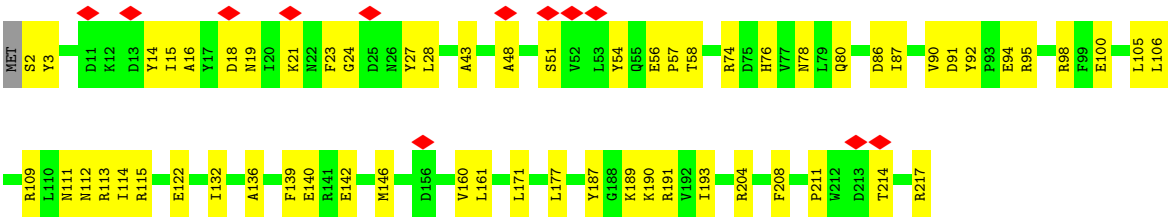
- Molecule 1: PSST

Chain B:



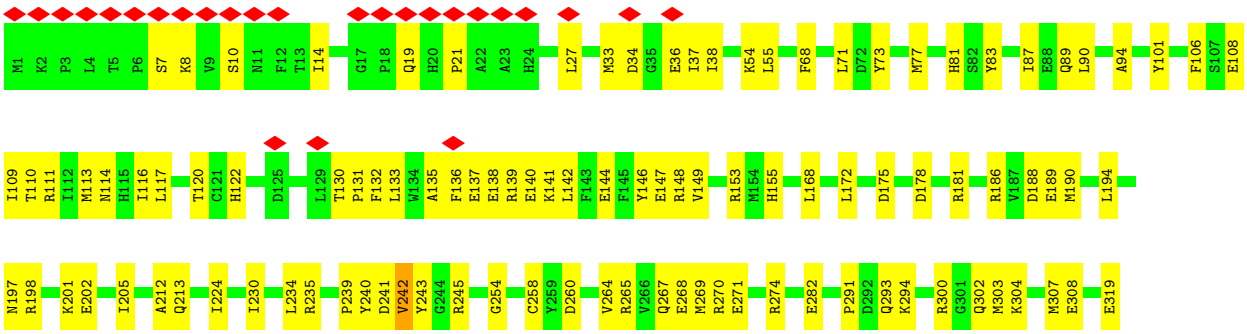
- Molecule 2: ND9

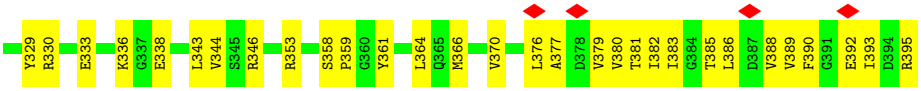
Chain C:



- Molecule 3: ND7

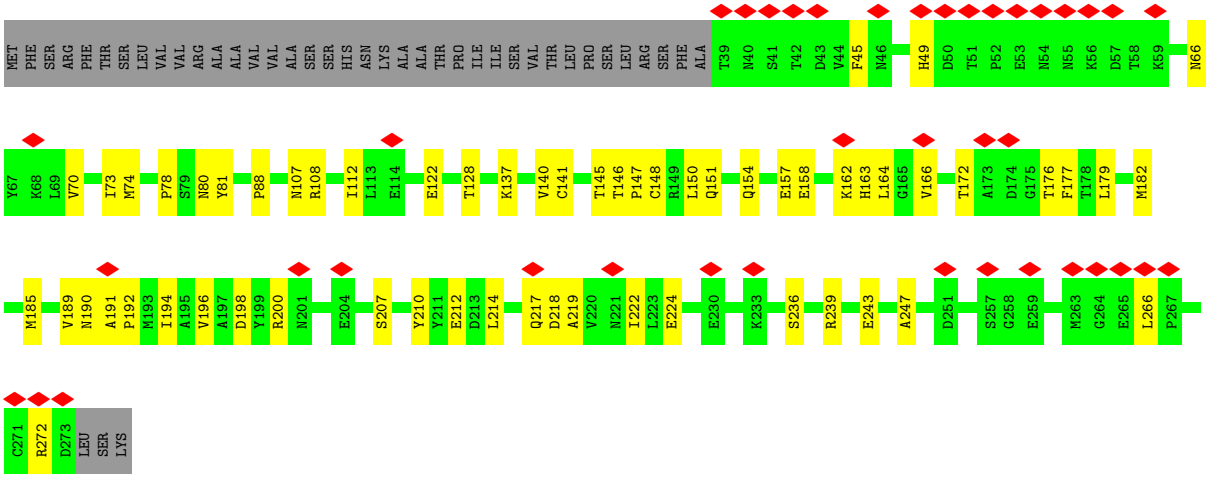
Chain D:





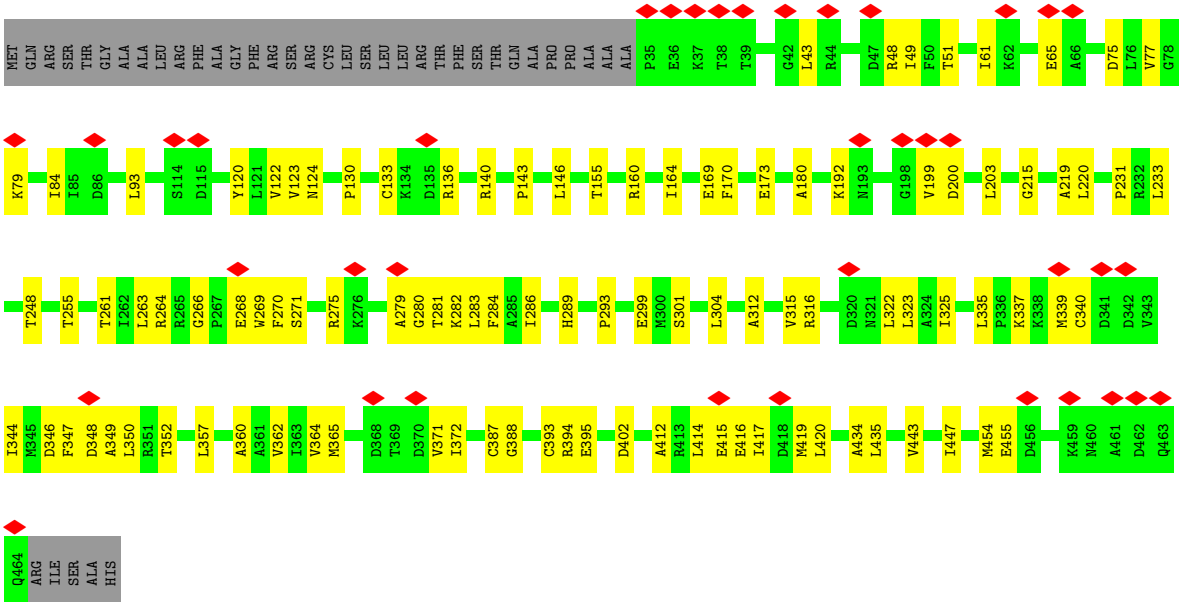
• Molecule 4: 24 kDa

Chain E:



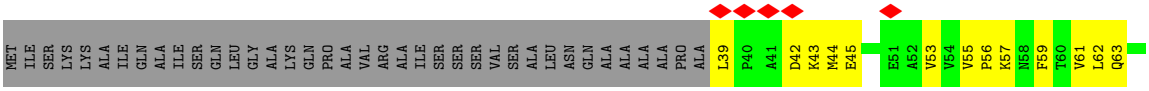
• Molecule 5: 51 kDa

Chain F:



• Molecule 6: 75 kDa

Chain G:



A68 D71 R74 H78 Q79 R80 L81 N86 C87 R88 E95 K96 G109 I114 D117 M129 E130 L133 I134 N135 H136 I142 C143 D144 Q145 G146 C149 D150 L151 Q152 R162 S163 R164 E167 D174 P179 G203 E206 I209 R212

V218 I222 E223 K224 L225 H226 S231 V234 V240 L244 S245 K246 F250 T251 A252 E261 D267 G270 V275 M283 R284 I285 D291 A292 I293 N294 E295 E296 R311 Q312 L318 K323 F334 G343 L349 K350 A351 K355 E360

L377 I378 H379 E380 D381 G382 S383 L386 A396 N397 T398 E404 D407 L410 G413 T414 N415 P416 L427 R428 K429 V430 L439 V440 G441 E442 K443 V444 D445 L446 T447 L460 K467 N479 P480 G485 S486 S487 V488 L489 R490 R491 D492 D493 R494 E495 A496

V501 V505 V510 E513 N516 N519 N524 R527 P537 N544 V550 D561 E562 A566 D567 A568 F569 R583 V587 E595 N602 R606 R611 V614 D623 I626 I627 R628 A629 E632 V633 Q637 D641 V646

A654 P655 H656 F657 A658 E659 K662 S665 Y673 F674 K675 G676 V677 K678 D679 L680 V681 A682 K683 A684 A685 R686 S687 T688 A689 R709 V717 R718 Q719 Q720

- Molecule 7: TYKY

Chain I:

MET SER LEU ILE ASN ARG ALA ALA GLN ARG LEU LEU SER MET PRO SER VAL SER SER MET GLY GLY LEU THR GLN PHE THR ARG SER MET G31 T32 E33 R34 R35 P36 G37 Q38 W42 K43 Q44 V45 D46 K47 Q48 R49 Y50 S51 S52 E53 W54 E55 Q56 D57 F60 K61 Q62 V63

P64 K65 N66 V67 S68 E69 V70 L71 D72 D73 S74 V75 S76 V77 L78 F79 L80 T81 D82 I83 V84 R85 G86 M87 M88 Y89 S90 A91 S92 G93 F94 F95 D96 D97 K98 V99 T100 I101 L102 Y103 P104 F105 E106 K107 G108 A109 V110 S111 P112 R121 I131 E137 P141 E148 A149

E150 E153 D154 G155 S156 R157 K158 T159 T160 R161 K168 C169 I170 C175 P180 T196 R197 E198 E199 L200 L201 K204 E209 I218 E225 S226 L227 Y228 R229

- Molecule 8: 39 kDa

Chain P:

MET S2 T3 L4 K5 P6 N10 N13 A14 V15 R16 N17 G18 P19 S24 Y42 E46 Y58 R59 C60 N61 V65 K69 Q70 D73 L74 I85 I95 S96 R97 V100 F123 P124 T125 R126 I130 E133 R139 Q142 A148 D149 V150

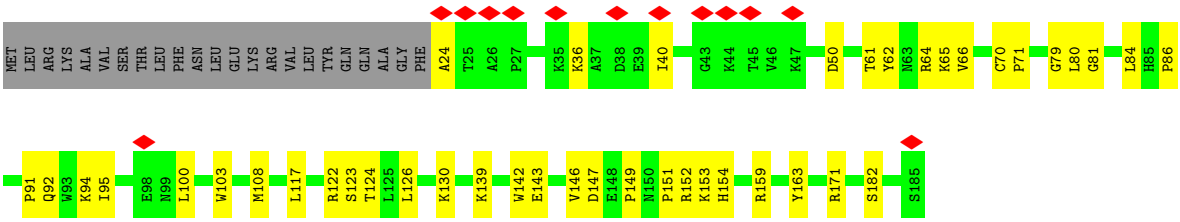
L157 D164 I167 I176 I177 R178 P179 V182 Y188 F189 N192 L193 I201 V202 A203 P204 N208 G209 A210 N211 P215 A222 D223 A224 V225 V226 K227 I228 D231 T234 P244 E245 T246 L247 T248 M249 R250 Q251 I257 D258 R261 L262 S263 N264

D265 D266 T267 V268 N269 L270 R271 Y272 E273 K276 M277 K280 D283 T284 L285 R286 E291 F292 P293 F294 L295 M298 N299 S300 Q307 A315 G316 I325 S326 P327 V330 T331 E332 G333 L334 E337 R340 F341 I342 R343 V344 G345 G346 Y347 D348 TRP GLY ASP MET

ASN LYS VAL SER SER ASN ILE PRO GLU HIS ILE ARG LYS TYR TYR ASN LEU LYS

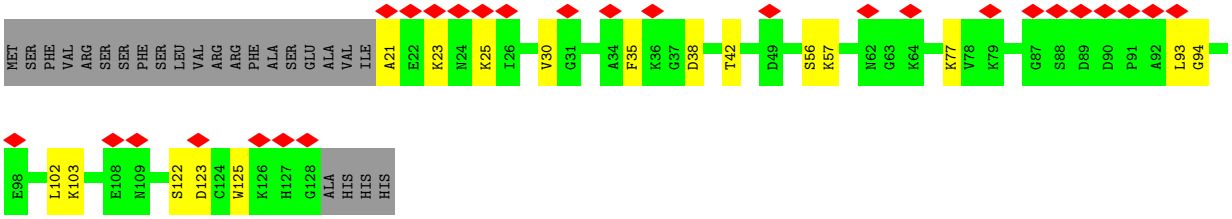
- Molecule 9: 18 kDa

Chain Q:



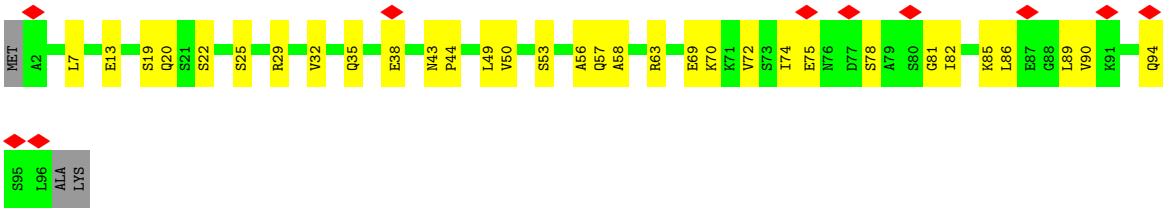
- Molecule 10: 13 kDa

Chain R:



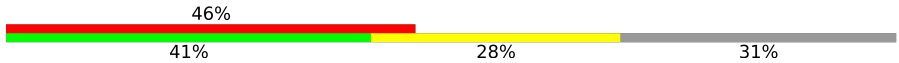
- Molecule 11: B8

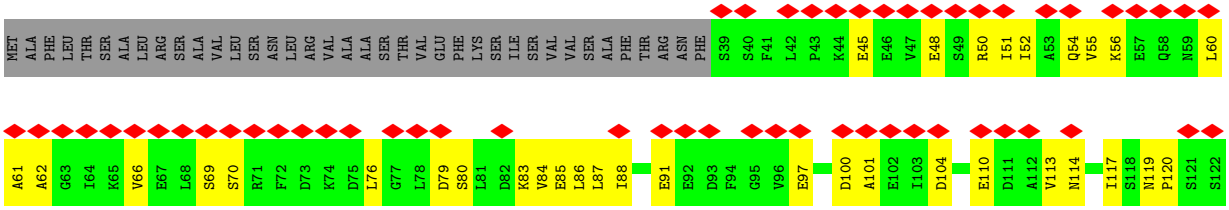
Chain S:



- Molecule 12: SDAP2

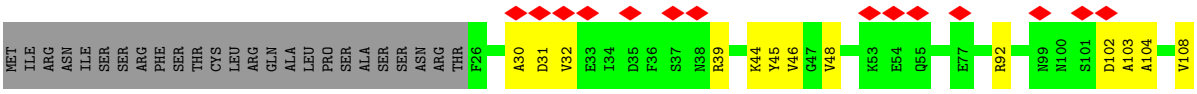
Chain U:

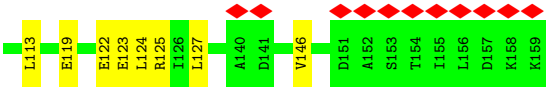




- Molecule 13: B13

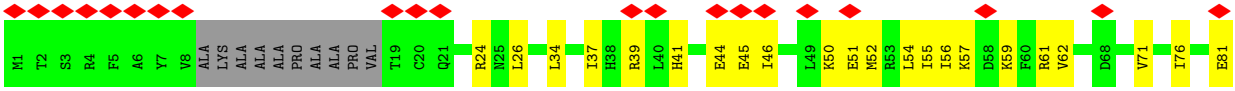
Chain V:

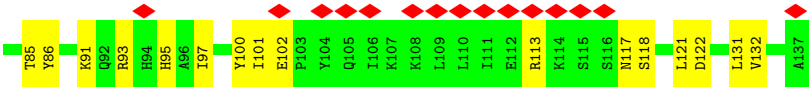




- Molecule 14: B14

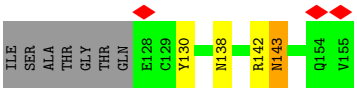
Chain W:





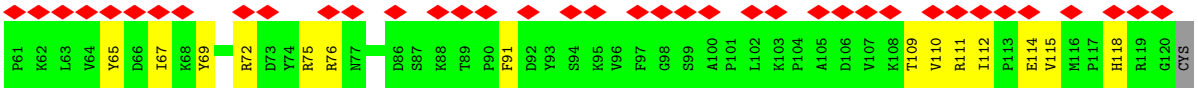
- Molecule 15: B17.2

Chain q:



- Molecule 16: B14.5a

Chain r:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42350	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	64	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.119	Depositor
Minimum map value	-0.060	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	502.2, 502.2, 502.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, NDP, FMN, SF4, 8Q1, FES

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	B	0.19	0/1240	0.42	0/1685
2	C	0.19	0/1862	0.37	0/2537
3	D	0.20	0/3257	0.42	0/4406
4	E	0.15	0/1843	0.39	0/2497
5	F	0.17	0/3394	0.38	0/4577
6	G	0.16	0/5254	0.34	0/7114
7	I	0.17	0/1634	0.41	0/2204
8	P	0.16	0/2750	0.37	0/3726
9	Q	0.16	0/1311	0.33	0/1774
10	R	0.13	0/832	0.33	0/1125
11	S	0.15	0/725	0.35	0/979
12	U	0.15	0/663	0.40	0/895
13	V	0.13	0/1069	0.31	0/1448
14	W	0.15	0/1097	0.34	0/1472
15	q	0.16	0/254	0.40	0/346
16	r	0.11	0/507	0.30	0/685
All	All	0.17	0/27692	0.37	0/37470

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	B	1206	0	1193	34	0
2	C	1808	0	1750	51	0
3	D	3178	0	3148	105	0
4	E	1806	0	1769	50	0
5	F	3322	0	3278	75	0
6	G	5166	0	5193	109	0
7	I	1602	0	1534	38	0
8	P	2701	0	2719	61	0
9	Q	1276	0	1264	32	0
10	R	812	0	781	16	0
11	S	716	0	730	23	0
12	U	655	0	647	24	0
13	V	1052	0	1059	18	0
14	W	1074	0	1101	27	0
15	q	243	0	233	5	0
16	r	493	0	498	17	0
17	B	8	0	0	1	0
17	F	8	0	0	2	0
17	G	16	0	0	0	0
17	I	16	0	0	1	0
18	E	4	0	0	0	0
18	G	4	0	0	0	0
19	F	31	0	19	2	0
20	P	48	0	26	1	0
21	R	1	0	0	0	0
22	W	35	0	0	1	0
23	B	14	0	0	0	0
23	C	36	0	0	3	0
23	D	44	0	0	2	0
23	E	12	0	0	2	0
23	F	17	0	0	1	0
23	G	113	0	0	2	0
23	I	36	0	0	2	0
23	P	56	0	0	4	0
23	Q	36	0	0	2	0
23	R	9	0	0	1	0
23	S	8	0	0	1	0
23	V	10	0	0	1	0
23	W	12	0	0	0	0
23	q	8	0	0	0	0
23	r	7	0	0	0	0
All	All	27699	0	26942	576	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 11.

All (576) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ARG:HE	1:B:63:PRO:HD2	1.35	0.92
5:F:271:SER:HA	5:F:279:ALA:HB1	1.58	0.85
3:D:101:TYR:OH	3:D:245:ARG:NH1	2.10	0.83
3:D:201:LYS:HE2	3:D:205:ILE:HD11	1.60	0.81
5:F:120:TYR:HB2	5:F:248:THR:HG22	1.64	0.80
6:G:295:GLU:OE2	6:G:429:LYS:NZ	2.13	0.79
3:D:307:MET:HE2	6:G:136:HIS:HD2	1.46	0.79
3:D:388:VAL:HB	3:D:393:ILE:HD11	1.64	0.79
6:G:709:ARG:NH2	10:R:23:LYS:O	2.15	0.78
2:C:24:GLY:HA2	2:C:28:LEU:HB2	1.65	0.78
2:C:95:ARG:NH1	2:C:100:GLU:OE2	2.15	0.78
5:F:447:ILE:HD13	5:F:454:MET:HE1	1.67	0.76
1:B:51:ARG:NH2	3:D:140:GLU:OE2	2.18	0.76
4:E:266:LEU:HD12	5:F:51:THR:HB	1.68	0.75
5:F:412:ALA:HB1	5:F:416:GLU:HG3	1.69	0.74
9:Q:61:THR:HG23	9:Q:117:LEU:HD11	1.70	0.74
6:G:709:ARG:NH1	10:R:25:LYS:O	2.21	0.74
6:G:665:SER:O	11:S:20:GLN:NE2	2.20	0.74
11:S:13:GLU:OE1	11:S:63:ARG:NH1	2.21	0.73
8:P:177:ILE:HG22	8:P:179:PRO:HD3	1.68	0.73
5:F:420:LEU:HD23	5:F:447:ILE:HD11	1.70	0.73
6:G:311:ARG:HE	6:G:709:ARG:HH21	1.36	0.73
5:F:315:VAL:HG21	5:F:322:LEU:HD21	1.69	0.73
6:G:222:ILE:HD11	6:G:224:LYS:HE2	1.71	0.72
2:C:106:LEU:HD13	2:C:113:ARG:HE	1.53	0.72
8:P:245:GLU:HG3	8:P:247:LEU:HD11	1.69	0.72
6:G:398:THR:OG1	6:G:516:ASN:O	2.08	0.72
1:B:110:TYR:HB2	7:I:170:ILE:HG21	1.72	0.71
4:E:163:HIS:NE2	4:E:224:GLU:OE2	2.22	0.71
6:G:164:ARG:HH21	16:r:67:ILE:HG12	1.54	0.71
2:C:177:LEU:HD11	3:D:55:LEU:HD23	1.71	0.71
5:F:395:GLU:HB3	6:G:134:ILE:HD11	1.72	0.71
6:G:495:GLU:HB3	6:G:681:VAL:HG12	1.73	0.71
8:P:227:LYS:HG3	8:P:325:ILE:HD11	1.72	0.71
7:I:197:ARG:HD3	8:P:74:LEU:HD21	1.72	0.71
1:B:62:ARG:NE	1:B:63:PRO:HD2	2.05	0.71
5:F:350:LEU:HD12	5:F:357:LEU:HB2	1.73	0.71
3:D:111:ARG:NH2	3:D:333:GLU:O	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:381:ASP:OD1	6:G:524:ASN:ND2	2.24	0.70
15:q:143:ASN:O	15:q:143:ASN:ND2	2.25	0.69
1:B:110:TYR:HE1	7:I:141:PRO:HB2	1.58	0.69
4:E:166:VAL:HG11	4:E:172:THR:HA	1.73	0.69
6:G:398:THR:HB	6:G:519:ASN:HD21	1.56	0.69
5:F:402:ASP:HB3	6:G:167:GLU:HG2	1.75	0.69
6:G:209:ILE:HD13	6:G:218:VAL:HG22	1.75	0.68
6:G:63:GLN:HG2	9:Q:154:HIS:CD2	2.29	0.68
8:P:6:PRO:HB3	8:P:16:ARG:NH1	2.08	0.68
12:U:104:ASP:OD1	14:W:24:ARG:NH2	2.27	0.68
8:P:244:PRO:HD3	8:P:327:PRO:HB2	1.76	0.68
22:W:200:8Q1:O40	22:W:200:8Q1:N36	2.26	0.67
11:S:29:ARG:NH1	23:S:101:HOH:O	2.25	0.67
4:E:151:GLN:NE2	23:E:601:HOH:O	2.29	0.66
9:Q:66:VAL:HG13	9:Q:95:ILE:HG23	1.78	0.66
5:F:140:ARG:HB3	5:F:173:GLU:HG3	1.76	0.66
8:P:46:GLU:HG3	8:P:222:ALA:HB1	1.76	0.66
3:D:239:PRO:HG3	16:r:112:ILE:HG23	1.77	0.66
3:D:178:ASP:O	3:D:181:ARG:HG2	1.95	0.66
4:E:236:SER:OG	4:E:239:ARG:O	2.14	0.66
8:P:164:ASP:OD2	23:P:601:HOH:O	2.13	0.65
4:E:137:LYS:HD2	4:E:200:ARG:HG2	1.79	0.65
8:P:307:GLN:NE2	23:P:608:HOH:O	2.29	0.65
2:C:214:THR:O	2:C:217:ARG:NH1	2.30	0.64
6:G:566:ALA:HA	6:G:583:ARG:HH21	1.63	0.64
9:Q:65:LYS:NZ	9:Q:143:GLU:OE1	2.29	0.64
12:U:60:LEU:HG	12:U:61:ALA:H	1.62	0.64
5:F:395:GLU:OE1	23:F:601:HOH:O	2.15	0.64
6:G:611:ARG:NH2	9:Q:147:ASP:OD2	2.31	0.64
13:V:102:ASP:HB2	13:V:113:LEU:HD11	1.80	0.63
3:D:68:PHE:HA	3:D:71:LEU:HD12	1.80	0.63
3:D:304:LYS:NZ	7:I:180:PRO:O	2.31	0.63
8:P:189:PHE:HE1	8:P:249:MET:HE1	1.64	0.63
3:D:19:GLN:NE2	3:D:21:PRO:HD2	2.13	0.63
6:G:80:ARG:NH2	6:G:291:ASP:OD1	2.32	0.63
4:E:164:LEU:HD12	4:E:179:LEU:HD21	1.79	0.63
4:E:214:LEU:HD13	4:E:219:ALA:HB2	1.81	0.63
6:G:480:PRO:HG2	6:G:510:VAL:HA	1.81	0.63
3:D:358:SER:HB3	3:D:361:TYR:HB2	1.81	0.63
5:F:417:ILE:HG23	5:F:447:ILE:HD12	1.81	0.63
8:P:188:TYR:O	8:P:192:ASN:ND2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:GLU:OE2	3:D:153:ARG:NH2	2.32	0.62
3:D:109:ILE:HG23	3:D:142:LEU:HD22	1.80	0.62
5:F:346:ASP:OD1	5:F:347:PHE:N	2.31	0.62
12:U:70:SER:HB3	12:U:76:LEU:HD11	1.81	0.62
3:D:33:MET:HG2	3:D:38:ILE:HA	1.82	0.62
6:G:275:VAL:HG22	6:G:285:ILE:HG12	1.81	0.62
11:S:57:GLN:NE2	11:S:75:GLU:OE2	2.30	0.62
5:F:84:ILE:HG23	5:F:263:LEU:HD21	1.80	0.62
13:V:122:GLU:HG2	13:V:125:ARG:HH22	1.64	0.62
7:I:35:ARG:HB2	7:I:38:GLN:HG2	1.82	0.62
8:P:262:LEU:HD23	8:P:343:ARG:HH22	1.65	0.61
6:G:74:ARG:HH22	9:Q:80:LEU:HD23	1.64	0.61
2:C:177:LEU:HA	3:D:54:LYS:HE3	1.82	0.61
6:G:293:ILE:HD11	6:G:606:ARG:HD2	1.82	0.61
9:Q:100:LEU:HD13	14:W:132:VAL:HG22	1.82	0.61
9:Q:122:ARG:NH2	23:Q:203:HOH:O	2.34	0.60
1:B:110:TYR:HB2	7:I:170:ILE:CG2	2.31	0.60
2:C:48:ALA:HB3	2:C:51:SER:O	2.01	0.60
2:C:74:ARG:NH1	2:C:132:ILE:O	2.34	0.60
3:D:271:GLU:OE1	3:D:274:ARG:NH1	2.33	0.60
2:C:191:ARG:NH2	14:W:102:GLU:OE1	2.25	0.60
8:P:257:ILE:HG12	8:P:262:LEU:HD12	1.82	0.60
6:G:146:GLY:O	6:G:152:GLN:NE2	2.29	0.60
3:D:293:GLN:HE22	3:D:302:GLN:HE22	1.49	0.60
8:P:100:VAL:HG12	8:P:139:ARG:HB2	1.83	0.60
14:W:34:LEU:HD23	14:W:37:ILE:HD11	1.83	0.60
8:P:257:ILE:HG23	8:P:262:LEU:HB2	1.82	0.60
8:P:258:ASP:O	8:P:261:ARG:HD3	2.01	0.60
12:U:61:ALA:HB1	12:U:76:LEU:HD23	1.83	0.60
3:D:186:ARG:NH2	3:D:189:GLU:OE2	2.30	0.60
3:D:234:LEU:HD11	3:D:338:GLU:HG3	1.83	0.60
6:G:628:ARG:HH12	6:G:637:GLN:HG3	1.67	0.60
3:D:14:ILE:HD12	3:D:33:MET:HE2	1.84	0.59
6:G:383:SER:O	6:G:527:ARG:NH2	2.35	0.59
2:C:18:ASP:OD1	2:C:19:ASN:N	2.35	0.59
3:D:141:LYS:O	3:D:144:GLU:HG3	2.02	0.59
9:Q:64:ARG:HD2	14:W:131:LEU:HD13	1.83	0.59
6:G:496:ALA:HB3	6:G:686:ARG:NH2	2.17	0.59
9:Q:130:LYS:HE3	9:Q:146:VAL:HG11	1.85	0.59
3:D:111:ARG:NH1	23:D:405:HOH:O	2.35	0.59
4:E:247:ALA:HB2	5:F:293:PRO:HD3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:142:GLU:OE2	3:D:395:ARG:NH2	2.36	0.58
3:D:113:MET:HG2	3:D:142:LEU:HD13	1.83	0.58
6:G:443:LYS:NZ	23:G:908:HOH:O	2.30	0.58
11:S:90:VAL:O	11:S:94:GLN:HG2	2.04	0.58
1:B:15:VAL:HG23	1:B:158:THR:HG22	1.86	0.58
3:D:33:MET:HE1	3:D:376:LEU:HD21	1.85	0.58
4:E:150:LEU:HD21	5:F:365:MET:HG2	1.85	0.58
14:W:97:ILE:HD13	14:W:101:ILE:HD12	1.86	0.57
2:C:187:TYR:O	2:C:190:LYS:NZ	2.36	0.57
5:F:286:ILE:HG21	5:F:312:ALA:HB2	1.86	0.57
12:U:79:ASP:OD1	12:U:80:SER:N	2.35	0.57
5:F:275:ARG:NH2	5:F:346:ASP:OD2	2.36	0.57
4:E:217:GLN:CD	4:E:217:GLN:H	2.13	0.57
4:E:145:THR:HG22	4:E:146:THR:H	1.70	0.57
6:G:410:LEU:HD11	6:G:440:VAL:HG23	1.87	0.56
8:P:124:PRO:HB3	8:P:167:ILE:HD11	1.85	0.56
9:Q:152:ARG:NH2	23:Q:205:HOH:O	2.38	0.56
3:D:264:VAL:O	3:D:268:GLU:HG3	2.06	0.56
7:I:201:LEU:HD11	8:P:74:LEU:HD13	1.86	0.56
3:D:188:ASP:OD1	3:D:270:ARG:NH2	2.34	0.56
3:D:241:ASP:C	3:D:243:TYR:H	2.14	0.56
3:D:389:VAL:O	3:D:393:ILE:HG13	2.05	0.56
4:E:141:CYS:SG	4:E:182:MET:HE3	2.45	0.56
8:P:224:ALA:O	8:P:228:ILE:HG12	2.06	0.56
6:G:659:GLU:HB3	6:G:662:LYS:HE2	1.87	0.56
2:C:136:ALA:O	2:C:140:GLU:HG3	2.06	0.56
13:V:92:ARG:NH1	23:V:202:HOH:O	2.36	0.55
3:D:393:ILE:O	3:D:395:ARG:NH1	2.39	0.55
2:C:43:ALA:HB3	13:V:146:VAL:HG22	1.89	0.55
5:F:155:THR:HG22	5:F:199:VAL:HG21	1.88	0.55
12:U:88:ILE:O	12:U:91:GLU:HB2	2.07	0.55
1:B:19:ASP:OD1	1:B:20:THR:N	2.40	0.55
1:B:132:PRO:HG3	7:I:200:LEU:HD11	1.89	0.55
3:D:147:GLU:HB2	3:D:153:ARG:HG2	1.89	0.55
3:D:307:MET:HE2	6:G:136:HIS:CD2	2.36	0.55
1:B:51:ARG:HD3	7:I:101:ILE:HD12	1.88	0.55
3:D:186:ARG:HH21	3:D:189:GLU:CD	2.13	0.55
7:I:229:ARG:NH2	23:I:605:HOH:O	2.38	0.55
2:C:16:ALA:HB3	2:C:21:LYS:HE3	1.87	0.55
4:E:190:ASN:OD1	4:E:239:ARG:NH2	2.33	0.55
7:I:153:GLU:HB3	10:R:30:VAL:HG23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:146:MET:HB3	2:C:171:LEU:HD12	1.88	0.55
3:D:27:LEU:HD13	3:D:390:PHE:CE2	2.42	0.55
4:E:74:MET:HE1	4:E:112:ILE:HG22	1.88	0.54
2:C:106:LEU:HD13	2:C:113:ARG:NE	2.21	0.54
9:Q:36:LYS:HZ2	9:Q:40:ILE:HD11	1.72	0.54
3:D:291:PRO:O	6:G:162:ARG:NH2	2.40	0.54
9:Q:91:PRO:HB2	9:Q:126:LEU:HB3	1.87	0.54
6:G:378:ILE:HG22	6:G:537:PRO:HG3	1.89	0.54
6:G:396:ALA:HB1	6:G:519:ASN:HD22	1.73	0.54
5:F:61:ILE:O	5:F:65:GLU:HG2	2.07	0.54
6:G:61:VAL:HG13	6:G:114:ILE:HD13	1.90	0.54
2:C:23:PHE:HE2	2:C:78:ASN:HB3	1.73	0.54
2:C:28:LEU:HD23	2:C:57:PRO:HG2	1.89	0.54
8:P:286:ARG:NH1	8:P:300:SER:HB3	2.23	0.54
2:C:122:GLU:OE2	9:Q:139:LYS:NZ	2.40	0.54
6:G:206:GLU:OE1	6:G:226:HIS:HA	2.08	0.54
4:E:198:ASP:OD2	4:E:207:SER:OG	2.27	0.53
8:P:95:ILE:HD11	8:P:130:ILE:HG22	1.90	0.53
4:E:191:ALA:HB3	4:E:192:PRO:HD3	1.89	0.53
6:G:583:ARG:O	6:G:583:ARG:HG3	2.09	0.53
1:B:37:LEU:HB2	1:B:75:GLY:HA3	1.90	0.53
1:B:160:LEU:HD22	8:P:60:CYS:O	2.07	0.53
6:G:680:LEU:HD11	11:S:44:PRO:HB3	1.90	0.53
8:P:42:TYR:O	8:P:46:GLU:HG2	2.08	0.53
1:B:137:THR:HA	3:D:153:ARG:HH21	1.72	0.53
2:C:204:ARG:NH1	23:C:305:HOH:O	2.33	0.53
7:I:201:LEU:HB3	9:Q:108:MET:HE2	1.89	0.53
9:Q:81:GLY:O	9:Q:92:GLN:NE2	2.42	0.53
3:D:130:THR:HG23	3:D:131:PRO:HD3	1.91	0.53
4:E:247:ALA:HB1	5:F:316:ARG:HH21	1.73	0.53
8:P:69:LYS:NZ	23:P:612:HOH:O	2.39	0.53
9:Q:71:PRO:HG3	9:Q:94:LYS:HE2	1.90	0.53
14:W:50:LYS:O	14:W:54:LEU:HG	2.09	0.53
14:W:57:LYS:O	14:W:61:ARG:HG2	2.08	0.53
5:F:219:ALA:HB2	5:F:231:PRO:HG3	1.91	0.53
6:G:355:LYS:HG3	6:G:380:GLU:OE2	2.07	0.53
7:I:148:GLU:HG2	7:I:161:ARG:HB3	1.90	0.53
10:R:35:PHE:HB2	10:R:38:ASP:OD2	2.09	0.52
14:W:81:GLU:O	14:W:85:THR:HG23	2.10	0.52
9:Q:84:LEU:HD12	9:Q:149:PRO:HG3	1.91	0.52
5:F:282:LYS:HE3	5:F:360:ALA:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:505:VAL:HG13	6:G:510:VAL:HG22	1.91	0.52
4:E:128:THR:HG23	6:G:212:ARG:HH12	1.74	0.52
5:F:170:PHE:HB3	5:F:173:GLU:HB2	1.91	0.52
6:G:56:PRO:HD2	6:G:59:PHE:CE2	2.44	0.52
6:G:270:GLY:HA3	6:G:602:ASN:HD21	1.75	0.52
7:I:56:GLN:HB3	13:V:44:LYS:NZ	2.25	0.52
12:U:83:LYS:O	12:U:86:LEU:HG	2.10	0.52
3:D:7:SER:C	3:D:8:LYS:HD3	2.35	0.51
8:P:209:GLY:O	8:P:248:THR:OG1	2.24	0.51
1:B:32:PRO:HD2	1:B:60:ILE:O	2.11	0.51
2:C:208:PHE:HB3	3:D:319:GLU:HG3	1.93	0.51
3:D:234:LEU:HB2	3:D:333:GLU:HB2	1.92	0.51
12:U:50:ARG:O	12:U:54:GLN:HG2	2.11	0.51
1:B:32:PRO:HA	1:B:70:VAL:O	2.10	0.51
3:D:168:LEU:HD22	3:D:172:LEU:HD23	1.93	0.51
6:G:252:ALA:HB2	6:G:283:MET:HE2	1.93	0.51
8:P:17:ASN:ND2	9:Q:103:TRP:HB3	2.25	0.51
13:V:122:GLU:HG2	13:V:125:ARG:NH2	2.26	0.51
12:U:91:GLU:OE1	12:U:97:GLU:HA	2.11	0.51
6:G:261:GLU:O	6:G:611:ARG:HD3	2.10	0.51
2:C:160:VAL:HG23	2:C:161:LEU:HG	1.93	0.51
3:D:110:THR:HB	3:D:146:TYR:OH	2.10	0.51
7:I:112:PRO:HB2	7:I:225:GLU:OE2	2.11	0.51
13:V:104:ALA:O	13:V:108:VAL:HG23	2.11	0.51
2:C:86:ASP:OD2	23:C:301:HOH:O	2.19	0.51
3:D:106:PHE:CZ	3:D:149:VAL:HG11	2.45	0.51
3:D:212:ALA:HB1	3:D:230:ILE:HD11	1.93	0.50
3:D:366:MET:HE3	3:D:370:VAL:HG21	1.92	0.50
5:F:77:VAL:HG11	5:F:199:VAL:HG11	1.93	0.50
8:P:340:ARG:HD3	14:W:45:GLU:HG3	1.92	0.50
2:C:87:ILE:HB	2:C:139:PHE:HB3	1.92	0.50
3:D:106:PHE:HZ	3:D:149:VAL:HG11	1.76	0.50
8:P:177:ILE:HD11	8:P:228:ILE:HG13	1.92	0.50
6:G:130:GLU:O	6:G:134:ILE:HG23	2.12	0.50
6:G:550:VAL:HG22	6:G:569:PHE:HB3	1.92	0.50
11:S:81:GLY:O	11:S:85:LYS:HG3	2.11	0.50
2:C:112:ASN:OD1	2:C:113:ARG:N	2.45	0.50
3:D:304:LYS:NZ	10:R:94:GLY:O	2.37	0.50
3:D:258:CYS:SG	3:D:385:THR:HG21	2.50	0.50
4:E:154:GLN:O	4:E:157:GLU:HG3	2.11	0.50
5:F:443:VAL:O	5:F:447:ILE:HG12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:231:SER:O	6:G:234:VAL:HG22	2.11	0.50
7:I:150:GLU:HG2	10:R:42:THR:HA	1.93	0.50
3:D:197:ASN:O	3:D:201:LYS:HG2	2.12	0.50
4:E:190:ASN:HB3	4:E:212:GLU:HB3	1.94	0.50
4:E:218:ASP:O	4:E:222:ILE:HG12	2.12	0.50
8:P:245:GLU:HG3	8:P:247:LEU:CD1	2.41	0.50
11:S:74:ILE:HB	11:S:82:ILE:HD12	1.94	0.50
6:G:311:ARG:HG2	6:G:312:GLN:HG2	1.94	0.50
3:D:10:SER:HB3	3:D:34:ASP:HB3	1.94	0.49
4:E:176:THR:HG23	4:E:177:PHE:CD2	2.47	0.49
5:F:49:ILE:HG23	5:F:261:THR:HG21	1.94	0.49
5:F:335:LEU:HD22	5:F:339:MET:HG2	1.94	0.49
5:F:348:ASP:OD1	5:F:349:ALA:N	2.45	0.49
11:S:13:GLU:OE2	11:S:49:LEU:HD11	2.12	0.49
2:C:211:PRO:HB2	9:Q:79:GLY:HA3	1.94	0.49
6:G:42:ASP:O	6:G:57:LYS:HG3	2.12	0.49
10:R:21:ALA:O	10:R:25:LYS:HG3	2.11	0.49
8:P:248:THR:HG22	8:P:251:GLN:OE1	2.13	0.49
8:P:46:GLU:CG	8:P:222:ALA:HB1	2.41	0.49
8:P:222:ALA:O	8:P:226:VAL:HG23	2.13	0.49
16:r:111:ARG:HH22	16:r:114:GLU:CD	2.20	0.49
5:F:415:GLU:HG3	16:r:65:TYR:HD1	1.78	0.49
10:R:56:SER:O	23:R:301:HOH:O	2.19	0.49
14:W:59:LYS:O	14:W:62:VAL:HG12	2.12	0.49
3:D:242:VAL:HG12	16:r:115:VAL:HG12	1.94	0.49
19:F:500:FMN:H3'	19:F:500:FMN:N1	2.27	0.49
6:G:440:VAL:HG12	6:G:440:VAL:O	2.13	0.49
5:F:304:LEU:HD11	5:F:362:VAL:HG21	1.94	0.49
3:D:245:ARG:HG2	16:r:114:GLU:HB3	1.95	0.49
3:D:377:ALA:O	3:D:380:VAL:HG22	2.13	0.49
4:E:189:VAL:HG23	5:F:133:CYS:SG	2.53	0.48
4:E:239:ARG:NH1	4:E:243:GLU:O	2.46	0.48
9:Q:123:SER:OG	9:Q:124:THR:HG23	2.13	0.48
1:B:19:ASP:HB3	1:B:158:THR:HB	1.95	0.48
1:B:123:ARG:O	8:P:70:GLN:NE2	2.44	0.48
5:F:393:CYS:HB2	17:F:501:SF4:S3	2.52	0.48
2:C:204:ARG:NH1	7:I:137:GLU:OE2	2.46	0.48
6:G:86:ASN:O	6:G:88:ARG:HG2	2.14	0.48
6:G:718:ARG:NH2	23:G:901:HOH:O	2.20	0.48
8:P:3:THR:HG21	14:W:122:ASP:HB3	1.95	0.48
11:S:22:SER:O	11:S:29:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:145:THR:HG22	4:E:146:THR:N	2.27	0.48
6:G:250:PHE:HB3	7:I:157:ARG:HG3	1.96	0.48
12:U:119:ASN:OD1	12:U:120:PRO:HD2	2.13	0.48
2:C:27:TYR:HB3	16:r:91:PHE:HZ	1.78	0.48
5:F:414:LEU:HD22	5:F:455:GLU:HG3	1.96	0.48
5:F:419:MET:HG3	6:G:164:ARG:HD3	1.96	0.48
12:U:85:GLU:OE2	14:W:50:LYS:NZ	2.28	0.48
1:B:43:GLU:HG3	1:B:135:PRO:HB2	1.94	0.47
4:E:80:ASN:OD1	4:E:81:TYR:N	2.46	0.47
1:B:32:PRO:HG3	1:B:59:ILE:HG23	1.97	0.47
14:W:26:LEU:HD22	14:W:76:ILE:HG23	1.97	0.47
3:D:114:ASN:HD21	3:D:336:LYS:HE3	1.78	0.47
7:I:154:ASP:OD1	7:I:155:GLY:N	2.47	0.47
2:C:48:ALA:HB2	2:C:54:TYR:C	2.40	0.47
2:C:80:GLN:HE22	13:V:119:GLU:CD	2.23	0.47
4:E:66:ASN:O	4:E:70:VAL:HG23	2.14	0.47
2:C:94:GLU:OE2	3:D:346:ARG:NH1	2.47	0.47
3:D:148:ARG:NH1	3:D:175:ASP:OD2	2.44	0.47
7:I:57:ASP:HB3	7:I:60:PHE:CD2	2.50	0.47
11:S:35:GLN:O	11:S:38:GLU:HG2	2.15	0.47
4:E:272:ARG:HG3	5:F:264:ARG:O	2.15	0.47
14:W:45:GLU:HG2	14:W:46:ILE:N	2.29	0.47
1:B:30:MET:O	1:B:32:PRO:HD3	2.15	0.47
3:D:198:ARG:HH22	7:I:80:LEU:HA	1.79	0.47
4:E:194:ILE:HG12	4:E:214:LEU:HD21	1.96	0.47
4:E:239:ARG:HB2	4:E:243:GLU:OE2	2.15	0.47
5:F:75:ASP:O	5:F:79:LYS:HG3	2.14	0.47
5:F:143:PRO:HB2	5:F:180:ALA:HB2	1.97	0.47
8:P:5:LYS:HE2	14:W:113:ARG:HH21	1.80	0.47
3:D:265:ARG:NH2	3:D:385:THR:O	2.48	0.47
14:W:39:ARG:HA	14:W:44:GLU:OE2	2.15	0.47
2:C:48:ALA:HB2	2:C:54:TYR:O	2.15	0.46
2:C:189:LYS:HD2	2:C:193:ILE:HG21	1.96	0.46
3:D:117:LEU:HD22	3:D:139:ARG:NH1	2.30	0.46
3:D:300:ARG:HA	3:D:303:MET:HG2	1.98	0.46
3:D:366:MET:HG2	3:D:370:VAL:HG23	1.97	0.46
7:I:121:ARG:HD3	7:I:218:ILE:HG21	1.98	0.46
13:V:124:LEU:HD12	13:V:127:LEU:HD12	1.96	0.46
6:G:349:LEU:HD23	6:G:550:VAL:HB	1.96	0.46
6:G:489:LEU:O	6:G:494:ARG:HD3	2.14	0.46
8:P:178:ARG:NH1	23:P:601:HOH:O	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:413:GLY:O	6:G:487:SER:OG	2.28	0.46
4:E:182:MET:SD	4:E:185:MET:HE1	2.56	0.46
1:B:138:ALA:O	1:B:142:LEU:HG	2.15	0.46
2:C:58:THR:HG23	2:C:115:ARG:HG2	1.98	0.46
4:E:272:ARG:NH1	5:F:263:LEU:O	2.47	0.46
6:G:53:VAL:HG21	6:G:68:ALA:HB2	1.97	0.46
6:G:439:LEU:HG	6:G:441:GLY:H	1.81	0.46
8:P:340:ARG:HG2	8:P:344:VAL:HG11	1.98	0.46
10:R:21:ALA:HB1	10:R:25:LYS:HE2	1.97	0.46
14:W:41:HIS:O	14:W:93:ARG:HD2	2.16	0.46
6:G:53:VAL:HG12	6:G:55:VAL:HG13	1.97	0.46
12:U:51:ILE:O	12:U:55:VAL:HG23	2.15	0.46
12:U:100:ASP:OD1	12:U:101:ALA:N	2.49	0.46
4:E:78:PRO:HG2	4:E:81:TYR:HB2	1.98	0.46
6:G:129:MET:HE1	6:G:151:LEU:HD12	1.98	0.46
7:I:84:VAL:HG12	7:I:88:MET:HE1	1.96	0.46
4:E:140:VAL:HG22	4:E:196:VAL:HG22	1.97	0.46
5:F:322:LEU:HB2	5:F:337:LYS:HD2	1.97	0.46
5:F:323:LEU:HD23	5:F:371:VAL:HG13	1.97	0.46
6:G:623:ASP:HA	6:G:626:ILE:HD12	1.97	0.46
8:P:202:VAL:O	8:P:204:PRO:HD3	2.16	0.46
6:G:628:ARG:NH2	6:G:641:ASP:OD1	2.42	0.45
8:P:211:ASN:HD21	8:P:249:MET:HG3	1.81	0.45
10:R:125:TRP:CD1	10:R:125:TRP:H	2.33	0.45
3:D:260:ASP:O	3:D:264:VAL:HG23	2.16	0.45
3:D:359:PRO:HD2	3:D:392:GLU:OE2	2.17	0.45
6:G:78:HIS:HB3	6:G:81:LEU:HB2	1.98	0.45
6:G:673:TYR:O	6:G:677:VAL:HG22	2.17	0.45
7:I:159:THR:O	7:I:204:LYS:NZ	2.44	0.45
8:P:6:PRO:HB3	8:P:16:ARG:HH11	1.79	0.45
14:W:117:ASN:HB3	14:W:121:LEU:HB3	1.98	0.45
1:B:135:PRO:HD3	3:D:155:HIS:CD2	2.51	0.45
11:S:72:VAL:CG1	11:S:85:LYS:HE3	2.45	0.45
14:W:52:MET:O	14:W:56:ILE:HG12	2.17	0.45
16:r:75:ARG:HD2	16:r:76:ARG:HD3	1.98	0.45
3:D:245:ARG:NH1	3:D:282:GLU:OE2	2.44	0.45
3:D:300:ARG:O	3:D:303:MET:HG2	2.17	0.45
6:G:44:MET:HE1	6:G:109:GLY:C	2.41	0.45
6:G:427:LEU:HA	6:G:430:VAL:HG22	1.97	0.45
7:I:226:SER:HB3	10:R:93:LEU:HD21	1.98	0.45
8:P:215:PRO:HB2	8:P:330:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:382:ILE:O	3:D:386:LEU:HG	2.17	0.45
4:E:158:GLU:O	4:E:162:LYS:HG2	2.17	0.45
5:F:200:ASP:OD1	5:F:200:ASP:N	2.49	0.45
8:P:19:PRO:HD2	8:P:24:SER:OG	2.17	0.45
8:P:73:ASP:OD1	8:P:74:LEU:N	2.38	0.45
9:Q:159:ARG:HH22	9:Q:171:ARG:HG2	1.82	0.45
5:F:283:LEU:O	5:F:360:ALA:HB3	2.17	0.45
6:G:595:GLU:HG2	6:G:614:VAL:HG23	1.99	0.45
6:G:679:ASP:O	6:G:683:LYS:HG2	2.16	0.45
7:I:175:CYS:HB3	17:I:500:SF4:S2	2.57	0.45
9:Q:24:ALA:HB2	9:Q:86:PRO:HB2	1.98	0.45
9:Q:66:VAL:CG1	9:Q:95:ILE:HG23	2.46	0.45
5:F:192:LYS:HG3	9:Q:182:SER:HB3	1.98	0.45
5:F:419:MET:SD	6:G:164:ARG:HD3	2.57	0.45
6:G:407:ASP:OD2	6:G:479:ASN:N	2.48	0.45
8:P:189:PHE:O	8:P:193:LEU:HG	2.16	0.45
9:Q:70:CYS:SG	9:Q:84:LEU:HG	2.57	0.45
3:D:37:ILE:HD11	7:I:42:TRP:CZ3	2.52	0.45
5:F:301:SER:O	5:F:344:ILE:HD11	2.17	0.45
12:U:114:ASN:HA	12:U:117:ILE:HG12	1.99	0.45
3:D:94:ALA:HB1	16:r:118:HIS:HA	1.99	0.44
5:F:164:ILE:HD11	5:F:203:LEU:HD21	1.99	0.44
11:S:63:ARG:HG3	11:S:69:GLU:HG2	1.99	0.44
14:W:59:LYS:HE2	14:W:100:TYR:CE1	2.52	0.44
3:D:379:VAL:HG12	3:D:383:ILE:HD12	1.99	0.44
8:P:61:ASN:O	8:P:65:VAL:HG22	2.17	0.44
6:G:318:LEU:HB2	6:G:587:VAL:HB	2.00	0.44
7:I:89:TYR:O	7:I:92:SER:OG	2.23	0.44
1:B:109:GLY:HA2	7:I:168:LYS:HA	1.98	0.44
3:D:109:ILE:O	3:D:113:MET:HG3	2.17	0.44
5:F:124:ASN:ND2	5:F:215:GLY:O	2.51	0.44
5:F:233:LEU:HB2	9:Q:163:TYR:CE2	2.53	0.44
2:C:2:SER:N	2:C:109:ARG:HB2	2.33	0.44
6:G:428:ARG:HH11	6:G:447:THR:HG22	1.82	0.44
12:U:87:LEU:O	12:U:91:GLU:HG2	2.18	0.44
6:G:675:LYS:O	6:G:678:LYS:HG3	2.17	0.44
14:W:91:LYS:HE3	14:W:95:HIS:HB3	1.99	0.44
5:F:435:LEU:HD23	17:F:501:SF4:S1	2.58	0.44
6:G:151:LEU:HB2	6:G:240:VAL:HG12	2.00	0.44
8:P:340:ARG:HG2	8:P:344:VAL:CG1	2.48	0.44
2:C:2:SER:OG	2:C:3:TYR:N	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:21:LYS:NZ	2:C:111:ASN:HB3	2.33	0.44
2:C:105:LEU:HB2	2:C:114:ILE:HG22	1.99	0.44
3:D:267:GLN:O	3:D:271:GLU:HG2	2.18	0.44
4:E:122:GLU:OE1	6:G:209:ILE:N	2.48	0.44
11:S:7:LEU:HB2	11:S:43:ASN:ND2	2.33	0.44
1:B:160:LEU:HD21	8:P:60:CYS:HB2	2.00	0.44
3:D:83:TYR:CZ	3:D:87:ILE:HD11	2.53	0.44
3:D:245:ARG:CG	16:r:114:GLU:HB3	2.48	0.44
6:G:270:GLY:HA3	6:G:602:ASN:ND2	2.31	0.44
6:G:360:GLU:HB3	6:G:646:VAL:HG11	1.99	0.44
8:P:58:TYR:HE2	8:P:61:ASN:H	1.66	0.44
11:S:74:ILE:HB	11:S:82:ILE:CD1	2.48	0.44
23:C:310:HOH:O	9:Q:122:ARG:NH2	2.50	0.43
4:E:200:ARG:HE	4:E:200:ARG:HB2	1.66	0.43
6:G:42:ASP:OD1	6:G:43:LYS:N	2.51	0.43
6:G:144:ASP:HB2	6:G:244:LEU:HD13	2.00	0.43
6:G:209:ILE:CD1	6:G:218:VAL:HG22	2.46	0.43
8:P:149:ASP:OD1	8:P:150:VAL:N	2.51	0.43
11:S:86:LEU:O	11:S:90:VAL:HG23	2.19	0.43
1:B:45:MET:HE3	3:D:132:PHE:CZ	2.53	0.43
6:G:717:VAL:O	6:G:720:GLN:HG2	2.18	0.43
13:V:92:ARG:HH12	13:V:119:GLU:CD	2.27	0.43
2:C:21:LYS:HE2	2:C:21:LYS:HA	2.00	0.43
3:D:137:GLU:OE2	3:D:138:GLU:HG2	2.19	0.43
4:E:108:ARG:O	4:E:112:ILE:HG13	2.17	0.43
6:G:414:THR:HB	6:G:485:GLY:HA3	2.01	0.43
3:D:117:LEU:HD22	3:D:139:ARG:HH12	1.84	0.43
5:F:93:LEU:HD21	5:F:255:THR:HG23	2.00	0.43
5:F:447:ILE:CD1	5:F:454:MET:HE1	2.44	0.43
6:G:334:PHE:HB3	6:G:633:VAL:HG11	2.01	0.43
6:G:416:PRO:HD2	6:G:446:LEU:HD21	2.00	0.43
12:U:69:SER:H	12:U:110:GLU:CD	2.26	0.43
3:D:90:LEU:HD12	3:D:343:LEU:HD23	2.00	0.43
3:D:194:LEU:HD23	3:D:194:LEU:HA	1.83	0.43
3:D:364:LEU:HD12	3:D:364:LEU:HA	1.81	0.43
4:E:150:LEU:HD23	5:F:289:HIS:CD2	2.54	0.43
6:G:179:PRO:O	6:G:246:LYS:HD2	2.18	0.43
6:G:491:ARG:HH21	6:G:493:ASP:CG	2.27	0.43
9:Q:50:ASP:HB3	14:W:71:VAL:HG21	2.00	0.43
13:V:39:ARG:O	13:V:39:ARG:HG2	2.18	0.43
1:B:39:CYS:HB3	17:B:500:SF4:S1	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:293:GLN:HE22	3:D:302:GLN:NE2	2.15	0.43
4:E:45:PHE:CE2	10:R:103:LYS:HB3	2.53	0.43
8:P:231:ASP:HB3	8:P:234:THR:HG23	2.01	0.43
11:S:53:SER:HB3	11:S:56:ALA:HB2	2.01	0.43
5:F:284:PHE:CD2	5:F:360:ALA:HB1	2.54	0.43
5:F:325:ILE:HB	5:F:340:CYS:SG	2.58	0.43
4:E:145:THR:HG21	5:F:130:PRO:HB3	2.01	0.43
4:E:189:VAL:HG12	4:E:239:ARG:HH22	1.84	0.43
6:G:39:LEU:HD11	6:G:45:GLU:HB2	2.00	0.43
6:G:164:ARG:HH21	16:r:67:ILE:H	1.67	0.43
6:G:428:ARG:NH1	6:G:447:THR:HG22	2.34	0.43
6:G:501:VAL:O	6:G:505:VAL:HG23	2.19	0.43
2:C:113:ARG:HH12	3:D:329:TYR:HE2	1.67	0.42
5:F:136:ARG:O	5:F:140:ARG:HG2	2.18	0.42
5:F:387:CYS:HA	6:G:212:ARG:HG3	2.01	0.42
5:F:434:ALA:HB3	19:F:500:FMN:HM81	2.00	0.42
8:P:13:ASN:OD1	8:P:14:ALA:N	2.52	0.42
11:S:70:LYS:HD3	11:S:89:LEU:HD23	2.00	0.42
13:V:46:VAL:HG23	13:V:48:VAL:HG23	2.00	0.42
2:C:28:LEU:HD22	2:C:112:ASN:ND2	2.34	0.42
2:C:91:ASP:CG	2:C:98:ARG:HH21	2.26	0.42
2:C:92:TYR:CB	2:C:95:ARG:HD2	2.49	0.42
3:D:224:ILE:HD12	3:D:224:ILE:H	1.84	0.42
9:Q:62:TYR:HA	9:Q:142:TRP:CD1	2.55	0.42
4:E:147:PRO:HG2	5:F:130:PRO:O	2.19	0.42
11:S:78:SER:O	11:S:82:ILE:HG12	2.20	0.42
12:U:70:SER:HB3	12:U:76:LEU:CD1	2.48	0.42
4:E:107:ASN:ND2	23:E:602:HOH:O	2.41	0.42
4:E:148:CYS:HA	4:E:191:ALA:HB1	2.02	0.42
5:F:281:THR:HA	5:F:299:GLU:HA	2.02	0.42
5:F:372:ILE:HD11	5:F:454:MET:HG2	2.01	0.42
16:r:111:ARG:NH2	16:r:114:GLU:OE2	2.43	0.42
6:G:142:ILE:HG23	7:I:131:ILE:HD12	2.01	0.42
7:I:56:GLN:HB3	13:V:44:LYS:HZ1	1.84	0.42
14:W:86:TYR:CE2	14:W:100:TYR:HE2	2.37	0.42
3:D:120:THR:HG21	3:D:135:ALA:HB2	2.02	0.42
4:E:272:ARG:NH1	5:F:266:GLY:HA2	2.34	0.42
6:G:654:ALA:HB3	6:G:657:PHE:HD2	1.84	0.42
12:U:62:ALA:HA	12:U:66:VAL:CG2	2.50	0.42
2:C:90:VAL:HG22	3:D:353:ARG:HG2	2.02	0.42
3:D:81:HIS:CE1	3:D:240:TYR:HE2	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:108:GLU:OE2	3:D:243:TYR:OH	2.29	0.42
5:F:160:ARG:HH22	9:Q:182:SER:HB2	1.85	0.42
7:I:196:THR:OG1	7:I:198:GLU:OE1	2.36	0.42
8:P:123:PHE:HB3	8:P:124:PRO:HD3	2.02	0.42
12:U:60:LEU:O	12:U:61:ALA:HB3	2.19	0.42
1:B:39:CYS:SG	3:D:73:TYR:HB3	2.59	0.42
4:E:210:TYR:OH	5:F:169:GLU:HB3	2.19	0.41
5:F:388:GLY:HA2	5:F:394:ARG:HB2	2.01	0.41
6:G:203:GLY:HA3	6:G:447:THR:CG2	2.50	0.41
7:I:150:GLU:OE2	10:R:57:LYS:NZ	2.53	0.41
8:P:182:VAL:HG23	20:P:500:NDP:H42N	2.01	0.41
10:R:57:LYS:O	15:q:142:ARG:NH1	2.29	0.41
12:U:48:GLU:HA	12:U:51:ILE:HG12	2.02	0.41
12:U:84:VAL:O	12:U:88:ILE:HG12	2.20	0.41
5:F:123:VAL:HG11	5:F:146:LEU:HD11	2.01	0.41
5:F:348:ASP:O	5:F:352:THR:HG23	2.19	0.41
6:G:386:LEU:HD13	6:G:494:ARG:HD2	2.01	0.41
6:G:655:PRO:HB2	11:S:53:SER:HB3	2.02	0.41
7:I:32:THR:HG21	13:V:30:ALA:HA	2.01	0.41
2:C:160:VAL:HG23	2:C:161:LEU:N	2.35	0.41
5:F:268:GLU:HG2	5:F:269:TRP:N	2.35	0.41
9:Q:151:PRO:HB2	9:Q:153:LYS:HE3	2.02	0.41
13:V:31:ASP:OD1	13:V:32:VAL:N	2.53	0.41
4:E:272:ARG:HH11	5:F:266:GLY:HA2	1.86	0.41
5:F:270:PHE:CZ	5:F:280:GLY:HA3	2.56	0.41
11:S:32:VAL:HG11	11:S:50:VAL:HG11	2.02	0.41
2:C:15:ILE:HG22	16:r:110:VAL:O	2.21	0.41
3:D:89:GLN:OE1	3:D:330:ARG:HD3	2.19	0.41
3:D:202:GLU:HG2	7:I:38:GLN:HB2	2.02	0.41
3:D:308:GLU:HG3	6:G:133:LEU:HD13	2.02	0.41
4:E:73:ILE:HD13	4:E:88:PRO:HB2	2.03	0.41
16:r:67:ILE:HG13	16:r:67:ILE:O	2.19	0.41
1:B:46:HIS:ND1	3:D:140:GLU:OE1	2.53	0.41
2:C:48:ALA:HA	2:C:56:GLU:OE1	2.20	0.41
3:D:77:MET:HB2	3:D:110:THR:HG21	2.02	0.41
6:G:654:ALA:HB1	6:G:656:HIS:NE2	2.35	0.41
6:G:656:HIS:CD2	6:G:656:HIS:H	2.39	0.41
6:G:145:GLN:O	6:G:149:CYS:HB2	2.20	0.41
7:I:199:GLU:HG2	15:q:130:TYR:O	2.20	0.41
10:R:77:LYS:NZ	10:R:123:ASP:OD1	2.53	0.41
11:S:19:SER:HB3	11:S:25:SER:OG	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:U:45:GLU:O	12:U:48:GLU:HG3	2.21	0.41
6:G:467:LYS:HD2	6:G:467:LYS:O	2.20	0.41
6:G:632:GLU:OE2	14:W:118:SER:OG	2.39	0.41
11:S:58:ALA:HB1	11:S:74:ILE:HG13	2.02	0.41
12:U:52:ILE:O	12:U:56:LYS:HG3	2.21	0.41
3:D:122:HIS:NE2	3:D:381:THR:HG23	2.36	0.41
3:D:235:ARG:NH2	23:D:408:HOH:O	2.53	0.41
3:D:254:GLY:HA3	13:V:45:TYR:O	2.21	0.41
5:F:122:VAL:HG11	5:F:220:LEU:HD21	2.02	0.41
5:F:315:VAL:HG22	5:F:364:VAL:HG11	2.02	0.41
6:G:62:LEU:HD11	6:G:74:ARG:HD3	2.02	0.41
6:G:351:ALA:HB3	6:G:377:LEU:HD23	2.03	0.41
6:G:440:VAL:HG11	6:G:460:LEU:HB2	2.02	0.41
7:I:209:GLU:OE1	23:I:601:HOH:O	2.22	0.41
8:P:97:ARG:NH2	15:q:138:ASN:O	2.53	0.41
12:U:51:ILE:HD13	12:U:113:VAL:HB	2.03	0.41
13:V:102:ASP:OD1	13:V:103:ALA:N	2.54	0.41
1:B:76:THR:HA	1:B:104:CYS:HB3	2.03	0.41
2:C:14:TYR:HB3	16:r:109:THR:HB	2.02	0.41
3:D:190:MET:HE1	3:D:269:MET:HE1	2.03	0.41
3:D:294:LYS:HD2	16:r:69:TYR:CE2	2.56	0.41
7:I:45:VAL:O	7:I:49:ARG:HG3	2.21	0.41
8:P:148:ALA:HA	8:P:157:LEU:HB3	2.02	0.41
8:P:286:ARG:HH12	8:P:300:SER:HB3	1.86	0.41
1:B:30:MET:HE2	1:B:149:GLN:HE21	1.87	0.40
10:R:102:LEU:HB3	10:R:122:SER:HB3	2.03	0.40
1:B:23:ASN:ND2	1:B:155:SER:O	2.53	0.40
1:B:160:LEU:O	1:B:164:LYS:HB2	2.21	0.40
3:D:36:GLU:OE1	3:D:36:GLU:N	2.55	0.40
3:D:116:ILE:CG2	3:D:135:ALA:HB1	2.51	0.40
8:P:85:ILE:O	8:P:126:ARG:HD2	2.21	0.40
16:r:72:ARG:HG2	16:r:72:ARG:O	2.22	0.40
2:C:3:TYR:CZ	3:D:213:GLN:HG2	2.56	0.40
3:D:133:LEU:HA	3:D:136:PHE:HD2	1.86	0.40
3:D:344:VAL:HB	3:D:353:ARG:HB3	2.03	0.40
6:G:78:HIS:CE1	6:G:296:GLU:OE2	2.74	0.40
8:P:142:GLN:HB3	8:P:176:ILE:HD13	2.03	0.40
14:W:51:GLU:O	14:W:55:ILE:HG13	2.22	0.40
1:B:161:TRP:NE1	8:P:291:GLU:O	2.54	0.40
15:q:143:ASN:HD22	15:q:143:ASN:C	2.17	0.40
2:C:76:HIS:HA	13:V:123:GLU:OE1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:43:LEU:HD23	5:F:48:ARG:HG2	2.03	0.40
6:G:629:ALA:O	6:G:633:VAL:HG23	2.22	0.40
8:P:13:ASN:HA	8:P:16:ARG:NE	2.37	0.40
8:P:189:PHE:CE1	8:P:249:MET:HE1	2.50	0.40
14:W:46:ILE:HD11	14:W:93:ARG:HH21	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	B	152/164 (93%)	146 (96%)	6 (4%)	0	100	100
2	C	214/217 (99%)	211 (99%)	3 (1%)	0	100	100
3	D	393/395 (100%)	386 (98%)	6 (2%)	1 (0%)	36	62
4	E	233/276 (84%)	226 (97%)	7 (3%)	0	100	100
5	F	428/469 (91%)	415 (97%)	13 (3%)	0	100	100
6	G	680/720 (94%)	664 (98%)	16 (2%)	0	100	100
7	I	197/229 (86%)	195 (99%)	2 (1%)	0	100	100
8	P	345/370 (93%)	333 (96%)	12 (4%)	0	100	100
9	Q	160/185 (86%)	154 (96%)	6 (4%)	0	100	100
10	R	106/132 (80%)	103 (97%)	3 (3%)	0	100	100
11	S	93/98 (95%)	92 (99%)	1 (1%)	0	100	100
12	U	82/122 (67%)	71 (87%)	11 (13%)	0	100	100
13	V	132/159 (83%)	129 (98%)	3 (2%)	0	100	100
14	W	123/137 (90%)	121 (98%)	2 (2%)	0	100	100
15	q	26/155 (17%)	26 (100%)	0	0	100	100
16	r	58/121 (48%)	58 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3422/3949 (87%)	3330 (97%)	91 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	242	VAL

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	B	129/134 (96%)	129 (100%)	0	100	100
2	C	199/200 (100%)	199 (100%)	0	100	100
3	D	339/339 (100%)	339 (100%)	0	100	100
4	E	197/232 (85%)	196 (100%)	1 (0%)	81	93
5	F	343/372 (92%)	343 (100%)	0	100	100
6	G	544/570 (95%)	544 (100%)	0	100	100
7	I	175/201 (87%)	175 (100%)	0	100	100
8	P	296/318 (93%)	296 (100%)	0	100	100
9	Q	134/154 (87%)	134 (100%)	0	100	100
10	R	86/107 (80%)	86 (100%)	0	100	100
11	S	77/79 (98%)	77 (100%)	0	100	100
12	U	76/108 (70%)	76 (100%)	0	100	100
13	V	116/139 (84%)	116 (100%)	0	100	100
14	W	119/123 (97%)	119 (100%)	0	100	100
15	q	26/138 (19%)	25 (96%)	1 (4%)	29	61
16	r	55/109 (50%)	55 (100%)	0	100	100
All	All	2911/3323 (88%)	2909 (100%)	2 (0%)	87	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	49	HIS
15	q	143	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	149	GLN
2	C	49	GLN
2	C	80	GLN
2	C	154	HIS
3	D	166	GLN
3	D	213	GLN
3	D	214	GLN
3	D	293	GLN
4	E	66	ASN
5	F	193	ASN
6	G	424	ASN
6	G	502	ASN
6	G	519	ASN
6	G	608	GLN
6	G	643	GLN
6	G	656	HIS
7	I	56	GLN
7	I	66	ASN
7	I	176	GLN
7	I	210	ASN
8	P	76	GLN
8	P	181	ASN
8	P	255	HIS
8	P	264	ASN
9	Q	150	ASN
9	Q	154	HIS
11	S	20	GLN
11	S	54	ASN
12	U	58	GLN
13	V	50	HIS
14	W	63	ASN
14	W	94	HIS
15	q	143	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	SF4	G	803	6	0,12,12	-	-	-		
17	SF4	B	500	1	0,12,12	-	-	-		
17	SF4	F	501	5	0,12,12	-	-	-		
20	NDP	P	500	-	49,52,52	2.15	6 (12%)	66,80,80	1.64	13 (19%)
18	FES	E	500	4	0,4,4	-	-	-		
22	8Q1	W	200	-	31,34,34	1.68	6 (19%)	40,43,43	1.56	5 (12%)
17	SF4	G	802	6	0,12,12	-	-	-		
18	FES	G	801	6	0,4,4	-	-	-		
19	FMN	F	500	-	33,33,33	1.07	2 (6%)	48,50,50	1.25	7 (14%)
17	SF4	I	500	7	0,12,12	-	-	-		
17	SF4	I	501	7	0,12,12	-	-	-		

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
17	SF4	G	803	6	-	-	0/6/5/5
17	SF4	B	500	1	-	-	0/6/5/5
17	SF4	F	501	5	-	-	0/6/5/5
20	NDP	P	500	-	-	10/34/77/77	0/5/5/5
18	FES	E	500	4	-	-	0/1/1/1
22	8Q1	W	200	-	-	11/41/41/41	-
17	SF4	G	802	6	-	-	0/6/5/5
18	FES	G	801	6	-	-	0/1/1/1
19	FMN	F	500	-	-	9/18/18/18	0/3/3/3
17	SF4	I	500	7	-	-	0/6/5/5
17	SF4	I	501	7	-	-	0/6/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	P	500	NDP	P2B-O2B	12.13	1.82	1.59
22	W	200	8Q1	C34-N36	5.48	1.45	1.33
22	W	200	8Q1	C39-N41	5.26	1.45	1.33
20	P	500	NDP	PN-O5D	3.89	1.75	1.59
19	F	500	FMN	C4A-N5	3.74	1.38	1.30
20	P	500	NDP	O2B-C2B	-3.05	1.33	1.44
22	W	200	8Q1	C1-S44	2.35	1.81	1.76
22	W	200	8Q1	O40-C39	-2.20	1.18	1.23
22	W	200	8Q1	O35-C34	-2.18	1.19	1.23
20	P	500	NDP	C5A-C4A	2.15	1.43	1.39
19	F	500	FMN	C10-N1	2.15	1.37	1.33
20	P	500	NDP	C2A-N1A	2.03	1.37	1.33
20	P	500	NDP	O5D-C5D	-2.01	1.37	1.44
22	W	200	8Q1	C6-C1	2.01	1.52	1.50

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	P	500	NDP	PN-O3-PA	-7.01	108.77	132.83
22	W	200	8Q1	C6-C1-S44	5.77	120.17	113.46
22	W	200	8Q1	O4-C1-C6	-3.35	120.04	123.99
20	P	500	NDP	O2B-P2B-O1X	-3.30	96.65	109.39
19	F	500	FMN	C4-N3-C2	-3.22	119.69	125.64
20	P	500	NDP	PA-O5B-C5B	-3.04	103.83	121.68
19	F	500	FMN	C4A-C10-N10	2.87	120.68	116.48
20	P	500	NDP	O4B-C4B-C3B	2.72	110.50	105.11
20	P	500	NDP	PN-O5D-C5D	-2.71	105.80	121.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	F	500	FMN	C4A-C4-N3	2.63	119.88	113.19
19	F	500	FMN	O4-C4-C4A	-2.60	119.72	126.60
20	P	500	NDP	O3X-P2B-O2X	2.56	117.41	107.64
20	P	500	NDP	O5D-PN-O1N	-2.52	99.24	109.07
20	P	500	NDP	N3A-C4A-N9A	2.45	131.13	127.08
20	P	500	NDP	O2N-PN-O1N	2.34	123.79	112.24
20	P	500	NDP	C2A-N1A-C6A	-2.33	114.77	118.77
20	P	500	NDP	C5A-C4A-N3A	-2.29	123.76	126.75
19	F	500	FMN	C10-C4A-N5	-2.26	120.06	124.86
20	P	500	NDP	C5B-C4B-C3B	-2.19	106.99	115.18
22	W	200	8Q1	O4-C1-S44	-2.17	119.80	122.61
19	F	500	FMN	C4A-C10-N1	-2.14	119.78	124.73
20	P	500	NDP	C3N-C2N-N1N	-2.13	120.05	123.10
22	W	200	8Q1	C38-C39-N41	2.13	120.01	116.42
19	F	500	FMN	C5A-C9A-N10	2.11	120.13	117.95
22	W	200	8Q1	C43-S44-C1	2.09	108.37	101.87

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	F	500	FMN	N10-C1'-C2'-O2'
19	F	500	FMN	N10-C1'-C2'-C3'
19	F	500	FMN	C1'-C2'-C3'-O3'
19	F	500	FMN	C1'-C2'-C3'-C4'
19	F	500	FMN	C5'-O5'-P-O2P
19	F	500	FMN	C5'-O5'-P-O3P
20	P	500	NDP	C5B-O5B-PA-O1A
20	P	500	NDP	C5D-O5D-PN-O1N
20	P	500	NDP	O4D-C4D-C5D-O5D
20	P	500	NDP	C2N-C3N-C7N-O7N
22	W	200	8Q1	O27-C28-C29-C30
22	W	200	8Q1	O27-C28-C29-C31
22	W	200	8Q1	O27-C28-C29-C32
22	W	200	8Q1	N36-C37-C38-C39
22	W	200	8Q1	C42-C43-S44-C1
22	W	200	8Q1	C28-O27-P24-O3
22	W	200	8Q1	C28-O27-P24-O2
22	W	200	8Q1	C28-O27-P24-O1
22	W	200	8Q1	C38-C39-N41-C42
19	F	500	FMN	O2'-C2'-C3'-C4'
22	W	200	8Q1	O40-C39-N41-C42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	P	500	NDP	C3D-C4D-C5D-O5D
19	F	500	FMN	O2'-C2'-C3'-O3'
22	W	200	8Q1	C6-C7-C8-C9
20	P	500	NDP	C5D-O5D-PN-O3
20	P	500	NDP	O4B-C4B-C5B-O5B
20	P	500	NDP	C2N-C3N-C7N-N7N
20	P	500	NDP	O4D-C1D-N1N-C6N
20	P	500	NDP	C2D-C1D-N1N-C6N
19	F	500	FMN	C5'-O5'-P-O1P

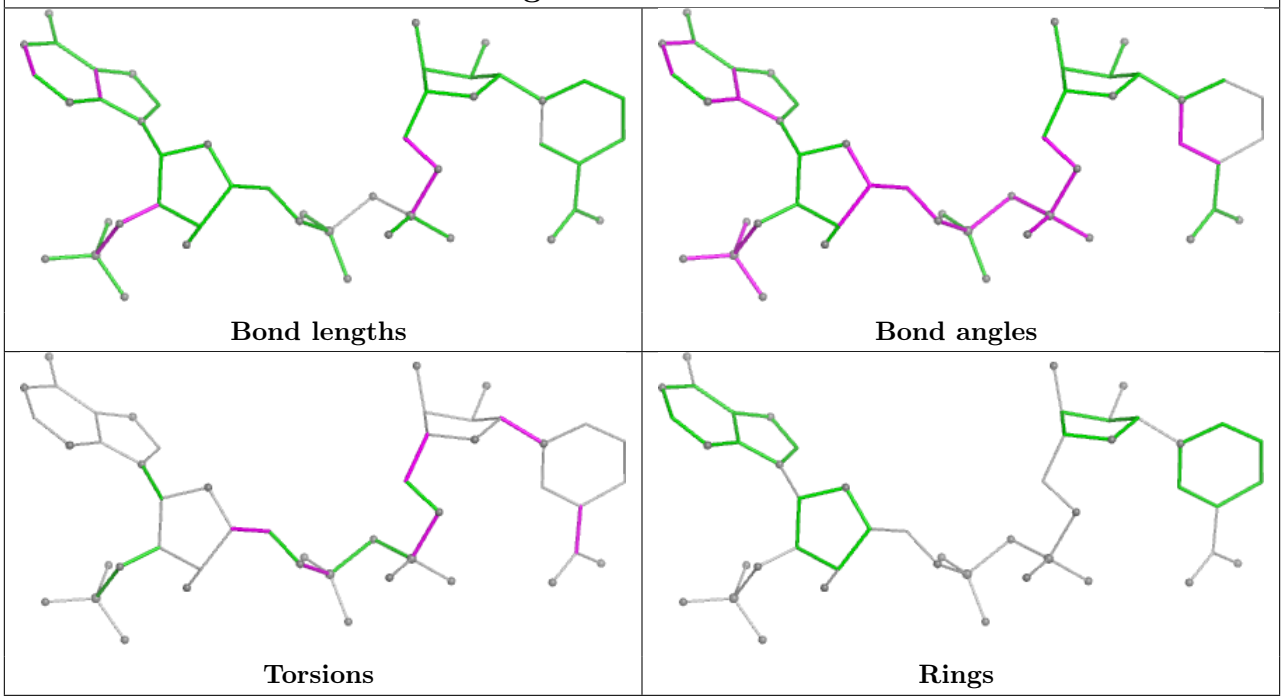
There are no ring outliers.

6 monomers are involved in 8 short contacts:

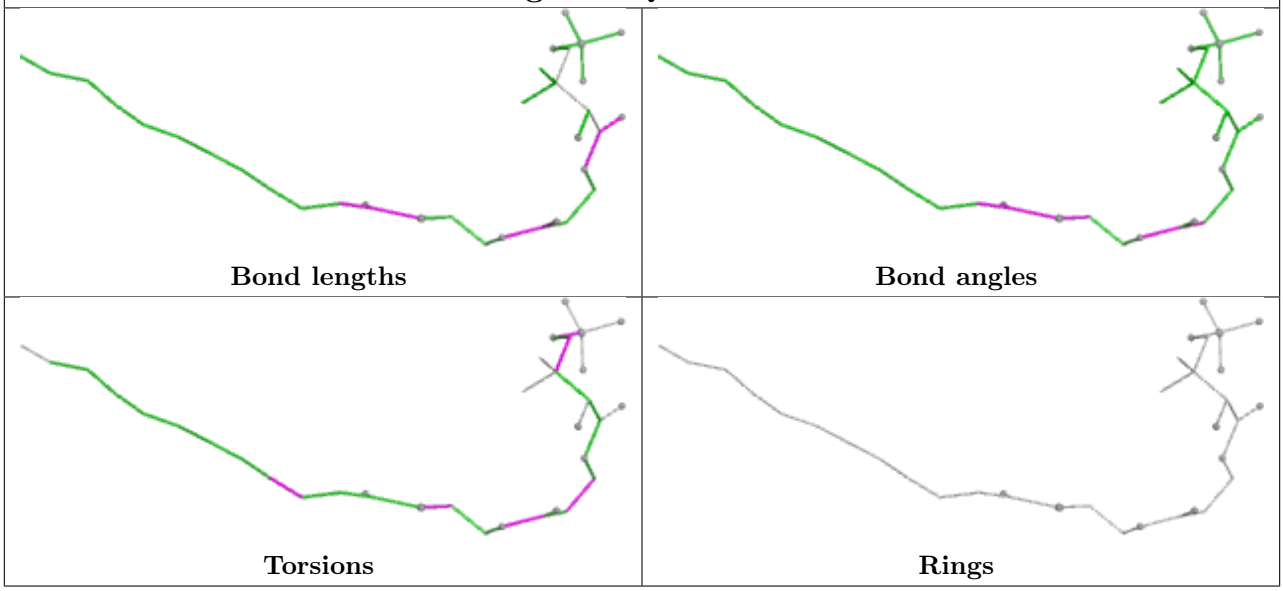
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	500	SF4	1	0
17	F	501	SF4	2	0
20	P	500	NDP	1	0
22	W	200	8Q1	1	0
19	F	500	FMN	2	0
17	I	500	SF4	1	0

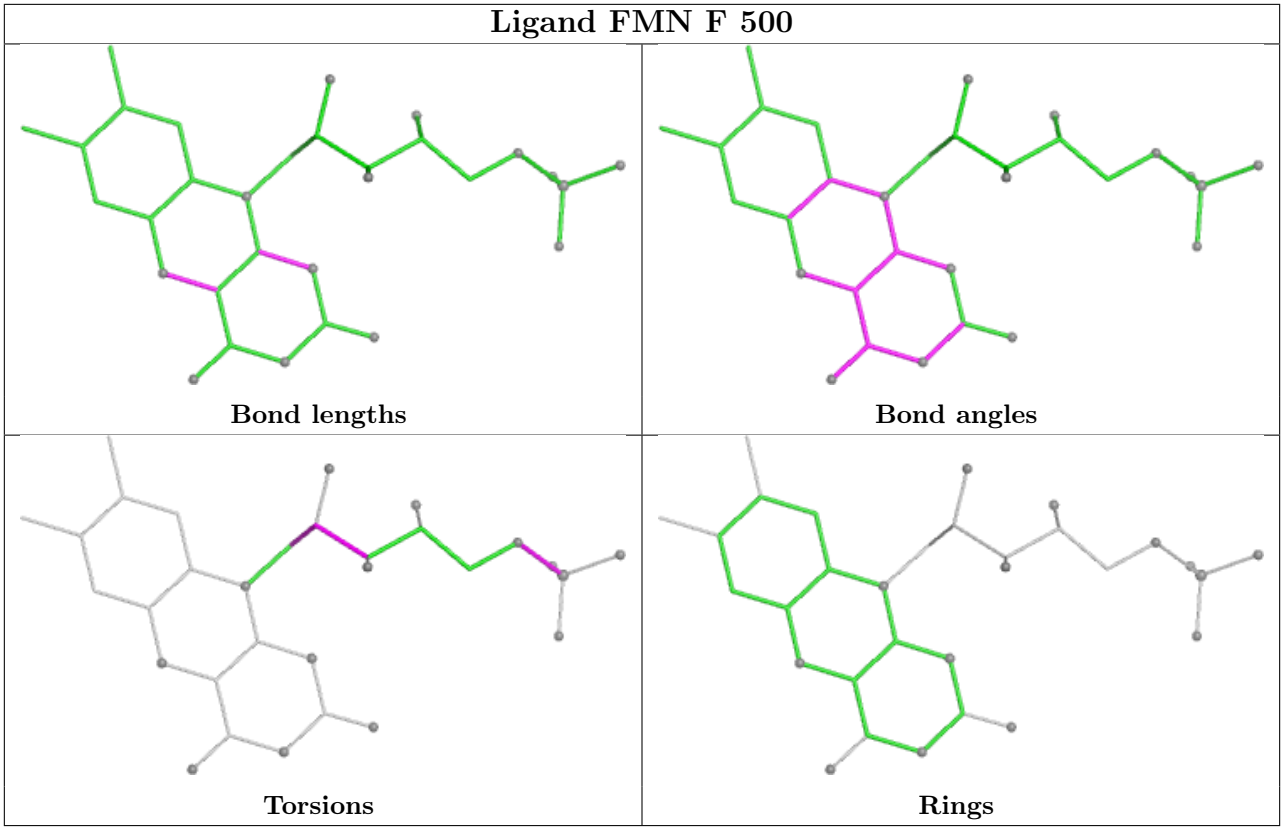
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand NDP P 500



Ligand 8Q1 W 200





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.

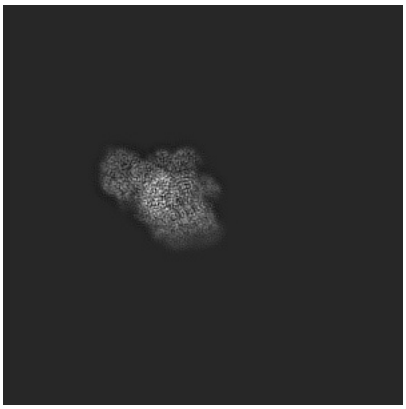
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11879. These allow visual inspection of the internal detail of the map and identification of artifacts.

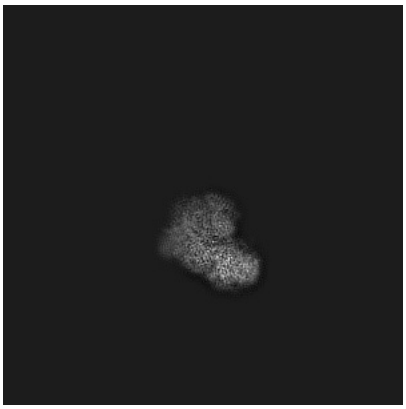
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

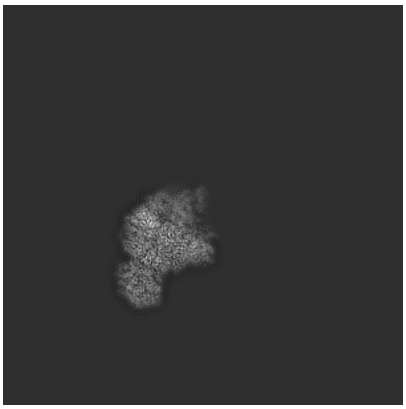
6.1.1 Primary map



X

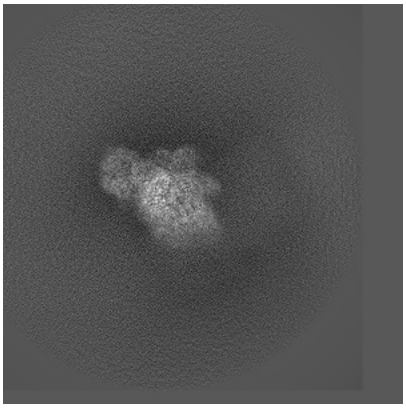


Y

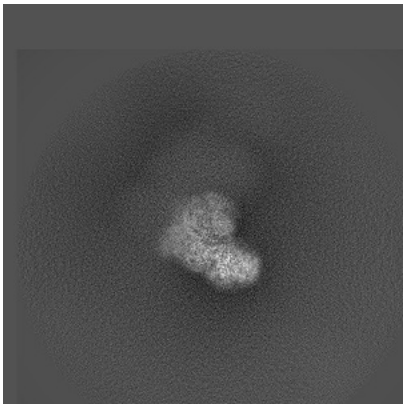


Z

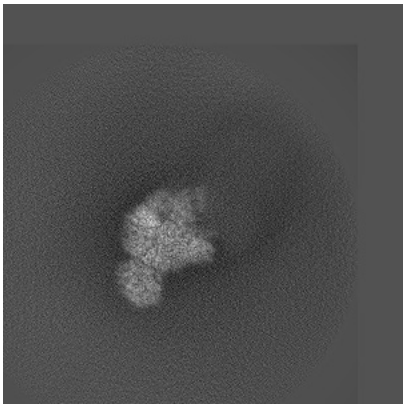
6.1.2 Raw map



X



Y



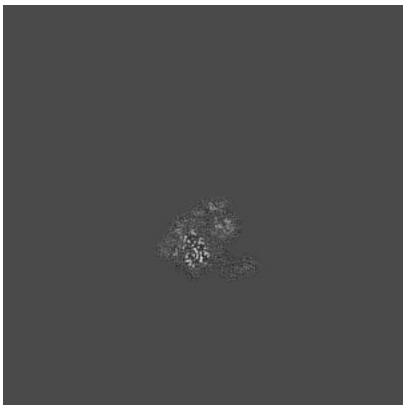
Z

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

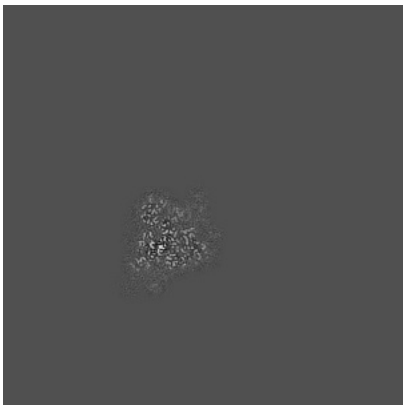
6.2 Central slices (i)

6.2.1 Primary map

X Index: 300

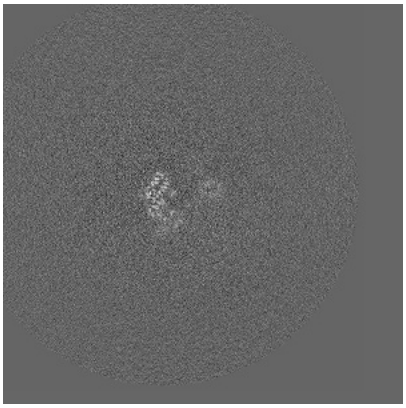


Y Index: 300

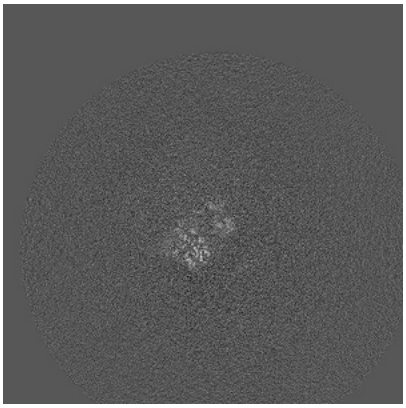


Z Index: 300

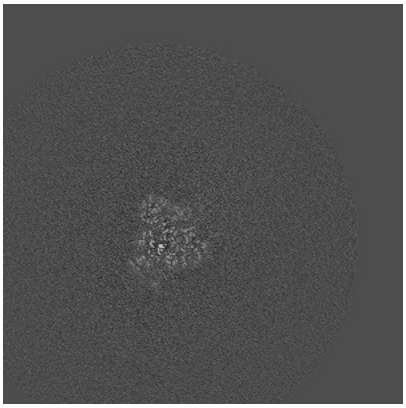
6.2.2 Raw map



X Index: 300



Y Index: 300

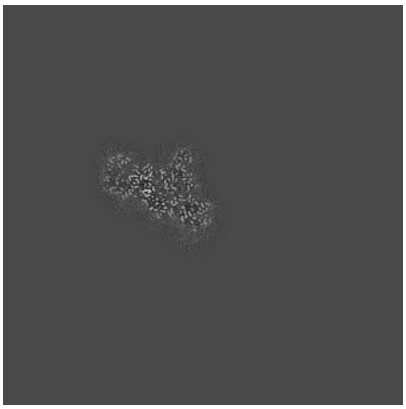


Z Index: 300

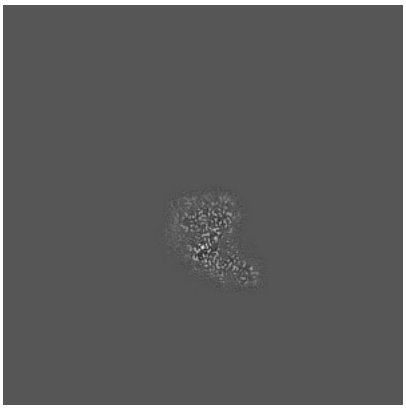
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

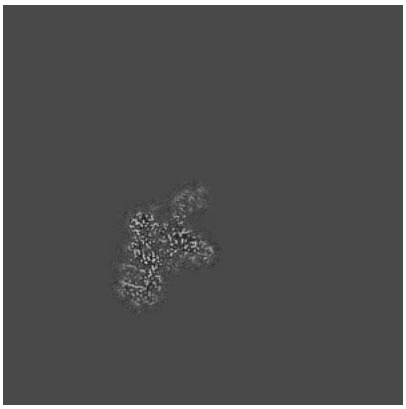
6.3.1 Primary map



X Index: 220

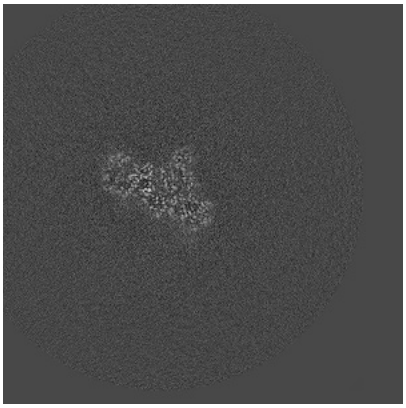


Y Index: 236

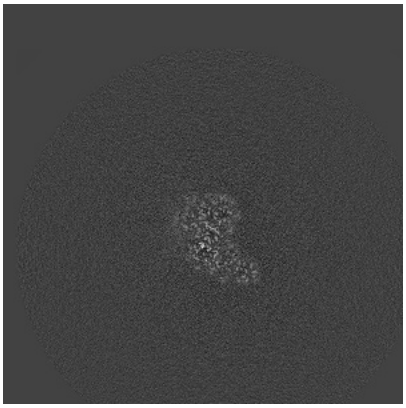


Z Index: 326

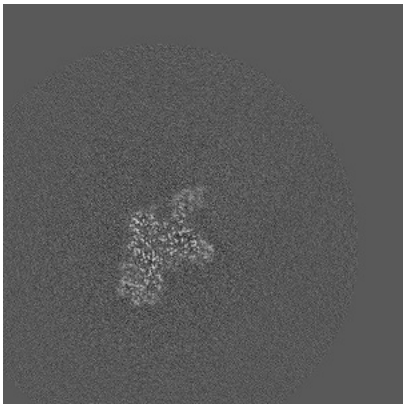
6.3.2 Raw map



X Index: 220



Y Index: 235

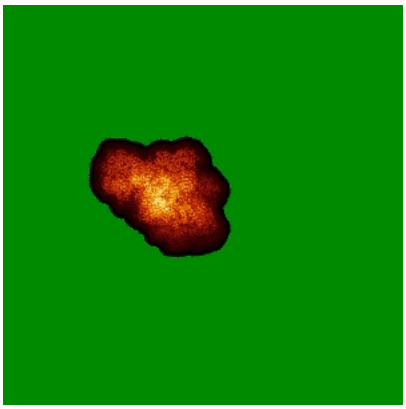


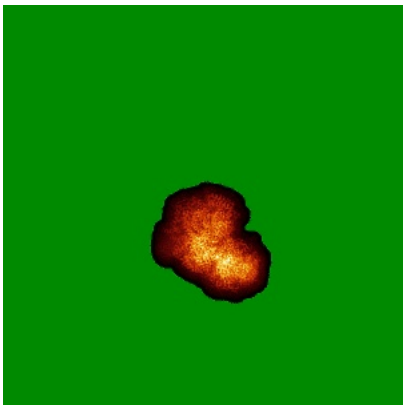
Z Index: 326

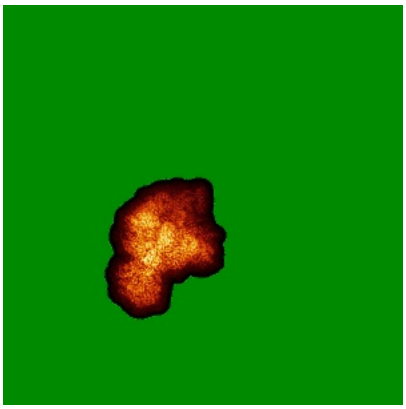
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

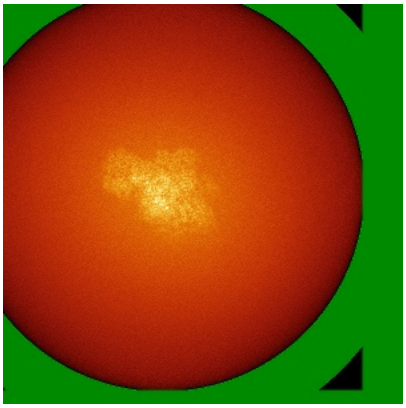
6.4.1 Primary map

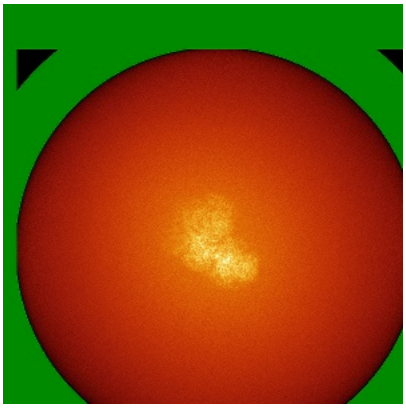

X

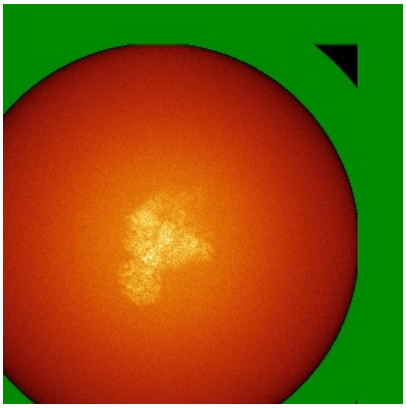

Y


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.

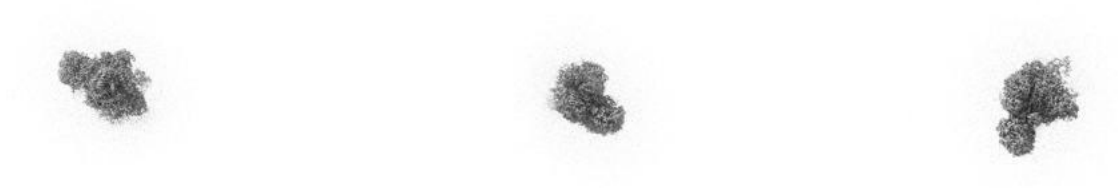
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.018. 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



X Y Z

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.

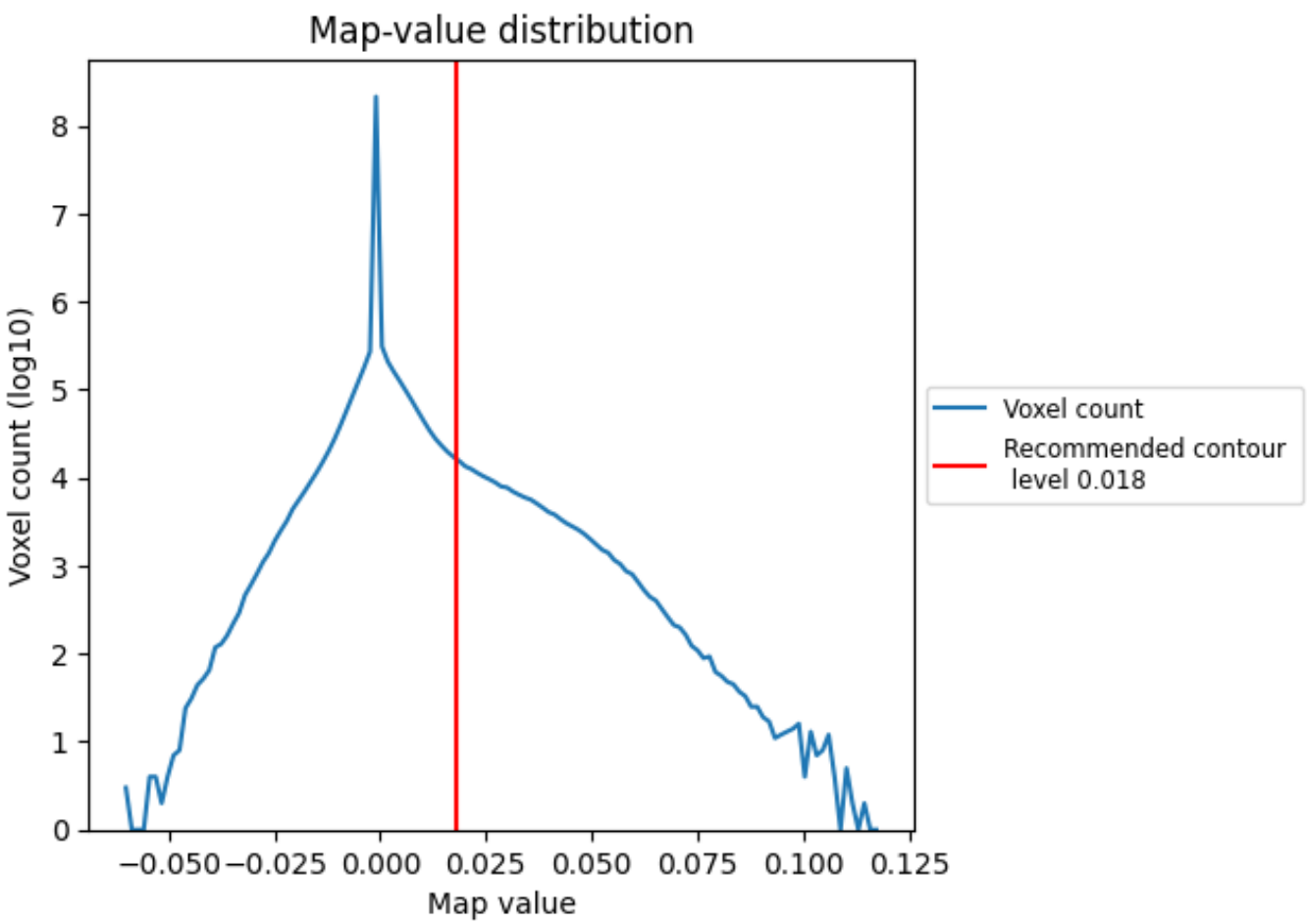
6.6 Mask visualisation (i)

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

7 Map analysis (i)

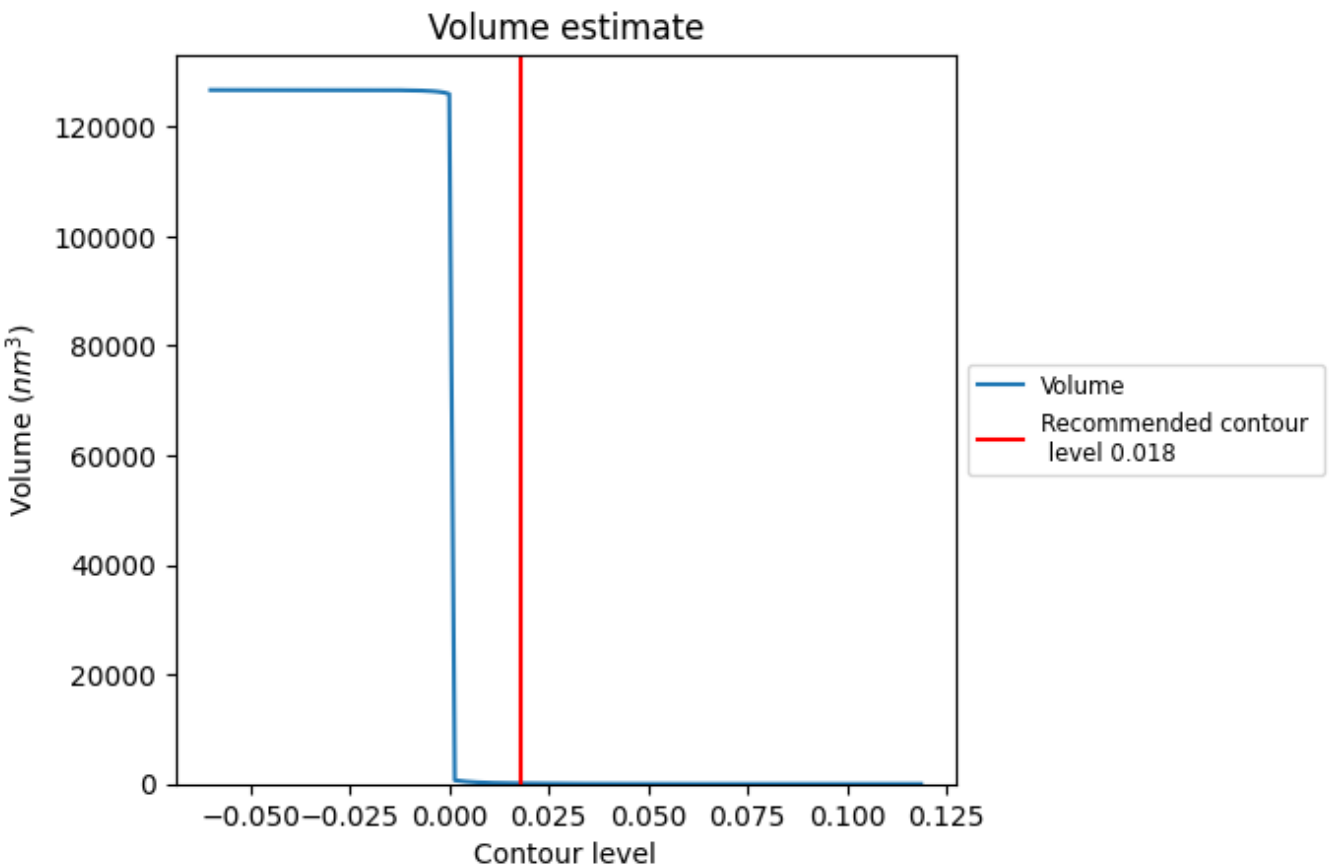
This section contains the results of statistical analysis of the map.

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.

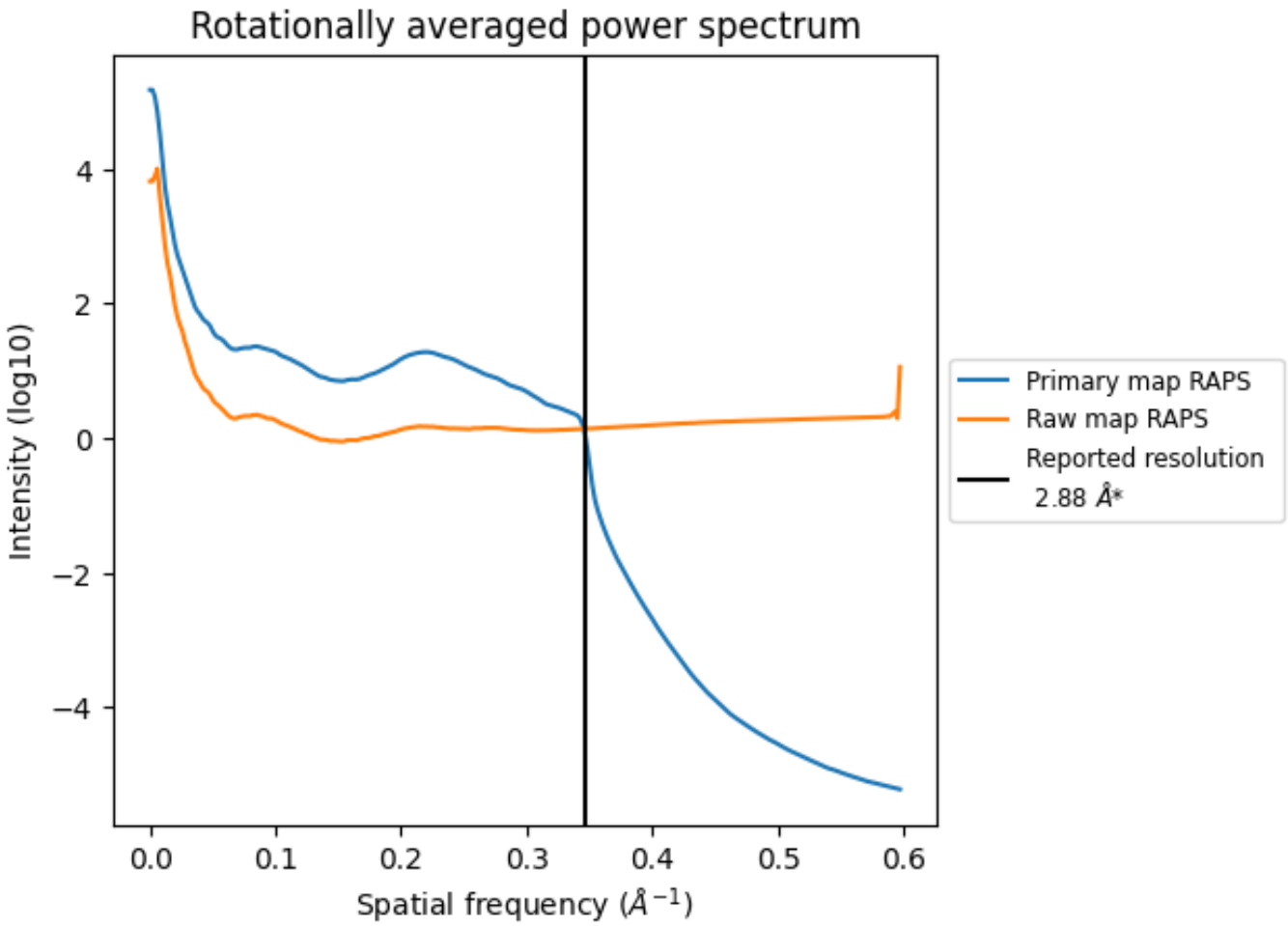
7.2 Volume estimate (i)



The volume at the recommended contour level is 104 nm^3; this corresponds to an approximate mass of 94 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)

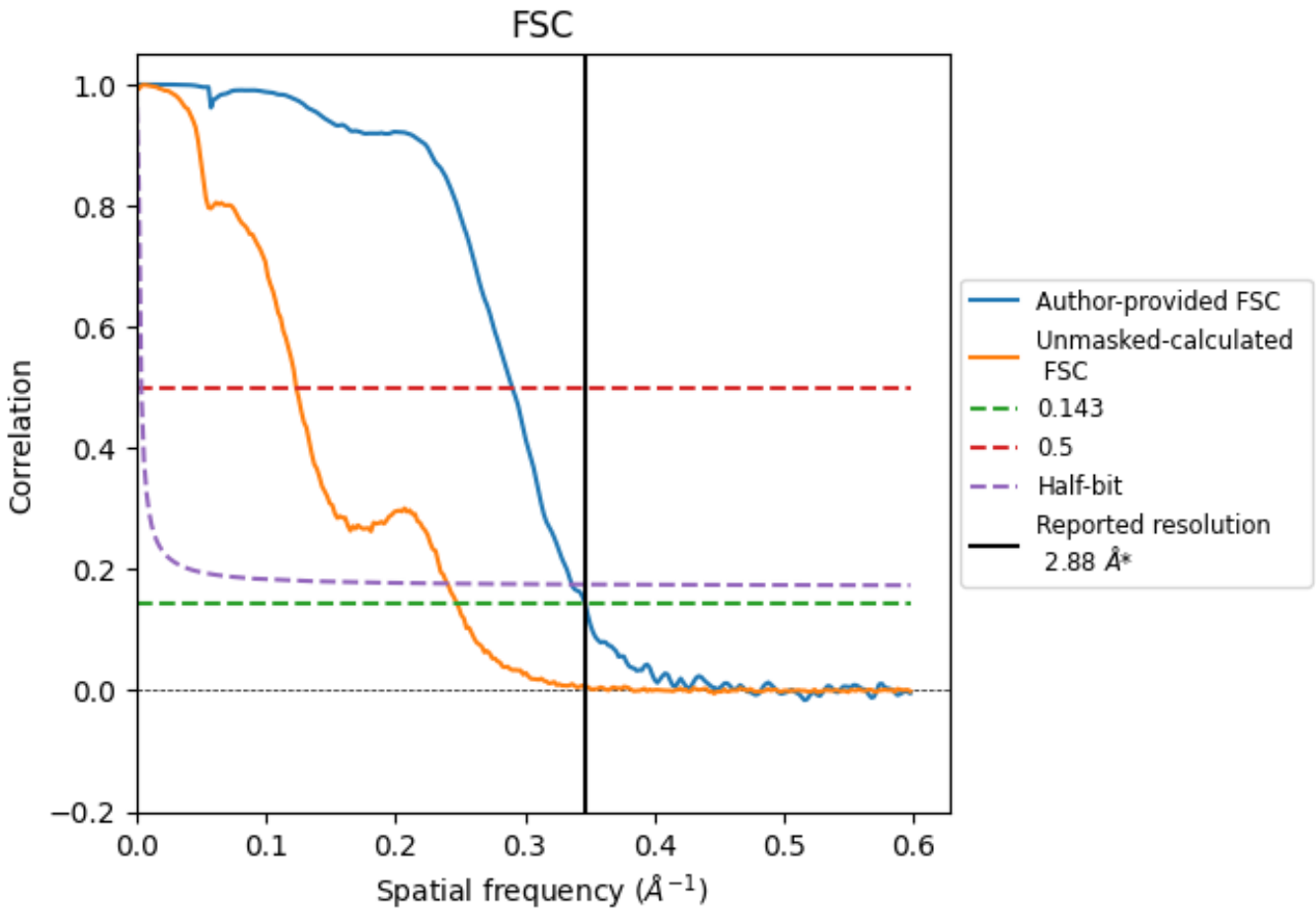


*Reported resolution corresponds to spatial frequency of 0.347 Å^{-1}

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 0.347 Å^{-1}

8.2 Resolution estimates (i)

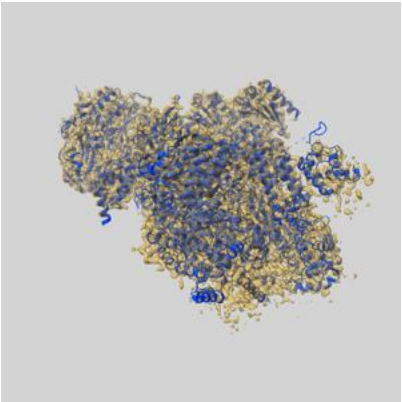
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.88	-	-
Author-provided FSC curve	2.89	3.45	2.98
Unmasked-calculated*	4.04	8.10	4.16

*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 4.04 differs from the reported value 2.88 by more than 10 %

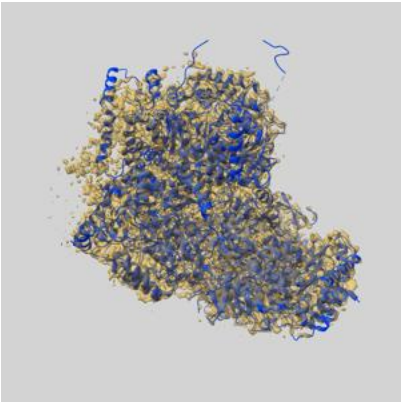
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11879 and PDB model 7ARC. Per-residue inclusion information can be found in section 3 on page 11.

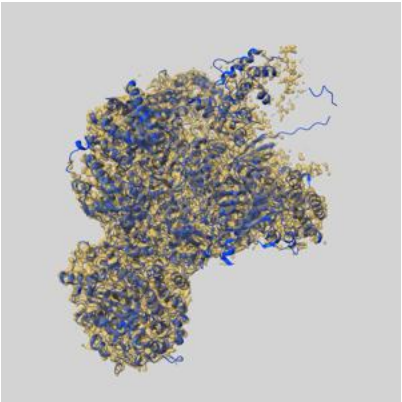
9.1 Map-model overlay (i)



X



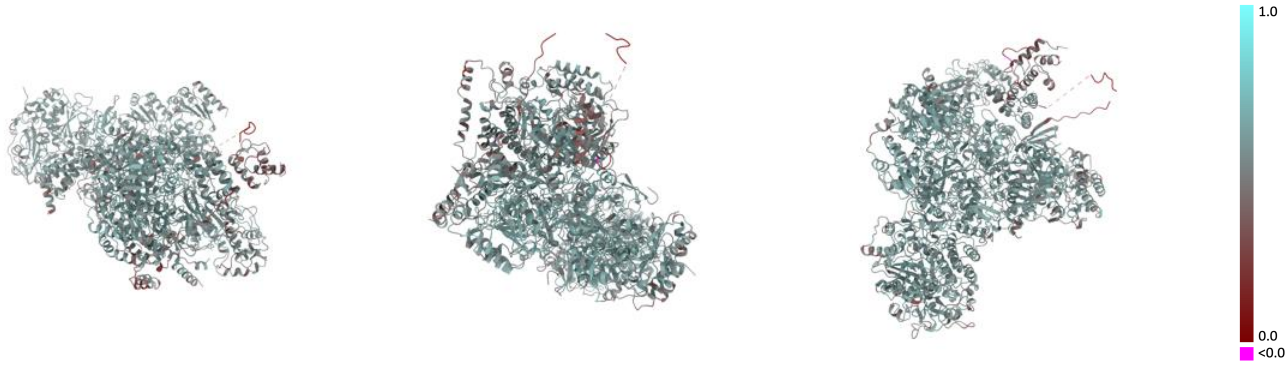
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.018 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.

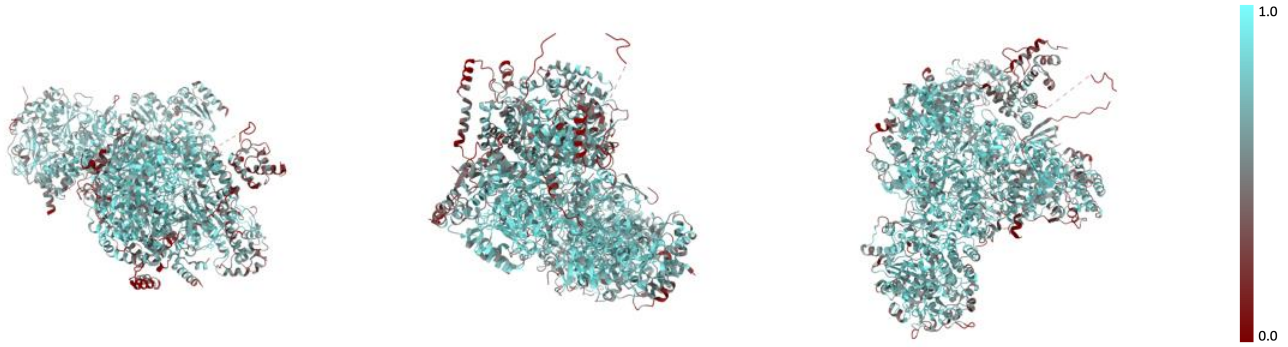
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

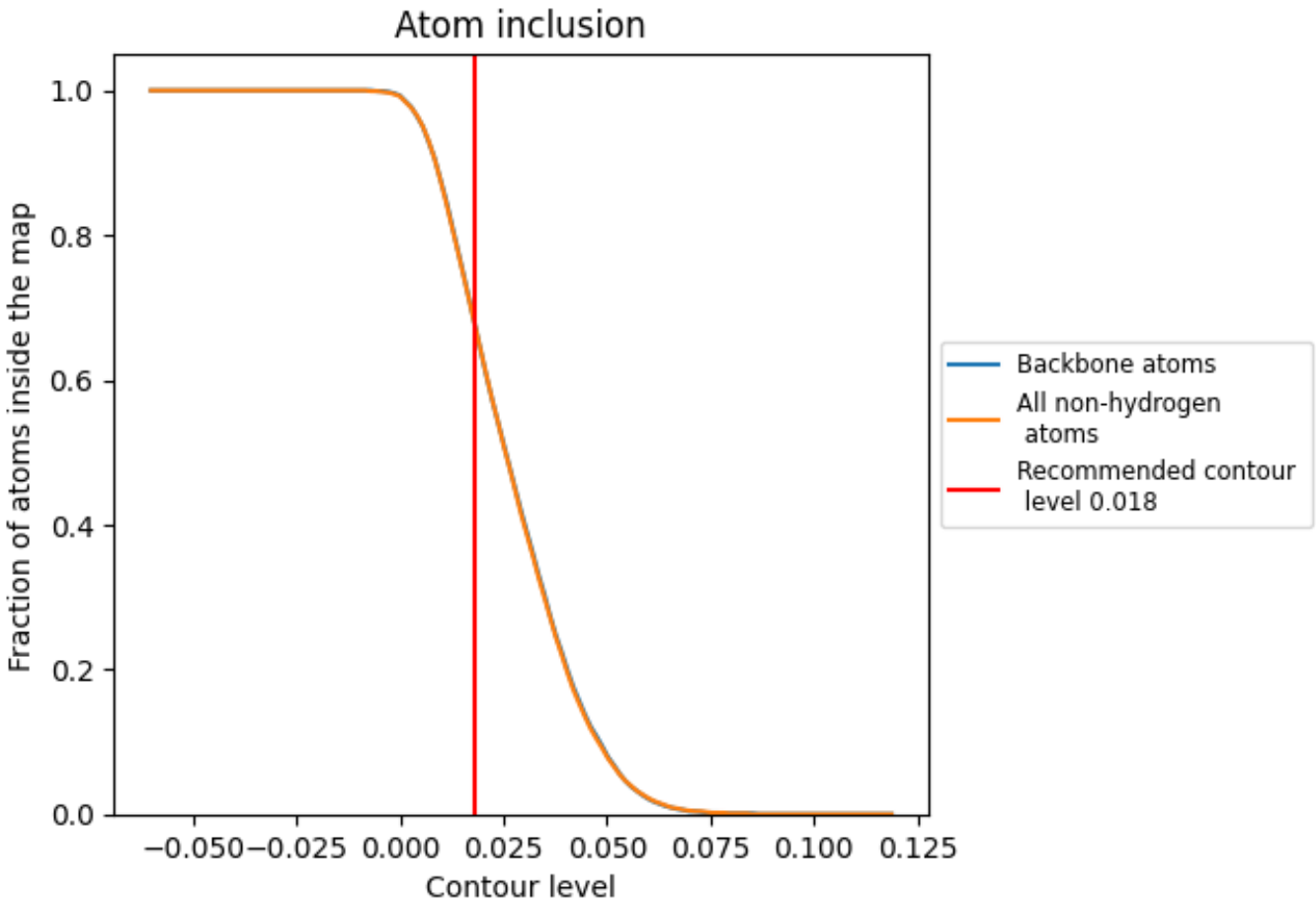
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.018).

9.4 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6780	0.5630
B	0.6900	0.5560
C	0.8000	0.6040
D	0.7530	0.5750
E	0.6500	0.5490
F	0.7060	0.5660
G	0.7680	0.5940
I	0.6070	0.5440
P	0.6770	0.5580
Q	0.7170	0.5900
R	0.5940	0.5410
S	0.6610	0.5540
U	0.3070	0.3960
V	0.5870	0.5320
W	0.5620	0.5080
q	0.7340	0.5870
r	0.3170	0.5150