



Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 09:34 AM EST

PDB ID : 7K36
EMDB ID : EMD-22650
Title : Cryo-EM structure of STRIPAK complex
Authors : Jeong, B.-C.; Bai, X.C.
Deposited on : 2020-09-10
Resolution : 3.30 Å(reported)
Based on initial models : 4N6J, 2NPP, 2YMU, 5YF4

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
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) : 2.31.2

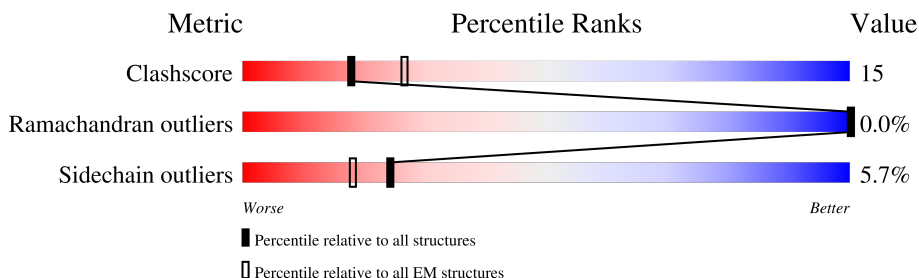
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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 ≥ 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	589	<div> <div>47%</div> <div>69%</div> <div>24%</div> <div>6%</div> </div>
2	B	713	<div> <div>9%</div> <div>22%</div> <div>19%</div> <div>58%</div> </div>
2	D	713	<div> <div>7%</div> <div>90%</div> </div>
2	E	713	<div> <div>6%</div> <div>91%</div> </div>
2	F	713	<div> <div>6%</div> <div>91%</div> </div>
2	G	713	<div> <div>6%</div> <div>92%</div> </div>
3	C	309	<div> <div>63%</div> <div>29%</div> <div>5%</div> </div>
4	H	225	<div> <div>10%</div> <div>45%</div> <div>32%</div> <div>21%</div> </div>

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Mol	Chain	Length	Quality of chain
5	I	837	 <div> <div></div> <div>51%</div> <div>19%</div> <div>28%</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 16613 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 Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	554	Total	C	N	O	S	0	0
			3515	2209	625	671	10		

- Molecule 2 is a protein called Striatin-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	298	Total	C	N	O	S	0	0
			2296	1462	388	434	12		
2	D	74	Total	C	N	O	S	0	0
			621	394	118	107	2		
2	E	66	Total	C	N	O	S	0	0
			563	360	105	96	2		
2	F	62	Total	C	N	O	S	0	0
			510	327	94	87	2		
2	G	60	Total	C	N	O	S	0	0
			457	295	83	78	1		

- Molecule 3 is a protein called Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	293	Total	C	N	O	S	0	0
			2360	1494	402	449	15		

- Molecule 4 is a protein called MOB-like protein phocein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	177	Total	C	N	O	S	0	0
			1422	907	249	255	11		

- Molecule 5 is a protein called Striatin-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	599	Total	C	N	O	S	0	0
			4829	3107	831	859	32		

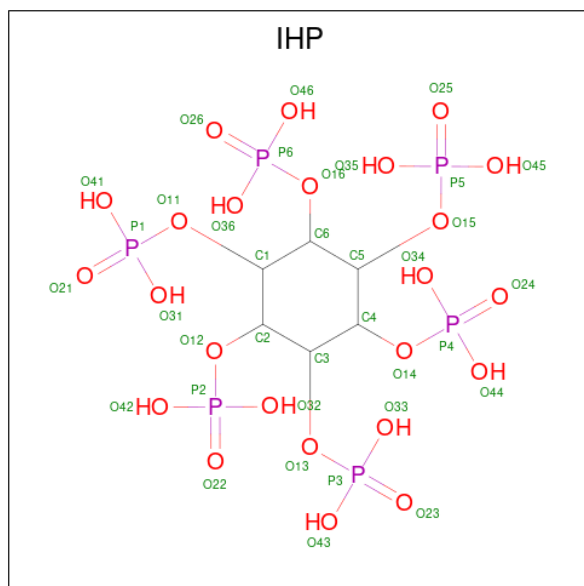
- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
6	C	2	Total	Mn	0
			2	2	

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
7	H	2	Total	Zn	0
			2	2	

- Molecule 8 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).

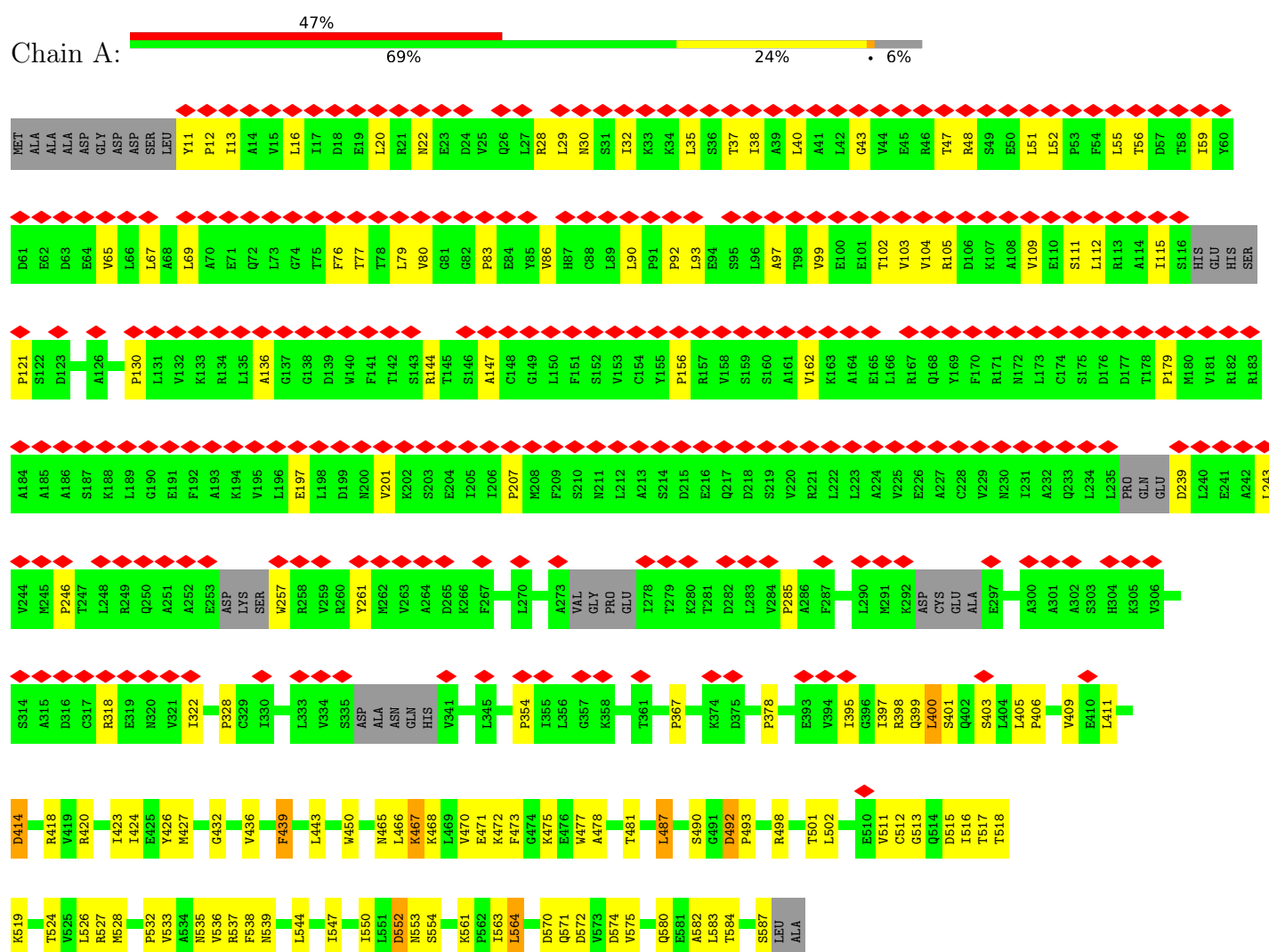


Mol	Chain	Residues	Atoms				AltConf
8	I	1	Total	C	O	P	0
			36	6	24	6	

3 Residue-property plots

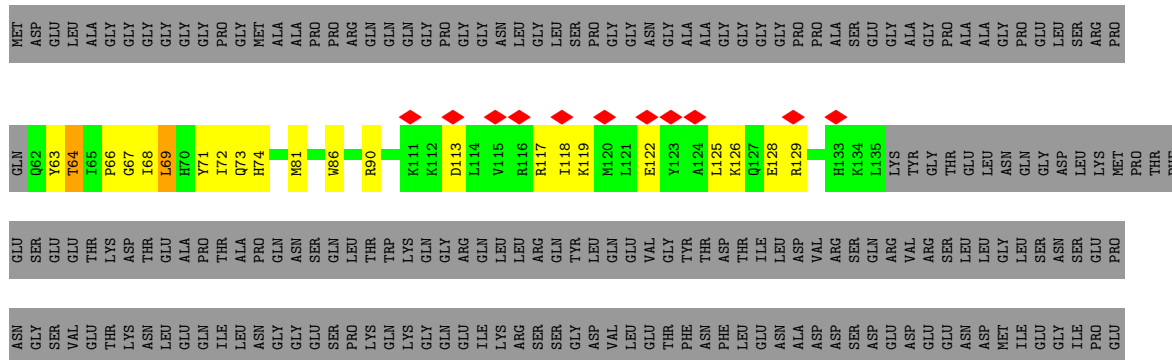
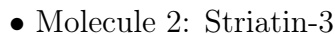
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform



- Molecule 2: Striatin-3





- Molecule 2: Striatin-3

MET	VAL	THR	THR	SER	PHE	ASN	THR	GLY	SER	ALA	VAL	ILE	TYR	ASP	LEU	GLU	THR	SER	GLN	SER	SER	LEU	VAL	VAL	ILE	LEU	SER	SER	GLN	ASP	VAL	SER	GLY	LEU	GLN	SER	SER	ASN	ASN	HIS	ILE	ASN	ARG	VAL	VAL	SER	HIS	PRO	THR	THR	LEU	PRO	VAL	THR	THR	THR	ALA	HIS	GLU	ASP	ARG	HIS	ARG	ILE	YS
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- Molecule 2: Striatin-3

[illegible]

- Molecule 2: Striatin-3



GLN	MET
Q62	ASP
Y63	LEU
T64	ALA
P66	GLY
G67	GLY
I68	GLY
L69	GLY
H70	GLY
Y71	PRO
I72	PRO
E75	MET
E76	MET
E82	ALA
W86	PRO
R90	ARG
A91	GLN
E92	GLN
L93	GLN
Q94	PRO
A95	GLY
R96	ASN
I97	LEU
A98	GLY
F99	LEU
L100	SER
Q101	PRO
G102	GLY
E103	GLY
R104	ASN
K105	ALA
G106	ALA
Q107	GLY
E108	GLY
N109	PRO
L110	PRO
K111	ALA
K112	SER
D113	GLY
L114	ALA
V115	GLY
R116	ALA
R117	ALA
I118	GLY
K119	PRO
M120	GLU
L121	LEU
G122	SER
T123	ARG
G124	PRO
T125	TYR
ALA	ALA
LEU	LEU
LYS	LYS
GLN	GLN
ARG	ARG
ALA	ALA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	87779	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	59524	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.042	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	298.8, 298.8, 298.8	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.30	0/3546	0.49	11/4874 (0.2%)
2	B	0.30	0/2356	0.49	1/3218 (0.0%)
2	D	0.35	0/633	0.40	0/848
2	E	0.38	0/575	0.41	0/771
2	F	0.31	0/522	0.39	0/705
2	G	0.35	0/468	0.37	0/637
3	C	0.49	0/2417	0.49	0/3278
4	H	0.31	0/1456	0.42	0/1968
5	I	0.44	0/4923	0.45	0/6645
All	All	0.38	0/16896	0.46	12/22944 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	PRO	N-CA-CB	5.96	110.45	103.30
1	A	354	PRO	N-CA-CB	5.94	110.43	103.30
1	A	130	PRO	N-CA-CB	5.85	110.32	103.30
1	A	179	PRO	N-CA-CB	5.79	110.25	103.30
1	A	367	PRO	N-CA-CB	5.74	110.19	103.30
1	A	207	PRO	N-CA-CB	5.70	110.14	103.30
1	A	285	PRO	N-CA-CB	5.69	110.12	103.30
1	A	246	PRO	N-CA-CB	5.67	110.10	103.30
1	A	156	PRO	N-CA-CB	5.66	110.10	103.30
1	A	328	PRO	N-CA-CB	5.64	110.07	103.30
1	A	378	PRO	N-CA-CB	5.52	109.92	103.30
2	B	685	ASP	CB-CG-OD2	5.21	122.99	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3515	0	2859	93	0
2	B	2296	0	2217	102	0
2	D	621	0	608	16	0
2	E	563	0	557	20	0
2	F	510	0	479	17	0
2	G	457	0	403	16	0
3	C	2360	0	2258	71	0
4	H	1422	0	1361	59	0
5	I	4829	0	4877	126	0
6	C	2	0	0	0	0
7	H	2	0	0	0	0
8	I	36	0	6	5	0
All	All	16613	0	15625	480	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 15.

All (480) 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)
4:H:110:CYS:HB3	4:H:119:CYS:SG	2.04	0.98
5:I:452:ASP:OD2	5:I:455:THR:HG22	1.66	0.95
4:H:13:ASN:N	4:H:13:ASN:HD22	1.65	0.93
5:I:452:ASP:OD2	5:I:455:THR:CG2	2.17	0.92
4:H:13:ASN:HD22	4:H:13:ASN:H	1.18	0.89
4:H:97:CYS:SG	4:H:174:HIS:CE1	2.66	0.88
4:H:110:CYS:SG	4:H:113:HIS:HD2	1.97	0.87
5:I:215:ASP:OD1	5:I:215:ASP:N	2.08	0.83
2:B:694:HIS:HD2	2:B:696:SER:H	1.22	0.80
2:F:100:LEU:HG	2:G:100:LEU:HB3	1.65	0.78
2:B:649:PRO:HG3	2:B:695:SER:HA	1.67	0.76
5:I:565:VAL:HG23	5:I:629:ASN:HD22	1.51	0.76
4:H:109:LEU:HD23	5:I:136:THR:HA	1.69	0.75
3:C:117:ASN:OD1	3:C:241:HIS:CE1	2.39	0.75
5:I:666:PHE:O	5:I:670:ASN:ND2	2.18	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:THR:HG23	1:A:51:LEU:HD12	1.69	0.74
1:A:424:ILE:O	1:A:465:ASN:ND2	2.22	0.73
3:C:167:HIS:CE1	3:C:241:HIS:ND1	2.56	0.73
2:B:463:GLN:HG2	2:B:475:TRP:HE1	1.53	0.73
2:B:667:ASN:HB2	2:B:674:VAL:HG21	1.70	0.72
1:A:136:ALA:HB2	1:A:147:ALA:HB3	1.70	0.72
2:B:489:TYR:OH	4:H:89:GLN:NE2	2.24	0.71
2:E:86:TRP:HE1	2:E:90:ARG:HH21	1.38	0.70
4:H:13:ASN:N	4:H:13:ASN:ND2	2.39	0.70
5:I:477:SER:N	5:I:480:GLU:OE1	2.24	0.70
2:E:68:ILE:HD12	2:G:68:ILE:HG12	1.74	0.69
2:F:112:LYS:O	2:F:116:ARG:HG3	1.92	0.69
4:H:195:VAL:O	4:H:199:ASN:N	2.23	0.69
3:C:168:GLY:O	3:C:239:ARG:NE	2.21	0.69
2:B:549:ILE:HG13	2:B:567:PHE:HD1	1.57	0.69
5:I:233:GLU:HB2	5:I:245:ARG:HH21	1.58	0.69
2:B:528:LEU:O	2:B:538:ILE:HA	1.93	0.68
3:C:57:ASP:OD2	3:C:59:HIS:CD2	2.47	0.68
2:B:598:ASN:ND2	2:B:618:ASP:OD2	2.27	0.68
5:I:706:GLN:OE1	5:I:708:MET:N	2.27	0.68
3:C:20:CYS:SG	3:C:63:HIS:NE2	2.66	0.67
1:A:537:ARG:NH1	1:A:570:ASP:OD2	2.27	0.67
2:D:128:GLU:OE1	2:D:129:ARG:NH2	2.25	0.67
5:I:744:ARG:NH1	8:I:901:IHP:O33	2.28	0.67
3:C:223:ASP:OD1	3:C:223:ASP:N	2.26	0.67
2:B:602:ARG:HG2	2:B:645:LEU:H	1.60	0.66
1:A:16:LEU:HD11	1:A:38:ILE:HG21	1.75	0.66
2:D:125:LEU:HD21	2:E:125:LEU:HD21	1.78	0.66
1:A:48:ARG:HA	1:A:52:LEU:HD23	1.77	0.66
2:F:64:THR:HG22	2:F:66:PRO:HD2	1.77	0.66
2:B:688:ILE:HA	2:B:704:GLY:HA2	1.77	0.65
2:B:390:TYR:HB2	2:B:711:VAL:HB	1.77	0.65
2:B:524:GLY:HA2	2:B:550:PRO:HD3	1.78	0.65
3:C:14:ILE:O	3:C:18:ASN:ND2	2.29	0.65
1:A:67:LEU:HG	1:A:104:VAL:HG22	1.79	0.65
2:B:659:HIS:HA	2:B:687:SER:HB3	1.79	0.65
5:I:438:GLU:OE1	5:I:448:THR:OG1	2.15	0.65
2:B:694:HIS:CD2	2:B:695:SER:H	2.14	0.64
4:H:140:LYS:HE2	5:I:256:LEU:HD22	1.78	0.64
5:I:231:HIS:HA	5:I:234:CYS:HB2	1.79	0.64
2:B:621:ILE:HD11	2:B:642:VAL:HG11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:VAL:HA	1:A:112:LEU:HD12	1.80	0.63
5:I:83:SER:O	5:I:569:ARG:NH1	2.32	0.63
2:B:516:GLN:HA	2:B:529:TRP:O	1.99	0.62
5:I:427:LYS:HG3	5:I:744:ARG:HD3	1.81	0.62
2:B:442:ILE:HA	2:B:485:PRO:HG3	1.81	0.62
2:F:97:ILE:HD11	2:G:93:LEU:HD22	1.81	0.62
1:A:492:ASP:O	1:A:498:ARG:NH1	2.31	0.62
2:F:83:ARG:HG2	2:G:86:TRP:CH2	2.35	0.62
2:B:516:GLN:HB3	2:B:528:LEU:HD11	1.81	0.61
3:C:188:GLU:OE1	3:C:189:VAL:N	2.33	0.61
5:I:84:GLU:OE2	5:I:663:ARG:NH1	2.33	0.61
2:D:71:TYR:HD2	2:D:72:ILE:HD13	1.64	0.61
4:H:161:ARG:HD3	5:I:131:ASP:HA	1.82	0.61
5:I:75:THR:OG1	5:I:81:GLU:OE2	2.18	0.61
1:A:77:THR:HB	1:A:115:ILE:HG22	1.82	0.61
1:A:20:LEU:O	1:A:28:ARG:NH1	2.33	0.61
2:B:526:VAL:HG11	2:B:553:VAL:HG11	1.83	0.61
2:B:664:ARG:NH1	2:B:676:GLU:OE1	2.34	0.61
2:B:484:ASP:HB3	2:B:487:ASP:HB3	1.83	0.61
1:A:470:VAL:HG23	1:A:478:ALA:HB2	1.82	0.60
1:A:32:ILE:HG23	1:A:69:LEU:HD23	1.83	0.60
4:H:54:ILE:HG23	4:H:190:ARG:HA	1.83	0.60
1:A:28:ARG:O	1:A:32:ILE:HG12	2.02	0.60
2:B:625:ASP:OD1	2:B:629:GLY:N	2.35	0.60
5:I:283:MET:N	5:I:547:ASP:OD1	2.33	0.60
3:C:49:ARG:NH1	3:C:160:ASP:OD1	2.35	0.59
3:C:117:ASN:H	3:C:167:HIS:CD2	2.19	0.59
3:C:237:VAL:HG13	3:C:256:VAL:HG13	1.84	0.59
1:A:475:LYS:NZ	1:A:511:VAL:O	2.26	0.59
4:H:110:CYS:SG	4:H:111:ALA:N	2.76	0.59
3:C:115:ARG:HH12	3:C:151:ASP:HA	1.67	0.59
2:B:640:ASP:HB3	2:B:659:HIS:HB2	1.85	0.59
4:H:133:ALA:O	4:H:137:ASN:ND2	2.33	0.59
4:H:41:GLN:N	4:H:41:GLN:OE1	2.35	0.59
5:I:715:LYS:NZ	8:I:901:IHP:O32	2.30	0.58
1:A:439:PHE:HB2	1:A:443:LEU:HD22	1.84	0.58
4:H:159:VAL:O	4:H:163:ILE:HG12	2.02	0.58
5:I:452:ASP:OD2	5:I:455:THR:HG21	2.04	0.58
2:B:446:ARG:NH1	4:H:130:ASP:OD2	2.36	0.58
1:A:32:ILE:HD12	1:A:69:LEU:HD21	1.86	0.58
1:A:411:LEU:HB3	1:A:423:ILE:HG13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:518:LEU:HD11	2:B:563:MET:HG2	1.85	0.58
2:B:394:SER:HB3	2:B:423:TRP:HH2	1.68	0.58
4:H:72:GLU:OE1	4:H:145:ARG:NH2	2.37	0.58
4:H:87:LYS:O	4:H:90:SER:OG	2.18	0.58
5:I:679:THR:O	5:I:679:THR:OG1	2.17	0.57
2:B:501:HIS:HE1	2:B:505:VAL:HG22	1.68	0.57
2:D:64:THR:HG23	2:D:67:GLY:HA3	1.86	0.57
2:B:394:SER:HB3	2:B:423:TRP:CH2	2.39	0.57
2:D:86:TRP:HZ3	2:E:82:GLU:HB3	1.69	0.57
2:G:64:THR:OG1	2:G:66:PRO:HD2	2.05	0.57
5:I:210:LEU:N	5:I:549:LEU:O	2.38	0.57
2:B:573:VAL:HG12	2:B:585:ILE:HG22	1.87	0.56
5:I:170:ARG:NE	5:I:233:GLU:OE2	2.34	0.56
5:I:322:GLU:OE2	5:I:425:ALA:N	2.28	0.56
1:A:83:PRO:HA	1:A:86:VAL:HG13	1.88	0.56
1:A:397:ILE:HD12	1:A:400:LEU:HD13	1.86	0.56
1:A:574:ASP:OD2	3:C:110:ARG:NH1	2.37	0.56
2:B:399:VAL:HA	2:B:415:SER:HA	1.87	0.56
2:E:92:GLU:HA	5:I:495:SER:HB3	1.87	0.56
2:B:422:LEU:HD23	2:B:442:ILE:HB	1.87	0.56
2:B:669:ASP:OD1	2:B:669:ASP:N	2.38	0.56
2:E:100:LEU:HD21	5:I:792:PHE:HE1	1.72	0.55
5:I:214:THR:HG22	5:I:217:ARG:HH22	1.71	0.55
4:H:149:LYS:O	4:H:152:SER:OG	2.22	0.55
1:A:532:PRO:O	1:A:537:ARG:NH2	2.39	0.55
2:D:125:LEU:HD11	2:E:125:LEU:HD21	1.89	0.55
5:I:76:ASP:OD1	5:I:77:LYS:N	2.37	0.55
2:B:521:SER:OG	2:B:522:ALA:N	2.40	0.55
3:C:263:PRO:HB2	3:C:291:PRO:HD3	1.89	0.55
5:I:97:ASN:HB3	5:I:150:TYR:HB2	1.87	0.55
2:B:477:ASN:HD21	2:B:495:ALA:HB2	1.71	0.55
3:C:202:ASP:OD1	3:C:202:ASP:N	2.39	0.55
1:A:400:LEU:O	1:A:403:SER:OG	2.14	0.55
1:A:564:LEU:HD11	1:A:582:ALA:HB3	1.87	0.55
3:C:60:GLY:N	3:C:86:TYR:O	2.40	0.55
1:A:56:THR:HA	1:A:92:PRO:HB3	1.87	0.55
2:B:527:ARG:HG2	2:B:540:THR:HG22	1.88	0.55
5:I:490:LEU:HD13	5:I:777:ARG:HE	1.73	0.54
2:B:506:TRP:CZ2	4:H:15:PRO:HA	2.42	0.54
1:A:43:GLY:O	1:A:47:THR:N	2.28	0.54
3:C:134:LEU:O	3:C:138:GLY:N	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:473:ILE:HB	2:B:498:LEU:HB2	1.88	0.54
4:H:112:ALA:HB3	4:H:127:HIS:HB3	1.90	0.54
4:H:113:HIS:CD2	4:H:113:HIS:H	2.26	0.54
5:I:669:ILE:O	5:I:673:ARG:HG3	2.08	0.54
4:H:201:MET:HG2	4:H:205:ASN:HD22	1.73	0.54
3:C:117:ASN:HD22	3:C:118:HIS:CD2	2.26	0.53
3:C:223:ASP:O	3:C:227:THR:HG23	2.08	0.53
1:A:535:ASN:HA	1:A:538:PHE:CE2	2.44	0.53
4:H:55:ASP:HB3	4:H:193:LYS:HE2	1.89	0.53
5:I:486:GLU:OE1	5:I:781:ARG:NH1	2.42	0.53
5:I:74:ASP:OD2	5:I:301:PHE:N	2.27	0.53
2:B:503:ASP:HB3	2:B:521:SER:OG	2.08	0.53
3:C:94:VAL:HG11	3:C:136:LYS:HD2	1.89	0.53
1:A:513:GLY:O	1:A:517:THR:HG23	2.09	0.53
2:B:417:ASP:HB2	2:B:419:THR:HG22	1.90	0.53
2:B:447:ALA:HB1	2:B:494:LEU:HD22	1.90	0.53
3:C:16:GLN:NE2	3:C:22:GLN:O	2.40	0.53
5:I:702:LEU:HD21	5:I:714:LEU:HD21	1.90	0.53
2:B:475:TRP:CE3	2:B:496:GLY:HA3	2.44	0.53
1:A:16:LEU:HD21	1:A:38:ILE:HG13	1.91	0.52
3:C:167:HIS:ND1	3:C:240:ALA:O	2.41	0.52
1:A:197:GLU:O	1:A:201:VAL:N	2.36	0.52
2:B:656:SER:HB3	2:B:666:TRP:HE1	1.73	0.52
3:C:261:SER:HA	3:C:273:ALA:HB1	1.92	0.52
4:H:81:LEU:HD22	4:H:129:LEU:HD21	1.89	0.52
5:I:710:GLN:O	5:I:714:LEU:HG	2.10	0.52
5:I:93:GLU:OE1	5:I:146:ARG:NH2	2.42	0.52
1:A:400:LEU:HD12	1:A:400:LEU:H	1.74	0.52
3:C:117:ASN:H	3:C:167:HIS:HD2	1.57	0.52
1:A:418:ARG:NH2	3:C:67:GLU:OE1	2.43	0.52
2:B:559:ASP:OD1	2:B:562:HIS:N	2.30	0.52
2:D:63:TYR:HD1	2:D:68:ILE:HD11	1.75	0.52
1:A:32:ILE:HG13	1:A:65:VAL:HG13	1.92	0.52
1:A:52:LEU:HD21	1:A:80:VAL:HG22	1.91	0.52
2:B:399:VAL:HG12	2:B:415:SER:HB3	1.92	0.52
5:I:213:SER:O	5:I:217:ARG:NH1	2.43	0.52
5:I:445:ILE:HD11	5:I:459:LEU:HD23	1.91	0.51
5:I:746:ARG:NH2	8:I:901:IHP:O44	2.43	0.51
1:A:67:LEU:HD11	1:A:103:VAL:HG23	1.92	0.51
1:A:515:ASP:N	1:A:515:ASP:OD1	2.41	0.51
5:I:173:ILE:HG21	5:I:229:THR:OG1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:677:LYS:NZ	8:I:901:IHP:O36	2.42	0.51
1:A:55:LEU:HA	1:A:59:ILE:HD11	1.92	0.51
2:F:65:ILE:HD12	2:F:68:ILE:HD12	1.90	0.51
5:I:449:LEU:CD2	5:I:455:THR:HG21	2.41	0.51
3:C:141:ASN:OD1	3:C:141:ASN:N	2.44	0.51
3:C:171:SER:HB3	3:C:197:ASP:HB2	1.92	0.51
3:C:178:ASP:OD2	5:I:473:HIS:NE2	2.39	0.51
4:H:13:ASN:H	4:H:13:ASN:ND2	1.95	0.51
4:H:93:HIS:CD2	4:H:94:PRO:HD2	2.46	0.51
5:I:750:ASP:OD1	5:I:750:ASP:N	2.43	0.51
2:B:659:HIS:CE1	2:B:686:GLU:HG3	2.46	0.51
5:I:492:SER:O	5:I:492:SER:OG	2.26	0.51
2:B:619:ARG:HH21	2:B:639:LEU:HA	1.76	0.50
2:F:75:GLU:HA	2:F:78:ARG:HG2	1.92	0.50
1:A:93:LEU:O	1:A:97:ALA:N	2.44	0.50
3:C:46:GLN:O	3:C:158:LEU:N	2.41	0.50
1:A:13:ILE:HA	1:A:16:LEU:HD12	1.94	0.50
1:A:493:PRO:O	1:A:498:ARG:NH1	2.44	0.50
5:I:78:TRP:HB2	5:I:232:GLN:HG3	1.93	0.50
3:C:121:ARG:NH2	3:C:151:ASP:OD2	2.44	0.50
2:E:68:ILE:HG23	2:G:68:ILE:HD13	1.94	0.50
4:H:88:LEU:O	4:H:92:CYS:N	2.45	0.50
1:A:239:ASP:O	1:A:243:LEU:N	2.40	0.50
3:C:167:HIS:HE1	3:C:241:HIS:HA	1.76	0.50
1:A:395:ILE:O	1:A:399:GLN:NE2	2.45	0.50
2:D:90:ARG:HB2	2:E:86:TRP:CZ3	2.46	0.50
1:A:257:TRP:O	1:A:261:TYR:N	2.36	0.50
2:B:449:ILE:O	2:B:470:ASP:HB2	2.12	0.50
1:A:105:ARG:O	1:A:109:VAL:HG23	2.12	0.49
5:I:87:SER:HB2	5:I:548:VAL:HG23	1.94	0.49
1:A:318:ARG:O	1:A:322:ILE:N	2.41	0.49
5:I:704:VAL:HG21	5:I:709:MET:SD	2.52	0.49
5:I:706:GLN:OE1	5:I:707:ALA:N	2.45	0.49
2:G:82:GLU:HG2	2:G:86:TRP:CZ2	2.47	0.49
5:I:70:PHE:HE2	5:I:72:TYR:HB2	1.76	0.49
2:G:82:GLU:HG2	2:G:86:TRP:CE2	2.47	0.49
1:A:11:TYR:HB3	1:A:12:PRO:HD3	1.94	0.49
5:I:534:THR:O	5:I:615:LYS:NZ	2.44	0.49
5:I:729:ARG:NH2	5:I:754:GLY:O	2.46	0.49
1:A:22:ASN:HB3	1:A:28:ARG:HG2	1.94	0.49
2:B:663:ILE:HD13	2:B:691:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:132:GLU:N	3:C:132:GLU:OE1	2.45	0.49
2:F:86:TRP:CZ3	2:G:90:ARG:HD2	2.48	0.49
4:H:44:GLN:OE1	4:H:48:ARG:NE	2.46	0.49
2:B:620:HIS:HB2	2:B:622:LYS:HZ1	1.77	0.49
5:I:486:GLU:OE2	5:I:781:ARG:NH2	2.45	0.48
2:B:549:ILE:HD12	2:B:568:ASN:HB3	1.93	0.48
5:I:716:LEU:O	5:I:719:VAL:HG12	2.12	0.48
2:B:683:LYS:NZ	4:H:40:GLN:OE1	2.30	0.48
2:E:74:HIS:HB2	5:I:449:LEU:HD21	1.94	0.48
5:I:123:ARG:NE	5:I:178:GLU:OE2	2.46	0.48
5:I:155:THR:O	5:I:155:THR:OG1	2.24	0.48
2:B:586:LEU:HD13	2:B:624:PHE:CD1	2.49	0.48
3:C:212:SER:OG	3:C:217:GLY:O	2.30	0.48
3:C:250:TRP:CE3	3:C:254:ARG:HD2	2.49	0.48
4:H:115:THR:HG21	5:I:194:ASP:OD2	2.14	0.48
5:I:108:HIS:CD2	5:I:128:ARG:HH11	2.32	0.48
5:I:460:PRO:HB2	5:I:462:PRO:HD2	1.95	0.48
1:A:29:LEU:HD13	1:A:65:VAL:HG22	1.95	0.48
1:A:405:LEU:O	1:A:409:VAL:HG13	2.13	0.48
1:A:515:ASP:HB2	1:A:519:LYS:NZ	2.29	0.48
1:A:490:SER:HA	1:A:501:THR:HG21	1.96	0.48
2:B:402:LEU:HD13	2:B:703:ALA:HB2	1.95	0.48
2:B:558:CYS:SG	2:B:609:LEU:HB2	2.54	0.48
2:B:503:ASP:HB2	2:B:523:ASP:CG	2.34	0.48
2:B:610:PRO:O	2:B:625:ASP:HA	2.14	0.48
5:I:130:LEU:HD21	5:I:181:THR:HG23	1.96	0.48
5:I:168:TRP:HA	5:I:168:TRP:CE3	2.49	0.48
5:I:170:ARG:HD3	5:I:241:TRP:HZ3	1.79	0.48
2:B:621:ILE:HG12	2:B:637:ALA:HB2	1.96	0.47
3:C:177:LEU:HD11	3:C:234:LEU:HD21	1.96	0.47
3:C:290:ASP:HB3	3:C:291:PRO:HD2	1.96	0.47
1:A:512:CYS:SG	1:A:516:ILE:HB	2.54	0.47
2:B:659:HIS:CE1	2:B:687:SER:H	2.32	0.47
2:B:469:ILE:HD11	4:H:22:PHE:CE1	2.49	0.47
2:B:470:ASP:HB3	2:B:472:THR:HG22	1.97	0.47
2:B:694:HIS:CD2	2:B:697:LYS:H	2.32	0.47
3:C:117:ASN:OD1	3:C:241:HIS:ND1	2.48	0.47
3:C:187:GLN:HB3	5:I:443:LYS:NZ	2.30	0.47
3:C:207:GLY:HA2	3:C:221:GLY:HA3	1.95	0.47
2:E:64:THR:O	2:E:68:ILE:HG12	2.15	0.47
5:I:452:ASP:CG	5:I:455:THR:CG2	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:53:ASN:HB2	4:H:56:LYS:HB3	1.97	0.47
5:I:78:TRP:CH2	5:I:166:GLN:HB2	2.49	0.47
1:A:406:PRO:O	1:A:409:VAL:HG22	2.15	0.47
3:C:252:HIS:O	3:C:255:ASN:ND2	2.44	0.47
2:B:527:ARG:HB2	2:B:529:TRP:HE1	1.80	0.47
4:H:70:LYS:HE2	4:H:198:TYR:CD1	2.49	0.47
5:I:717:LEU:HA	5:I:717:LEU:HD23	1.79	0.47
2:B:527:ARG:HB2	2:B:529:TRP:NE1	2.30	0.46
5:I:547:ASP:HB2	5:I:570:HIS:CE1	2.50	0.46
1:A:432:GLY:HA3	1:A:472:LYS:HD3	1.96	0.46
1:A:552:ASP:OD2	1:A:554:SER:OG	2.30	0.46
2:D:118:ILE:HD11	2:E:118:ILE:HG12	1.96	0.46
4:H:190:ARG:HG2	4:H:191:PHE:CD1	2.49	0.46
5:I:452:ASP:CG	5:I:455:THR:HG22	2.34	0.46
2:G:118:ILE:HD13	2:G:121:LEU:HD21	1.97	0.46
5:I:326:LYS:HG2	5:I:329:ARG:HH11	1.81	0.46
5:I:622:MET:O	5:I:626:THR:HG22	2.14	0.46
2:B:394:SER:O	2:B:394:SER:OG	2.33	0.46
2:B:623:PHE:CD2	2:B:633:HIS:HB3	2.51	0.46
2:B:689:TYR:CE2	2:B:705:ALA:HA	2.50	0.46
5:I:801:SER:O	5:I:804:GLY:N	2.46	0.46
2:E:118:ILE:O	2:E:122:GLU:HG2	2.15	0.46
5:I:230:VAL:HG11	5:I:248:PHE:CD2	2.51	0.46
2:B:404:PHE:CE1	2:B:411:LEU:HB2	2.51	0.46
4:H:44:GLN:HG3	4:H:48:ARG:HD2	1.98	0.46
5:I:433:ILE:HD13	5:I:471:LYS:HG2	1.98	0.46
1:A:487:LEU:HD13	1:A:487:LEU:HA	1.74	0.46
2:B:476:TRP:CD1	2:B:493:VAL:HG12	2.51	0.46
5:I:248:PHE:O	5:I:251:GLU:HG3	2.15	0.46
2:B:523:ASP:HB3	2:B:525:THR:HG22	1.97	0.46
5:I:258:ASN:OD1	5:I:258:ASN:N	2.48	0.46
3:C:20:CYS:HG	3:C:63:HIS:CE1	2.33	0.46
3:C:239:ARG:NH1	3:C:258:THR:OG1	2.49	0.46
4:H:46:ASN:HB3	4:H:57:ILE:HG12	1.98	0.46
2:B:599:HIS:HD2	2:B:600:ILE:H	1.64	0.45
4:H:204:ASP:HB2	5:I:128:ARG:NH2	2.31	0.45
1:A:526:LEU:HD22	1:A:563:ILE:HG13	1.98	0.45
2:B:566:SER:OG	2:B:567:PHE:N	2.49	0.45
2:F:83:ARG:HG2	2:G:86:TRP:HH2	1.81	0.45
4:H:65:ASP:OD2	4:H:66:GLU:N	2.49	0.45
4:H:71:TYR:OH	4:H:75:ARG:NH1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:633:HIS:CE1	2:B:635:MET:HB3	2.52	0.45
5:I:545:LEU:H	5:I:545:LEU:HG	1.49	0.45
1:A:564:LEU:HB3	1:A:583:LEU:HD21	1.98	0.45
2:B:559:ASP:OD2	2:B:609:LEU:HD11	2.16	0.45
4:H:50:ASP:HB3	4:H:53:ASN:HD22	1.80	0.45
4:H:50:ASP:HB3	4:H:53:ASN:ND2	2.32	0.45
2:D:118:ILE:O	2:D:122:GLU:HG2	2.17	0.45
5:I:523:ALA:O	5:I:527:ILE:HG13	2.16	0.45
2:B:486:TYR:HA	4:H:127:HIS:CD2	2.52	0.45
3:C:117:ASN:CG	3:C:241:HIS:CE1	2.90	0.45
5:I:211:ALA:HA	5:I:214:THR:HG23	1.98	0.45
5:I:545:LEU:O	5:I:549:LEU:HG	2.16	0.45
1:A:93:LEU:HD21	1:A:111:SER:HB2	1.99	0.45
1:A:467:LYS:HB3	1:A:467:LYS:HE3	1.67	0.45
2:B:399:VAL:HG23	2:B:703:ALA:HB1	1.98	0.45
3:C:49:ARG:HD2	3:C:49:ARG:HA	1.70	0.45
3:C:45:VAL:O	3:C:45:VAL:HG13	2.16	0.45
1:A:414:ASP:OD1	1:A:420:ARG:HG3	2.16	0.45
1:A:32:ILE:O	1:A:35:LEU:HG	2.16	0.45
2:B:628:THR:HG23	2:B:630:LYS:HG2	1.99	0.45
2:F:100:LEU:HD13	2:F:100:LEU:HA	1.81	0.45
5:I:441:ARG:NH1	5:I:452:ASP:O	2.37	0.45
2:E:74:HIS:CG	5:I:449:LEU:HD11	2.52	0.44
5:I:661:CYS:HB3	5:I:664:ASN:HD22	1.82	0.44
1:A:502:LEU:HD12	1:A:502:LEU:HA	1.78	0.44
1:A:424:ILE:HG12	1:A:450:TRP:CD2	2.51	0.44
2:B:655:MET:SD	2:B:665:LEU:HG	2.58	0.44
3:C:124:THR:HB	3:C:129:PHE:HB3	1.98	0.44
5:I:151:VAL:HG12	5:I:176:LEU:HD11	1.98	0.44
1:A:52:LEU:HD13	1:A:55:LEU:HD21	2.00	0.44
4:H:55:ASP:O	4:H:59:GLU:N	2.51	0.44
2:B:416:GLU:HB3	2:B:451:PRO:HB3	2.00	0.44
5:I:85:LEU:HD22	5:I:224:TYR:CD2	2.53	0.44
5:I:610:ILE:HB	5:I:611:PRO:HD3	1.98	0.44
3:C:239:ARG:O	3:C:258:THR:HA	2.18	0.44
3:C:250:TRP:HE3	3:C:254:ARG:HA	1.83	0.44
5:I:118:ASP:OD1	5:I:119:THR:N	2.47	0.44
1:A:487:LEU:HG	1:A:524:THR:HG21	2.00	0.44
1:A:547:ILE:HA	1:A:550:ILE:HD13	2.00	0.44
2:F:93:LEU:HD23	2:F:93:LEU:HA	1.86	0.44
5:I:722:LYS:HG3	5:I:754:GLY:HA3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:464:CYS:SG	2:B:476:TRP:HB2	2.58	0.44
3:C:277:GLU:O	3:C:284:TYR:HA	2.18	0.44
1:A:561:LYS:HE2	1:A:587:SER:HB3	1.99	0.43
2:B:476:TRP:HD1	2:B:493:VAL:HG12	1.83	0.43
4:H:125:THR:HG22	4:H:166:ILE:HG12	2.00	0.43
2:B:446:ARG:O	4:H:86:VAL:HG23	2.18	0.43
2:B:587:SER:O	2:B:587:SER:OG	2.31	0.43
3:C:94:VAL:O	3:C:98:THR:OG1	2.28	0.43
5:I:661:CYS:SG	5:I:664:ASN:ND2	2.92	0.43
1:A:48:ARG:HB2	1:A:80:VAL:HG13	1.99	0.43
3:C:51:PRO:HA	3:C:278:LEU:O	2.18	0.43
2:B:447:ALA:HB3	2:B:476:TRP:HZ2	1.84	0.43
2:D:64:THR:OG1	2:D:66:PRO:HD2	2.18	0.43
5:I:250:ALA:O	5:I:254:SER:OG	2.31	0.43
2:E:111:LYS:O	2:E:115:VAL:HG13	2.18	0.43
1:A:571:GLN:OE1	1:A:571:GLN:N	2.51	0.43
2:B:399:VAL:O	2:B:689:TYR:HD2	2.01	0.43
5:I:424:TRP:HB3	5:I:744:ARG:HE	1.84	0.43
5:I:427:LYS:NZ	8:I:901:IHP:O33	2.43	0.43
5:I:486:GLU:O	5:I:490:LEU:HG	2.18	0.43
5:I:556:THR:HG22	5:I:558:LEU:H	1.84	0.43
1:A:427:MET:SD	1:A:443:LEU:HD23	2.59	0.43
1:A:572:ASP:HB3	1:A:575:VAL:HG12	2.00	0.43
4:H:72:GLU:OE2	4:H:145:ARG:NH1	2.51	0.43
5:I:177:LEU:HD11	5:I:230:VAL:HG21	2.01	0.43
1:A:524:THR:O	1:A:528:MET:HG3	2.19	0.43
4:H:156:LEU:HA	4:H:159:VAL:HG22	2.00	0.43
5:I:614:LEU:HD23	5:I:614:LEU:HA	1.86	0.43
5:I:724:LEU:HD23	5:I:724:LEU:HA	1.77	0.43
3:C:120:SER:O	3:C:124:THR:HG23	2.18	0.43
3:C:237:VAL:O	3:C:256:VAL:HA	2.19	0.43
5:I:599:TYR:HA	5:I:775:ILE:HD13	1.99	0.43
3:C:167:HIS:CE1	3:C:241:HIS:HA	2.53	0.43
1:A:517:THR:OG1	1:A:518:THR:N	2.52	0.42
4:H:47:ILE:HD13	4:H:57:ILE:HD13	2.01	0.42
2:B:420:LEU:HG	2:B:445:PHE:CD2	2.54	0.42
3:C:187:GLN:HB3	5:I:443:LYS:HZ1	1.82	0.42
1:A:29:LEU:HD12	1:A:29:LEU:HA	1.88	0.42
2:B:619:ARG:NH2	2:B:639:LEU:HA	2.33	0.42
3:C:131:ASP:OD1	3:C:131:ASP:N	2.51	0.42
3:C:211:ILE:HD13	3:C:211:ILE:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:69:LEU:HD21	2:G:72:ILE:HG21	2.01	0.42
2:F:84:ALA:O	2:F:87:GLU:HG3	2.19	0.42
5:I:547:ASP:HB2	5:I:570:HIS:HE1	1.84	0.42
1:A:99:VAL:HG21	1:A:104:VAL:HB	2.01	0.42
1:A:544:LEU:HD23	1:A:544:LEU:HA	1.87	0.42
3:C:39:LEU:HD12	3:C:149:LEU:HD11	2.01	0.42
3:C:42:GLU:O	3:C:185:ARG:NH1	2.52	0.42
3:C:239:ARG:NH2	3:C:241:HIS:HB3	2.35	0.42
3:C:248:TYR:HA	3:C:258:THR:O	2.19	0.42
3:C:283:LYS:HD2	3:C:283:LYS:HA	1.83	0.42
2:D:69:LEU:HA	2:D:69:LEU:HD22	1.65	0.42
2:G:96:ARG:HA	2:G:96:ARG:HD2	1.76	0.42
1:A:465:ASN:HA	1:A:468:LYS:HD2	2.02	0.42
2:B:562:HIS:HD2	2:B:626:ASN:HD22	1.68	0.42
5:I:291:TRP:CZ3	5:I:576:LYS:HE2	2.55	0.42
1:A:86:VAL:O	1:A:90:LEU:HD23	2.20	0.42
2:B:503:ASP:HB3	2:B:521:SER:HG	1.85	0.42
2:B:399:VAL:HG22	2:B:707:ALA:HA	2.02	0.42
2:B:501:HIS:CE1	2:B:505:VAL:HG22	2.53	0.42
2:E:65:ILE:O	2:E:69:LEU:HG	2.20	0.42
2:E:65:ILE:HG13	2:F:76:TRP:CD1	2.54	0.42
5:I:185:LEU:HD23	5:I:185:LEU:HA	1.82	0.42
3:C:76:PRO:HB3	3:C:107:TYR:CE1	2.55	0.42
2:D:119:LYS:HB2	2:D:119:LYS:HE3	1.81	0.42
4:H:75:ARG:CZ	4:H:145:ARG:HE	2.32	0.42
5:I:620:ASN:O	5:I:623:SER:OG	2.37	0.42
2:B:449:ILE:HB	2:B:470:ASP:OD2	2.20	0.42
2:D:63:TYR:CD1	2:D:68:ILE:HD11	2.54	0.42
2:E:85:HIS:O	2:E:89:GLU:HG2	2.19	0.42
4:H:149:LYS:HE2	4:H:149:LYS:HB2	1.88	0.42
5:I:802:VAL:O	5:I:803:LEU:HD23	2.19	0.42
2:D:126:LYS:HB3	2:D:126:LYS:HE2	1.83	0.42
2:F:87:GLU:OE1	2:F:90:ARG:NH2	2.53	0.42
2:G:97:ILE:HG13	2:G:98:ALA:N	2.35	0.42
2:G:114:LEU:O	2:G:118:ILE:HG12	2.20	0.42
1:A:535:ASN:ND2	3:C:77:ASP:O	2.53	0.41
5:I:70:PHE:CE2	5:I:72:TYR:HB2	2.54	0.41
3:C:87:VAL:CG1	3:C:97:VAL:HB	2.50	0.41
5:I:301:PHE:HA	5:I:304:LEU:HB2	2.01	0.41
1:A:580:GLN:O	1:A:584:THR:HG23	2.20	0.41
5:I:143:LYS:HE2	5:I:143:LYS:HB2	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:702:LEU:HD12	5:I:702:LEU:HA	1.78	0.41
1:A:136:ALA:HB1	1:A:144:ARG:HA	2.02	0.41
1:A:420:ARG:O	1:A:424:ILE:HG13	2.20	0.41
1:A:436:VAL:HG22	1:A:473:PHE:CD2	2.56	0.41
2:B:695:SER:O	5:I:803:LEU:HD12	2.21	0.41
5:I:547:ASP:N	5:I:547:ASP:OD2	2.53	0.41
1:A:398:ARG:O	1:A:401:SER:OG	2.30	0.41
1:A:502:LEU:HD23	1:A:539:ASN:HB3	2.02	0.41
2:B:541:TYR:HE2	2:B:580:SER:HA	1.85	0.41
2:B:680:HIS:CD2	2:B:704:GLY:HA3	2.56	0.41
4:H:84:LEU:HB2	4:H:181:TYR:CE2	2.55	0.41
5:I:549:LEU:HA	5:I:550:PRO:HD3	1.90	0.41
2:B:466:SER:O	2:B:473:ILE:HA	2.20	0.41
2:B:700:ILE:HG23	2:B:712:PHE:HD2	1.85	0.41
3:C:36:LYS:HB2	3:C:36:LYS:HE3	1.84	0.41
2:F:76:TRP:CZ2	2:G:75:GLU:HG2	2.56	0.41
5:I:240:GLU:OE1	5:I:240:GLU:N	2.54	0.41
2:B:518:LEU:HD13	2:B:553:VAL:HG12	2.01	0.41
3:C:159:VAL:HB	3:C:163:ILE:HB	2.03	0.41
4:H:76:GLN:O	4:H:80:GLU:HG3	2.21	0.41
4:H:204:ASP:HB2	5:I:128:ARG:CZ	2.51	0.41
1:A:37:THR:O	1:A:40:LEU:HG	2.21	0.41
1:A:439:PHE:HD2	1:A:443:LEU:HB2	1.86	0.41
3:C:160:ASP:O	3:C:162:GLN:HG2	2.21	0.41
1:A:59:ILE:HD12	1:A:69:LEU:HD13	2.03	0.41
1:A:102:THR:HA	1:A:105:ARG:CZ	2.51	0.41
1:A:424:ILE:HG12	1:A:450:TRP:CE3	2.56	0.41
1:A:477:TRP:O	1:A:481:THR:OG1	2.31	0.41
2:B:646:ALA:HB3	2:B:655:MET:HB2	2.02	0.41
3:C:83:MET:SD	3:C:165:CYS:HB3	2.61	0.41
5:I:76:ASP:OD1	5:I:77:LYS:HG2	2.21	0.41
5:I:177:LEU:HD23	5:I:177:LEU:HA	1.77	0.41
5:I:302:GLU:OE1	5:I:302:GLU:N	2.50	0.41
4:H:97:CYS:HA	4:H:173:HIS:HD2	1.84	0.41
5:I:105:PHE:HD1	5:I:125:HIS:NE2	2.19	0.41
5:I:604:LEU:HD12	5:I:604:LEU:HA	1.82	0.41
5:I:699:LYS:HZ3	5:I:728:TRP:HE1	1.68	0.41
2:B:410:VAL:HG21	2:B:481:PRO:HG3	2.02	0.40
2:B:708:LEU:HD12	2:B:708:LEU:HA	1.94	0.40
2:F:96:ARG:HH21	2:F:99:PHE:HE2	1.69	0.40
3:C:56:GLY:N	3:C:261:SER:OG	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:69:LEU:HD22	2:F:69:LEU:HD22	2.03	0.40
4:H:37:LEU:HD21	4:H:146:VAL:HG12	2.03	0.40
4:H:80:GLU:O	4:H:181:TYR:OH	2.29	0.40
5:I:100:CYS:SG	5:I:143:LYS:NZ	2.70	0.40
2:B:551:THR:OG1	2:B:552:SER:N	2.55	0.40
3:C:89:ARG:HD3	3:C:265:TYR:OH	2.22	0.40
2:E:114:LEU:O	2:E:118:ILE:HG13	2.22	0.40
4:H:120:PRO:HD2	4:H:123:ASP:OD2	2.21	0.40
5:I:174:PHE:HD1	5:I:244:MET:HG2	1.86	0.40
1:A:533:VAL:HB	1:A:536:VAL:HG23	2.02	0.40
2:B:397:ASP:OD1	2:B:416:GLU:HB2	2.21	0.40
5:I:113:LYS:HE2	5:I:113:LYS:HB3	1.83	0.40
5:I:117:LEU:HD22	5:I:121:GLN:HG2	2.04	0.40
5:I:220:LEU:O	5:I:221:ASN:C	2.59	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	540/589 (92%)	515 (95%)	24 (4%)	1 (0%)	47	77
2	B	288/713 (40%)	258 (90%)	30 (10%)	0	100	100
2	D	72/713 (10%)	72 (100%)	0	0	100	100
2	E	64/713 (9%)	64 (100%)	0	0	100	100
2	F	60/713 (8%)	60 (100%)	0	0	100	100
2	G	58/713 (8%)	58 (100%)	0	0	100	100
3	C	291/309 (94%)	263 (90%)	28 (10%)	0	100	100
4	H	169/225 (75%)	159 (94%)	10 (6%)	0	100	100
5	I	579/837 (69%)	544 (94%)	35 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2121/5525 (38%)	1993 (94%)	127 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	240/512 (47%)	224 (93%)	16 (7%)	16	45
2	B	255/589 (43%)	238 (93%)	17 (7%)	16	45
2	D	59/589 (10%)	52 (88%)	7 (12%)	5	21
2	E	55/589 (9%)	50 (91%)	5 (9%)	9	31
2	F	47/589 (8%)	40 (85%)	7 (15%)	3	13
2	G	37/589 (6%)	35 (95%)	2 (5%)	22	53
3	C	258/274 (94%)	245 (95%)	13 (5%)	24	55
4	H	153/202 (76%)	147 (96%)	6 (4%)	32	62
5	I	522/739 (71%)	503 (96%)	19 (4%)	35	63
All	All	1626/4672 (35%)	1534 (94%)	92 (6%)	24	51

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	76	PHE
1	A	79	LEU
1	A	400	LEU
1	A	414	ASP
1	A	426	TYR
1	A	439	PHE

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Mol	Chain	Res	Type
1	A	466	LEU
1	A	467	LYS
1	A	471	GLU
1	A	487	LEU
1	A	492	ASP
1	A	527	ARG
1	A	552	ASP
1	A	553	ASN
1	A	564	LEU
2	B	404	PHE
2	B	418	HIS
2	B	422	LEU
2	B	477	ASN
2	B	480	SER
2	B	520	CYS
2	B	521	SER
2	B	555	PHE
2	B	559	ASP
2	B	576	ASP
2	B	604	VAL
2	B	628	THR
2	B	635	MET
2	B	643	THR
2	B	667	ASN
2	B	693	PHE
2	B	712	PHE
3	C	40	THR
3	C	50	CYS
3	C	52	VAL
3	C	57	ASP
3	C	88	ASP
3	C	117	ASN
3	C	141	ASN
3	C	160	ASP
3	C	170	LEU
3	C	188	GLU
3	C	223	ASP
3	C	244	VAL
3	C	282	LEU
2	D	64	THR
2	D	69	LEU
2	D	73	GLN

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Mol	Chain	Res	Type
2	D	74	HIS
2	D	81	MET
2	D	113	ASP
2	D	117	ARG
2	E	64	THR
2	E	76	TRP
2	E	78	ARG
2	E	83	ARG
2	E	112	LYS
2	F	64	THR
2	F	65	ILE
2	F	76	TRP
2	F	83	ARG
2	F	99	PHE
2	F	100	LEU
2	F	113	ASP
2	G	70	HIS
2	G	99	PHE
4	H	13	ASN
4	H	36	THR
4	H	42	TYR
4	H	119	CYS
4	H	185	THR
4	H	190	ARG
5	I	74	ASP
5	I	78	TRP
5	I	113	LYS
5	I	115	THR
5	I	119	THR
5	I	155	THR
5	I	168	TRP
5	I	215	ASP
5	I	258	ASN
5	I	280	HIS
5	I	310	GLU
5	I	455	THR
5	I	456	VAL
5	I	476	THR
5	I	545	LEU
5	I	547	ASP
5	I	719	VAL
5	I	735	THR

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Mol	Chain	Res	Type
5	I	737	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	433	GLN
1	A	535	ASN
2	B	477	ASN
2	B	501	HIS
2	B	562	HIS
2	B	568	ASN
2	B	599	HIS
2	B	616	HIS
2	B	694	HIS
3	C	79	ASN
3	C	118	HIS
3	C	249	ASN
2	D	70	HIS
2	E	101	GLN
2	F	74	HIS
4	H	13	ASN
4	H	82	ASN
4	H	89	GLN
4	H	173	HIS
4	H	205	ASN
5	I	305	GLN
5	I	570	HIS
5	I	629	ASN
5	I	664	ASN
5	I	720	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	$\# Z > 2$
8	IHP	I	901	-	36,36,36	1.38	6 (16%)	54,60,60	1.20	5 (9%)

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
8	IHP	I	901	-	-	5/30/54/54	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	901	IHP	P3-O13	3.30	1.65	1.59
8	I	901	IHP	P1-O11	2.93	1.64	1.59
8	I	901	IHP	P6-O16	2.61	1.64	1.59
8	I	901	IHP	P5-O15	2.47	1.64	1.59
8	I	901	IHP	P4-O14	2.37	1.63	1.59
8	I	901	IHP	P2-O12	2.01	1.63	1.59

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	901	IHP	C6-C5-C4	4.11	119.41	110.41
8	I	901	IHP	C5-C6-C1	3.63	118.36	110.41
8	I	901	IHP	C5-C4-C3	3.40	117.85	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	901	IHP	C3-C2-C1	2.52	115.92	110.41
8	I	901	IHP	O13-C3-C4	2.29	114.08	108.69

There are no chirality outliers.

All (5) torsion outliers are listed below:

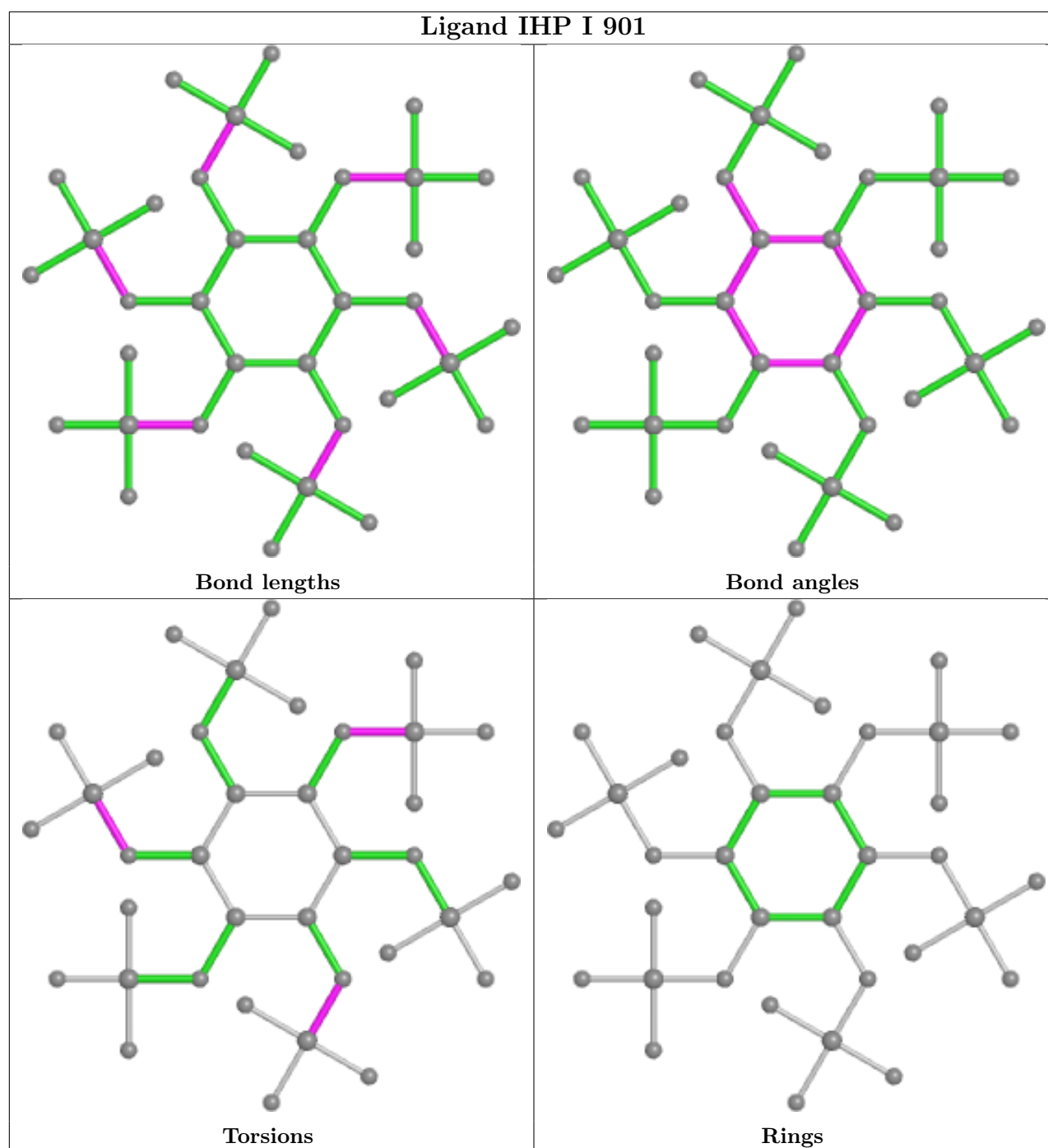
Mol	Chain	Res	Type	Atoms
8	I	901	IHP	C2-O12-P2-O42
8	I	901	IHP	C6-O16-P6-O36
8	I	901	IHP	C4-O14-P4-O44
8	I	901	IHP	C4-O14-P4-O34
8	I	901	IHP	C6-O16-P6-O46

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	I	901	IHP	5	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 than 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.



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.

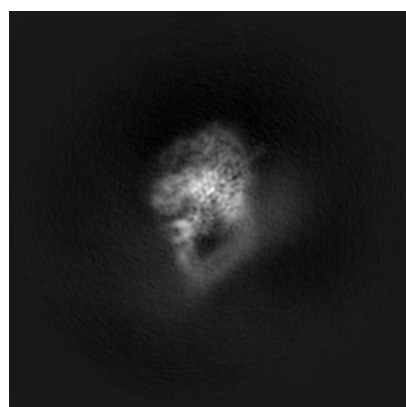
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22650. These allow visual inspection of the internal detail of the map and identification of artifacts.

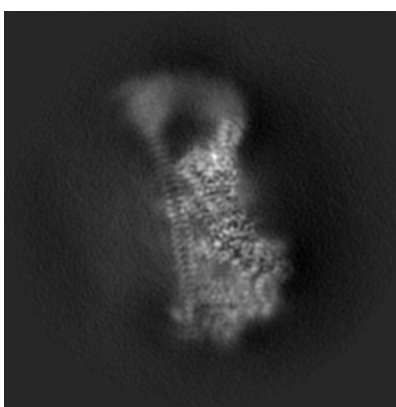
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

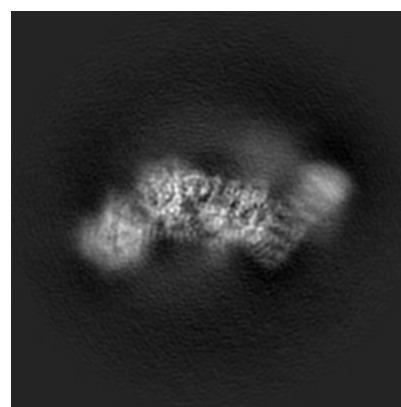
6.1.1 Primary map



X



Y

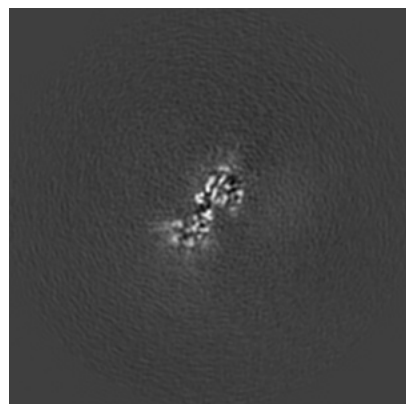


Z

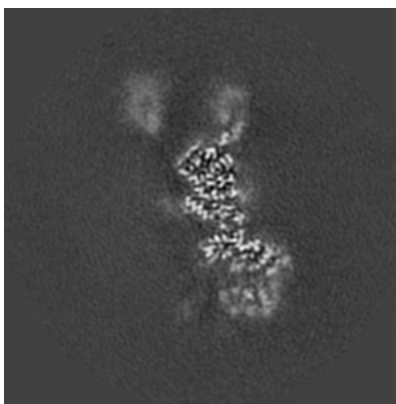
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

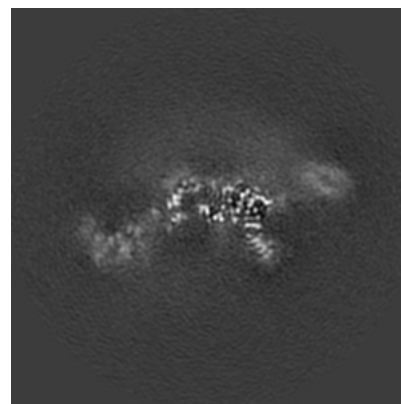
6.2.1 Primary map



X Index: 180



Y Index: 180

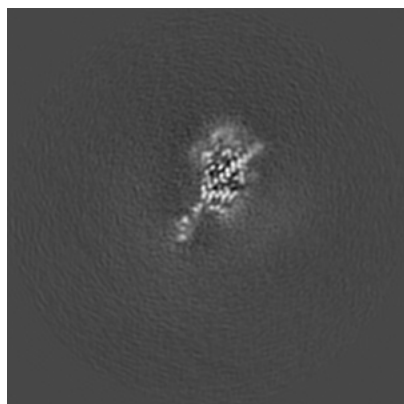


Z Index: 180

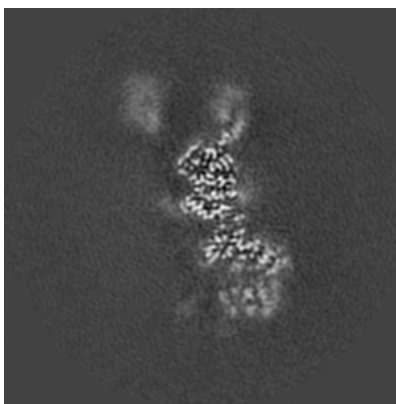
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

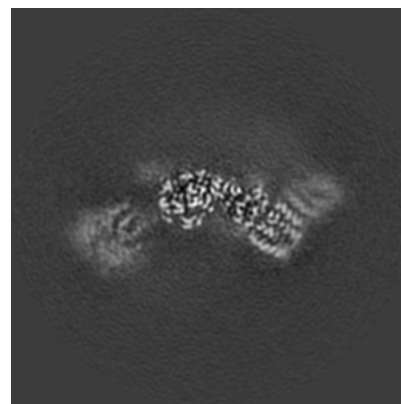
6.3.1 Primary map



X Index: 149



Y Index: 179

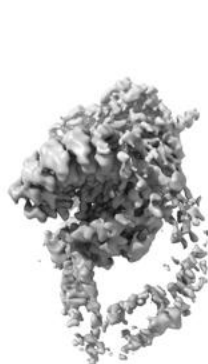


Z Index: 199

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

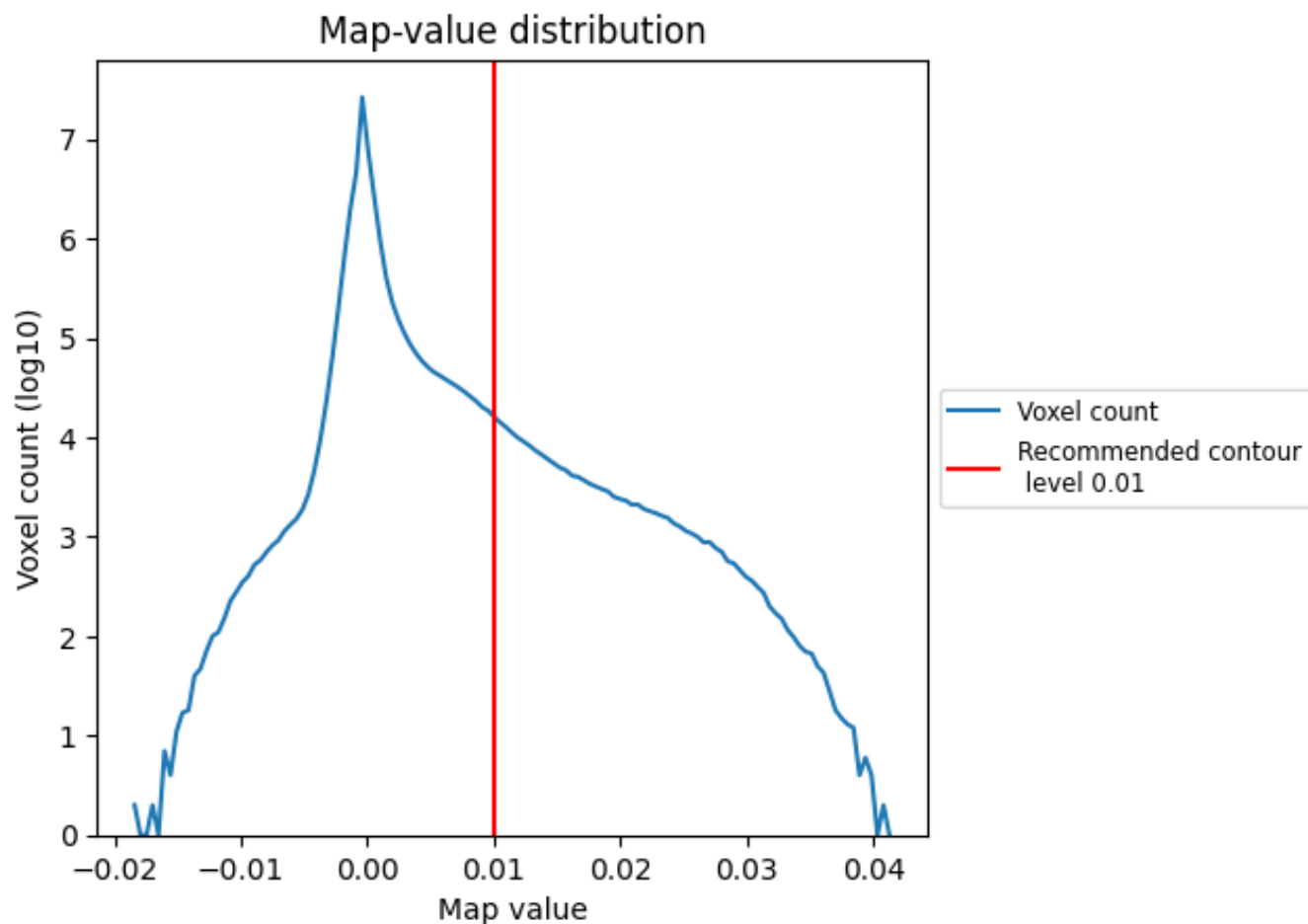
6.5 Mask visualisation

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

7 Map analysis [i](#)

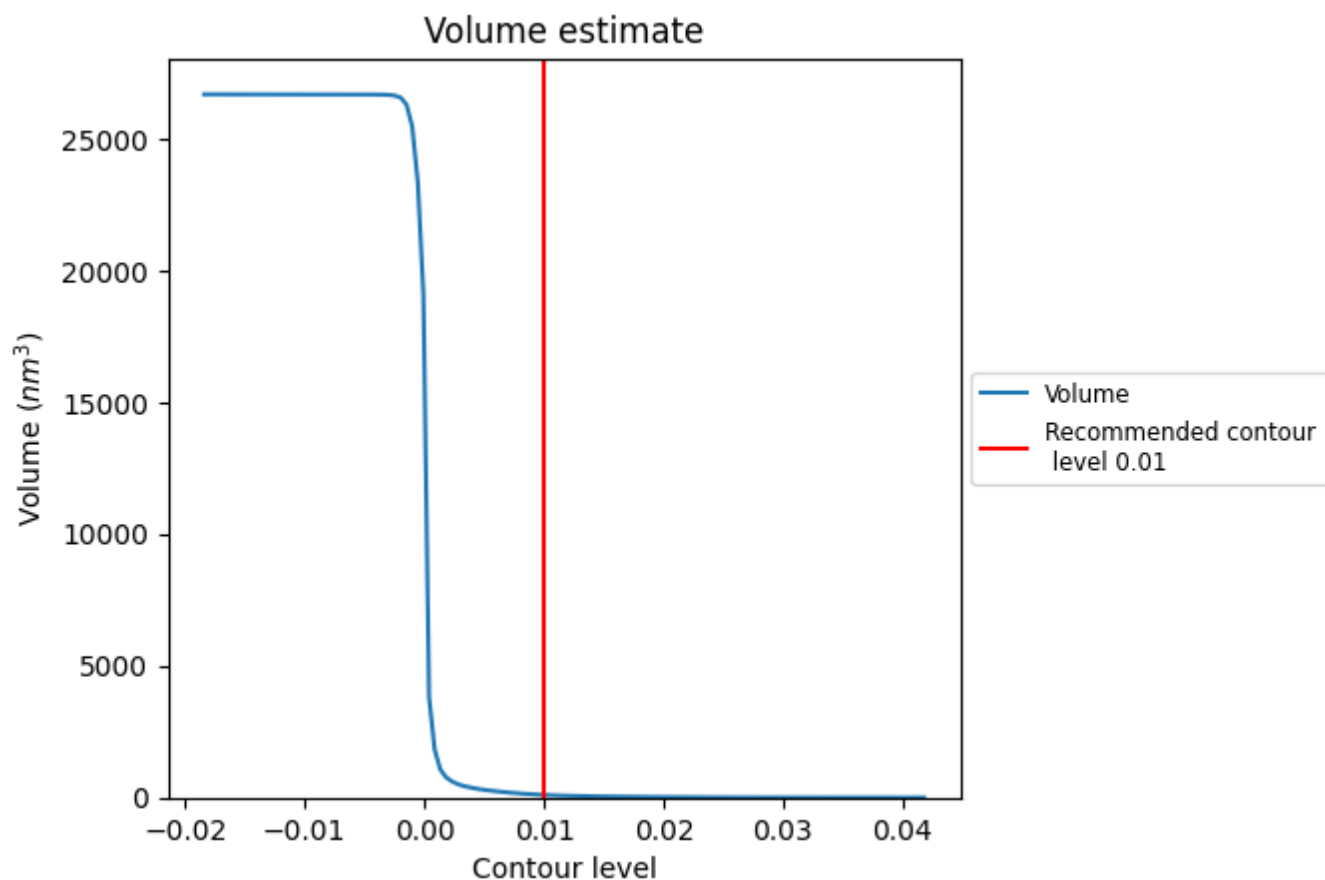
This section contains the results of statistical analysis of the map.

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.

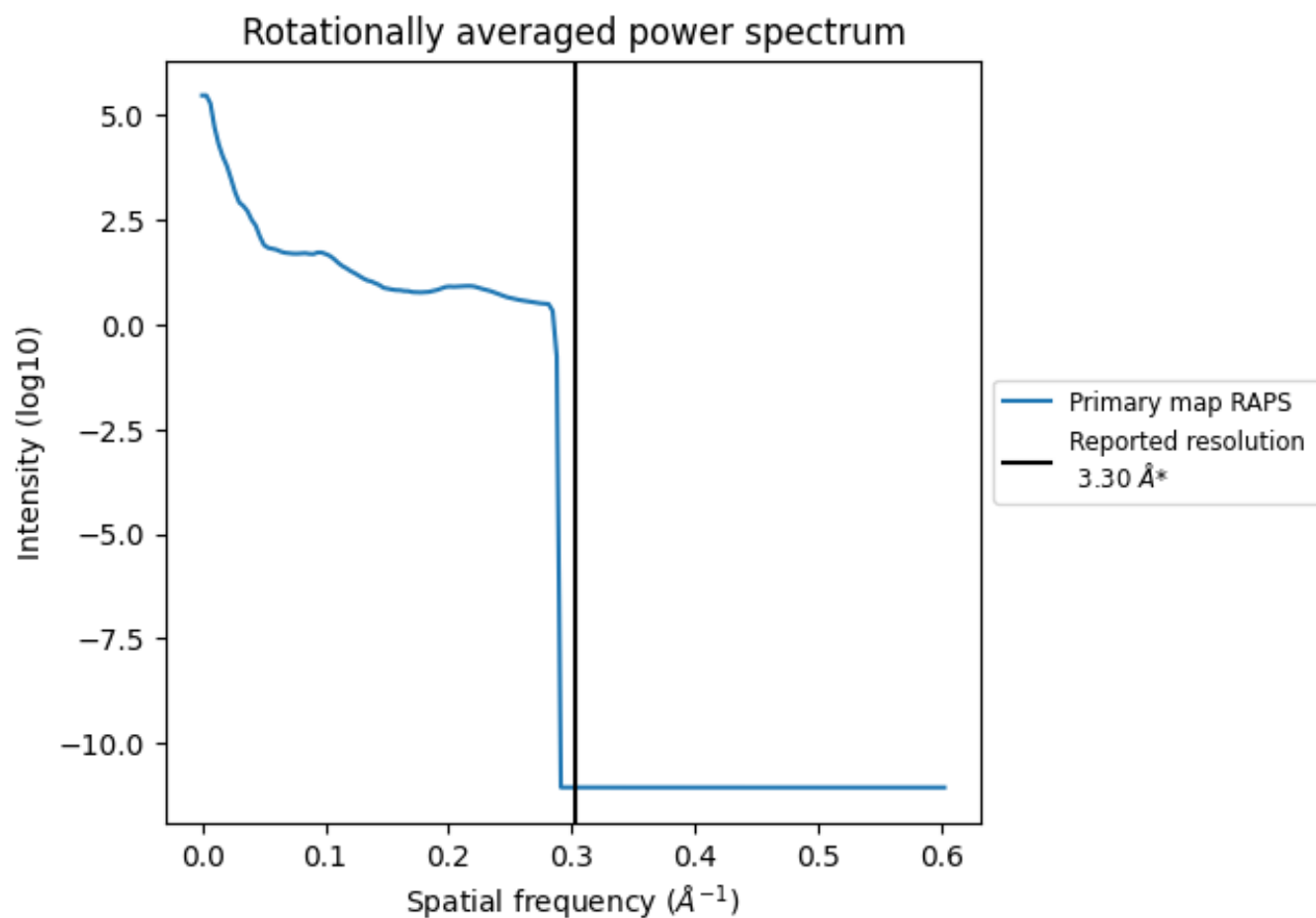
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 100 nm^3 ; this corresponds to an approximate mass of 90 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

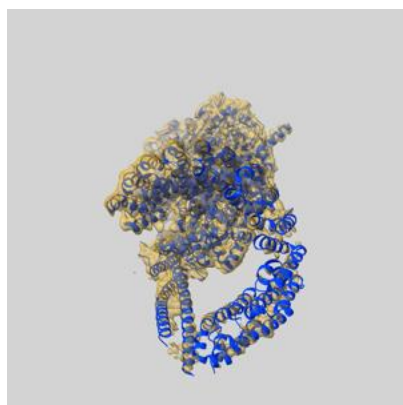
8 Fourier-Shell correlation ⓘ

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

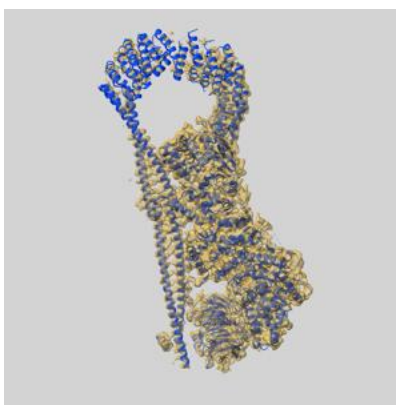
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22650 and PDB model 7K36. Per-residue inclusion information can be found in section [3](#) on page [6](#).

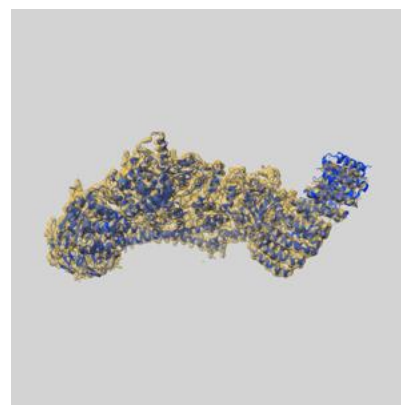
9.1 Map-model overlay [i](#)



X



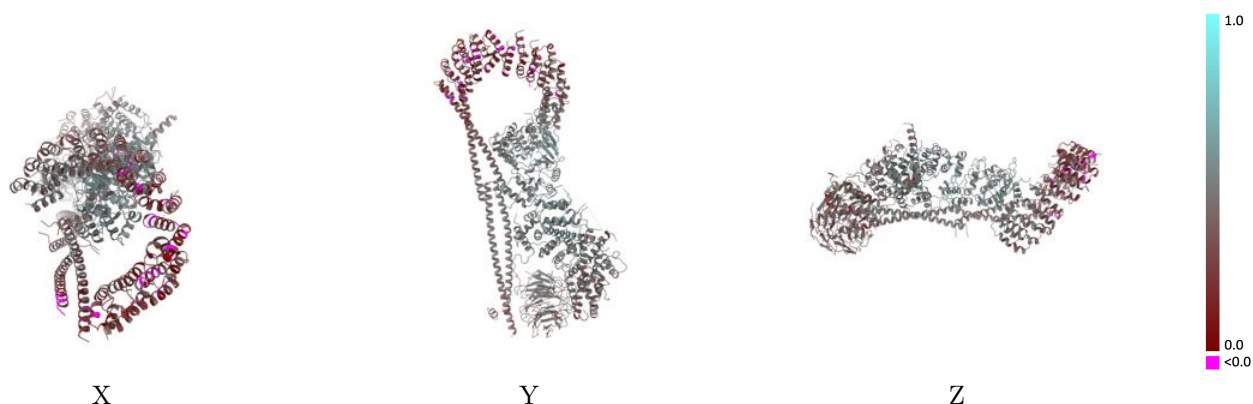
Y



Z

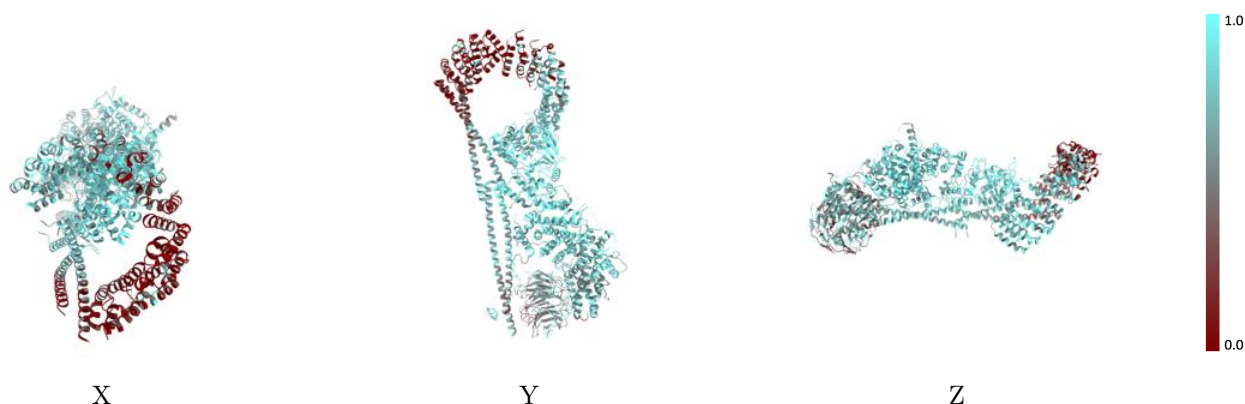
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



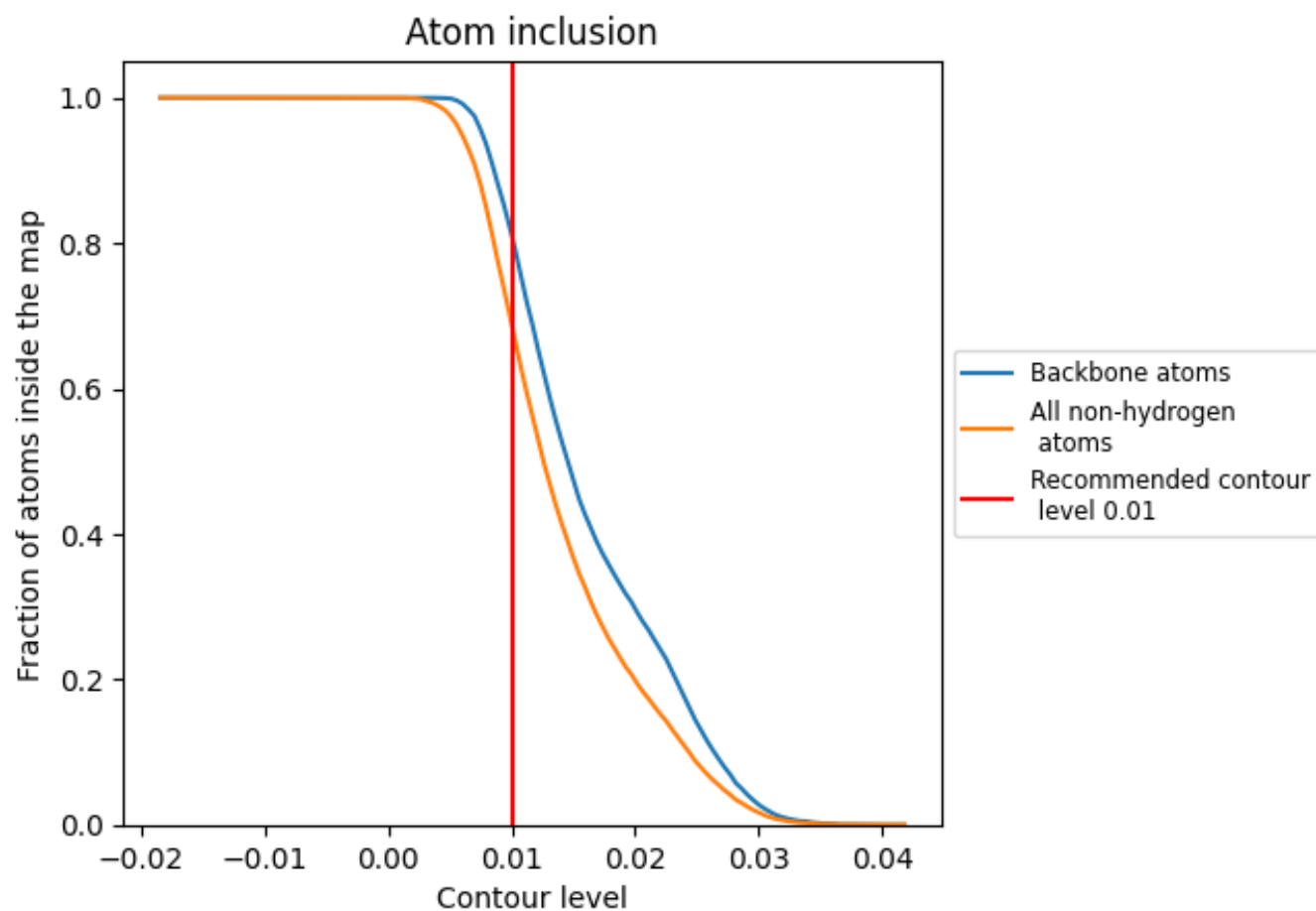
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 69% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6878	<div></div> 0.4300
A	<div></div> 0.4694	<div></div> 0.3250
B	<div></div> 0.5882	<div></div> 0.4170
C	<div></div> 0.8727	<div></div> 0.5170
D	<div></div> 0.6883	<div></div> 0.4200
E	<div></div> 0.7188	<div></div> 0.4350
F	<div></div> 0.5598	<div></div> 0.3450
G	<div></div> 0.5438	<div></div> 0.3310
H	<div></div> 0.6562	<div></div> 0.3900
I	<div></div> 0.8375	<div></div> 0.4990

1.0

0.0

<0.0