



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 03:09 AM EDT

PDB ID : 7T3B / pdb_00007t3b
EMDB ID : EMD-25653
Title : GATOR1-RAG-RAGULATOR - GAP Complex
Authors : Egri, S.B.; Shen, K.
Deposited on : 2021-12-07
Resolution : 3.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
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

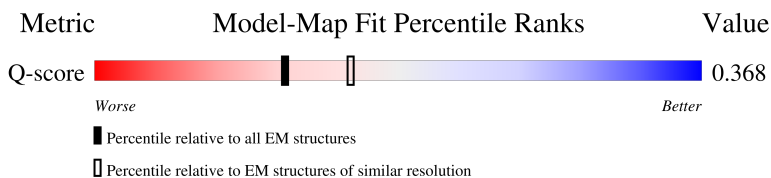
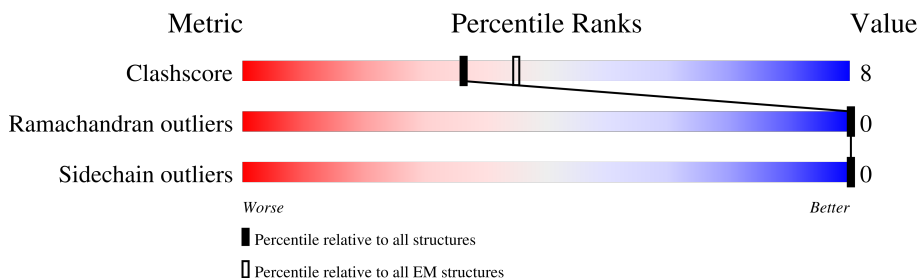
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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	8855 (3.40 - 4.40)

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	E	399	 59% 17% 24%
2	B	380	 72% 23% 5%
3	A	1603	 51% 10% 38%
4	H	124	 76% 21% .

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Mol	Chain	Length	Quality of chain
5	G	125	
6	J	91	
7	I	99	
8	F	161	
9	C	569	
10	D	313	

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
12	AF3	D	601	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 23294 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 Ras-related GTP-binding protein C.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	305	Total	C	N	O	S	0	0
			2464	1585	397	468	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	92	ALA	PHE	engineered mutation	UNP Q9HB90

- Molecule 2 is a protein called GATOR complex protein NPRL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	362	Total	C	N	O	S	0	0
			2918	1868	486	546	18		

- Molecule 3 is a protein called GATOR complex protein DEPDC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	989	Total	C	N	O	S	0	0
			8104	5231	1345	1483	45		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	775	ALA	TYR	engineered mutation	UNP O75140

- Molecule 4 is a protein called Regulator complex protein LAMTOR3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	120	Total	C	N	O	S	0	0
			934	601	157	175	1		

- Molecule 5 is a protein called Regulator complex protein LAMTOR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	124	Total	C	N	O	S	0	0
			936	588	161	181	6		

- Molecule 6 is a protein called Regulator complex protein LAMTOR5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	91	Total	C	N	O	S	1	0
			672	409	116	139	8		

- Molecule 7 is a protein called Regulator complex protein LAMTOR4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	89	Total	C	N	O	S	0	0
			678	424	124	128	2		

- Molecule 8 is a protein called Regulator complex protein LAMTOR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	111	Total	C	N	O	S	0	0
			861	541	148	170	2		

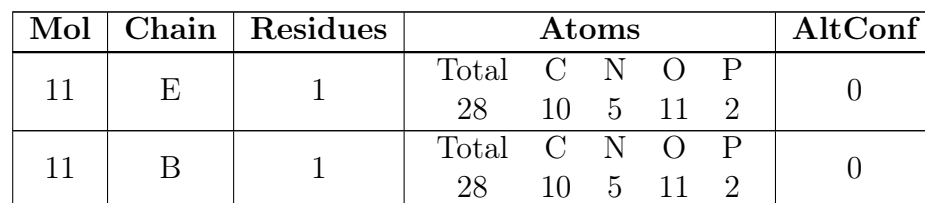
- Molecule 9 is a protein called GATOR complex protein NPRL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	405	Total	C	N	O	S	0	0
			3234	2081	567	567	19		

- Molecule 10 is a protein called Ras-related GTP-binding protein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	296	Total	C	N	O	S	0	0
			2429	1543	423	446	17		

- Molecule 11 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂) (labeled as "Ligand of Interest" by depositor).



- AF3
-
- The diagram illustrates the AF3 molecule. A central Aluminum (Al) atom is shown with a +3 charge. It is bonded to three Fluorine (F) atoms, each with a -1 charge. The bonds are labeled F1, F2, and F3. The central Al atom is labeled Al^{+3} . The Fluorine atoms are labeled F^- . The bonds are represented by lines connecting the central Al atom to each F atom.

Mol	Chain	Residues	Atoms			AltConf
12	E	1	Total 4	Al 1	F 3	0



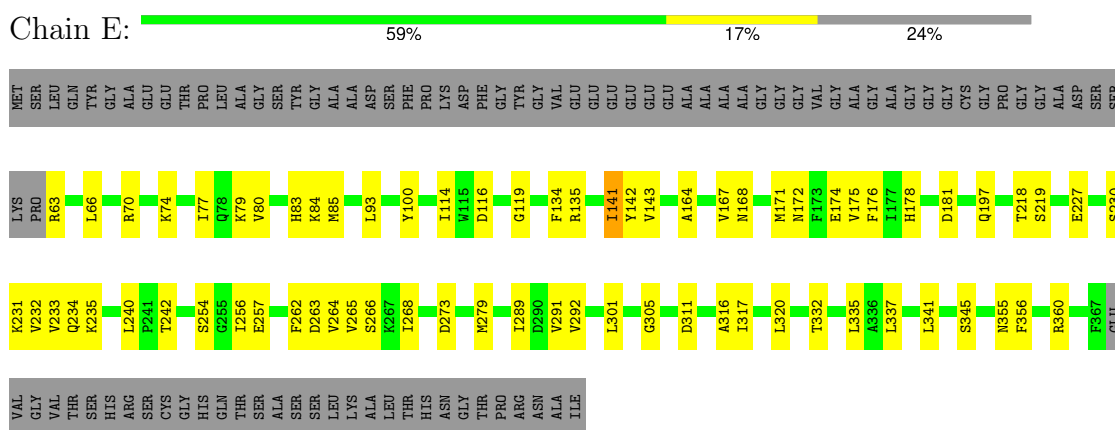
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Mol	Chain	Residues	Atoms			AltConf
			Total	Al	F	
12	D	1	4	1	3	0

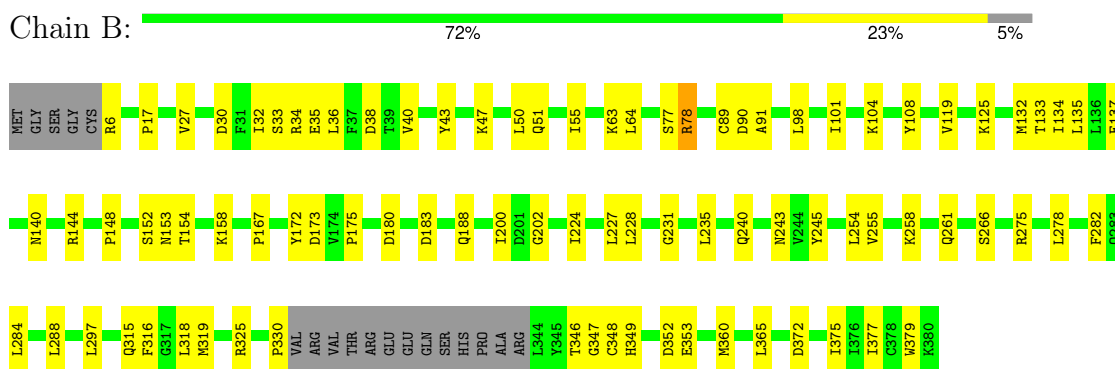
3 Residue-property plots

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.

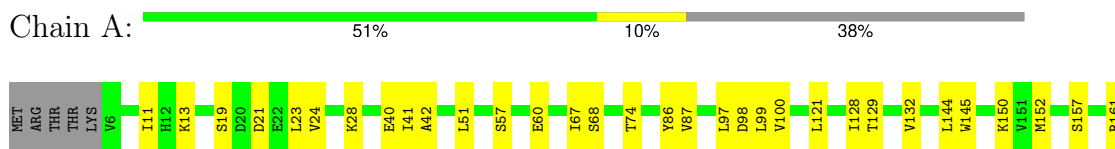
• Molecule 1: Ras-related GTP-binding protein C



• Molecule 2: GATOR complex protein NPRL2



• Molecule 3: GATOR complex protein DEPDC5



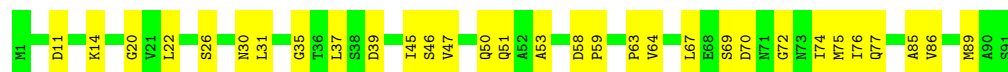
- Molecule 5: Regulator complex protein LAMTOR2

Chain G:  77% 22%



- Molecule 6: Regulator complex protein LAMTOR5

Chain J:  66% 34%



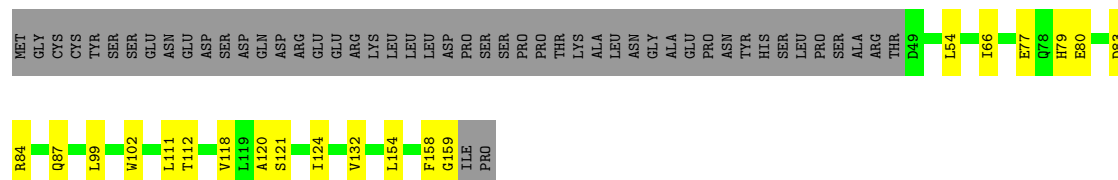
- Molecule 7: Regulator complex protein LAMTOR4

Chain I:  68% 22% 10%



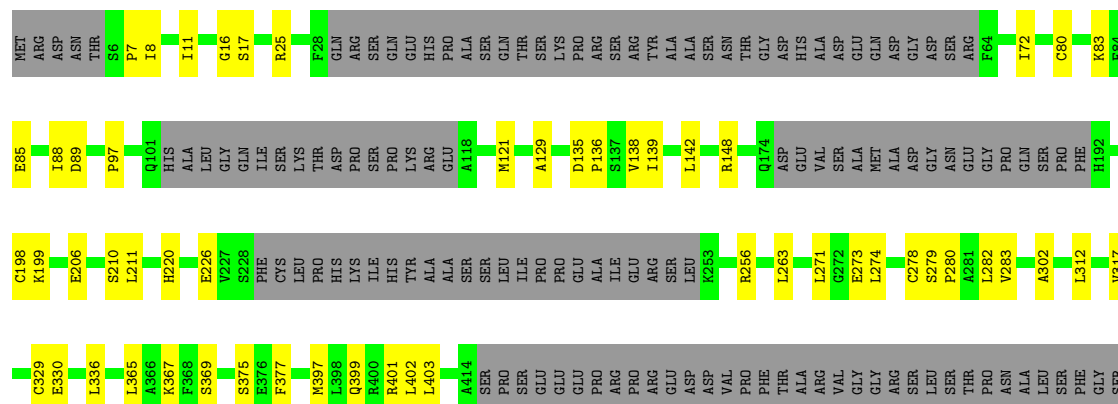
- Molecule 8: Regulator complex protein LAMTOR1

Chain F:  57% 12% 31%



- Molecule 9: GATOR complex protein NPRL3

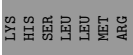
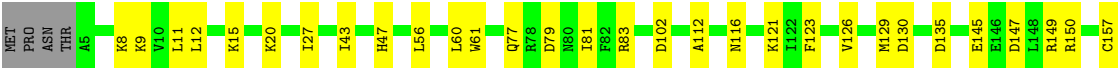
Chain C:  60% 11% 29%





● Molecule 10: Ras-related GTP-binding protein A

Chain D: 75% 19% 5%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	139231	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 ($e^-/\text{\AA}^2$)	54.2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.081	Depositor
Minimum map value	-0.497	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.092	Depositor
Recommended contour level	0.21	Depositor
Map size (Å)	315.4, 315.4, 315.4	wwPDB
Map dimensions	380, 380, 380	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: AF3, GDP

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	E	0.25	0/2515	0.65	0/3396
2	B	0.24	0/2977	0.64	5/4034 (0.1%)
3	A	0.23	0/8320	0.53	1/11283 (0.0%)
4	H	0.23	0/951	0.53	0/1290
5	G	0.25	0/947	0.66	0/1283
6	J	0.22	0/678	0.62	0/919
7	I	0.20	0/686	0.58	0/926
8	F	0.20	0/877	0.55	0/1192
9	C	0.20	0/3298	0.54	4/4472 (0.1%)
10	D	0.27	0/2474	0.66	0/3331
All	All	0.23	0/23723	0.58	10/32126 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	2
2	B	0	1
All	All	0	3

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	226	GLU	CA-CB-CG	5.55	125.20	114.10
9	C	88	ILE	N-CA-C	-5.53	104.03	110.05
9	C	302	ALA	CA-C-N	5.41	130.08	122.46
9	C	302	ALA	C-N-CA	5.41	130.08	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	78	ARG	CB-CG-CD	5.40	123.71	111.30
2	B	17	PRO	CA-C-N	5.28	131.63	121.54
2	B	17	PRO	C-N-CA	5.28	131.63	121.54
2	B	30	ASP	CA-C-N	5.09	129.56	122.08
2	B	30	ASP	C-N-CA	5.09	129.56	122.08
3	A	266	GLU	CA-CB-CG	5.04	124.19	114.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	200	ILE	Peptide
1	E	141	ILE	Peptide
1	E	66	LEU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2464	0	2436	49	0
2	B	2918	0	2945	47	0
3	A	8104	0	7881	99	0
4	H	934	0	958	18	0
5	G	936	0	943	20	0
6	J	672	0	670	21	0
7	I	678	0	689	31	0
8	F	861	0	858	36	0
9	C	3234	0	3331	36	0
10	D	2429	0	2426	45	0
11	B	28	0	12	1	0
11	E	28	0	12	1	0
12	D	4	0	0	2	0
12	E	4	0	0	1	0
All	All	23294	0	23161	358	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 8.

All (358) 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)
7:I:61:VAL:CG1	8:F:111:LEU:HD22	1.81	1.09
7:I:61:VAL:CG1	8:F:111:LEU:HD13	1.87	1.03
7:I:61:VAL:HG11	8:F:111:LEU:HD22	1.47	0.97
7:I:61:VAL:HG13	8:F:111:LEU:HD13	1.43	0.97
7:I:61:VAL:HG13	8:F:111:LEU:CD1	1.93	0.96
7:I:61:VAL:CG2	8:F:111:LEU:HD22	1.98	0.92
3:A:1464:THR:O	3:A:1468:ARG:HB2	1.75	0.87
7:I:61:VAL:CG1	8:F:111:LEU:CD2	2.56	0.82
7:I:61:VAL:CG2	8:F:111:LEU:CD2	2.63	0.76
3:A:277:LEU:O	3:A:281:TYR:HB2	1.89	0.72
7:I:61:VAL:HG21	8:F:111:LEU:HD22	1.68	0.72
7:I:61:VAL:CG1	8:F:111:LEU:CD1	2.60	0.71
1:E:256:ILE:HG13	1:E:341:LEU:HB3	1.73	0.70
1:E:79:LYS:O	1:E:83:HIS:HB2	1.91	0.70
7:I:61:VAL:HG13	8:F:111:LEU:CD2	2.21	0.68
5:G:72:ILE:HB	5:G:83:ILE:HB	1.77	0.66
3:A:242:ILE:HD11	3:A:249:ARG:HB2	1.80	0.64
7:I:61:VAL:HG11	8:F:111:LEU:CD2	2.25	0.64
4:H:59:GLN:HG2	8:F:66:ILE:HD13	1.81	0.63
7:I:61:VAL:CB	8:F:111:LEU:HD22	2.28	0.63
6:J:45:ILE:HG23	6:J:76:ILE:HG23	1.80	0.62
9:C:274:LEU:HD13	9:C:283:VAL:HG12	1.80	0.62
7:I:61:VAL:HG22	8:F:111:LEU:CD2	2.29	0.61
3:A:215:GLU:OE2	3:A:263:ARG:NH2	2.33	0.61
10:D:47:HIS:HA	10:D:60:LEU:O	1.99	0.61
3:A:372:GLN:HG2	3:A:377:VAL:HG11	1.82	0.61
6:J:47:VAL:O	6:J:51:GLN:HB2	2.01	0.60
3:A:1427:PRO:HB3	3:A:1434:PRO:HA	1.84	0.60
4:H:72:ILE:HB	5:G:73:LEU:HB2	1.84	0.59
3:A:219:VAL:HG12	3:A:257:VAL:HG12	1.83	0.59
2:B:266:SER:HA	2:B:275:ARG:HH12	1.68	0.58
10:D:266:PHE:HB3	10:D:270:THR:HG23	1.84	0.58
3:A:1201:SER:HG	3:A:1204:CYS:HG	1.51	0.58
2:B:325:ARG:NH1	2:B:352:ASP:OD2	2.37	0.57
3:A:128:ILE:HG13	3:A:129:THR:HG23	1.86	0.57
3:A:960:THR:HA	3:A:1571:ARG:HH22	1.69	0.57
6:J:75:MET:HG3	8:F:132:VAL:HG11	1.85	0.57
10:D:123:PHE:HA	10:D:157:CYS:HB2	1.85	0.57
7:I:65:ARG:NH1	8:F:118:VAL:O	2.36	0.57
1:E:135:ARG:HH22	1:E:167:VAL:HB	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:ASP:O	2:B:183:ASP:HB2	2.04	0.57
6:J:53:ALA:HA	6:J:63:PRO:HG2	1.87	0.57
1:E:142:TYR:O	1:E:175:VAL:HA	2.04	0.57
3:A:1313:LEU:HD12	3:A:1317:PRO:HG3	1.86	0.57
9:C:397:MET:HE2	9:C:402:LEU:HB2	1.85	0.57
2:B:77:SER:OG	2:B:78:ARG:N	2.38	0.56
6:J:75:MET:HE1	8:F:124:ILE:HG12	1.88	0.56
3:A:28:LYS:HE3	3:A:60:GLU:HB2	1.86	0.56
4:H:47:PRO:O	4:H:51:SER:HB3	2.05	0.56
10:D:203:VAL:HG22	10:D:274:VAL:HG12	1.87	0.56
2:B:89:CYS:SG	2:B:90:ASP:N	2.79	0.56
4:H:6:LYS:HE2	4:H:35:VAL:HG23	1.88	0.56
9:C:504:ALA:HB1	9:C:510:LEU:HD12	1.87	0.56
8:F:99:LEU:HD11	8:F:102:TRP:HB2	1.87	0.55
3:A:948:LEU:HB3	3:A:1384:PHE:HB3	1.88	0.55
4:H:99:ASN:ND2	6:J:46:SER:OG	2.38	0.55
3:A:786:ARG:HE	3:A:928:ALA:HB3	1.70	0.55
3:A:99:LEU:HB3	3:A:145:TRP:HB2	1.88	0.55
3:A:177:MET:HB2	3:A:222:SER:HB3	1.87	0.55
2:B:202:GLY:O	2:B:315:GLN:NE2	2.40	0.55
3:A:41:ILE:HG12	3:A:87:VAL:HG22	1.88	0.55
1:E:316:ALA:HA	10:D:253:GLU:O	2.07	0.55
10:D:251:SER:HA	10:D:263:ILE:O	2.07	0.55
3:A:97:LEU:HD11	3:A:144:LEU:HB3	1.89	0.55
5:G:80:ARG:NH1	5:G:99:VAL:O	2.39	0.55
3:A:340:VAL:HG13	3:A:373:PRO:HG3	1.88	0.54
7:I:61:VAL:HG21	8:F:111:LEU:CD2	2.33	0.54
3:A:152:MET:SD	3:A:152:MET:N	2.80	0.54
2:B:346:THR:OG1	2:B:347:GLY:N	2.40	0.54
3:A:771:THR:HG23	3:A:878:LYS:HG2	1.90	0.54
6:J:75:MET:O	6:J:85:ALA:HA	2.08	0.54
9:C:263:LEU:O	9:C:399:GLN:NE2	2.41	0.54
1:E:100:TYR:HB3	1:E:116:ASP:HB3	1.90	0.54
2:B:227:LEU:O	2:B:231:GLY:N	2.36	0.54
4:H:34:LYS:HE3	4:H:45:LEU:HB3	1.89	0.54
1:E:141:ILE:HG12	1:E:174:GLU:HB2	1.90	0.53
2:B:43:TYR:HB3	2:B:55:ILE:HG21	1.89	0.53
2:B:27:VAL:HG13	2:B:133:THR:HG22	1.90	0.53
7:I:19:LEU:HB2	7:I:33:LEU:HD13	1.90	0.53
2:B:188:GLN:HB3	3:A:423:ILE:HG21	1.90	0.53
6:J:30:ASN:ND2	6:J:39:ASP:OD1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:8:GLY:O	7:I:11:ARG:HB2	2.09	0.53
1:E:63:ARG:HH21	1:E:233:VAL:HA	1.73	0.53
1:E:141:ILE:HA	1:E:174:GLU:O	2.08	0.53
2:B:132:MET:HA	2:B:135:LEU:HB2	1.91	0.53
1:E:254:SER:OG	1:E:355:ASN:ND2	2.42	0.53
3:A:324:ARG:NH2	3:A:328:ARG:O	2.42	0.53
4:H:112:PRO:HB2	8:F:102:TRP:HZ2	1.74	0.53
1:E:74:LYS:NZ	1:E:116:ASP:OD1	2.41	0.52
2:B:379:TRP:HB2	9:C:369:SER:HB2	1.92	0.52
3:A:1256:TYR:OH	3:A:1352:ARG:NH2	2.42	0.52
2:B:119:VAL:O	2:B:125:LYS:NZ	2.41	0.52
3:A:165:ARG:HA	3:A:751:ALA:HA	1.90	0.52
3:A:213:SER:O	3:A:328:ARG:NH1	2.42	0.52
3:A:263:ARG:NH1	3:A:327:ASP:OD2	2.37	0.52
9:C:282:LEU:HD13	9:C:312:LEU:HD22	1.90	0.52
3:A:301:SER:HB3	3:A:344:GLU:HG3	1.92	0.52
3:A:24:VAL:HB	3:A:68:SER:HB3	1.92	0.52
7:I:21:LEU:HD13	7:I:43:ILE:HD13	1.92	0.52
2:B:33:SER:OG	2:B:34:ARG:N	2.41	0.52
9:C:401:ARG:NH2	9:C:564:PHE:O	2.43	0.52
4:H:24:VAL:O	4:H:32:VAL:N	2.42	0.52
5:G:118:PRO:HG2	8:F:154:LEU:HD12	1.92	0.52
2:B:32:ILE:HA	2:B:36:LEU:HD22	1.92	0.52
2:B:47:LYS:O	2:B:51:GLN:NE2	2.42	0.52
3:A:41:ILE:HD11	3:A:67:ILE:HD13	1.92	0.51
10:D:145:GLU:OE2	10:D:149:ARG:NH2	2.43	0.51
1:E:171:MET:HE3	1:E:172:ASN:H	1.74	0.51
1:E:218:THR:OG1	1:E:219:SER:N	2.42	0.51
9:C:198:CYS:SG	9:C:199:LYS:N	2.82	0.51
8:F:159:GLY:O	10:D:296:HIS:NE2	2.43	0.51
2:B:254:LEU:O	2:B:261:GLN:NE2	2.42	0.51
10:D:204:LEU:HB3	10:D:273:MET:HB3	1.91	0.51
3:A:327:ASP:OD1	3:A:327:ASP:N	2.44	0.51
3:A:240:ALA:O	3:A:303:GLN:NE2	2.44	0.51
3:A:1366:ARG:NH1	3:A:1368:GLU:OE2	2.44	0.51
10:D:206:PHE:HE1	10:D:213:VAL:HG12	1.76	0.51
2:B:35:GLU:HA	2:B:38:ASP:HB2	1.92	0.50
1:E:164:ALA:HB1	1:E:171:MET:HG2	1.94	0.50
3:A:758:ASP:N	3:A:758:ASP:OD1	2.44	0.50
5:G:32:LEU:HA	10:D:284:ALA:HB3	1.93	0.50
1:E:311:ASP:OD1	1:E:311:ASP:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:317:ILE:HG12	10:D:253:GLU:HB3	1.92	0.50
1:E:291:VAL:HG21	10:D:238:PHE:HB2	1.94	0.50
1:E:337:LEU:HD22	1:E:356:PHE:HE2	1.77	0.50
2:B:98:LEU:HA	2:B:101:ILE:HD12	1.94	0.50
10:D:130:ASP:OD1	10:D:130:ASP:N	2.42	0.50
10:D:173:TRP:HB3	10:D:212:LEU:HD21	1.92	0.50
5:G:47:ALA:HA	5:G:50:SER:HB3	1.93	0.50
6:J:22:LEU:HD22	6:J:37:LEU:HB3	1.93	0.50
2:B:148:PRO:HA	2:B:154:THR:HG22	1.93	0.50
3:A:98:ASP:OD1	3:A:98:ASP:N	2.43	0.50
3:A:860:PHE:HB2	3:A:875:TYR:HB2	1.94	0.50
3:A:923:GLN:O	3:A:927:SER:OG	2.30	0.50
3:A:942:TRP:O	3:A:1389:HIS:HA	2.12	0.50
7:I:12:ILE:HG13	8:F:120:ALA:HB2	1.93	0.50
9:C:278:CYS:SG	9:C:279:SER:N	2.84	0.50
5:G:74:MET:HB2	5:G:81:VAL:HB	1.93	0.49
9:C:336:LEU:HD21	9:C:365:LEU:HB3	1.94	0.49
1:E:257:GLU:HG2	1:E:341:LEU:HA	1.93	0.49
3:A:344:GLU:HB3	3:A:381:LYS:HB2	1.92	0.49
6:J:64:VAL:HG22	6:J:77:GLN:HG3	1.93	0.49
7:I:79:VAL:HG23	7:I:84:VAL:HG22	1.92	0.49
3:A:1181:LEU:HA	3:A:1184:MET:HE2	1.93	0.49
10:D:206:PHE:HB2	10:D:271:TYR:HB2	1.93	0.49
3:A:295:GLN:NE2	3:A:298:ASN:OD1	2.45	0.49
3:A:858:ARG:NH1	3:A:881:TYR:OH	2.45	0.49
10:D:147:ASP:OD1	10:D:150:ARG:NH2	2.45	0.49
3:A:329:THR:OG1	3:A:330:GLY:N	2.45	0.49
6:J:72:GLY:HA2	6:J:89:MET:HA	1.93	0.49
4:H:4:ASP:OD1	4:H:4:ASP:N	2.46	0.49
7:I:6:THR:HG22	7:I:9:LEU:HD12	1.95	0.49
3:A:894:PRO:HG3	3:A:1437:ALA:HB3	1.95	0.49
3:A:381:LYS:NZ	3:A:395:ASP:OD2	2.45	0.48
9:C:8:ILE:N	9:C:129:ALA:O	2.44	0.48
9:C:329:CYS:SG	9:C:330:GLU:N	2.85	0.48
2:B:6:ARG:N	2:B:140:ASN:OD1	2.46	0.48
10:D:8:LYS:HD2	10:D:56:LEU:HD11	1.95	0.48
1:E:332:THR:OG1	1:E:360:ARG:NH2	2.44	0.48
10:D:15:LYS:NZ	10:D:102:ASP:OD1	2.36	0.48
6:J:67:LEU:HB3	6:J:74:ILE:HB	1.94	0.48
10:D:9:LYS:HE2	10:D:11:LEU:HD11	1.95	0.48
3:A:208:LYS:HE2	3:A:266:GLU:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:89:ARG:NH1	8:F:121:SER:O	2.46	0.48
3:A:1499:LYS:NZ	3:A:1514:PRO:O	2.47	0.48
4:H:74:TYR:HB2	5:G:71:PHE:H	1.78	0.48
10:D:263:ILE:HA	10:D:272:VAL:O	2.13	0.48
2:B:245:TYR:HB2	2:B:288:LEU:HD22	1.96	0.48
7:I:61:VAL:HG22	8:F:111:LEU:HD21	1.95	0.48
10:D:79:ASP:N	10:D:79:ASP:OD1	2.47	0.48
10:D:207:GLU:OE1	10:D:210:THR:N	2.47	0.48
2:B:47:LYS:NZ	10:D:43:ILE:O	2.46	0.48
6:J:69:SER:OG	6:J:70:ASP:N	2.47	0.48
9:C:17:SER:O	10:D:9:LYS:NZ	2.45	0.48
10:D:27:ILE:HD12	10:D:212:LEU:HD11	1.95	0.47
6:J:26:SER:O	6:J:50:GLN:NE2	2.47	0.47
1:E:234:GLN:HB2	1:E:240:LEU:HD11	1.96	0.47
3:A:42:ALA:HB3	3:A:86:TYR:HB2	1.96	0.47
4:H:117:LEU:HD12	4:H:120:VAL:HG21	1.95	0.47
3:A:242:ILE:HG12	3:A:247:LYS:HD2	1.95	0.47
7:I:20:VAL:HG13	7:I:27:LEU:HB2	1.96	0.47
3:A:215:GLU:OE2	3:A:325:ASN:ND2	2.48	0.47
3:A:303:GLN:O	3:A:305:ASN:ND2	2.48	0.47
3:A:1565:ASP:N	3:A:1565:ASP:OD1	2.42	0.47
9:C:89:ASP:OD1	9:C:89:ASP:N	2.46	0.47
10:D:121:LYS:HD3	10:D:179:GLN:HG3	1.95	0.47
2:B:40:VAL:HG11	2:B:64:LEU:HG	1.95	0.47
3:A:927:SER:O	3:A:930:SER:OG	2.33	0.47
1:E:77:ILE:HA	1:E:80:VAL:HG12	1.97	0.47
3:A:23:LEU:HA	3:A:68:SER:O	2.15	0.47
3:A:890:TYR:OH	3:A:1434:PRO:O	2.33	0.47
9:C:136:PRO:HA	9:C:139:ILE:HD12	1.97	0.47
2:B:33:SER:H	2:B:36:LEU:HD13	1.80	0.47
2:B:167:PRO:HG2	2:B:228:LEU:HD21	1.96	0.47
6:J:11:ASP:HA	6:J:14:LYS:HG2	1.97	0.47
2:B:134:ILE:HA	2:B:137:GLU:HG3	1.97	0.46
2:B:348:CYS:O	2:B:349:HIS:ND1	2.49	0.46
4:H:16:VAL:HG21	4:H:106:LEU:HD22	1.97	0.46
3:A:319:LYS:NZ	3:A:1429:TYR:O	2.48	0.46
5:G:53:TRP:HB2	5:G:83:ILE:HG21	1.97	0.46
2:B:316:PHE:HA	2:B:319:MET:HE2	1.96	0.46
2:B:372:ASP:OD1	2:B:375:ILE:N	2.48	0.46
3:A:406:SER:HB2	3:A:742:VAL:HA	1.98	0.46
4:H:24:VAL:HG12	4:H:90:VAL:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:61:VAL:CG1	8:F:111:LEU:CG	2.93	0.46
10:D:224:ASP:OD1	10:D:224:ASP:N	2.47	0.46
1:E:84:LYS:HG3	1:E:265:VAL:HG11	1.98	0.46
4:H:57:THR:HG23	4:H:68:ASN:HB3	1.98	0.46
7:I:17:GLY:HA2	7:I:31:GLY:HA3	1.98	0.46
1:E:181:ASP:OD1	1:E:181:ASP:N	2.47	0.46
3:A:284:LEU:HD12	3:A:285:VAL:HG23	1.96	0.46
3:A:760:PHE:HB2	3:A:814:ILE:HG21	1.97	0.46
10:D:204:LEU:HD11	10:D:213:VAL:HB	1.95	0.46
1:E:264:VAL:HG13	1:E:266:SER:H	1.80	0.46
3:A:346:ASP:HB2	3:A:384:ASN:HD21	1.81	0.46
2:B:240:GLN:O	2:B:243:ASN:ND2	2.49	0.46
3:A:932:ASP:OD1	3:A:932:ASP:N	2.44	0.46
8:F:77:GLU:HG2	8:F:79:HIS:H	1.80	0.46
10:D:181:ILE:HG23	10:D:184:VAL:HB	1.98	0.46
2:B:175:PRO:HB3	2:B:224:ILE:HD11	1.97	0.46
1:E:231:LYS:HA	1:E:234:GLN:HG2	1.97	0.46
5:G:26:ASN:OD1	5:G:30:SER:N	2.49	0.46
1:E:174:GLU:HG3	1:E:232:VAL:HG22	1.98	0.45
9:C:135:ASP:HB3	9:C:138:VAL:HG23	1.98	0.45
9:C:397:MET:HE1	9:C:403:LEU:HG	1.99	0.45
3:A:1207:SER:OG	3:A:1254:GLY:O	2.32	0.45
3:A:1363:ARG:NH2	3:A:1400:GLU:OE1	2.49	0.45
9:C:271:LEU:HA	9:C:274:LEU:HD12	1.97	0.45
1:E:143:VAL:HG22	1:E:176:PHE:HB2	1.99	0.45
2:B:63:LYS:HG3	2:B:91:ALA:HA	1.97	0.45
3:A:121:LEU:HD21	3:A:132:VAL:HG11	1.97	0.45
2:B:360:MET:HB3	2:B:365:LEU:HB2	1.99	0.45
3:A:930:SER:OG	3:A:932:ASP:OD1	2.33	0.45
4:H:73:CYS:HB2	4:H:80:VAL:HG22	1.99	0.45
9:C:16:GLY:HA3	9:C:121:MET:HA	1.99	0.45
3:A:1223:THR:H	3:A:1226:MET:HE2	1.82	0.45
8:F:84:ARG:HA	8:F:87:GLN:HE21	1.82	0.45
10:D:129:MET:HE2	10:D:129:MET:HB3	1.76	0.45
1:E:135:ARG:NH1	1:E:167:VAL:O	2.50	0.45
5:G:69:LEU:HD23	5:G:72:ILE:HD11	1.98	0.45
10:D:79:ASP:HB2	10:D:83:ARG:HE	1.82	0.45
3:A:256:LYS:HE2	3:A:277:LEU:HD11	1.98	0.45
3:A:945:ARG:NE	3:A:1385:GLU:OE2	2.43	0.45
2:B:144:ARG:HH22	2:B:158:LYS:HE3	1.81	0.45
3:A:731:PRO:HB2	3:A:733:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:77:GLN:HB3	10:D:81:ILE:HG12	1.99	0.45
3:A:958:ARG:HE	3:A:968:ILE:HD12	1.82	0.45
4:H:55:LEU:O	4:H:59:GLN:NE2	2.44	0.45
2:B:255:VAL:O	2:B:258:LYS:NZ	2.50	0.44
3:A:998:ARG:NH2	3:A:1192:GLN:O	2.48	0.44
10:D:112:ALA:O	10:D:116:ASN:ND2	2.50	0.44
1:E:263:ASP:HB3	1:E:335:LEU:H	1.82	0.44
9:C:367:LYS:HB3	9:C:377:PHE:HZ	1.81	0.44
6:J:51:GLN:NE2	7:I:45:GLU:O	2.50	0.44
9:C:142:LEU:HD23	9:C:142:LEU:HA	1.84	0.44
3:A:281:TYR:HA	3:A:284:LEU:HG	1.99	0.44
7:I:7:GLN:O	7:I:11:ARG:NH1	2.51	0.44
3:A:145:TRP:HE1	3:A:150:LYS:HZ1	1.66	0.44
3:A:273:THR:HA	3:A:276:LYS:HG2	1.98	0.44
5:G:93:MET:HE3	5:G:104:LEU:HD12	2.00	0.44
10:D:126:VAL:HG13	10:D:129:MET:HE1	2.00	0.44
1:E:301:LEU:HD12	1:E:305:GLY:HA2	2.00	0.44
9:C:7:PRO:HD3	9:C:211:LEU:HD22	2.00	0.43
9:C:11:ILE:HG12	9:C:25:ARG:HG3	2.00	0.43
3:A:947:LEU:HD12	3:A:1419:VAL:HG11	2.00	0.43
2:B:330:PRO:HA	2:B:377:ILE:HA	2.00	0.43
1:E:141:ILE:HD11	1:E:232:VAL:HG11	2.01	0.43
1:E:262:PHE:HE1	1:E:289:ILE:HG21	1.83	0.43
5:G:41:ASP:OD1	5:G:41:ASP:N	2.48	0.43
10:D:249:PHE:O	10:D:271:TYR:OH	2.34	0.43
1:E:235:LYS:HB3	1:E:235:LYS:HE2	1.89	0.43
1:E:289:ILE:HA	1:E:292:VAL:HG12	1.99	0.43
2:B:50:LEU:HD11	9:C:72:ILE:HG12	2.00	0.43
3:A:100:VAL:HG23	3:A:144:LEU:HG	2.01	0.43
9:C:508:GLU:HG2	9:C:511:ARG:HH12	1.84	0.43
5:G:53:TRP:CE2	5:G:90:LEU:HD11	2.54	0.43
8:F:84:ARG:HA	8:F:84:ARG:HD3	1.79	0.43
3:A:241:SER:O	3:A:303:GLN:NE2	2.51	0.43
6:J:58:ASP:HA	6:J:59:PRO:HD3	1.90	0.43
10:D:135:ASP:N	10:D:135:ASP:OD1	2.47	0.43
3:A:1477:ALA:HB1	3:A:1482:PHE:HB2	2.01	0.43
6:J:75:MET:HB2	6:J:86:VAL:HG22	2.01	0.43
10:D:9:LYS:HE3	10:D:61:TRP:CE2	2.53	0.43
1:E:63:ARG:HD2	1:E:114:ILE:HD12	2.00	0.43
4:H:62:LYS:HD2	8:F:66:ILE:HD11	2.01	0.43
9:C:317:VAL:HG21	9:C:564:PHE:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:63:ARG:HB2	1:E:114:ILE:HD12	2.00	0.43
1:E:341:LEU:HD12	1:E:345:SER:HB2	2.01	0.43
2:B:284:LEU:HD22	2:B:297:LEU:HD21	2.01	0.43
5:G:105:LYS:HG3	5:G:109:GLN:HE22	1.84	0.43
10:D:20:LYS:NZ	12:D:601:AF3:F3	2.42	0.43
3:A:764:GLN:O	3:A:768:ASN:HB2	2.19	0.42
10:D:277:SER:OG	10:D:278:ASP:N	2.52	0.42
3:A:206:LYS:HA	3:A:209:GLU:HB2	2.01	0.42
5:G:10:VAL:HG21	8:F:154:LEU:HD21	1.99	0.42
1:E:227:GLU:HG3	1:E:279:MET:HE1	2.00	0.42
1:E:242:THR:HG21	8:F:54:LEU:HD13	2.01	0.42
3:A:334:VAL:HA	3:A:364:VAL:O	2.20	0.42
6:J:58:ASP:OD1	6:J:58:ASP:N	2.50	0.42
3:A:959:ILE:O	3:A:1571:ARG:NH1	2.49	0.42
3:A:169:ALA:O	3:A:214:HIS:ND1	2.53	0.42
5:G:39:ASP:OD1	5:G:39:ASP:N	2.51	0.42
1:E:197:GLN:HE22	3:A:1407:ARG:HD2	1.83	0.42
11:E:501:GDP:O1B	12:E:502:AF3:F2	2.28	0.42
3:A:11:ILE:HG12	3:A:74:THR:HG21	2.01	0.42
4:H:12:LYS:HA	4:H:12:LYS:HD3	1.88	0.42
9:C:256:ARG:HA	9:C:256:ARG:HD3	1.83	0.42
10:D:12:LEU:HD23	10:D:20:LYS:HB2	2.02	0.42
1:E:80:VAL:HA	1:E:85:MET:HG2	2.02	0.42
2:B:235:LEU:HD22	2:B:318:LEU:HB3	2.00	0.42
2:B:284:LEU:HD23	2:B:284:LEU:HA	1.91	0.42
3:A:21:ASP:OD2	3:A:57:SER:N	2.53	0.42
1:E:134:PHE:O	1:E:168:ASN:ND2	2.51	0.42
9:C:330:GLU:HB3	9:C:375:SER:HB3	2.00	0.42
10:D:262:PHE:HD2	10:D:274:VAL:HG23	1.83	0.42
1:E:85:MET:HE1	1:E:93:LEU:HD11	2.02	0.41
3:A:811:TYR:HA	3:A:856:MET:HB3	2.02	0.41
5:G:77:MET:SD	5:G:77:MET:N	2.93	0.41
1:E:273:ASP:OD1	1:E:273:ASP:N	2.42	0.41
3:A:1508:THR:HG22	3:A:1554:LEU:HD23	2.02	0.41
8:F:80:GLU:HA	8:F:83:ASP:HB3	2.02	0.41
9:C:206:GLU:O	9:C:210:SER:OG	2.31	0.41
11:B:501:GDP:O2B	12:D:601:AF3:F3	2.28	0.41
9:C:80:CYS:HA	9:C:97:PRO:HG2	2.02	0.41
9:C:83:LYS:HE2	9:C:85:GLU:HB2	2.02	0.41
9:C:498:ILE:HG23	9:C:547:PHE:HE1	1.84	0.41
3:A:801:GLU:OE1	3:A:1366:ARG:NH2	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:64:LYS:O	8:F:112:THR:OG1	2.38	0.41
9:C:148:ARG:NH2	9:C:567:LEU:O	2.54	0.41
1:E:320:LEU:HD23	1:E:320:LEU:HA	1.92	0.41
3:A:40:GLU:HA	3:A:51:LEU:O	2.20	0.41
3:A:157:SER:O	3:A:157:SER:OG	2.32	0.41
5:G:102:GLY:HA3	6:J:31:LEU:HA	2.02	0.41
7:I:12:ILE:HG21	7:I:87:VAL:HG11	2.03	0.41
10:D:204:LEU:HD13	10:D:216:HIS:HB3	2.03	0.41
3:A:98:ASP:O	3:A:161:ARG:N	2.54	0.41
3:A:794:THR:OG1	3:A:797:GLN:OE1	2.31	0.41
2:B:104:LYS:O	2:B:108:TYR:HB2	2.20	0.41
2:B:152:SER:OG	2:B:153:ASN:OD1	2.38	0.41
3:A:1228:ILE:HG23	3:A:1251:PHE:HD2	1.84	0.41
6:J:20:GLY:HA2	6:J:35:GLY:HA3	2.03	0.41
8:F:158:PHE:HB2	10:D:197:ILE:HD13	2.03	0.41
1:E:143:VAL:HG11	1:E:178:HIS:CE1	2.56	0.41
2:B:173:ASP:N	2:B:173:ASP:OD1	2.47	0.41
3:A:13:LYS:O	3:A:19:SER:OG	2.35	0.41
3:A:191:TYR:HE1	3:A:369:MET:HA	1.85	0.41
3:A:757:THR:OG1	3:A:758:ASP:N	2.53	0.41
5:G:15:ASN:OD1	5:G:35:SER:OG	2.29	0.41
3:A:239:ARG:O	3:A:250:PHE:HA	2.21	0.40
2:B:172:TYR:CE1	2:B:353:GLU:HA	2.57	0.40
3:A:1259:LYS:HB2	3:A:1259:LYS:HE3	1.83	0.40
9:C:280:PRO:HA	9:C:283:VAL:HG22	2.03	0.40
1:E:230:SER:HA	1:E:268:ILE:HG23	2.04	0.40
9:C:527:GLU:OE2	9:C:537:ARG:NH1	2.52	0.40
1:E:70:ARG:NH2	1:E:119:GLY:O	2.51	0.40
2:B:278:LEU:O	2:B:282:PHE:HB3	2.21	0.40
9:C:220:HIS:NE2	9:C:273:GLU:OE2	2.55	0.40
10:D:181:ILE:HD12	10:D:182:PRO:HD2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	303/399 (76%)	277 (91%)	26 (9%)	0	100	100
2	B	358/380 (94%)	316 (88%)	42 (12%)	0	100	100
3	A	973/1603 (61%)	905 (93%)	68 (7%)	0	100	100
4	H	118/124 (95%)	113 (96%)	5 (4%)	0	100	100
5	G	122/125 (98%)	111 (91%)	11 (9%)	0	100	100
6	J	90/91 (99%)	86 (96%)	4 (4%)	0	100	100
7	I	87/99 (88%)	78 (90%)	9 (10%)	0	100	100
8	F	109/161 (68%)	101 (93%)	8 (7%)	0	100	100
9	C	393/569 (69%)	375 (95%)	18 (5%)	0	100	100
10	D	294/313 (94%)	276 (94%)	18 (6%)	0	100	100
All	All	2847/3864 (74%)	2638 (93%)	209 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	E	278/339 (82%)	278 (100%)	0	100	100
2	B	334/351 (95%)	334 (100%)	0	100	100
3	A	889/1411 (63%)	889 (100%)	0	100	100
4	H	105/108 (97%)	105 (100%)	0	100	100
5	G	97/98 (99%)	97 (100%)	0	100	100
6	J	78/77 (101%)	78 (100%)	0	100	100
7	I	74/83 (89%)	74 (100%)	0	100	100
8	F	96/141 (68%)	96 (100%)	0	100	100
9	C	362/504 (72%)	362 (100%)	0	100	100

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	D	271/287 (94%)	271 (100%)	0	100	100
All	All	2584/3399 (76%)	2584 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	168	ASN
1	E	172	ASN
1	E	187	HIS
1	E	280	GLN
1	E	355	ASN
1	E	357	HIS
2	B	153	ASN
2	B	194	GLN
2	B	195	GLN
3	A	63	GLN
3	A	148	ASN
3	A	246	HIS
3	A	375	HIS
3	A	384	ASN
3	A	1381	ASN
3	A	1512	GLN
5	G	65	ASN
6	J	30	ASN
6	J	41	HIS
7	I	35	ASN
9	C	355	GLN
10	D	55	ASN
10	D	179	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	GDP	E	501	12	29,30,30	1.14	3 (10%)	45,47,47	1.82	7 (15%)
11	GDP	B	501	2,12	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
12	AF3	D	601	11	0,3,3	-	-	-		
12	AF3	E	502	11	0,3,3	-	-	-		

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
11	GDP	E	501	12	-	3/16/32/32	0/3/3/3
11	GDP	B	501	2,12	-	2/16/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	501	GDP	C5-C4	3.00	1.47	1.38
11	E	501	GDP	C5-C4	2.99	1.46	1.38
11	B	501	GDP	C6-N1	-2.73	1.33	1.38
11	E	501	GDP	C6-N1	-2.63	1.33	1.38
11	B	501	GDP	C5-N7	-2.35	1.34	1.39
11	E	501	GDP	C5-N7	-2.17	1.34	1.39

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	E	501	GDP	C5-C4-N3	-6.32	118.33	128.39
11	B	501	GDP	C5-C4-N3	-6.27	118.41	128.39
11	E	501	GDP	C2-N3-C4	5.01	120.94	112.30
11	B	501	GDP	C2-N3-C4	4.93	120.79	112.30
11	E	501	GDP	N9-C4-N3	4.90	135.75	125.95
11	B	501	GDP	N9-C4-N3	4.63	135.22	125.95
11	E	501	GDP	C6-C5-N7	2.94	135.65	130.29
11	B	501	GDP	C6-C5-N7	2.85	135.47	130.29
11	E	501	GDP	C3'-C2'-C1'	2.54	106.27	101.46
11	E	501	GDP	C4-C5-N7	-2.40	106.86	110.67
11	B	501	GDP	C4-C5-N7	-2.36	106.93	110.67
11	E	501	GDP	O6-C6-C5	-2.26	120.58	126.53
11	B	501	GDP	C3'-C2'-C1'	2.25	105.72	101.46
11	B	501	GDP	O6-C6-C5	-2.16	120.84	126.53

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	E	501	GDP	C5'-O5'-PA-O3A
11	E	501	GDP	C5'-O5'-PA-O2A
11	B	501	GDP	O4'-C4'-C5'-O5'
11	B	501	GDP	C3'-C4'-C5'-O5'
11	E	501	GDP	O4'-C4'-C5'-O5'

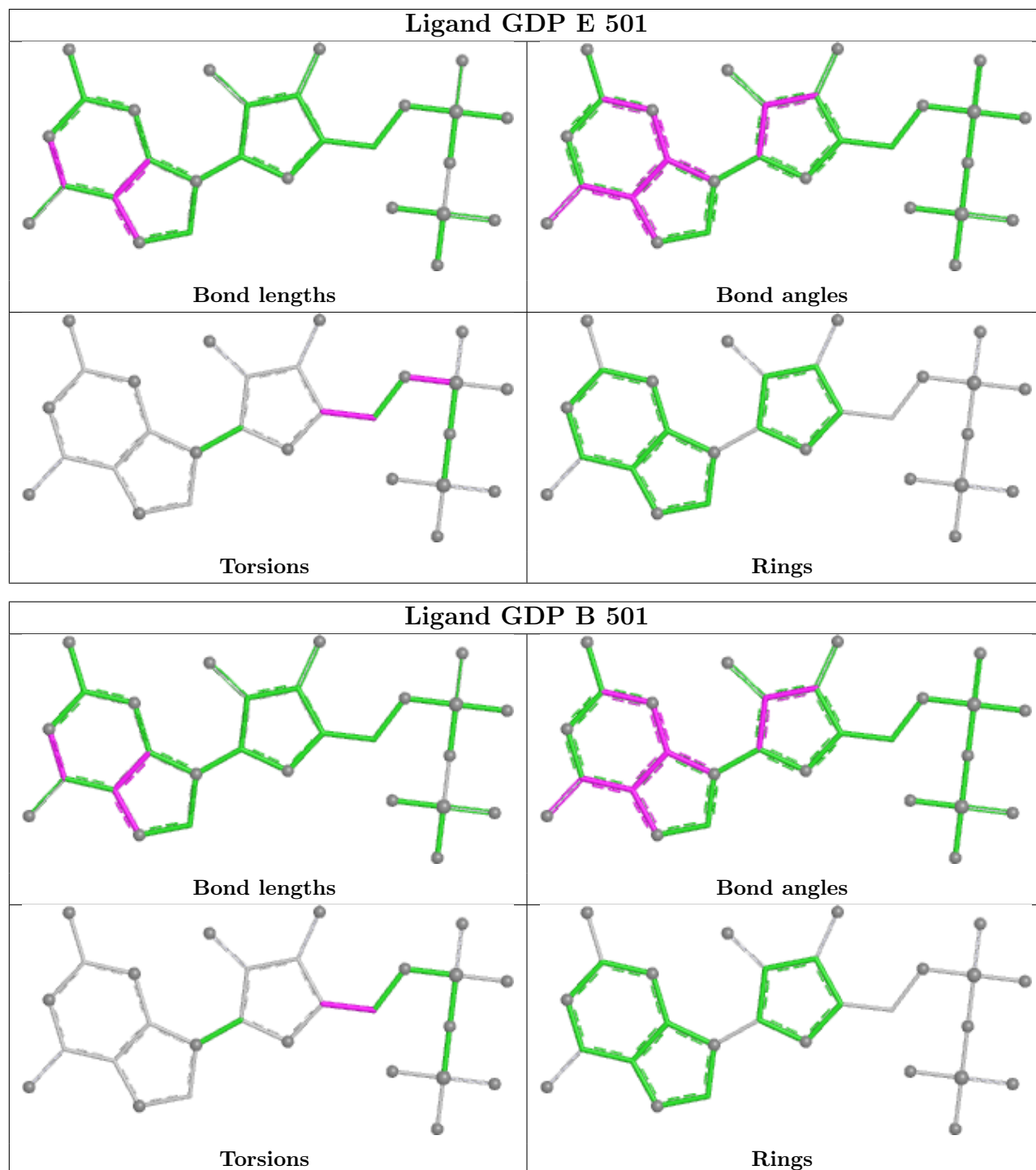
There are no ring outliers.

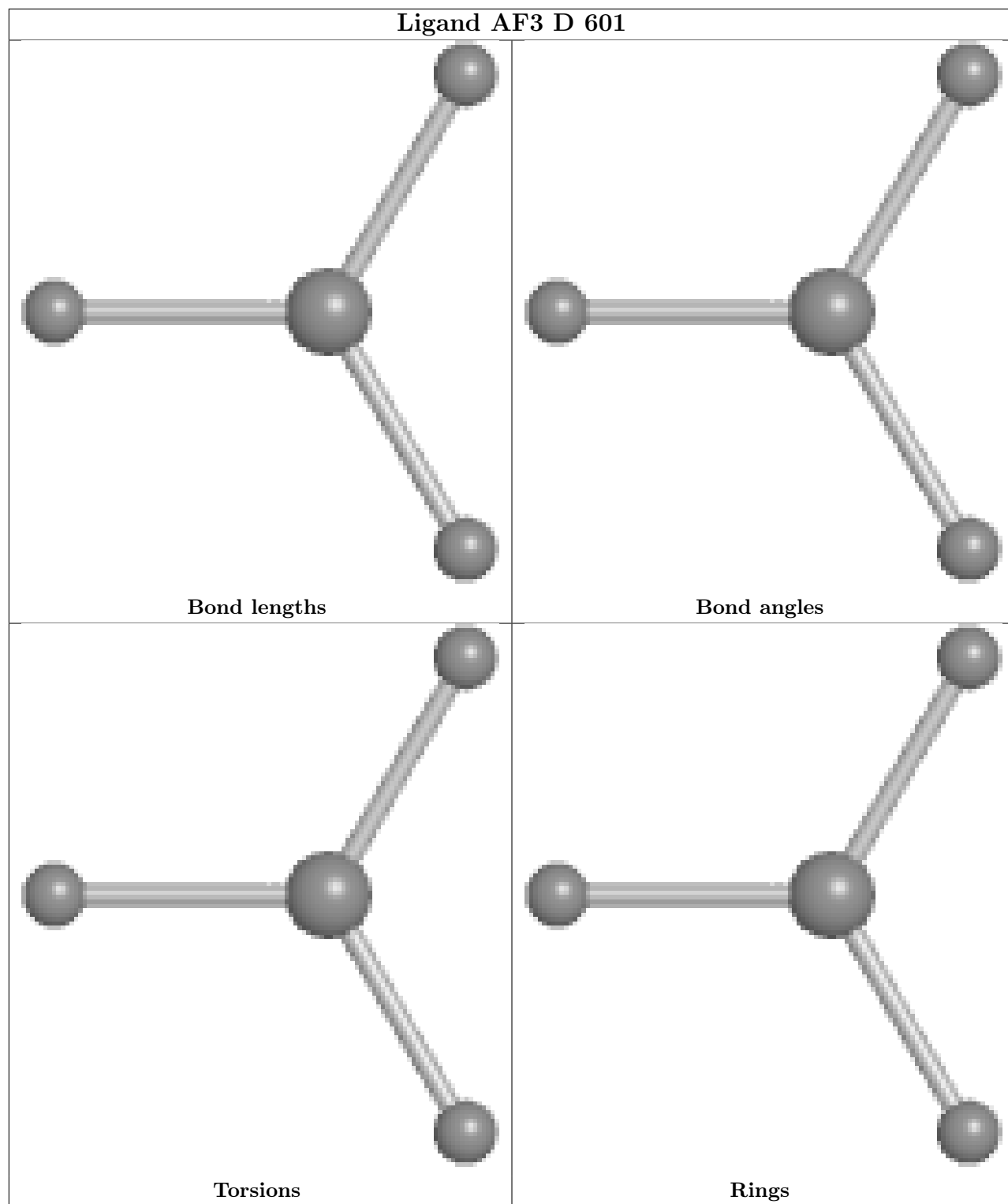
4 monomers are involved in 3 short contacts:

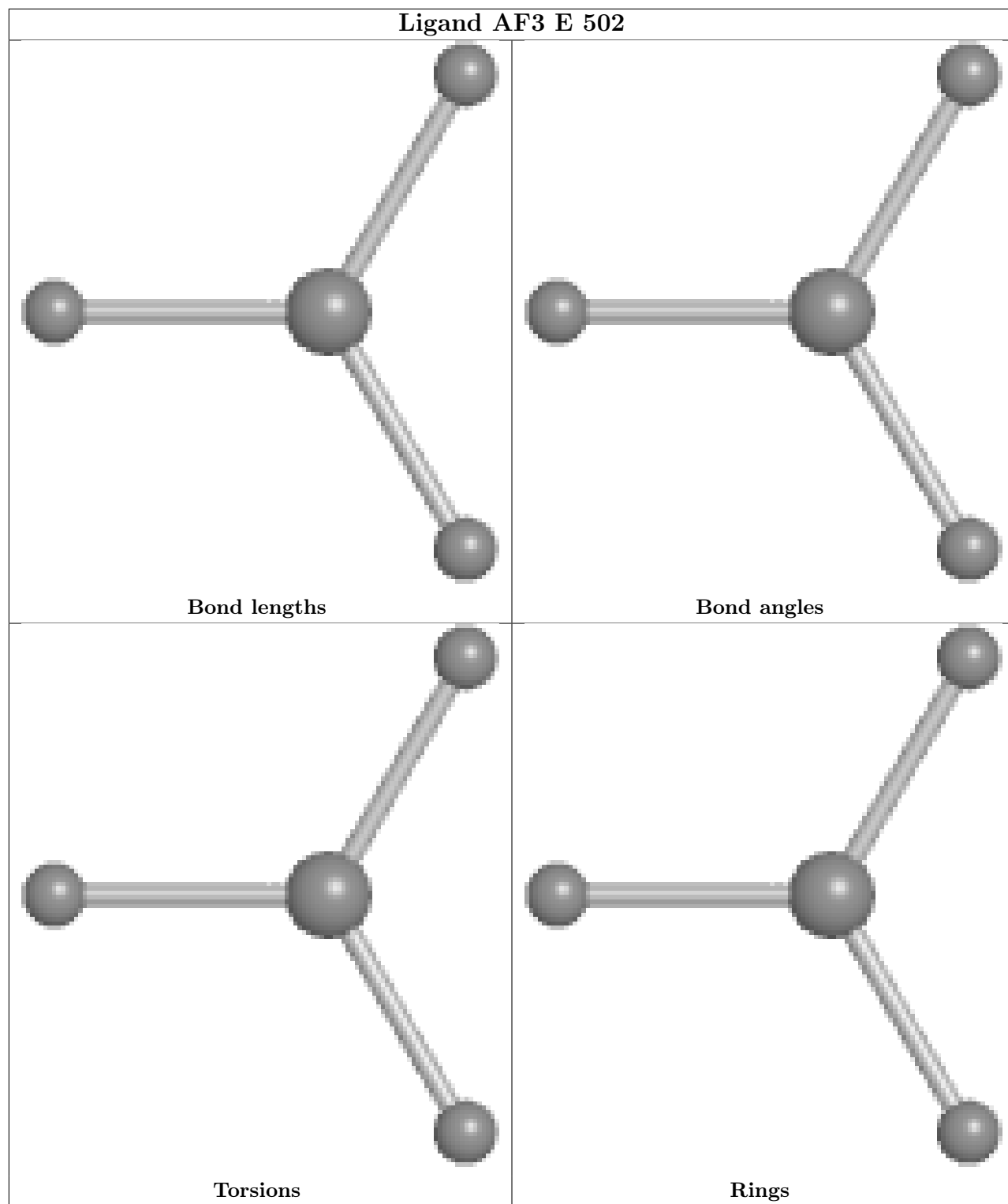
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	E	501	GDP	1	0
11	B	501	GDP	1	0
12	D	601	AF3	2	0
12	E	502	AF3	1	0

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 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 ⓘ

There are no chain breaks in this entry.

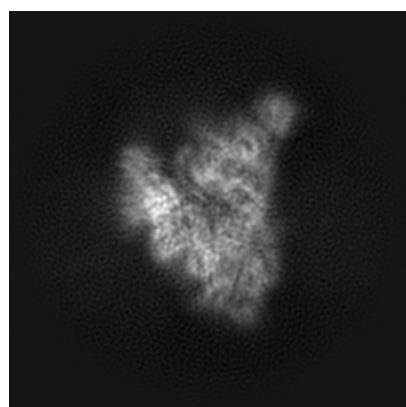
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25653. These allow visual inspection of the internal detail of the map and identification of artifacts.

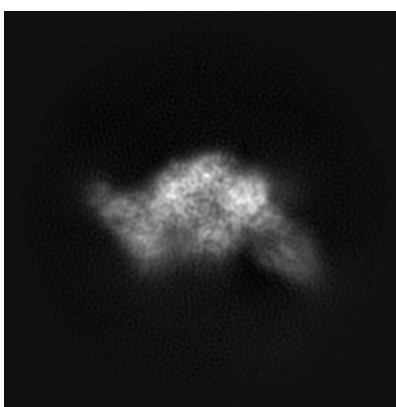
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

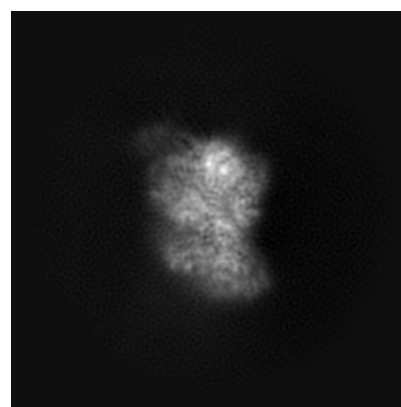
6.1.1 Primary map



X



Y

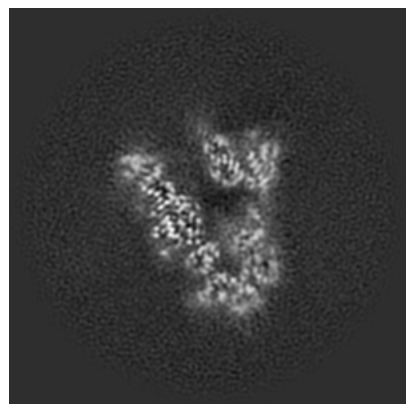


Z

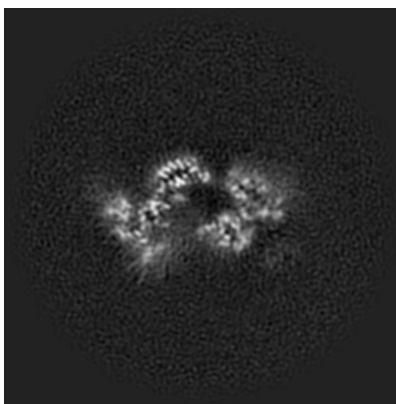
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

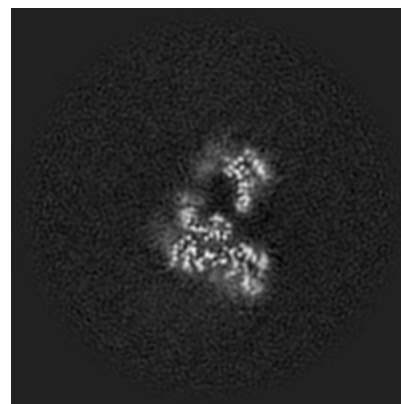
6.2.1 Primary map



X Index: 190



Y Index: 190

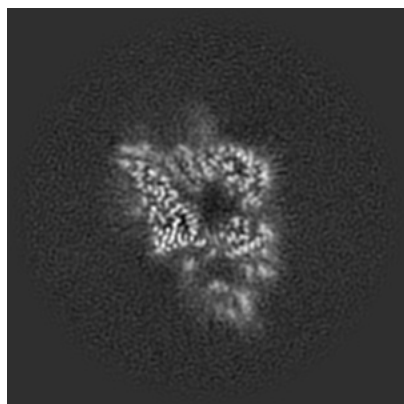


Z Index: 190

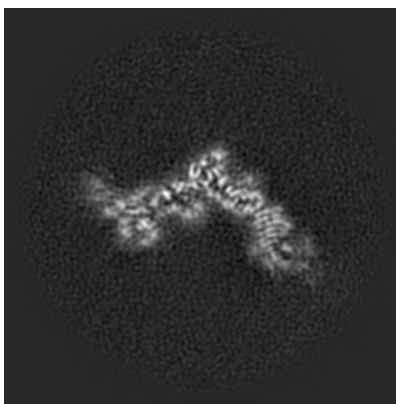
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

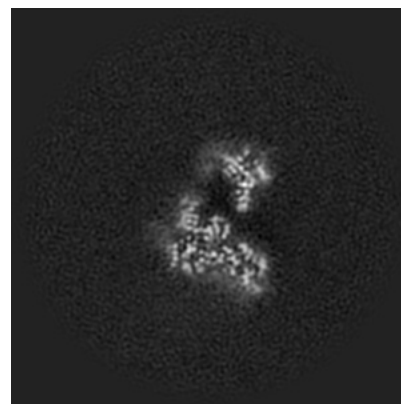
6.3.1 Primary map



X Index: 202



Y Index: 232

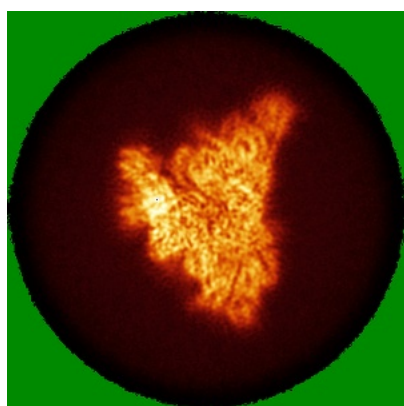


Z Index: 192

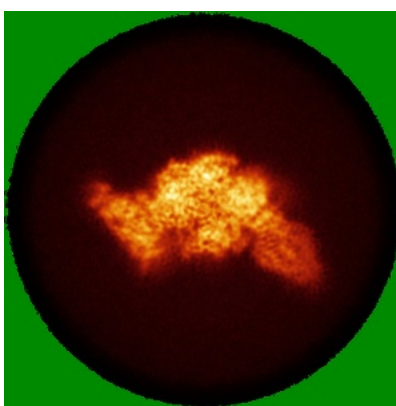
The images above show the largest variance slices of the map in three orthogonal directions.

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

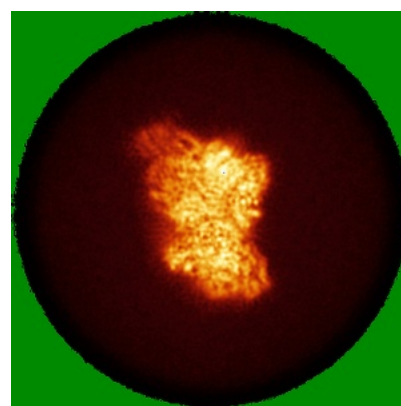
6.4.1 Primary map



X



Y

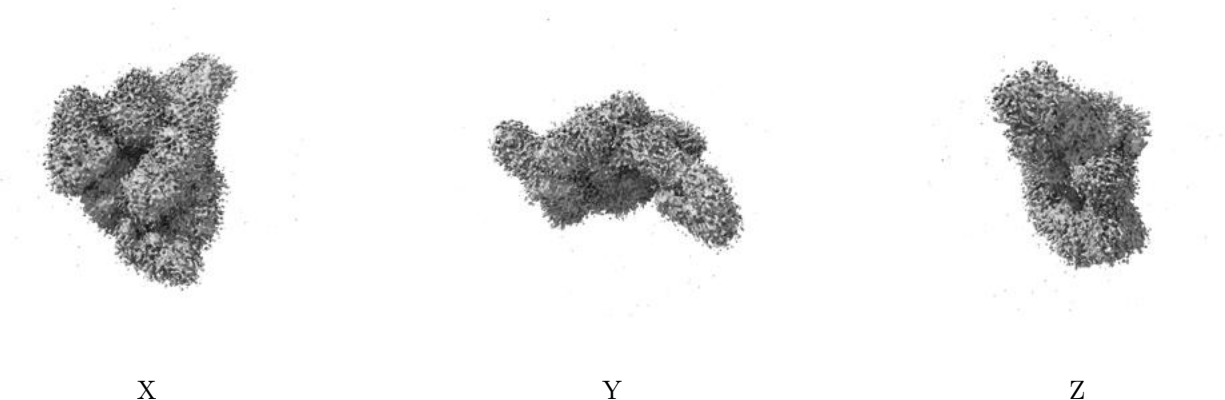


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.21. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

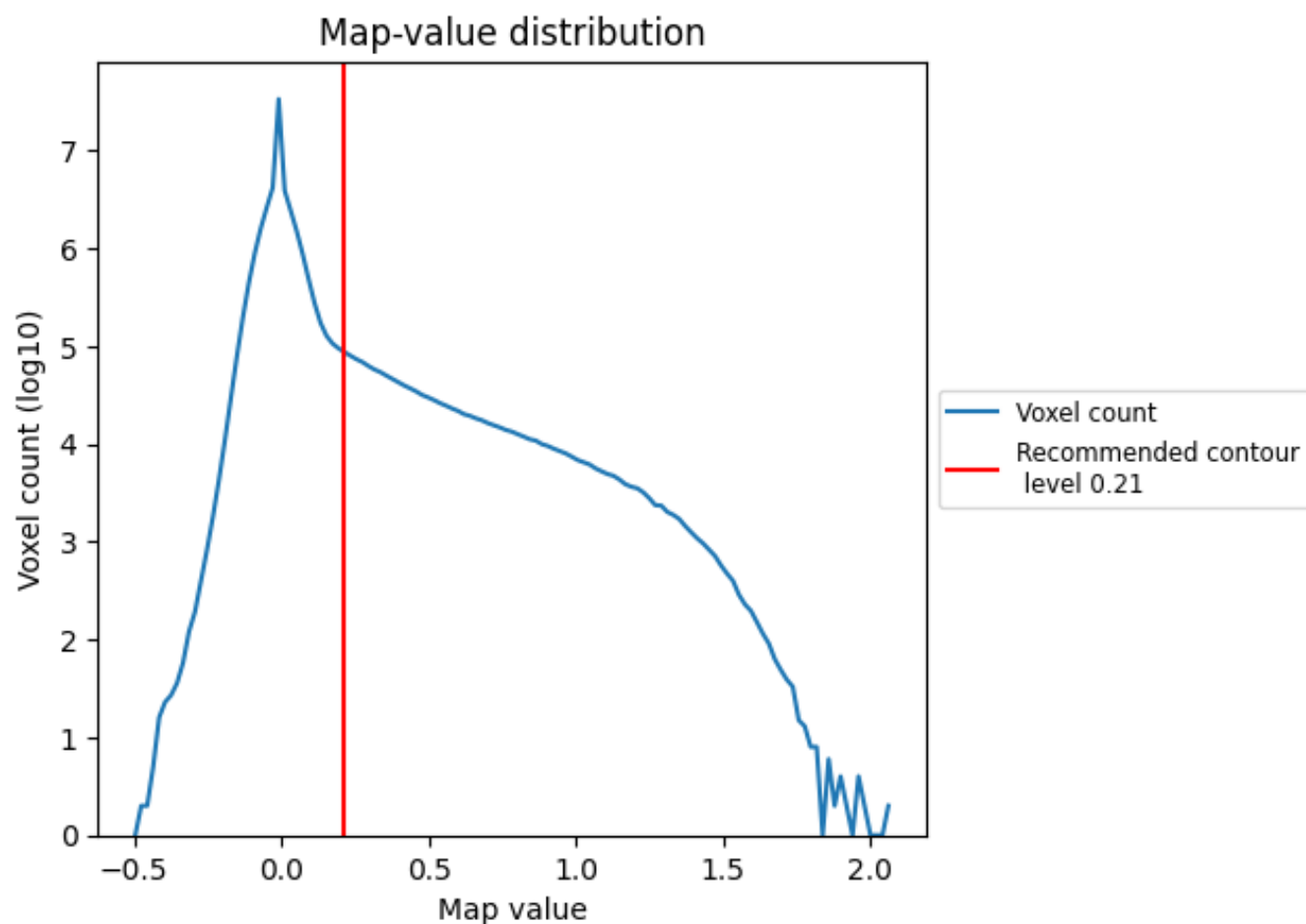
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

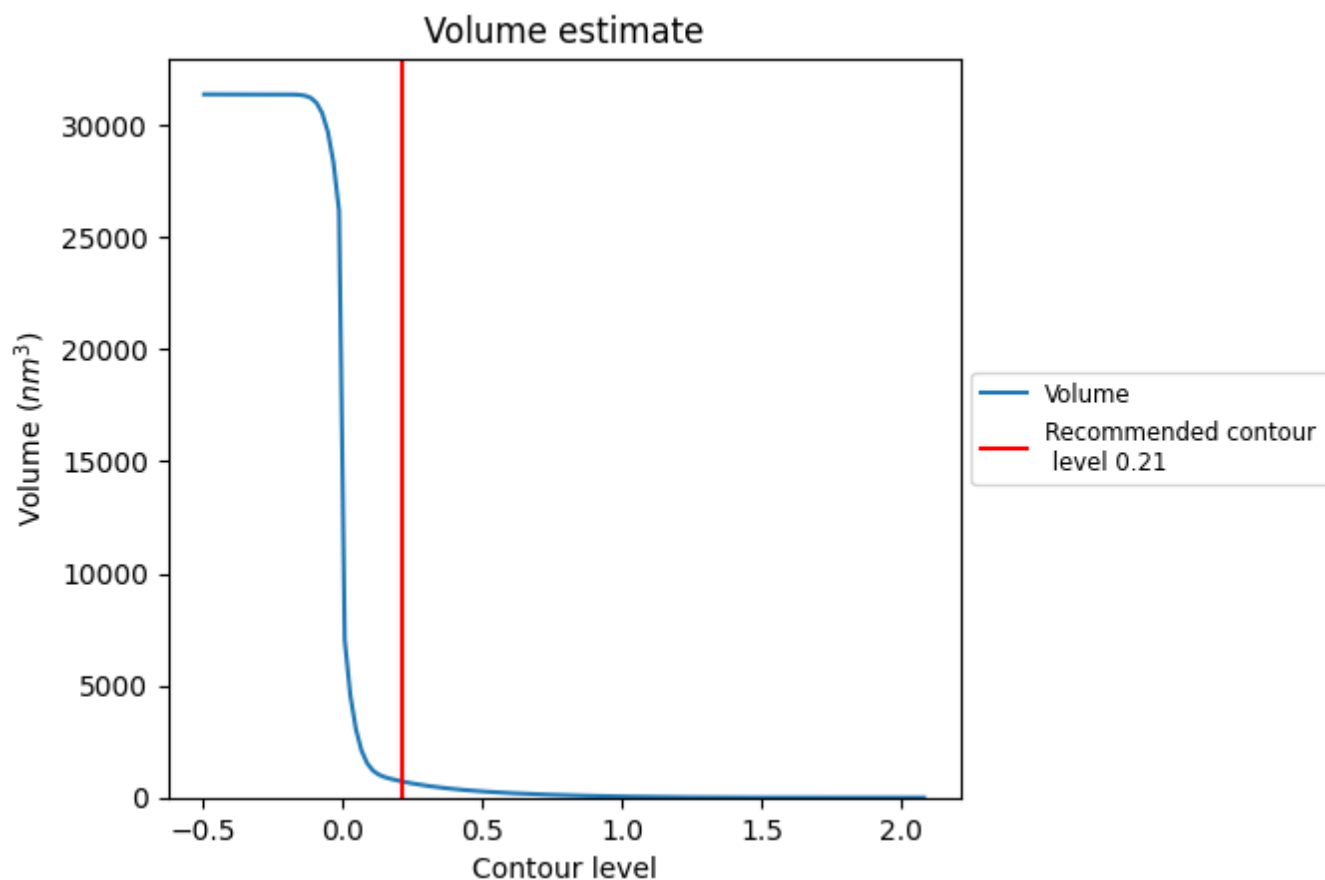
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

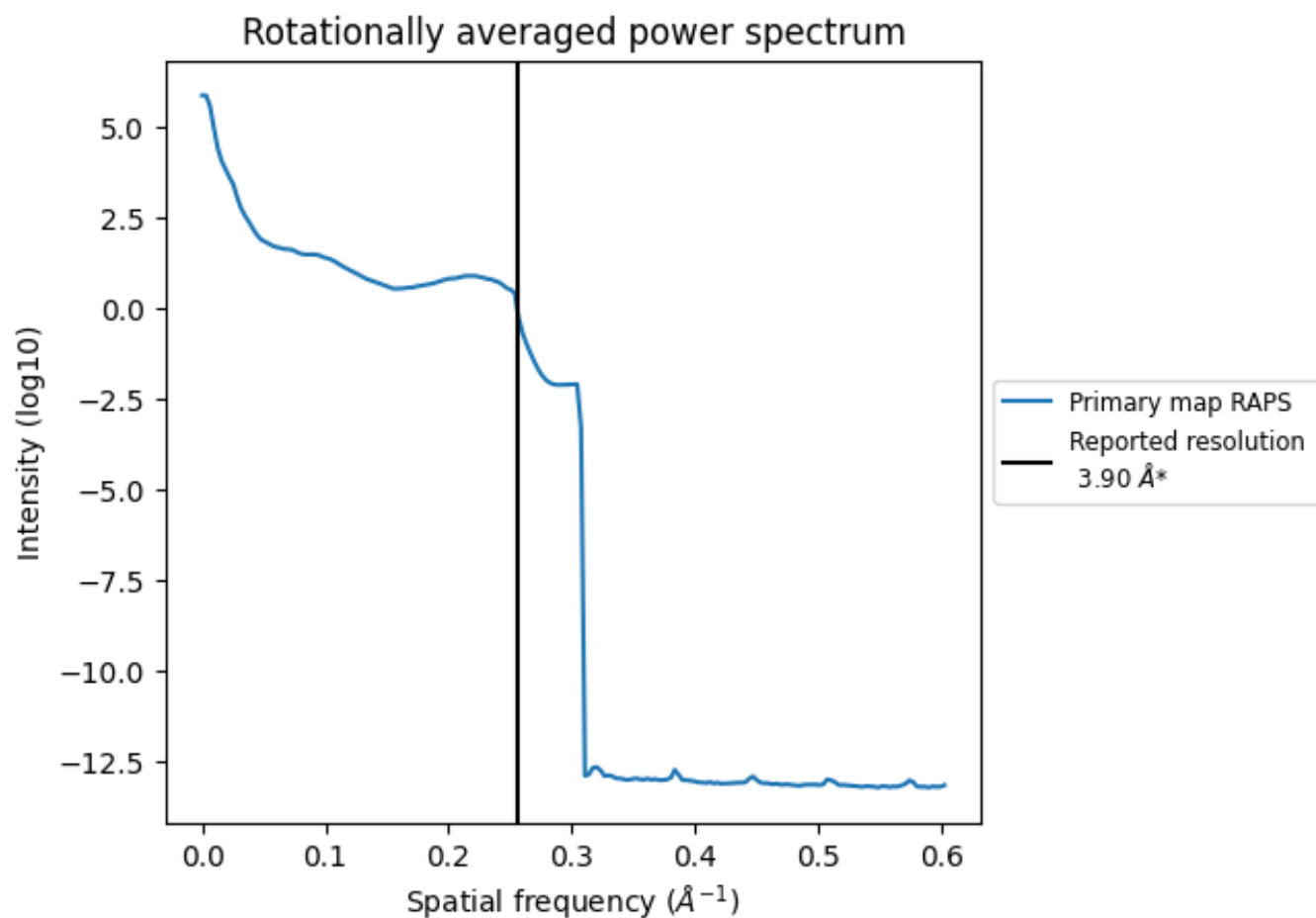
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 723 nm³; this corresponds to an approximate mass of 654 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 0.256 Å⁻¹

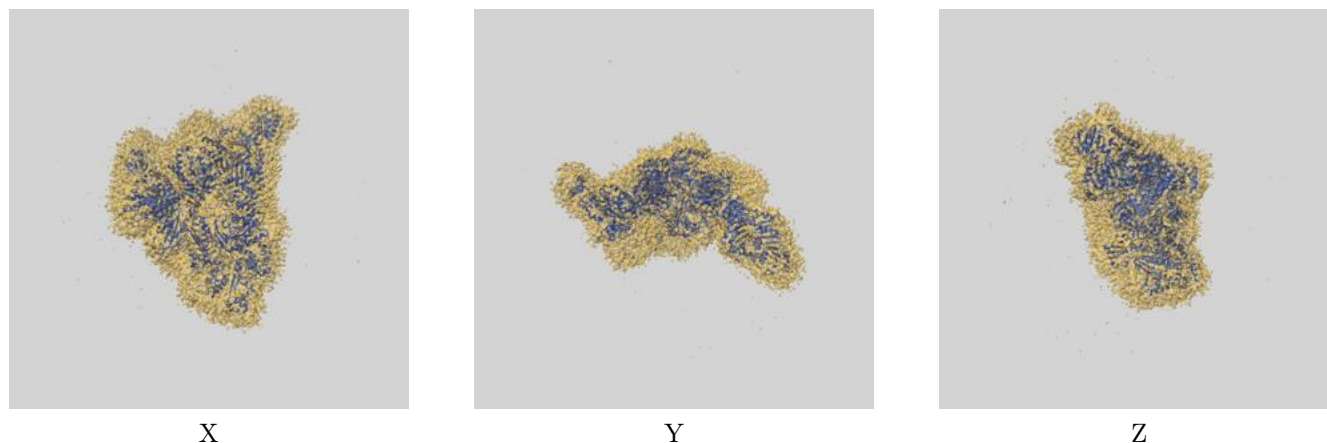
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

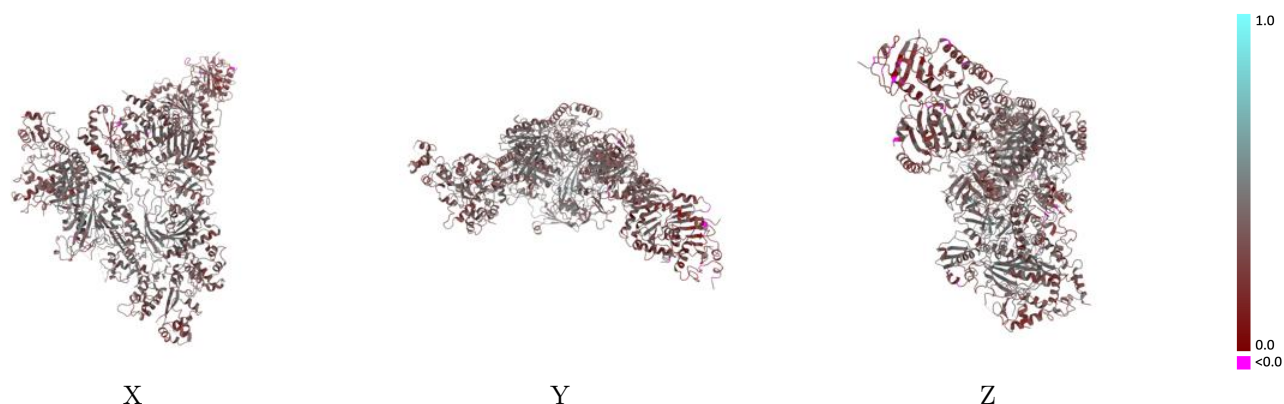
This section contains information regarding the fit between EMDB map EMD-25653 and PDB model 7T3B. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



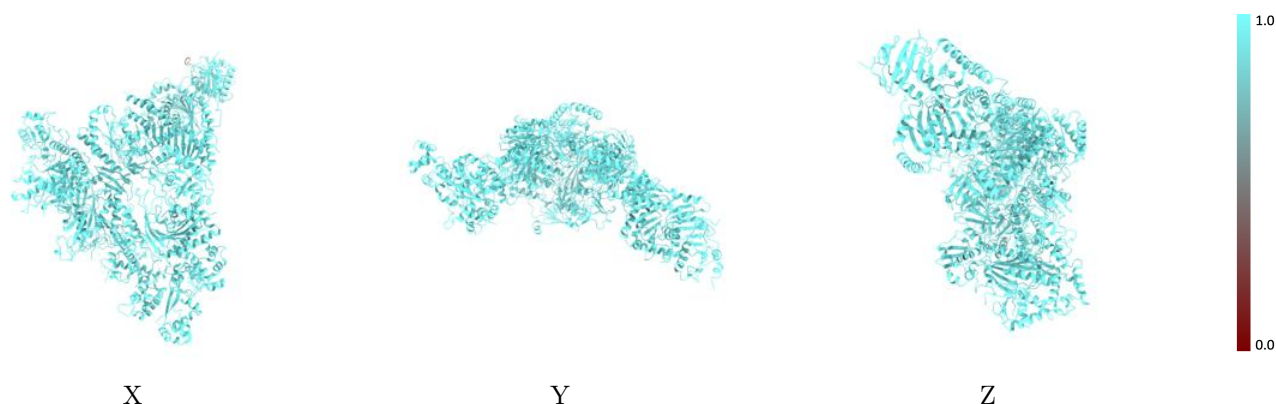
The images above show the 3D surface view of the map at the recommended contour level 0.21 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



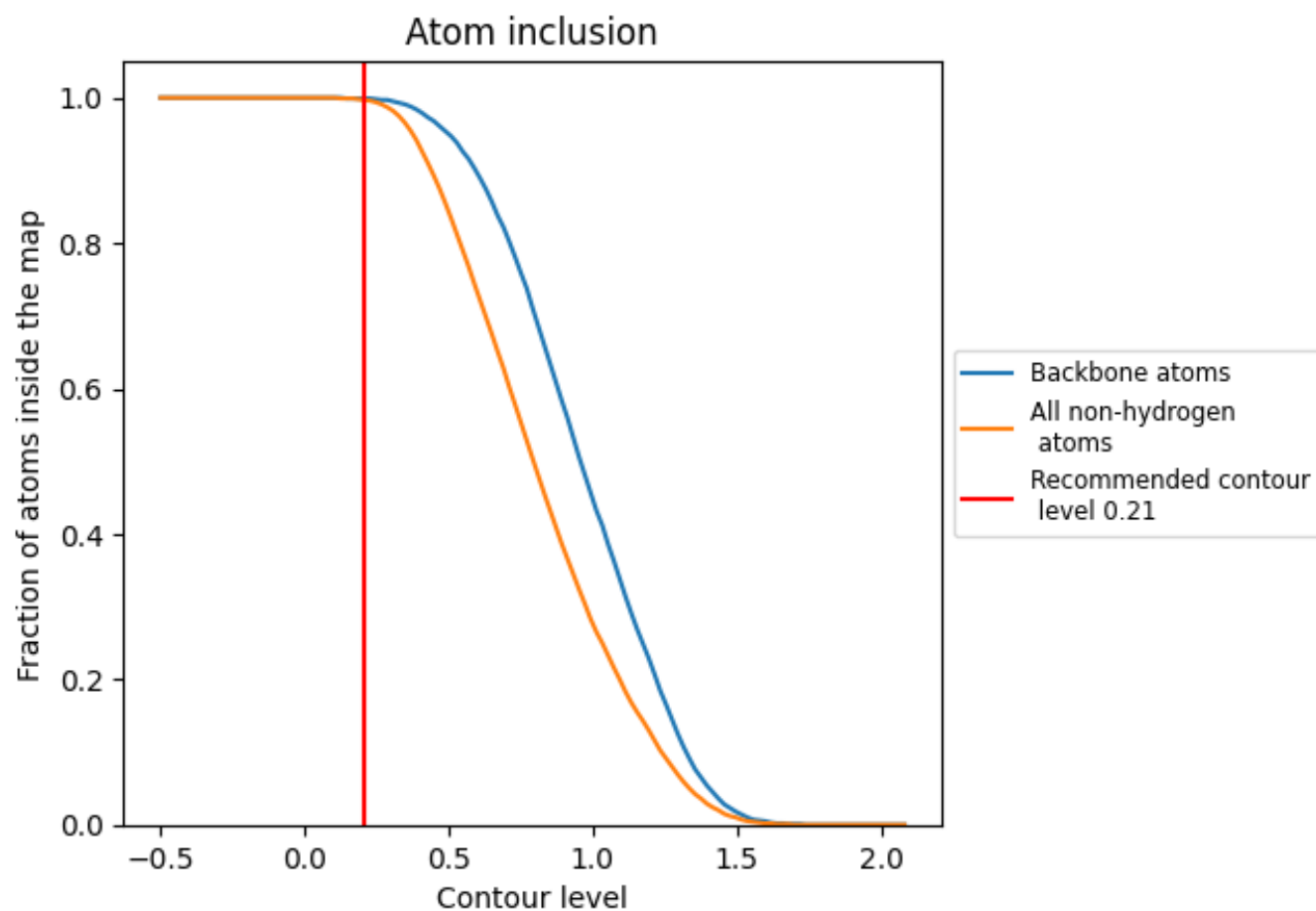
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.21).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.21) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9970	0.3680
A	0.9980	0.3920
B	1.0000	0.3980
C	1.0000	0.3740
D	1.0000	0.3900
E	0.9980	0.3380
F	0.9950	0.3070
G	0.9970	0.3410
H	0.9950	0.3260
I	0.9610	0.2190
J	0.9930	0.2810

1.0

0.0

<0.0