



## Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 06:12 AM UTC

PDB ID : 9CAE / pdb\_00009cae  
EMDB ID : EMD-45388  
Title : Cryo-EM structure of the reconstituted RuvBL lobe of the human TIP60 complex (composite structure)  
Authors : Louder, R.K.; Park, G.; Patel, A.B.  
Deposited on : 2024-06-17  
Resolution : 3.07 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132  
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) : 2.49

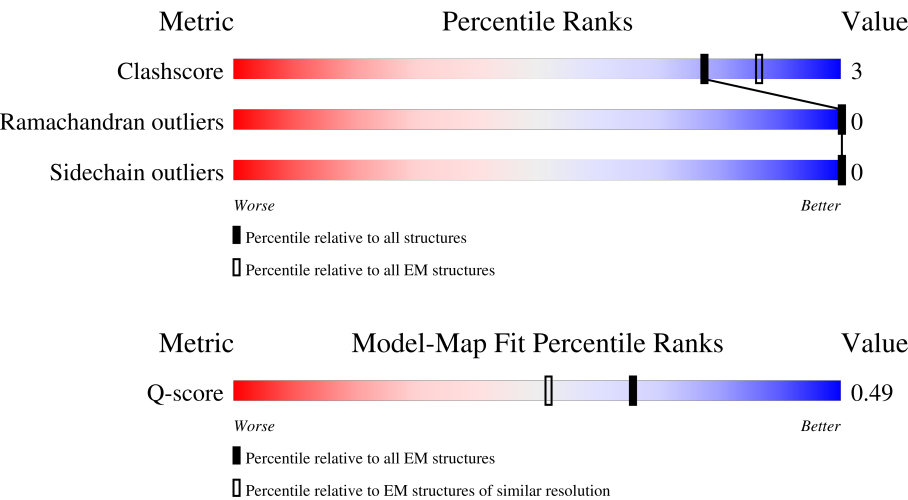


# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.07 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	13977 ( 2.57 - 3.57 )

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

Mol	Chain	Length	Quality of chain
1	A	2841	
2	B	364	
3	C	263	
4	E	456	

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Mol	Chain	Length	Quality of chain
4	G	456	
4	I	456	
5	F	857	
5	H	857	
5	J	857	
6	L	375	
7	M	429	
8	N	467	



## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 34005 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 E1A-binding protein p400,E1A-binding protein p400/Haloalkane dehalogenase chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	607	Total	C	N	O	S	0	0
			4975	3163	890	898	24		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	657	MET	-	initiating methionine	UNP Q96L91
A	2844	ALA	THR	conflict	UNP Q96L91

- Molecule 2 is a protein called Vacuolar protein sorting-associated protein 72 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	90	Total	C	N	O	S	0	0
			721	469	126	124	2		

- Molecule 3 is a protein called Enhancer of polycomb homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	93	Total	C	N	O	S	0	0
			769	485	154	127	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	358	MET	-	initiating methionine	UNP Q9H2F5

- Molecule 4 is a protein called RuvB-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	422	Total	C	N	O	S	0	0
			3249	2050	559	625	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	429	Total	C	N	O	S	0	0
			3308	2086	567	639	16		
4	I	425	Total	C	N	O	S	0	0
			3269	2060	562	631	16		

- Molecule 5 is a protein called RuvB-like 2,RuvB-like 2/Maltose/maltodextrin-binding periplasmic protein chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	435	Total	C	N	O	S	0	0
			3381	2113	593	659	16		
5	H	428	Total	C	N	O	S	0	0
			3327	2082	582	647	16		
5	J	412	Total	C	N	O	S	0	0
			3198	1999	558	626	15		

- Molecule 6 is a protein called Actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	357	Total	C	N	O	S	0	0
			2786	1769	465	532	20		

- Molecule 7 is a protein called Actin-like protein 6A.

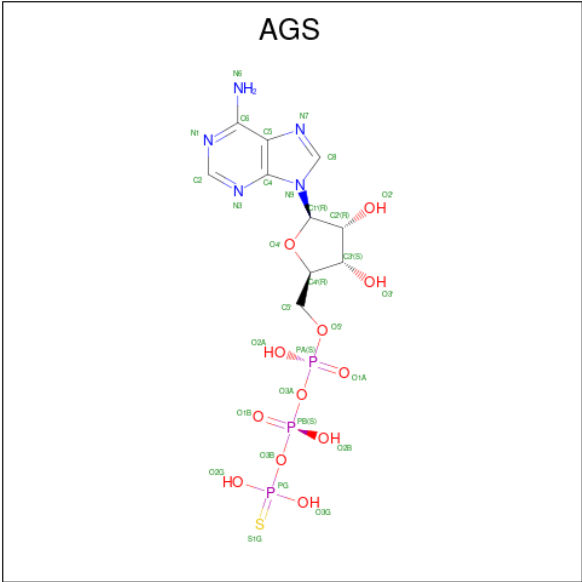
Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	401	Total	C	N	O	S	0	0
			3138	1987	532	595	24		

- Molecule 8 is a protein called DNA methyltransferase 1-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	190	Total	C	N	O	S	0	0
			1628	1040	297	288	3		

- Molecule 9 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>S).





Mol	Chain	Residues	Atoms					AltConf
9	E	1	Total	C	N	O	P	S
			31	10	5	12	3	1
9	F	1	Total	C	N	O	P	S
			31	10	5	12	3	1
9	G	1	Total	C	N	O	P	S
			31	10	5	12	3	1
9	H	1	Total	C	N	O	P	S
			31	10	5	12	3	1
9	I	1	Total	C	N	O	P	S
			31	10	5	12	3	1
9	J	1	Total	C	N	O	P	S
			31	10	5	12	3	1
9	L	1	Total	C	N	O	P	S
			31	10	5	12	3	1
9	M	1	Total	C	N	O	P	S
			31	10	5	12	3	1

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
10	E	1	Total	Mg	0
			1	1	
10	F	1	Total	Mg	0
			1	1	
10	G	1	Total	Mg	0
			1	1	
10	H	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
10	I	1	Total 1	Mg 1	0
10	J	1	Total 1	Mg 1	0
10	L	1	Total 1	Mg 1	0
10	M	1	Total 1	Mg 1	0











[illegible]

- Molecule 2: Vacuolar protein sorting-associated protein 72 homolog

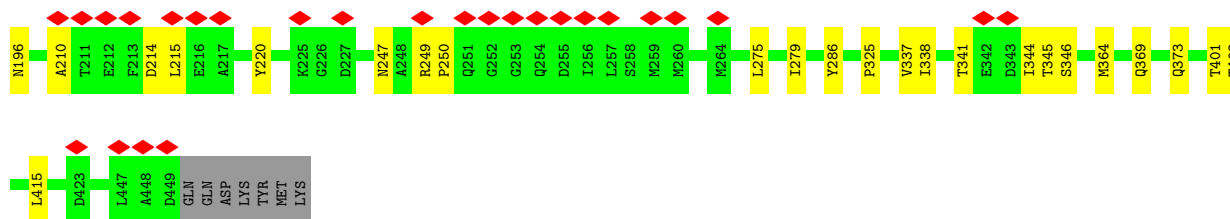
Chain B: 

[illegible]



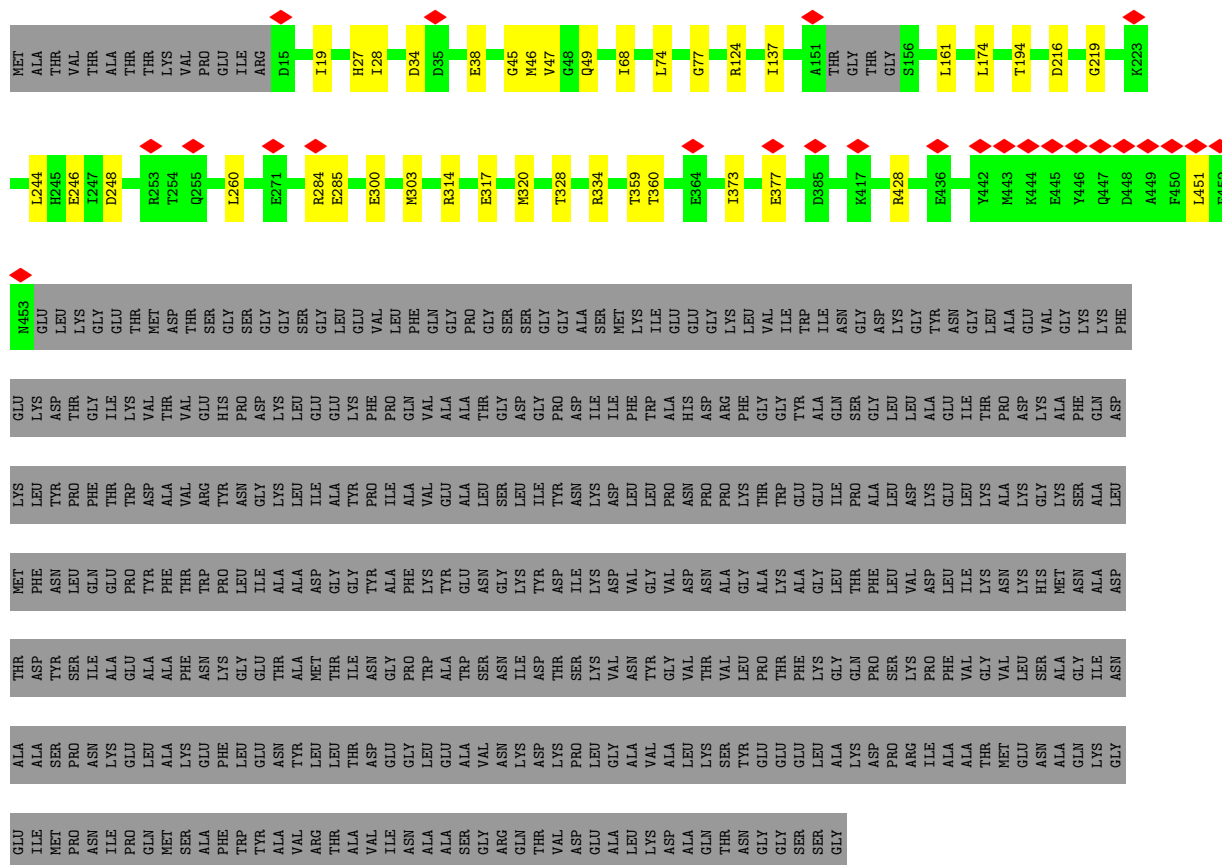






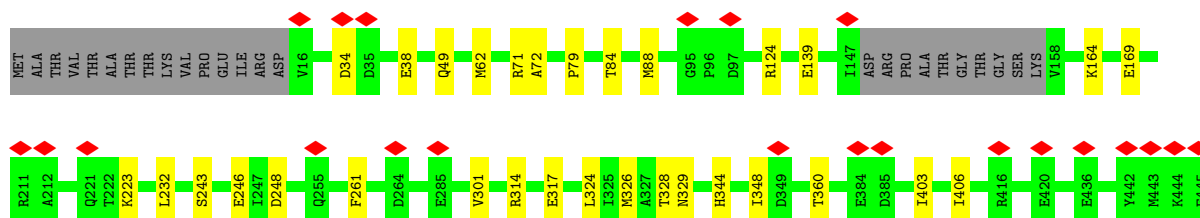
- Molecule 5: RuvB-like 2,RuvB-like 2/Maltose/maltodextrin-binding periplasmic protein chimera

Chain F: 46% 49%



- Molecule 5: RuvB-like 2,RuvB-like 2/Maltose/maltodextrin-binding periplasmic protein chimera

Chain H: 46% 50%

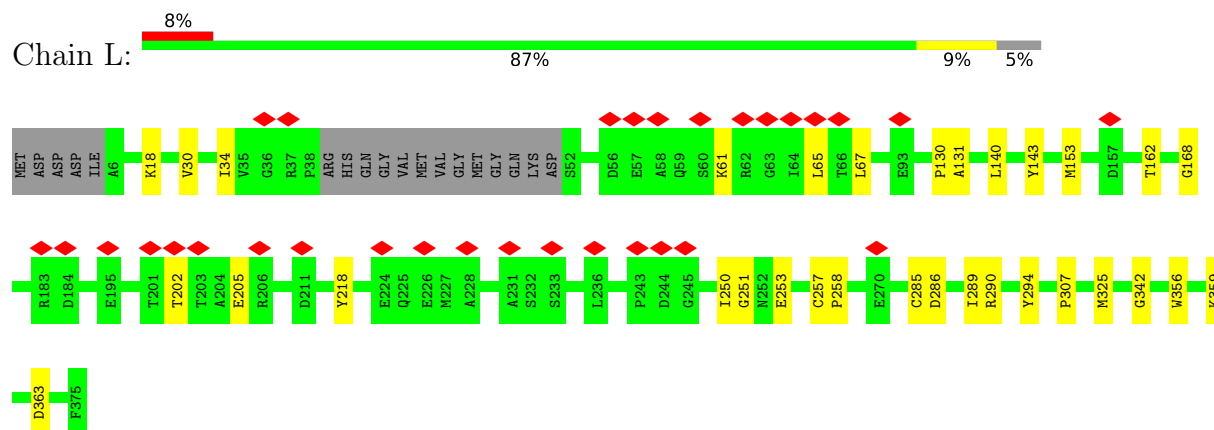




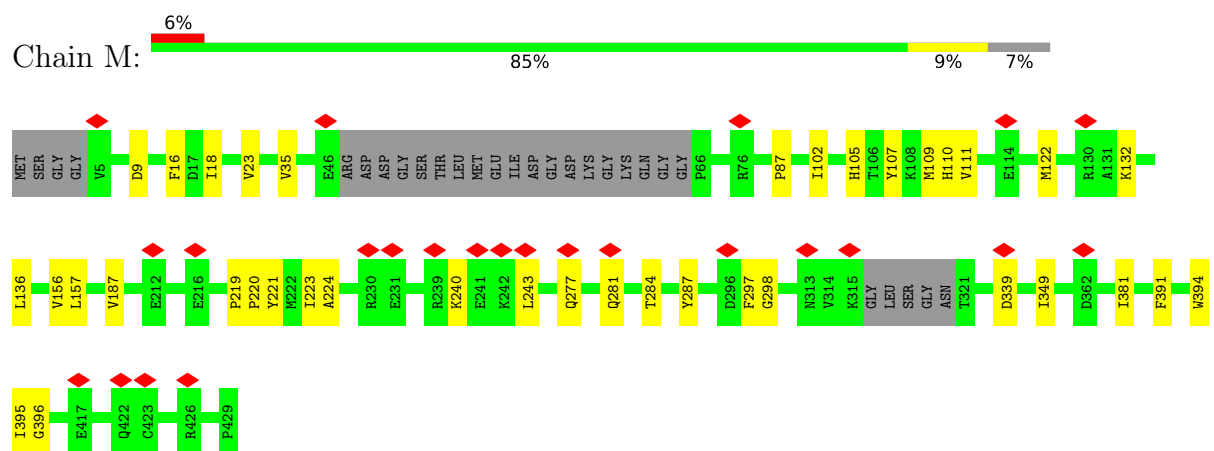




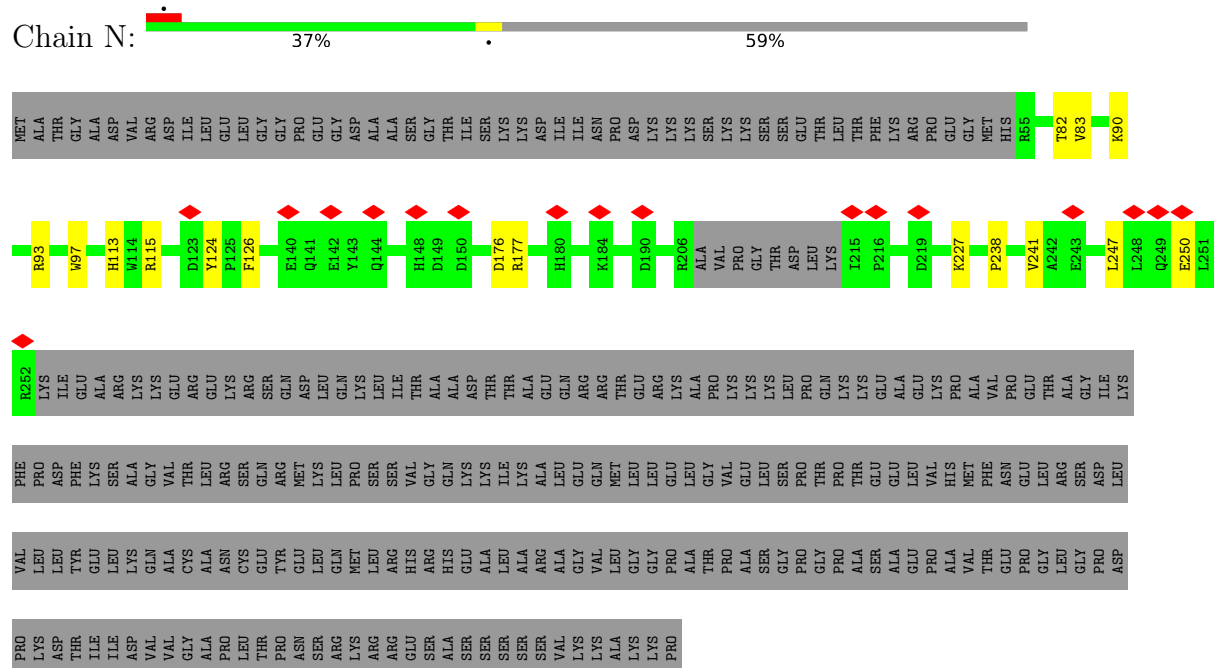
## Chain L:



## Chain M:



Chain N:





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45284	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	2.313	Depositor
Minimum map value	-0.112	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	348.48, 348.48, 348.48	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.726, 0.726, 0.726	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AGS, MG

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	0.15	0/5076	0.35	0/6861
2	B	0.14	0/746	0.28	0/1020
3	C	0.12	0/795	0.33	0/1076
4	E	0.14	0/3291	0.30	0/4436
4	G	0.15	0/3350	0.36	0/4516
4	I	0.14	0/3311	0.35	0/4463
5	F	0.16	0/3420	0.33	0/4603
5	H	0.15	0/3365	0.32	0/4529
5	J	0.15	0/3232	0.34	0/4349
6	L	0.14	0/2847	0.32	0/3858
7	M	0.13	0/3209	0.26	0/4351
8	N	0.13	0/1673	0.33	0/2255
All	All	0.14	0/34315	0.33	0/46317

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4975	0	5048	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	721	0	719	11	0
3	C	769	0	732	6	0
4	E	3249	0	3360	15	0
4	G	3308	0	3418	22	0
4	I	3269	0	3374	20	0
5	F	3381	0	3450	24	0
5	H	3327	0	3399	18	0
5	J	3198	0	3267	15	0
6	L	2786	0	2757	20	0
7	M	3138	0	3079	24	0
8	N	1628	0	1589	11	0
9	E	31	0	12	2	0
9	F	31	0	12	2	0
9	G	31	0	12	0	0
9	H	31	0	12	1	0
9	I	31	0	12	1	0
9	J	31	0	12	1	0
9	L	31	0	12	0	0
9	M	31	0	12	0	0
10	E	1	0	0	0	0
10	F	1	0	0	0	0
10	G	1	0	0	0	0
10	H	1	0	0	0	0
10	I	1	0	0	0	0
10	J	1	0	0	0	0
10	L	1	0	0	0	0
10	M	1	0	0	0	0
All	All	34005	0	34288	201	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 3.

All (201) 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)
6:L:34:ILE:HD11	6:L:67:LEU:HB3	1.65	0.77
7:M:16:PHE:HB2	7:M:122:MET:HG2	1.68	0.74
4:G:96:MET:SD	4:G:115:ASN:ND2	2.60	0.74
1:A:841:VAL:HG21	6:L:168:GLY:HA3	1.69	0.73
1:A:1369:ASN:HB3	1:A:1926:MET:HE3	1.73	0.69
4:I:215:LEU:HG	5:J:178:MET:HE3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:56:ILE:HD13	4:G:87:LEU:HD11	1.74	0.68
5:J:124:ARG:NE	5:J:248:ASP:OD2	2.24	0.68
1:A:841:VAL:HG22	6:L:143:TYR:HE1	1.60	0.67
4:I:96:MET:SD	4:I:115:ASN:ND2	2.68	0.67
9:I:501:AGS:H8	9:I:501:AGS:H5'1	1.78	0.66
5:H:301:VAL:HG21	5:H:326:MET:HE3	1.77	0.66
1:A:1436:PRO:HG2	1:A:1439:LEU:HD13	1.80	0.64
2:B:312:THR:HG23	2:B:315:ALA:H	1.63	0.62
1:A:1367:ILE:HG13	1:A:1374:VAL:HG21	1.80	0.62
5:H:124:ARG:NE	5:H:248:ASP:OD2	2.32	0.62
4:E:271:ILE:HG23	4:E:275:LEU:HD23	1.82	0.61
9:E:501:AGS:H8	9:E:501:AGS:H5'1	1.81	0.61
7:M:349:ILE:HG12	7:M:381:ILE:HD12	1.82	0.61
7:M:339:ASP:OD2	8:N:227:LYS:NZ	2.33	0.61
5:F:244:LEU:HD11	5:F:320:MET:HE3	1.81	0.61
2:B:321:GLU:HG2	2:B:324:LYS:HE3	1.82	0.61
7:M:18:ILE:HG23	7:M:23:VAL:HG22	1.83	0.60
4:E:163:THR:HG23	4:E:165:LYS:H	1.67	0.60
1:A:1976:ARG:NH2	1:A:1999:MET:SD	2.75	0.59
7:M:87:PRO:HG3	7:M:102:ILE:HD12	1.83	0.59
6:L:18:LYS:HG3	6:L:30:VAL:HG22	1.83	0.59
1:A:1990:PHE:HB2	1:A:2020:ARG:HD3	1.85	0.59
7:M:122:MET:HE1	7:M:136:LEU:HD11	1.85	0.58
5:F:124:ARG:NE	5:F:248:ASP:OD2	2.35	0.58
1:A:1858:MET:HE1	5:J:254:THR:HG23	1.86	0.57
2:B:210:PRO:HB3	2:B:273:THR:HG21	1.85	0.57
9:H:901:AGS:H5'1	9:H:901:AGS:H8	1.86	0.57
1:A:841:VAL:HG22	6:L:143:TYR:CE1	2.39	0.57
5:H:79:PRO:HG3	5:H:329:ASN:HD22	1.70	0.56
1:A:1928:ASP:OD1	1:A:1943:ARG:NH1	2.38	0.55
7:M:284:THR:HG22	7:M:298:GLY:HA2	1.87	0.55
4:G:172:LEU:HD13	4:G:176:ILE:HD13	1.88	0.55
7:M:220:PRO:HA	7:M:223:ILE:HD12	1.89	0.55
1:A:841:VAL:HG21	6:L:168:GLY:CA	2.36	0.55
7:M:18:ILE:HG12	7:M:23:VAL:HG13	1.89	0.55
1:A:1760:ARG:NH2	4:I:196:ASN:O	2.40	0.55
8:N:113:HIS:HB3	8:N:115:ARG:HG2	1.88	0.54
5:F:74:LEU:HD11	5:F:328:THR:HG22	1.90	0.54
4:I:119:ALA:HB3	4:I:325:PRO:HG3	1.89	0.54
1:A:2280:LEU:HD12	1:A:2281:PRO:HD2	1.88	0.54
6:L:285:CYS:HB3	6:L:289:ILE:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:107:TYR:HA	7:M:111:VAL:HB	1.90	0.54
2:B:258:PRO:O	2:B:260:ARG:NH1	2.41	0.53
6:L:153:MET:HG2	6:L:162:THR:HG22	1.89	0.53
1:A:1761:CYS:HB3	5:H:223:LYS:HE3	1.90	0.53
7:M:394:TRP:HE3	7:M:395:ILE:HD13	1.73	0.53
4:G:401:THR:OG1	4:G:402:THR:N	2.41	0.52
2:B:296:HIS:HD2	8:N:90:LYS:HE2	1.73	0.52
5:F:314:ARG:NH1	5:F:317:GLU:OE1	2.43	0.52
5:H:403:ILE:HA	5:H:406:ILE:HD12	1.92	0.52
4:E:180:LEU:HD23	4:E:200:VAL:HG11	1.90	0.52
1:A:1403:ASP:N	1:A:1403:ASP:OD1	2.43	0.52
5:J:382:MET:HG2	5:J:421:VAL:HB	1.91	0.52
1:A:1846:ARG:HH22	5:J:201:LYS:HZ2	1.58	0.51
5:H:49:GLN:NE2	5:H:360:THR:O	2.43	0.51
4:E:411:THR:HG21	5:F:68:ILE:HG13	1.90	0.51
5:J:94:LEU:HD21	5:J:98:THR:HB	1.92	0.51
1:A:1931:GLU:HB2	1:A:1941:TYR:CZ	2.46	0.51
1:A:1419:GLU:N	1:A:1419:GLU:OE1	2.44	0.51
5:F:284:ARG:NH1	5:F:285:GLU:OE2	2.40	0.50
5:F:161:LEU:HB2	5:F:174:LEU:HD11	1.91	0.50
4:E:140:PRO:HA	4:E:157:VAL:HG12	1.92	0.50
5:J:56:ALA:HB1	5:J:90:MET:HE2	1.92	0.50
8:N:238:PRO:HA	8:N:241:VAL:HG12	1.92	0.50
9:F:901:AGS:O2B	9:F:901:AGS:O1A	2.29	0.50
5:H:62:MET:HE1	5:H:71:ARG:HG2	1.94	0.50
1:A:2035:GLY:O	1:A:2039:LEU:HG	2.12	0.49
4:I:157:VAL:HG21	4:I:177:PHE:HB2	1.94	0.49
4:I:415:LEU:HD11	5:J:65:GLU:OE1	2.12	0.49
4:E:61:MET:HG3	5:J:407:THR:HG21	1.94	0.49
7:M:156:VAL:HG23	7:M:187:VAL:HG23	1.95	0.49
5:J:328:THR:HG22	5:J:330:ARG:H	1.78	0.49
2:B:302:ARG:HA	2:B:309:PRO:HA	1.94	0.49
2:B:284:PRO:HG2	4:G:205:ARG:HH22	1.78	0.48
5:J:246:GLU:HA	5:J:260:LEU:HD21	1.96	0.48
4:I:247:ASN:HD22	4:I:279:ILE:HD11	1.78	0.48
5:F:27:HIS:HB3	5:F:377:GLU:HG3	1.96	0.48
5:H:328:THR:HG21	5:H:344:HIS:HB3	1.96	0.48
4:E:157:VAL:HG11	4:E:177:PHE:CD1	2.49	0.48
5:F:451:LEU:HD22	5:H:348:ILE:HD11	1.96	0.47
5:F:246:GLU:HA	5:F:260:LEU:HD21	1.96	0.47
8:N:124:TYR:CE2	8:N:126:PHE:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:428:ARG:NH2	4:G:47:GLU:OE1	2.38	0.47
6:L:286:ASP:O	6:L:290:ARG:HG3	2.15	0.47
5:H:164:LYS:HB2	5:H:169:GLU:HG2	1.97	0.47
5:H:261:PHE:HD1	4:I:275:LEU:HD13	1.80	0.47
7:M:391:PHE:O	7:M:395:ILE:HG12	2.14	0.47
1:A:2280:LEU:HG	3:C:406:ARG:HD2	1.97	0.47
9:E:501:AGS:O1B	9:E:501:AGS:O2A	2.33	0.47
6:L:218:TYR:HA	6:L:307:PRO:HD2	1.97	0.47
7:M:9:ASP:OD1	8:N:115:ARG:NH2	2.43	0.47
1:A:1918:LEU:HD11	1:A:1983:VAL:HG11	1.97	0.46
1:A:1955:GLU:OE1	1:A:1958:ARG:NH1	2.48	0.46
4:E:107:LYS:HE2	4:E:110:GLU:HG2	1.96	0.46
5:F:34:ASP:OD1	5:F:38:GLU:N	2.47	0.46
1:A:1318:LYS:N	1:A:2015:ASP:OD1	2.49	0.46
4:E:156:HIS:N	4:E:174:PRO:HG3	2.31	0.46
7:M:157:LEU:O	7:M:396:GLY:HA3	2.16	0.46
7:M:240:LYS:HB2	7:M:243:LEU:HD11	1.98	0.46
4:I:97:VAL:HG12	4:I:100:GLU:HG3	1.98	0.46
5:J:166:THR:HG23	5:J:228:PRO:O	2.16	0.46
7:M:105:HIS:CE1	7:M:109:MET:HG3	2.50	0.45
5:H:243:SER:N	5:H:246:GLU:OE1	2.48	0.45
5:F:303:MET:SD	4:G:313:THR:HG21	2.57	0.45
8:N:247:LEU:HA	8:N:250:GLU:HG2	1.99	0.45
5:H:84:THR:O	5:H:88:MET:HG2	2.17	0.45
4:I:210:ALA:HA	4:I:220:TYR:CZ	2.52	0.45
5:F:219:GLY:H	4:G:195:ALA:HB1	1.82	0.45
7:M:132:LYS:HE2	7:M:132:LYS:HB2	1.85	0.45
2:B:260:ARG:HG3	2:B:260:ARG:HH11	1.82	0.45
7:M:224:ALA:HB2	7:M:240:LYS:HA	1.97	0.45
4:G:304:VAL:HG21	4:G:329:PHE:CD1	2.52	0.45
4:G:338:ILE:HD11	4:G:346:SER:HB2	1.99	0.45
4:I:341:THR:HG21	4:I:344:ILE:HD12	1.98	0.45
6:L:131:ALA:HB1	6:L:356:TRP:HB3	1.98	0.45
1:A:822:MET:HE1	3:C:461:ARG:HD3	1.99	0.44
4:I:214:ASP:HB2	5:J:173:ASP:H	1.82	0.44
4:I:338:ILE:HD11	4:I:346:SER:HB2	1.99	0.44
5:F:216:ASP:OD2	4:G:171:LYS:N	2.43	0.44
8:N:82:THR:HG23	8:N:83:VAL:HG13	2.00	0.44
5:H:34:ASP:OD1	5:H:38:GLU:N	2.50	0.44
4:E:411:THR:OG1	4:E:412:PRO:HD3	2.18	0.44
1:A:1839:VAL:HG21	1:A:1884:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:369:GLN:O	4:G:373:GLN:HG3	2.17	0.44
5:H:314:ARG:NH1	5:H:317:GLU:OE1	2.47	0.44
6:L:363:ASP:OD2	8:N:93:ARG:NH2	2.43	0.44
3:C:475:ASP:OD1	3:C:475:ASP:N	2.50	0.44
8:N:97:TRP:HA	8:N:113:HIS:O	2.17	0.44
1:A:1423:THR:O	1:A:1427:ALA:N	2.44	0.43
1:A:2039:LEU:O	1:A:2043:VAL:HG23	2.18	0.43
1:A:2276:PRO:HG2	1:A:2279:LYS:HG2	2.01	0.43
4:I:369:GLN:O	4:I:373:GLN:HG3	2.18	0.43
1:A:837:ALA:O	1:A:841:VAL:HG23	2.18	0.43
1:A:1321:GLU:HG2	1:A:2018:ILE:HD11	2.00	0.43
4:G:337:VAL:HA	4:G:345:THR:HA	2.00	0.43
5:F:137:ILE:HG23	5:F:194:THR:HG23	2.01	0.43
5:F:300:GLU:CD	4:G:313:THR:HB	2.44	0.43
4:G:53:VAL:HA	4:G:56:ILE:HD12	2.01	0.43
4:E:256:ILE:HG23	4:E:257:LEU:HD12	2.00	0.43
5:F:45:GLY:HA2	5:F:373:ILE:HD13	2.01	0.43
1:A:2008:ASP:OD1	1:A:2012:ARG:NE	2.51	0.42
6:L:130:PRO:HA	6:L:359:LYS:HD2	2.01	0.42
6:L:294:TYR:CD2	6:L:325:MET:HG2	2.55	0.42
2:B:303:ASP:OD2	2:B:320:ARG:NH1	2.48	0.42
4:G:155:SER:C	4:G:174:PRO:HG3	2.44	0.42
5:F:77:GLY:HA3	5:F:359:THR:OG1	2.19	0.42
6:L:257:CYS:HB3	6:L:258:PRO:HD3	2.01	0.42
1:A:1412:MET:HB2	4:I:286:TYR:CZ	2.54	0.42
4:E:64:ARG:HA	4:E:64:ARG:HD3	1.85	0.42
5:F:47:VAL:O	9:F:901:AGS:N6	2.52	0.42
5:H:139:GLU:O	5:H:232:LEU:HD23	2.20	0.42
4:I:71:PRO:HD2	4:I:74:THR:HG21	2.01	0.42
1:A:2245:MET:HE3	3:C:529:PHE:CD2	2.53	0.42
5:F:49:GLN:NE2	5:F:360:THR:O	2.49	0.42
7:M:277:GLN:O	7:M:281:GLN:HG2	2.19	0.42
1:A:2023:SER:HB3	1:A:2026:SER:OG	2.20	0.42
4:I:42:GLN:HE22	4:I:364:MET:H	1.67	0.42
6:L:251:GLY:C	6:L:253:GLU:H	2.28	0.42
7:M:394:TRP:CE3	7:M:395:ILE:HD13	2.54	0.42
2:B:213:THR:HB	2:B:267:THR:HB	2.02	0.41
4:E:110:GLU:HG3	4:E:270:GLU:HA	2.02	0.41
4:I:249:ARG:HG2	4:I:250:PRO:HD2	2.02	0.41
4:I:401:THR:OG1	4:I:402:THR:N	2.38	0.41
5:F:334:ARG:NH2	4:G:342:GLU:OE1	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:140:LEU:O	6:L:342:GLY:HA3	2.21	0.41
8:N:176:ASP:OD2	8:N:177:ARG:NH1	2.54	0.41
1:A:1438:LYS:HA	1:A:1438:LYS:HD3	1.95	0.41
5:F:28:ILE:HG23	5:F:46:MET:HE2	2.03	0.41
1:A:2268:LEU:HD11	3:C:423:TRP:CH2	2.54	0.41
4:G:159:ILE:HD11	4:G:180:LEU:HD11	2.03	0.41
1:A:1748:GLU:HG3	1:A:1752:GLN:HE21	1.85	0.41
1:A:1899:LYS:HZ1	1:A:2028:GLU:CD	2.27	0.41
6:L:250:ILE:O	6:L:250:ILE:HG13	2.20	0.41
1:A:1986:ASP:OD1	1:A:1986:ASP:N	2.53	0.41
2:B:302:ARG:NH1	2:B:307:ASP:OD1	2.48	0.41
5:H:62:MET:HE2	5:H:62:MET:HB3	1.88	0.41
6:L:61:LYS:HE3	6:L:65:LEU:HD11	2.02	0.41
1:A:1900:LEU:HD23	1:A:1900:LEU:HA	1.93	0.40
1:A:1924:ILE:HG23	1:A:1943:ARG:NH2	2.35	0.40
5:F:19:ILE:HD11	4:G:283:VAL:HG11	2.03	0.40
4:G:98:GLY:O	4:G:101:VAL:HG22	2.21	0.40
4:I:337:VAL:HG22	4:I:345:THR:HG22	2.03	0.40
6:L:202:THR:OG1	6:L:205:GLU:OE1	2.24	0.40
7:M:287:TYR:HB3	7:M:297:PHE:HE2	1.86	0.40
4:E:172:LEU:HD13	4:E:176:ILE:HG21	2.03	0.40
4:G:346:SER:OG	4:G:350:ILE:O	2.39	0.40
1:A:2248:TRP:CD1	3:C:437:ARG:HD3	2.57	0.40
4:E:256:ILE:O	4:E:260:MET:HG2	2.22	0.40
4:G:138:LEU:HD23	4:G:159:ILE:HG12	2.03	0.40
5:J:47:VAL:O	9:J:901:AGS:N6	2.53	0.40
7:M:219:PRO:HB2	7:M:221:TYR:CD1	2.57	0.40
1:A:1850:PRO:HA	1:A:1851:PRO:HD3	1.91	0.40
5:H:72:ALA:HA	5:H:324:LEU:O	2.22	0.40
5:J:138:ILE:O	5:J:194:THR:HA	2.22	0.40
7:M:35:VAL:HG21	7:M:110:HIS:CG	2.56	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	A	595/2841 (21%)	586 (98%)	9 (2%)	0	100	100
2	B	86/364 (24%)	85 (99%)	1 (1%)	0	100	100
3	C	89/263 (34%)	85 (96%)	4 (4%)	0	100	100
4	E	418/456 (92%)	415 (99%)	3 (1%)	0	100	100
4	G	423/456 (93%)	414 (98%)	9 (2%)	0	100	100
4	I	421/456 (92%)	417 (99%)	4 (1%)	0	100	100
5	F	431/857 (50%)	420 (97%)	11 (3%)	0	100	100
5	H	424/857 (50%)	415 (98%)	9 (2%)	0	100	100
5	J	406/857 (47%)	397 (98%)	9 (2%)	0	100	100
6	L	353/375 (94%)	349 (99%)	4 (1%)	0	100	100
7	M	395/429 (92%)	392 (99%)	3 (1%)	0	100	100
8	N	186/467 (40%)	183 (98%)	3 (2%)	0	100	100
All	All	4227/8678 (49%)	4158 (98%)	69 (2%)	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	A	543/2411 (22%)	543 (100%)	0	100	100
2	B	78/312 (25%)	78 (100%)	0	100	100
3	C	78/232 (34%)	78 (100%)	0	100	100
4	E	356/387 (92%)	356 (100%)	0	100	100
4	G	365/387 (94%)	365 (100%)	0	100	100
4	I	359/387 (93%)	359 (100%)	0	100	100
5	F	367/699 (52%)	367 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	H	361/699 (52%)	361 (100%)	0	100	100
5	J	348/699 (50%)	348 (100%)	0	100	100
6	L	303/318 (95%)	303 (100%)	0	100	100
7	M	345/364 (95%)	345 (100%)	0	100	100
8	N	170/400 (42%)	170 (100%)	0	100	100
All	All	3673/7295 (50%)	3673 (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 (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1425	HIS
1	A	1752	GLN
1	A	1875	GLN
1	A	1974	HIS
4	E	44	ASN
5	F	146	GLN
5	F	453	ASN
4	G	34	GLN
4	G	44	ASN
4	G	203	GLN
4	G	348	HIS
4	G	373	GLN
5	H	233	GLN
5	H	245	HIS
5	H	422	GLN
5	H	453	ASN
4	I	408	GLN
5	J	313	ASN
5	J	369	GLN
5	J	422	GLN
6	L	128	ASN
8	N	222	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	$\# Z  > 2$
9	AGS	F	901	10	32,33,33	0.63	1 (3%)	45,52,52	0.69	1 (2%)
9	AGS	M	501	10	32,33,33	0.56	1 (3%)	45,52,52	0.63	1 (2%)
9	AGS	J	901	10	32,33,33	0.57	1 (3%)	45,52,52	0.63	1 (2%)
9	AGS	E	501	10	32,33,33	0.53	1 (3%)	45,52,52	0.59	1 (2%)
9	AGS	I	501	10	32,33,33	0.63	1 (3%)	45,52,52	0.64	1 (2%)
9	AGS	L	401	10	32,33,33	0.58	1 (3%)	45,52,52	0.66	1 (2%)
9	AGS	G	501	10	32,33,33	0.53	1 (3%)	45,52,52	0.74	1 (2%)
9	AGS	H	901	10	32,33,33	0.56	0	45,52,52	0.80	1 (2%)

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
9	AGS	F	901	10	-	7/21/38/38	0/3/3/3
9	AGS	M	501	10	-	2/21/38/38	0/3/3/3
9	AGS	J	901	10	-	5/21/38/38	0/3/3/3
9	AGS	E	501	10	-	5/21/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	AGS	I	501	10	-	4/21/38/38	0/3/3/3
9	AGS	L	401	10	-	12/21/38/38	0/3/3/3
9	AGS	G	501	10	-	3/21/38/38	0/3/3/3
9	AGS	H	901	10	-	4/21/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	J	901	AGS	PG-S1G	2.20	1.95	1.90
9	E	501	AGS	PG-S1G	2.16	1.95	1.90
9	F	901	AGS	PG-S1G	2.15	1.95	1.90
9	I	501	AGS	PG-S1G	2.13	1.95	1.90
9	M	501	AGS	PG-S1G	2.10	1.95	1.90
9	L	401	AGS	PG-S1G	2.04	1.95	1.90
9	G	501	AGS	PG-S1G	2.01	1.95	1.90

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	F	901	AGS	PB-O3B-PG	-3.70	119.62	133.17
9	L	401	AGS	PB-O3B-PG	-3.57	120.11	133.17
9	M	501	AGS	PB-O3B-PG	-3.41	120.67	133.17
9	J	901	AGS	PB-O3B-PG	-3.37	120.84	133.17
9	H	901	AGS	PB-O3B-PG	-3.30	121.10	133.17
9	I	501	AGS	PB-O3B-PG	-3.15	121.63	133.17
9	G	501	AGS	PB-O3B-PG	-3.03	122.07	133.17
9	E	501	AGS	PB-O3B-PG	-2.89	122.59	133.17

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	F	901	AGS	C5'-O5'-PA-O1A
9	F	901	AGS	C5'-O5'-PA-O3A
9	J	901	AGS	C5'-O5'-PA-O2A
9	L	401	AGS	PB-O3B-PG-O2G
9	L	401	AGS	PB-O3B-PG-O3G
9	L	401	AGS	C5'-O5'-PA-O1A
9	L	401	AGS	C5'-O5'-PA-O2A
9	L	401	AGS	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
9	M	501	AGS	PB-O3B-PG-O2G
9	M	501	AGS	C5'-O5'-PA-O1A
9	E	501	AGS	O4'-C4'-C5'-O5'
9	F	901	AGS	O4'-C4'-C5'-O5'
9	F	901	AGS	C3'-C4'-C5'-O5'
9	I	501	AGS	O4'-C4'-C5'-O5'
9	L	401	AGS	PG-O3B-PB-O1B
9	L	401	AGS	O4'-C4'-C5'-O5'
9	L	401	AGS	C3'-C4'-C5'-O5'
9	G	501	AGS	PA-O3A-PB-O2B
9	J	901	AGS	PA-O3A-PB-O1B
9	L	401	AGS	PB-O3A-PA-O2A
9	E	501	AGS	C3'-C4'-C5'-O5'
9	F	901	AGS	C5'-O5'-PA-O2A
9	J	901	AGS	C5'-O5'-PA-O1A
9	J	901	AGS	C5'-O5'-PA-O3A
9	F	901	AGS	PA-O3A-PB-O2B
9	H	901	AGS	PA-O3A-PB-O1B
9	H	901	AGS	PG-O3B-PB-O2B
9	G	501	AGS	C4'-C5'-O5'-PA
9	L	401	AGS	C4'-C5'-O5'-PA
9	I	501	AGS	C3'-C4'-C5'-O5'
9	E	501	AGS	PG-O3B-PB-O2B
9	H	901	AGS	PG-O3B-PB-O1B
9	E	501	AGS	PA-O3A-PB-O1B
9	G	501	AGS	PA-O3A-PB-O1B
9	H	901	AGS	PA-O3A-PB-O2B
9	L	401	AGS	PB-O3A-PA-O1A
9	L	401	AGS	C2'-C1'-N9-C8
9	E	501	AGS	PA-O3A-PB-O2B
9	F	901	AGS	PA-O3A-PB-O1B
9	I	501	AGS	PA-O3A-PB-O1B
9	I	501	AGS	PB-O3A-PA-O2A
9	J	901	AGS	PA-O3A-PB-O2B

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	F	901	AGS	2	0
9	J	901	AGS	1	0
9	E	501	AGS	2	0

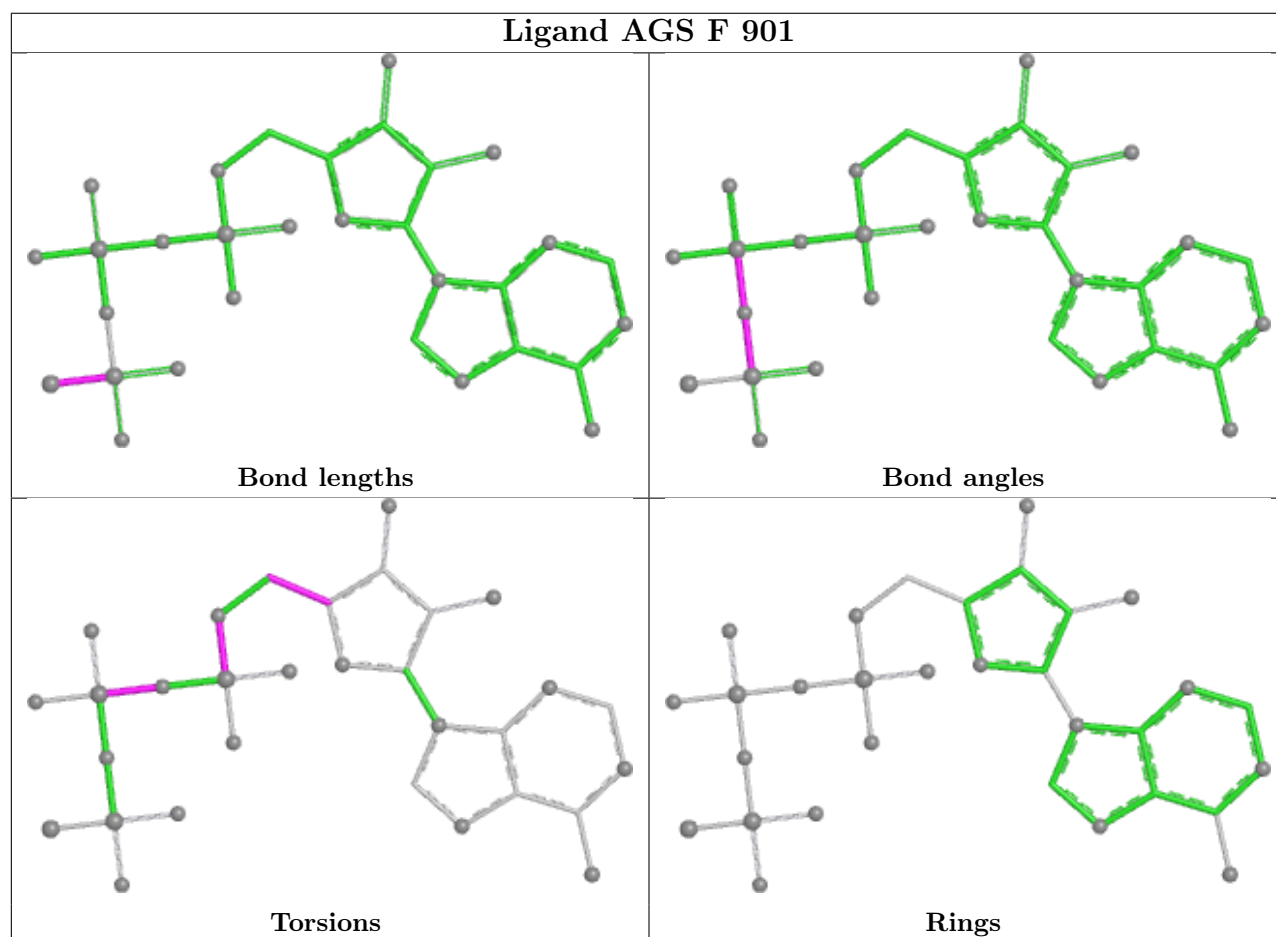
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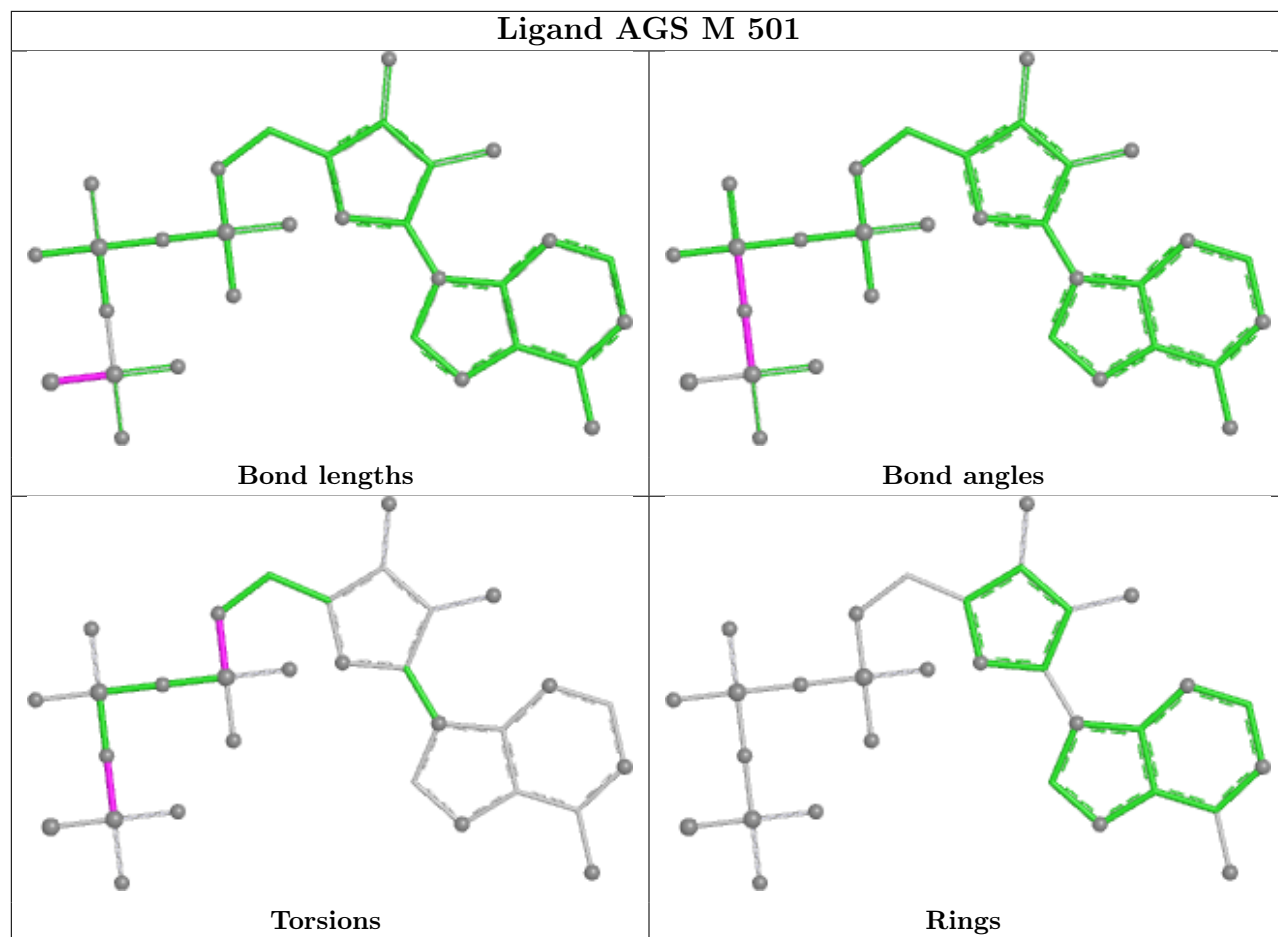
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	I	501	AGS	1	0
9	H	901	AGS	1	0

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.

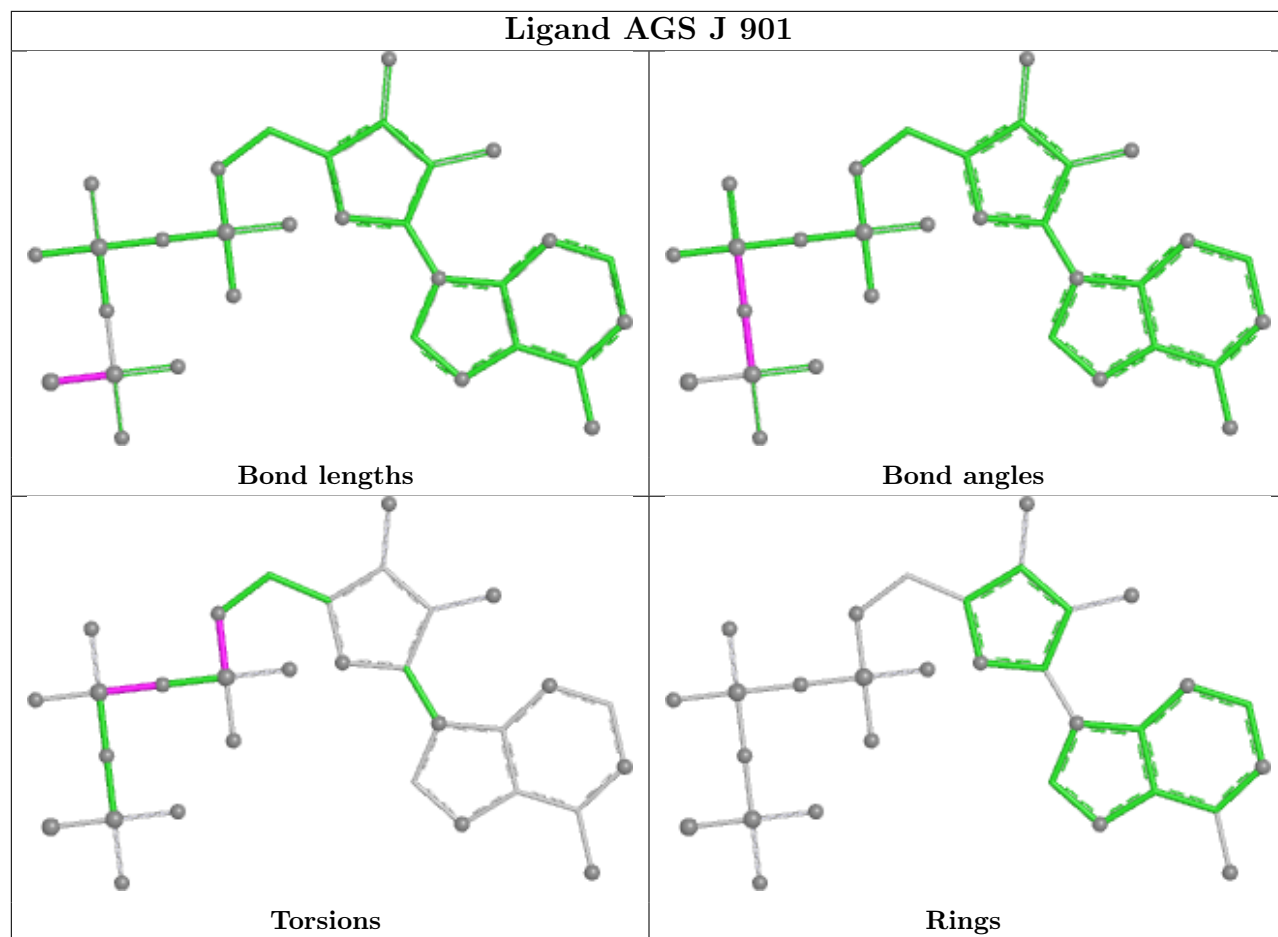






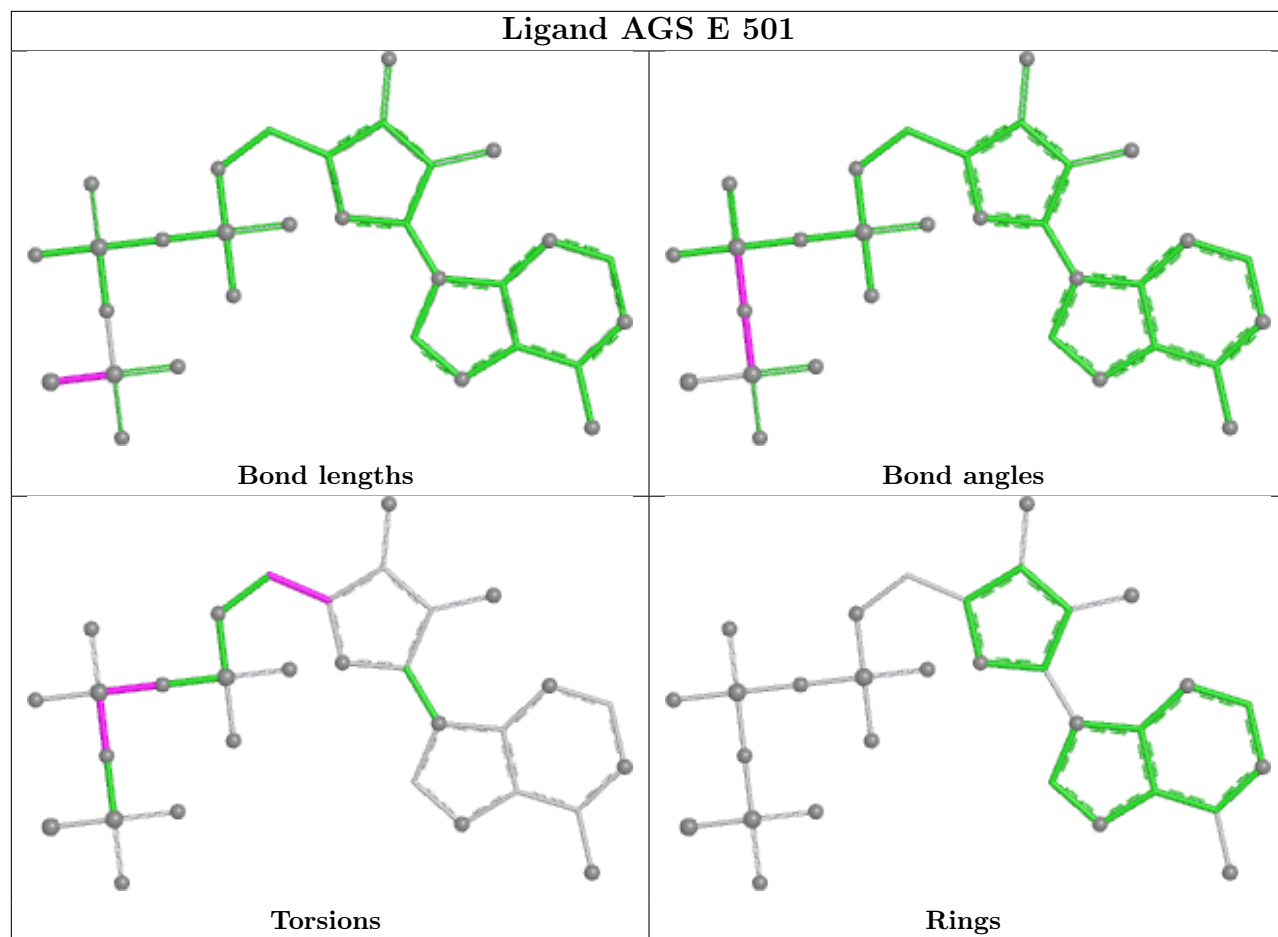


## Ligand AGS J 901



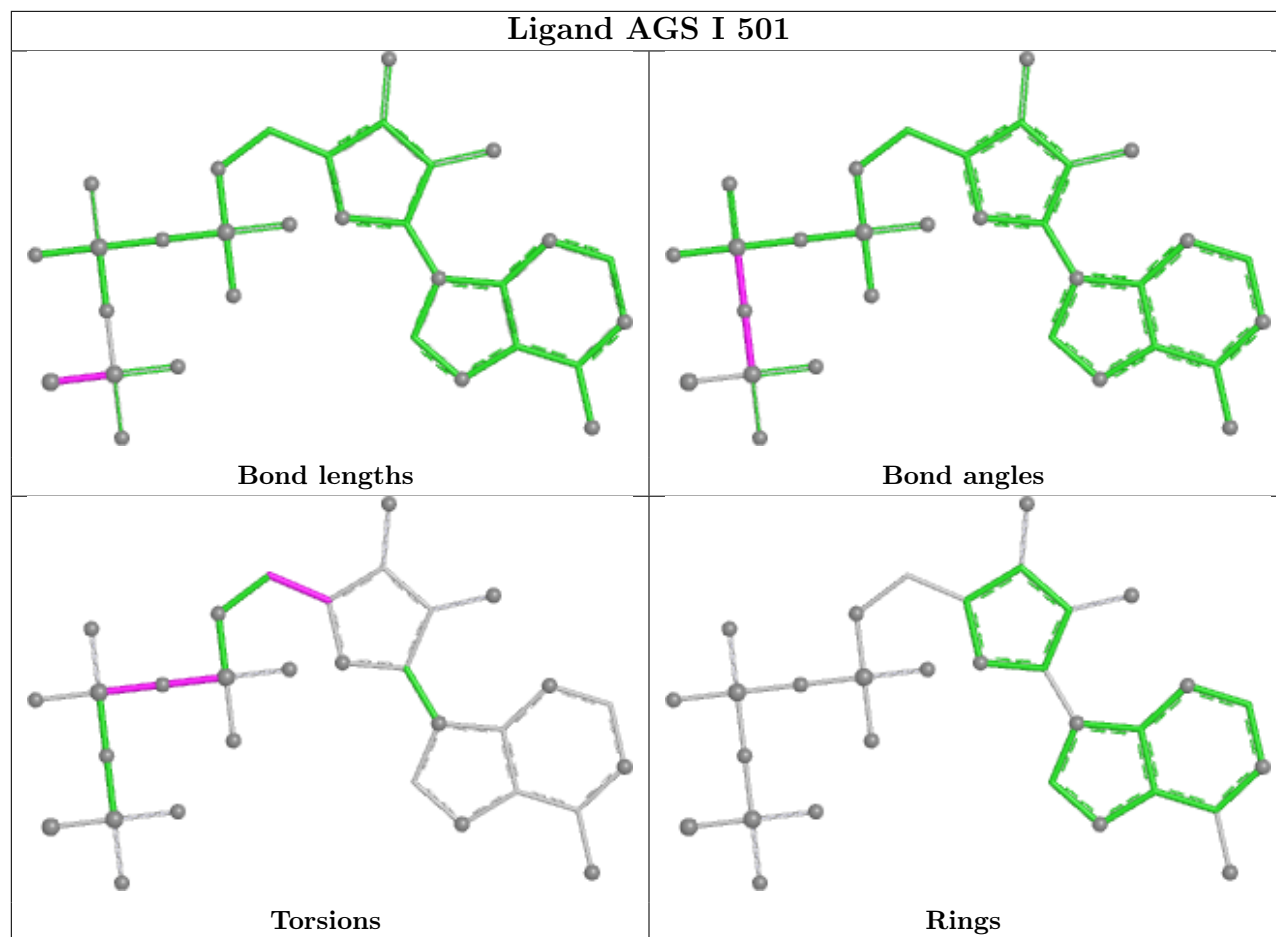


## Ligand AGS E 501



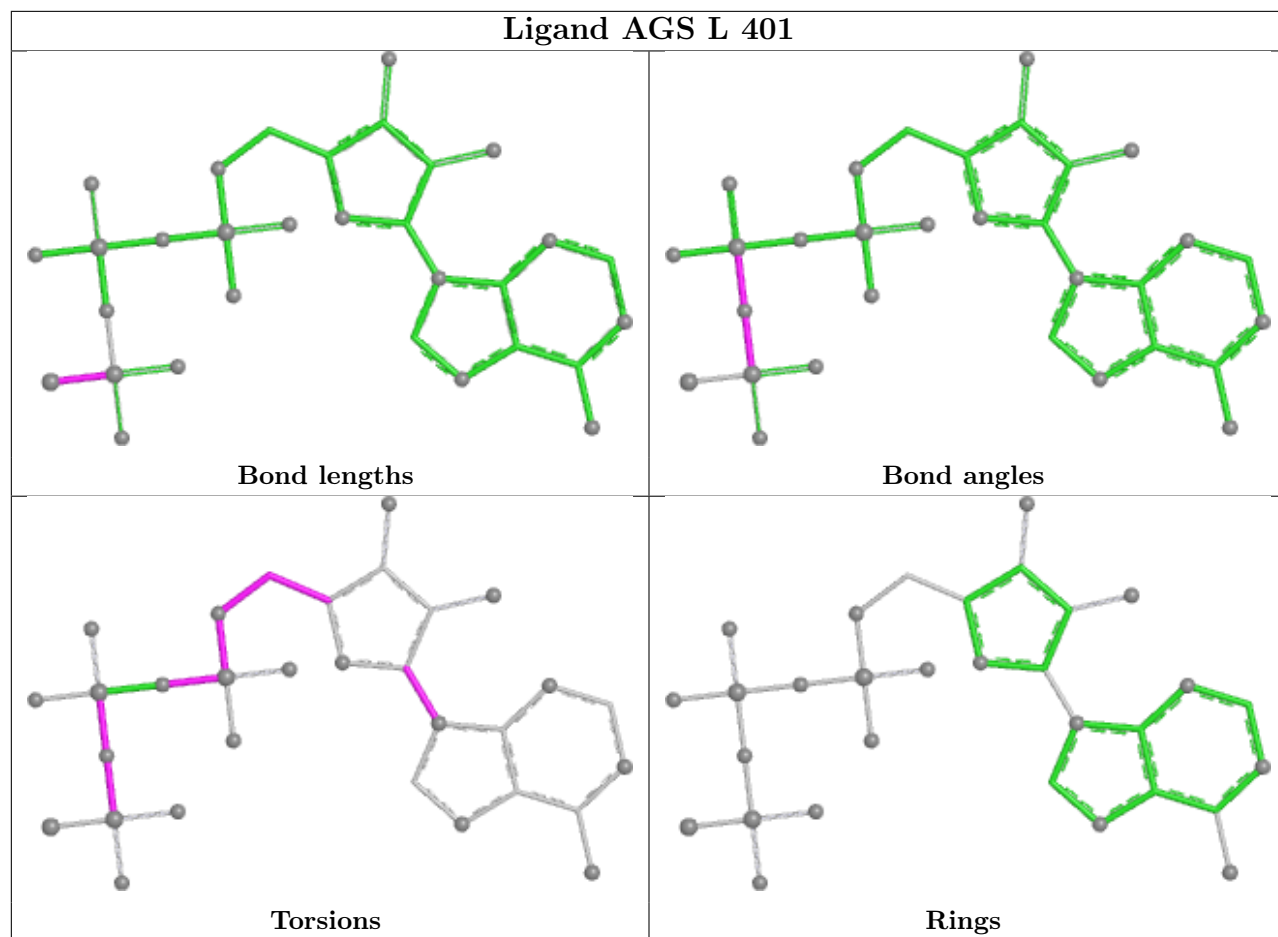


## Ligand AGS I 501

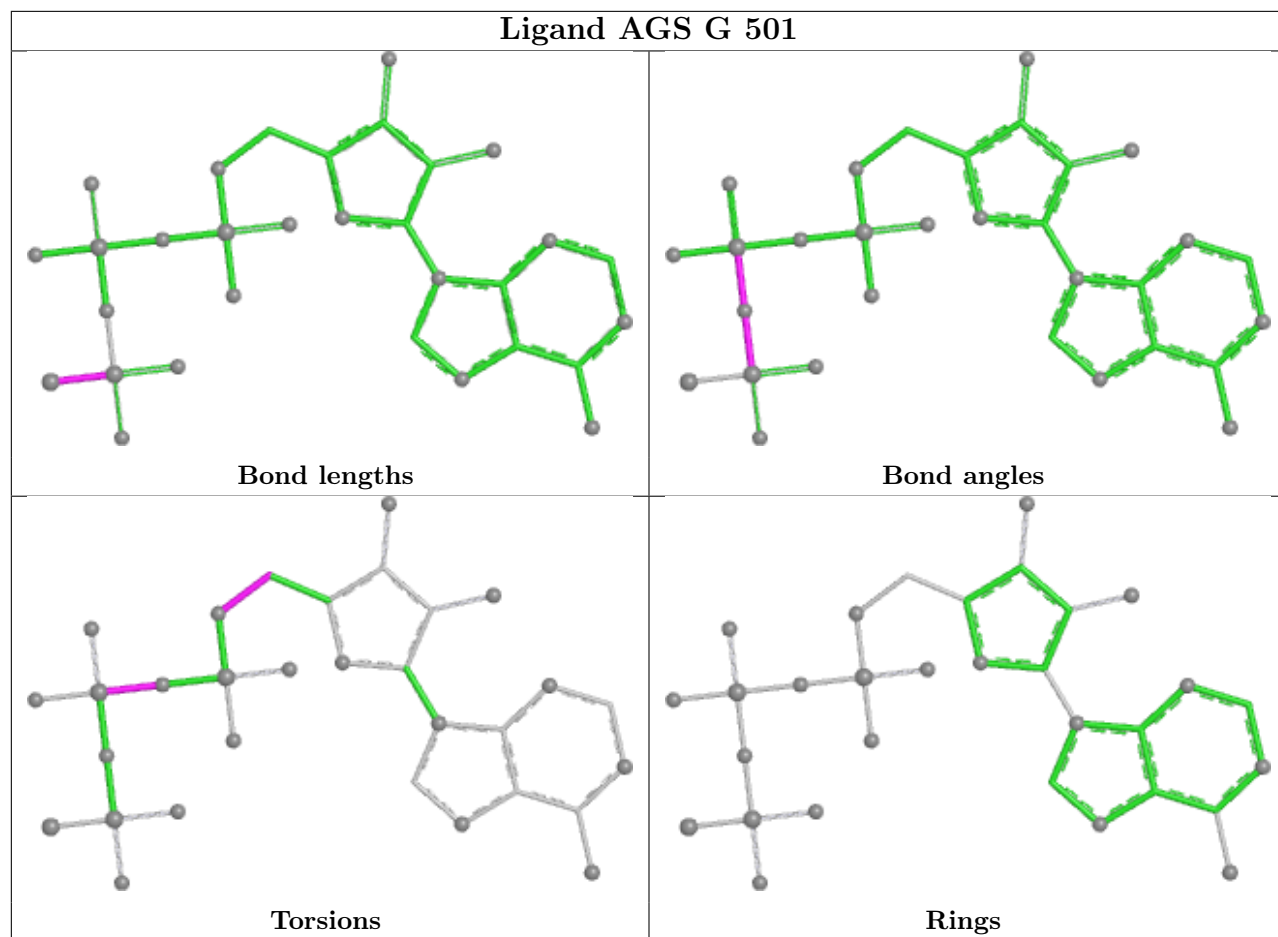




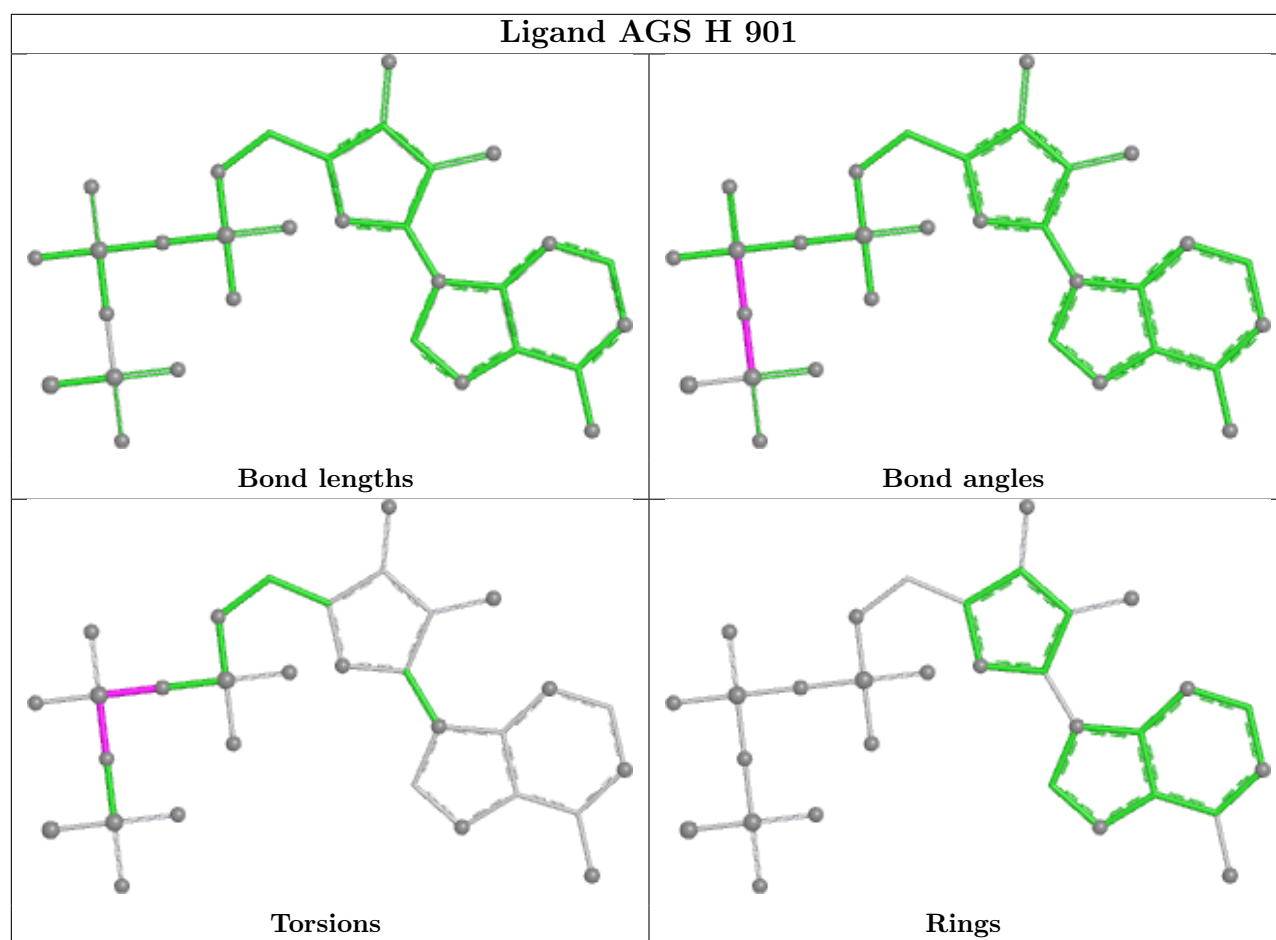
## Ligand AGS L 401











## 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.



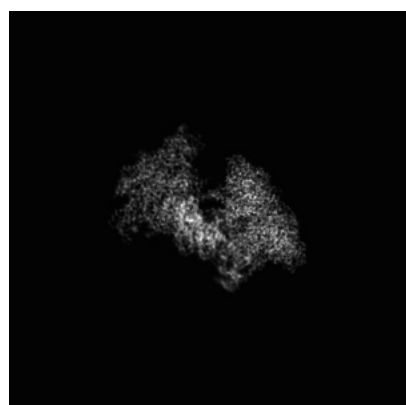
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45388. These allow visual inspection of the internal detail of the map and identification of artifacts.

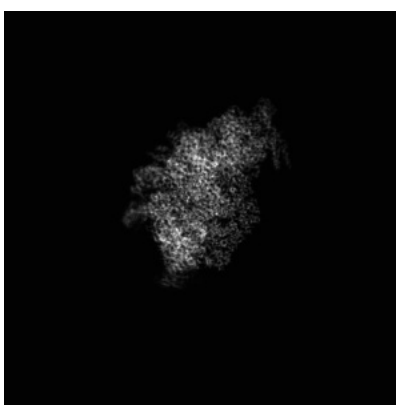
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

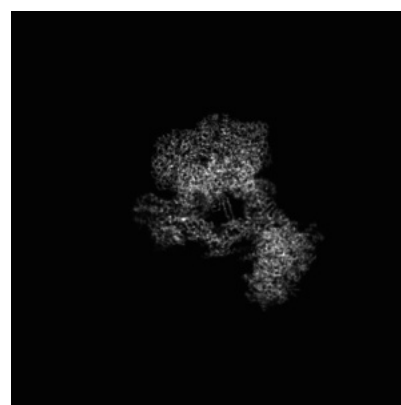
#### 6.1.1 Primary map



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: 240



Y Index: 240



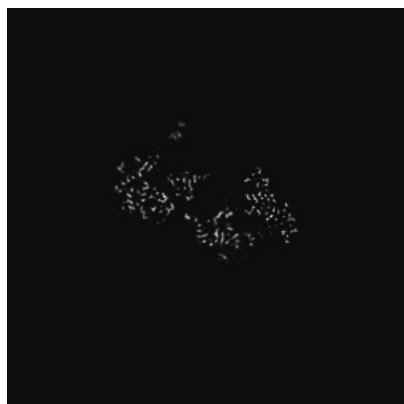
Z Index: 240



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: 296



Y Index: 287

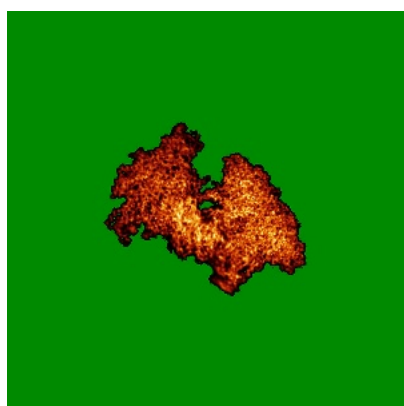


Z Index: 232

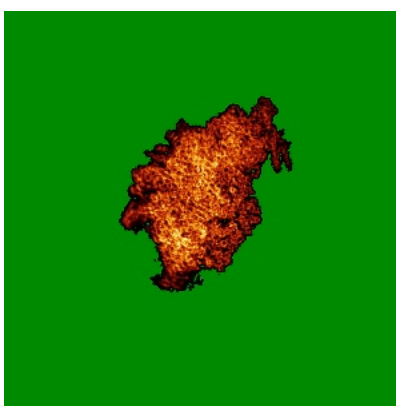
The images above show the largest variance slices of the map in three orthogonal directions.

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

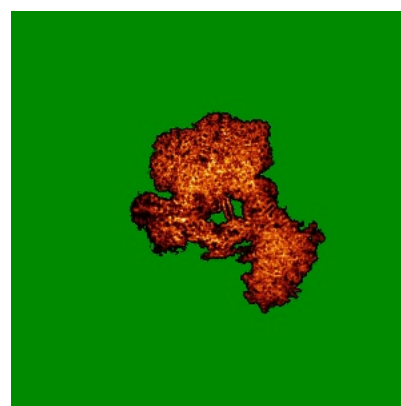
### 6.4.1 Primary map



X



Y



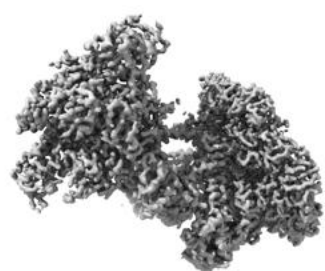
Z

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.

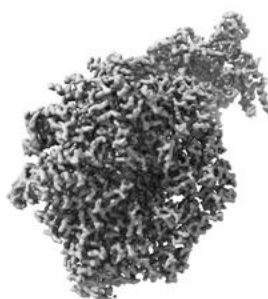


## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. 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](#)

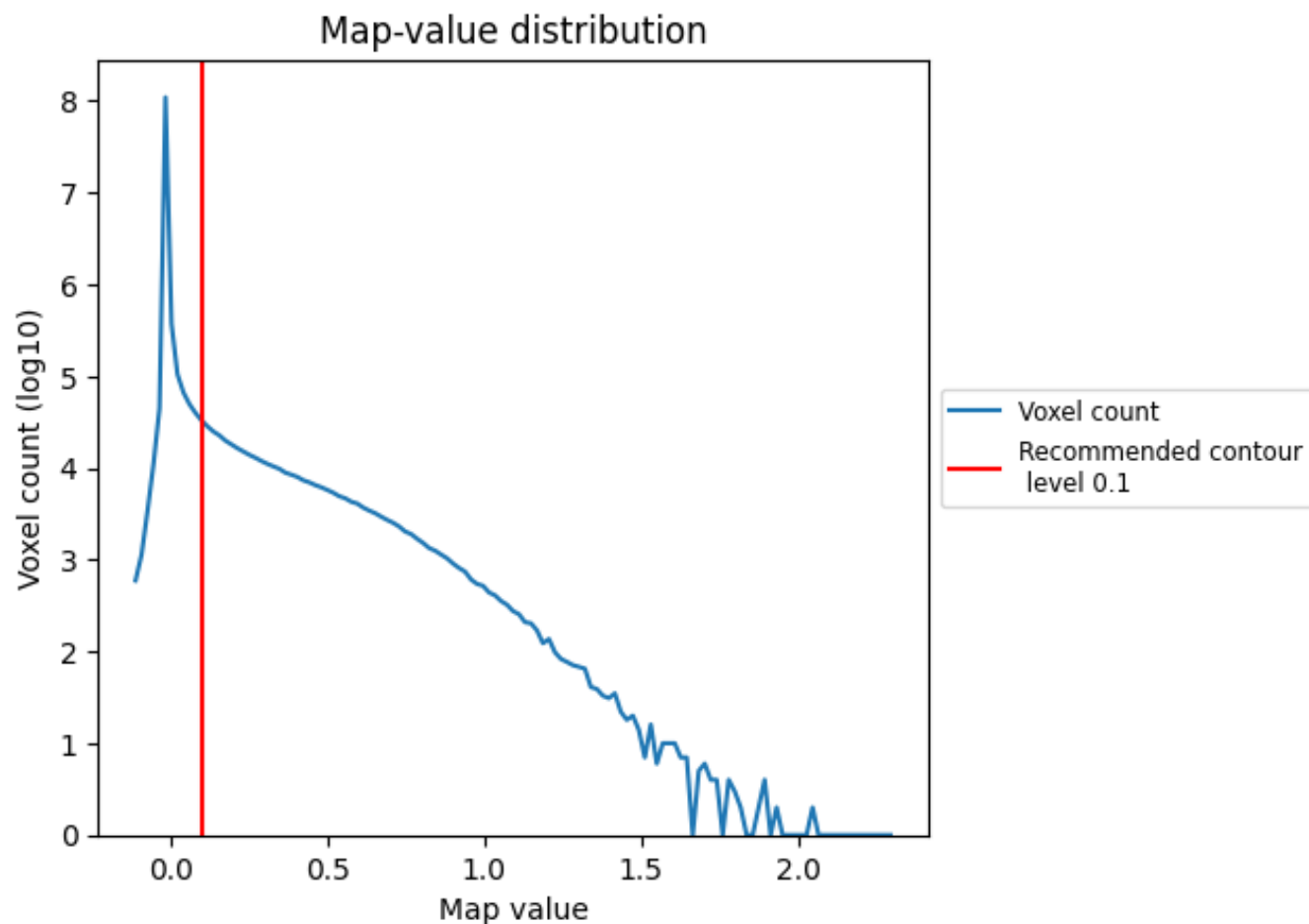
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

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

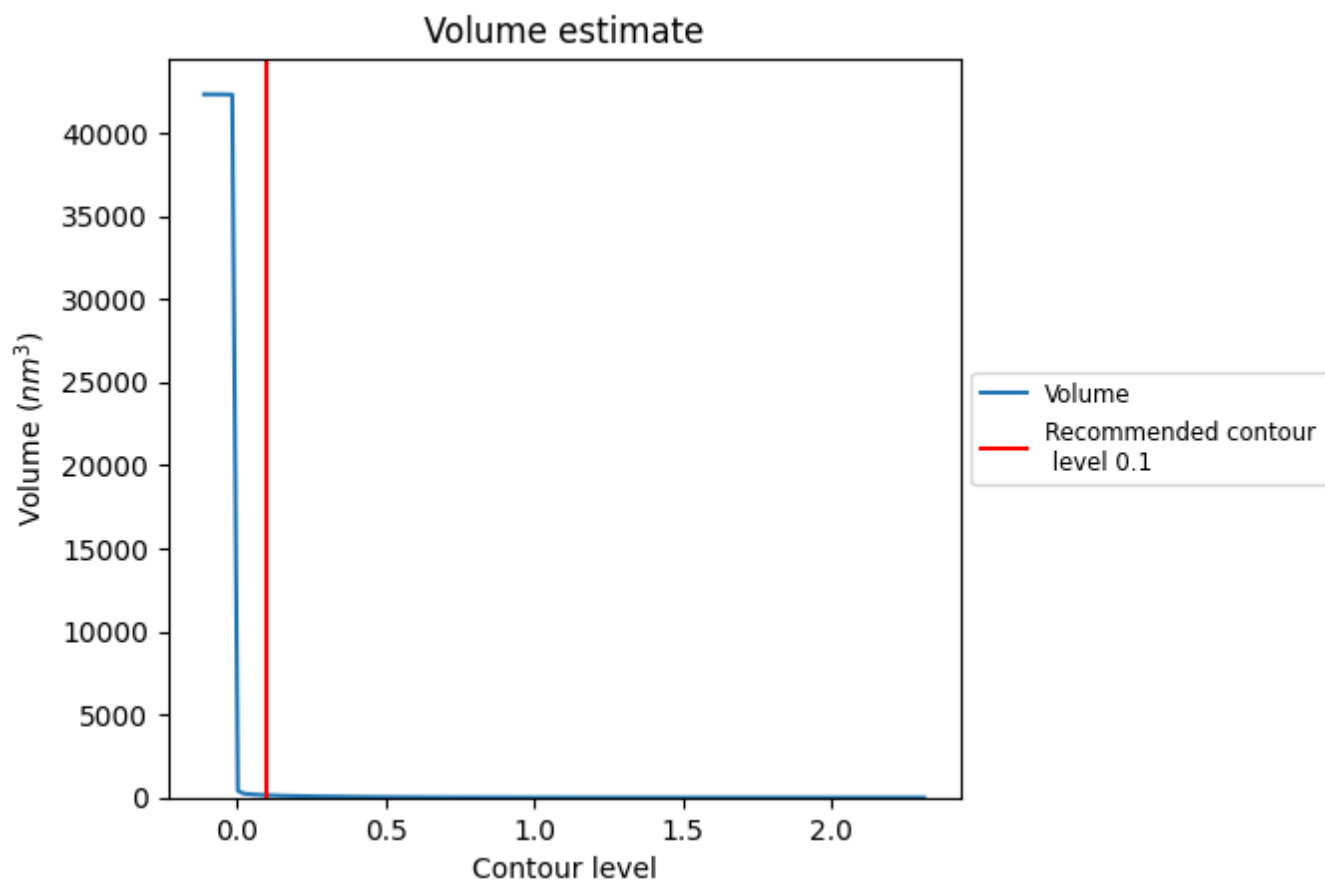
### 7.1 Map-value distribution [i](#)



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](#)

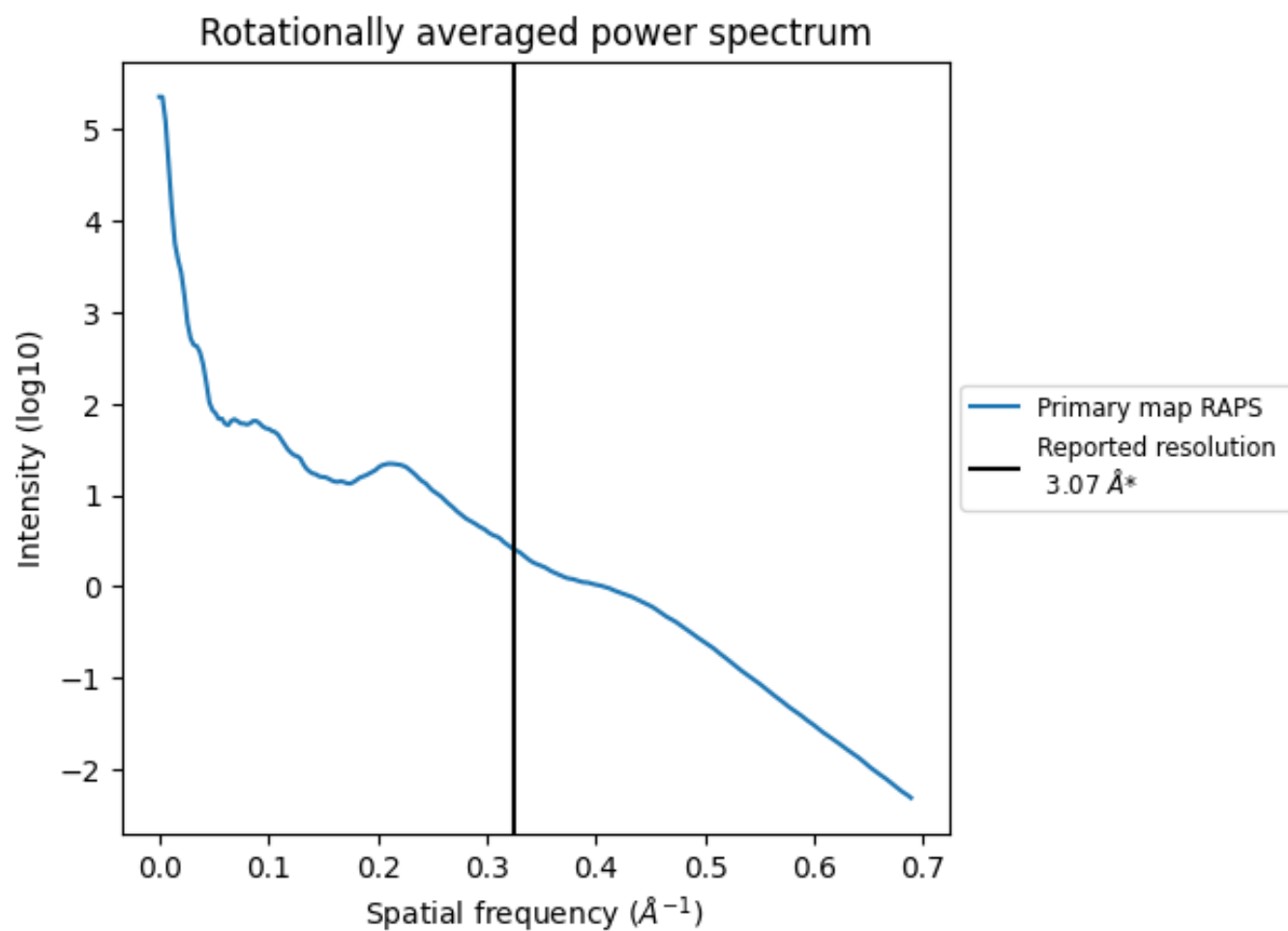


The volume at the recommended contour level is 141  $\text{nm}^3$ ; this corresponds to an approximate mass of 127 kDa.

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 0.326 Å<sup>-1</sup>



## 8 Fourier-Shell correlation ⓘ

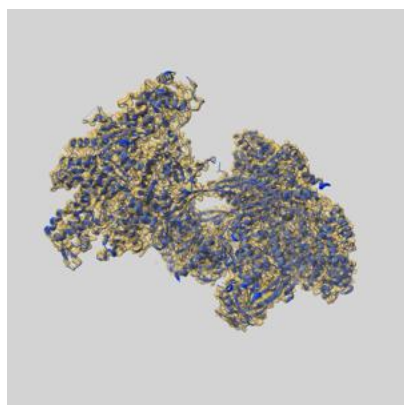
This section was not generated. No FSC curve or half-maps provided.



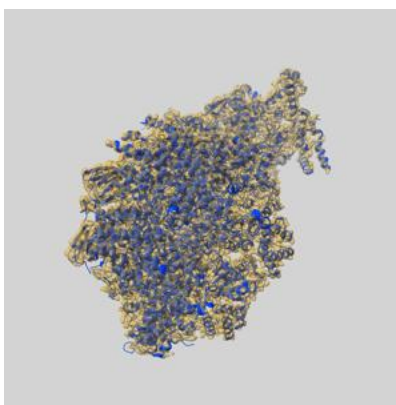
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45388 and PDB model 9CAE. Per-residue inclusion information can be found in section [3](#) on page [8](#).

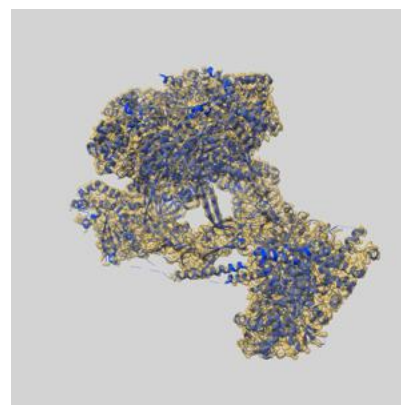
### 9.1 Map-model overlay [i](#)



X



Y

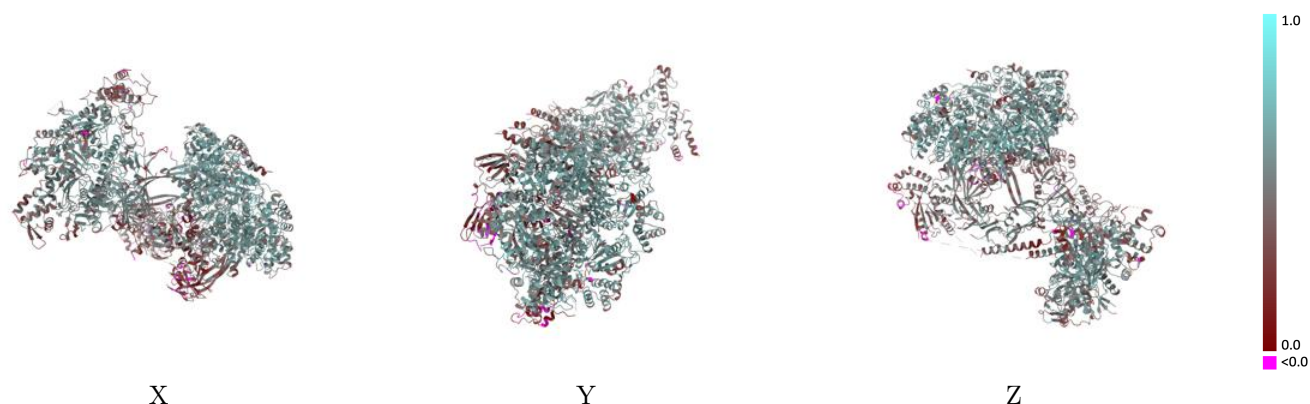


Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

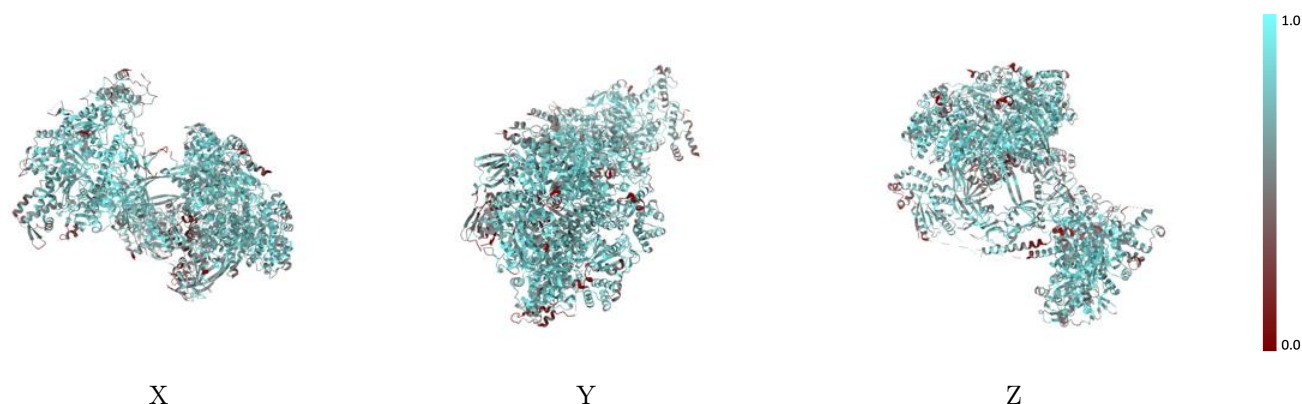


## 9.2 Q-score mapped to coordinate model [i](#)



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.

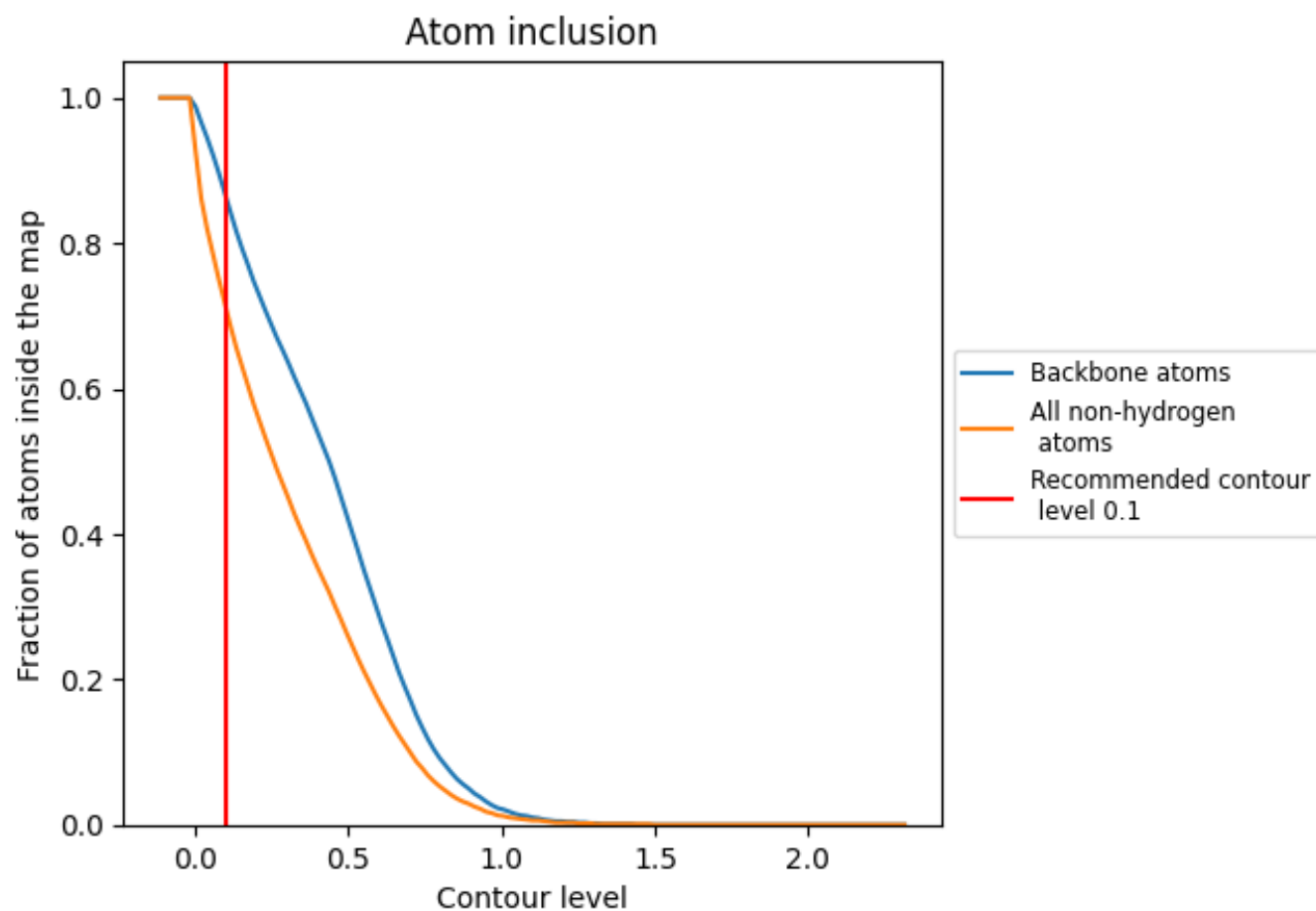
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.1).



## 9.4 Atom inclusion ⓘ



At the recommended contour level, 87% of all backbone atoms, 71% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7130	<div></div> 0.4900
A	<div></div> 0.6120	<div></div> 0.3560
B	<div></div> 0.7110	<div></div> 0.4320
C	<div></div> 0.7240	<div></div> 0.5040
E	<div></div> 0.7340	<div></div> 0.5270
F	<div></div> 0.7440	<div></div> 0.5350
G	<div></div> 0.7440	<div></div> 0.5420
H	<div></div> 0.7440	<div></div> 0.5330
I	<div></div> 0.7250	<div></div> 0.5030
J	<div></div> 0.6780	<div></div> 0.4830
L	<div></div> 0.7360	<div></div> 0.4970
M	<div></div> 0.7560	<div></div> 0.5190
N	<div></div> 0.6950	<div></div> 0.4640

