



## Full wwPDB EM Validation Report ⓘ

Mar 11, 2024 – 12:16 PM JST

PDB ID : 8WM7  
EMDB ID : EMD-37644  
Title : Cryo-EM structure of cyanobacterial nitrate/nitrite transporter NrtBCD in complex with signalling protein PII  
Authors : Li, B.; Zhou, C.Z.; Chen, Y.X.; Jiang, Y.L.  
Deposited on : 2023-10-03  
Resolution : 3.53 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:

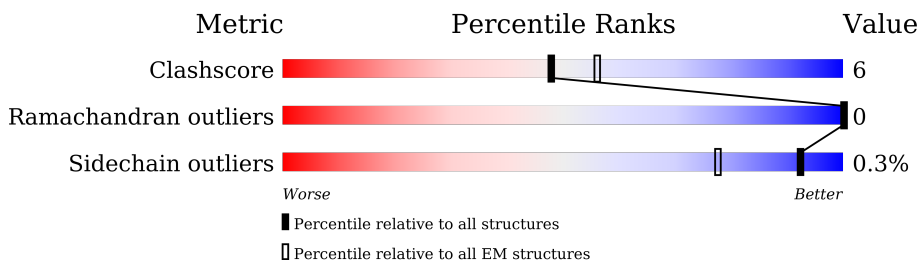
EMDB validation analysis : 0.0.1.dev70  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

# 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 3.53 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

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

Mol	Chain	Length	Quality of chain
1	A	279	76% 14% 9%
1	B	279	76% 15% 9%
2	C	682	85% 11% .
3	D	277	79% 14% 7%
4	E	118	74% 12% 14%
4	F	118	61% 18% 21%
4	G	118	59% 20% 20%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 27327 atoms, of which 13848 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 Nitrate transport permease protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	B	253	4016	1324	2058	304	328	2	0	0
1	A	253	4016	1324	2058	304	328	2	0	0

- Molecule 2 is a protein called Nitrate transport ATP-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	C	658	10386	3278	5227	903	957	21	0	0

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	658	SER	-	expression tag	UNP Q8YZ76
C	659	SER	-	expression tag	UNP Q8YZ76
C	660	GLY	-	expression tag	UNP Q8YZ76
C	661	ASP	-	expression tag	UNP Q8YZ76
C	662	TYR	-	expression tag	UNP Q8YZ76
C	663	LYS	-	expression tag	UNP Q8YZ76
C	664	ASP	-	expression tag	UNP Q8YZ76
C	665	HIS	-	expression tag	UNP Q8YZ76
C	666	ASP	-	expression tag	UNP Q8YZ76
C	667	GLY	-	expression tag	UNP Q8YZ76
C	668	ASP	-	expression tag	UNP Q8YZ76
C	669	TYR	-	expression tag	UNP Q8YZ76
C	670	LYS	-	expression tag	UNP Q8YZ76
C	671	ASP	-	expression tag	UNP Q8YZ76
C	672	HIS	-	expression tag	UNP Q8YZ76
C	673	ASP	-	expression tag	UNP Q8YZ76
C	674	ILE	-	expression tag	UNP Q8YZ76
C	675	ASP	-	expression tag	UNP Q8YZ76
C	676	TYR	-	expression tag	UNP Q8YZ76

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Chain	Residue	Modelled	Actual	Comment	Reference
C	677	LYS	-	expression tag	UNP Q8YZ76
C	678	ASP	-	expression tag	UNP Q8YZ76
C	679	ASP	-	expression tag	UNP Q8YZ76
C	680	ASP	-	expression tag	UNP Q8YZ76
C	681	ASP	-	expression tag	UNP Q8YZ76
C	682	LYS	-	expression tag	UNP Q8YZ76

- Molecule 3 is a protein called Nitrate transport ATP-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	D	257	4086	1304	2049	344	377	12	0	0

- Molecule 4 is a protein called Nitrogen regulatory protein P-II.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	E	101	1615	496	836	136	144	3	0	0
4	F	93	1498	461	776	126	132	3	0	0
4	G	94	1515	466	784	128	134	3	0	0

There are 18 discrepancies between the modelled and reference sequences:

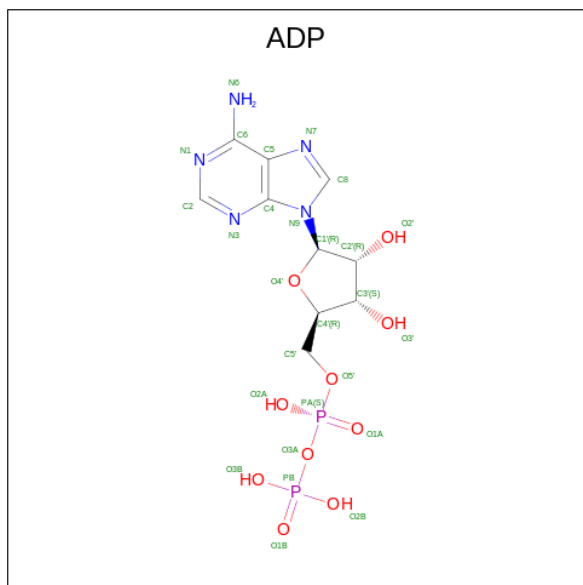
Chain	Residue	Modelled	Actual	Comment	Reference
E	113	HIS	-	expression tag	UNP Q9L422
E	114	HIS	-	expression tag	UNP Q9L422
E	115	HIS	-	expression tag	UNP Q9L422
E	116	HIS	-	expression tag	UNP Q9L422
E	117	HIS	-	expression tag	UNP Q9L422
E	118	HIS	-	expression tag	UNP Q9L422
F	113	HIS	-	expression tag	UNP Q9L422
F	114	HIS	-	expression tag	UNP Q9L422
F	115	HIS	-	expression tag	UNP Q9L422
F	116	HIS	-	expression tag	UNP Q9L422
F	117	HIS	-	expression tag	UNP Q9L422
F	118	HIS	-	expression tag	UNP Q9L422
G	113	HIS	-	expression tag	UNP Q9L422
G	114	HIS	-	expression tag	UNP Q9L422
G	115	HIS	-	expression tag	UNP Q9L422
G	116	HIS	-	expression tag	UNP Q9L422

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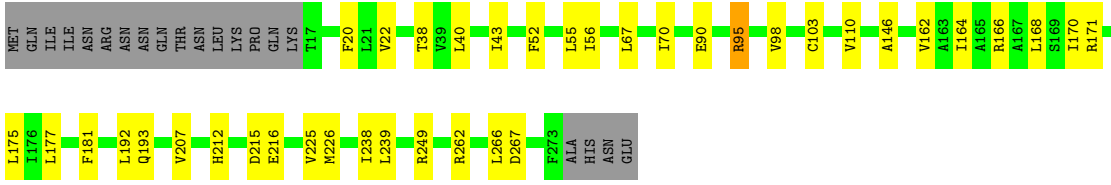
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Chain	Residue	Modelled	Actual	Comment	Reference
G	117	HIS	-	expression tag	UNP Q9L422
G	118	HIS	-	expression tag	UNP Q9L422

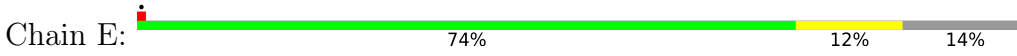
- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).



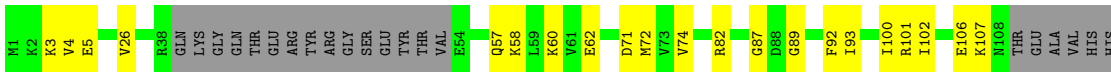




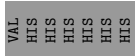
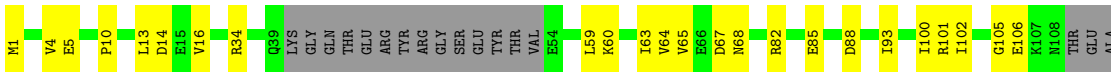
• Molecule 4: Nitrogen regulatory protein P-II



• Molecule 4: Nitrogen regulatory protein P-II



• Molecule 4: Nitrogen regulatory protein P-II



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	304482	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 ( $e^-/\text{\AA}^2$ )	55	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.945	Depositor
Minimum map value	-1.713	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.072	Depositor
Recommended contour level	0.243	Depositor
Map size (Å)	273.92, 273.92, 273.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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: ADP

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	0.25	0/2013	0.42	0/2761
1	B	0.25	0/2013	0.42	0/2761
2	C	0.24	0/5260	0.48	0/7141
3	D	0.24	0/2080	0.48	0/2823
4	E	0.24	0/783	0.50	0/1048
4	F	0.25	0/726	0.53	0/971
4	G	0.24	0/735	0.51	0/983
All	All	0.24	0/13610	0.47	0/18488

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	1958	2058	2058	31	0
1	B	1958	2058	2058	28	0
2	C	5159	5227	5227	53	0
3	D	2037	2049	2049	29	0
4	E	779	836	836	14	0
4	F	722	776	776	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	731	784	784	20	0
5	C	27	12	12	0	0
5	D	27	12	12	0	0
5	E	54	24	24	1	0
5	F	27	12	12	4	0
All	All	13479	13848	13848	173	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 6.

All (173) 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)
3:D:103:CYS:SG	3:D:166:ARG:NH2	2.50	0.84
4:G:1:MET:N	4:G:65:VAL:O	2.13	0.82
4:F:5:GLU:OE2	4:F:60:LYS:NZ	2.12	0.81
1:A:175:ASP:OD1	2:C:86:ASN:ND2	2.15	0.79
2:C:455:ASN:OD1	2:C:456:TYR:N	2.22	0.73
2:C:41:ILE:HD11	2:C:202:ALA:HB3	1.74	0.68
4:F:5:GLU:O	4:F:92:PHE:N	2.27	0.68
2:C:145:GLN:NE2	2:C:165:PRO:O	2.27	0.67
1:A:53:GLY:O	1:A:57:THR:HG23	1.95	0.66
4:F:4:VAL:HA	4:F:93:ILE:HG22	1.78	0.65
2:C:72:GLU:OE2	4:E:86:ILE:HD11	1.97	0.65
1:B:130:PRO:CG	1:A:219:VAL:HG11	2.26	0.65
2:C:59:ASP:OD1	2:C:60:ARG:N	2.30	0.65
1:B:130:PRO:CB	1:A:219:VAL:HG11	2.28	0.64
3:D:98:VAL:HB	3:D:177:LEU:HD23	1.80	0.64
1:A:222:GLU:O	1:A:226:GLY:N	2.30	0.63
3:D:20:PHE:O	3:D:22:VAL:HG23	1.96	0.63
2:C:11:ASP:OD1	2:C:27:ASN:N	2.28	0.63
4:E:62:GLU:OE1	4:G:60:LYS:NZ	2.31	0.63
2:C:11:ASP:O	2:C:13:ILE:HD12	1.97	0.63
4:F:5:GLU:N	4:F:92:PHE:O	2.31	0.62
4:F:71:ASP:OD1	4:F:72:MET:N	2.33	0.62
1:A:80:LEU:HD21	1:A:233:PHE:CE1	2.35	0.61
2:C:104:ASP:OD2	2:C:115:ARG:NH1	2.33	0.61
1:B:105:LEU:HD23	1:B:105:LEU:O	2.00	0.61
4:G:101:ARG:O	4:G:105:GLY:N	2.33	0.61
4:E:91:ILE:HD11	4:F:102:ILE:HD11	1.82	0.60
2:C:200:ASP:OD2	3:D:262:ARG:NH2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:82:ARG:NH2	4:G:88:ASP:OD2	2.35	0.59
2:C:72:GLU:HB2	4:E:86:ILE:HD11	1.85	0.59
3:D:55:LEU:HD23	3:D:225:VAL:CG2	2.33	0.58
4:G:67:ASP:OD1	4:G:68:ASN:N	2.35	0.58
1:A:152:VAL:O	1:A:156:THR:HG22	2.02	0.58
1:B:104:ILE:O	1:B:108:LEU:HD23	2.04	0.58
2:C:287:THR:HG22	2:C:453:PRO:HD3	1.86	0.58
3:D:225:VAL:HG12	3:D:238:ILE:HG23	1.85	0.58
2:C:178:GLN:OE1	2:C:234:ARG:NH1	2.38	0.57
1:B:130:PRO:HG3	1:A:219:VAL:HG11	1.86	0.57
1:A:98:ALA:O	1:A:102:GLY:N	2.38	0.57
1:A:153:ILE:HD11	1:A:218:ILE:HD13	1.86	0.57
1:A:217:ALA:O	1:A:221:ALA:N	2.37	0.57
4:F:89:GLY:O	4:G:102:ILE:HG22	2.05	0.56
2:C:161:LEU:O	2:C:162:LEU:HD12	2.03	0.56
2:C:199:VAL:HG23	2:C:250:ILE:HG21	1.86	0.56
3:D:181:PHE:CE1	3:D:192:LEU:HD22	2.39	0.56
3:D:193:GLN:OE1	3:D:249:ARG:NH1	2.38	0.56
4:F:87:GLY:N	5:F:201:ADP:O2A	2.39	0.56
3:D:55:LEU:HD11	3:D:67:LEU:HD21	1.88	0.56
2:C:25:LEU:HD21	2:C:47:GLY:HA3	1.87	0.55
4:G:4:VAL:HG22	4:G:93:ILE:CD1	2.36	0.55
3:D:162:VAL:HG13	3:D:162:VAL:O	2.07	0.55
1:B:52:PRO:HG2	1:B:250:ILE:HD12	1.89	0.55
2:C:226:VAL:O	2:C:226:VAL:HG23	2.07	0.55
2:C:398:LEU:HB2	2:C:428:LEU:HD23	1.87	0.55
1:B:126:LEU:O	1:B:129:VAL:HG12	2.08	0.54
1:B:224:LEU:HD21	1:A:224:LEU:HD23	1.90	0.54
1:B:255:TYR:O	1:B:259:VAL:HG23	2.08	0.53
1:A:236:ASP:OD1	1:A:237:ALA:N	2.42	0.53
2:C:41:ILE:HD12	2:C:209:VAL:CG1	2.38	0.53
5:F:201:ADP:O1A	4:G:101:ARG:NH1	2.42	0.53
2:C:495:THR:O	2:C:495:THR:HG22	2.07	0.52
4:E:29:THR:O	4:E:29:THR:HG22	2.08	0.52
1:A:87:SER:OG	1:A:230:ILE:N	2.39	0.52
4:E:104:THR:OG1	4:E:106:GLU:OE1	2.28	0.52
1:A:153:ILE:CD1	1:A:218:ILE:HD13	2.41	0.51
2:C:5:VAL:HG21	2:C:159:LEU:HD13	1.93	0.51
2:C:281:ILE:CG2	2:C:292:LEU:HD21	2.41	0.51
1:A:251:LEU:O	1:A:254:ILE:HG22	2.11	0.50
1:A:80:LEU:HD21	1:A:233:PHE:CZ	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:170:ILE:HG22	3:D:171:ARG:N	2.26	0.50
2:C:41:ILE:HD12	2:C:209:VAL:HG11	1.94	0.50
2:C:235:LEU:HD12	3:D:267:ASP:OD1	2.13	0.49
1:B:54:PRO:HA	1:B:57:THR:HG22	1.95	0.49
4:F:92:PHE:CE1	4:G:64:VAL:HG21	2.48	0.49
1:B:123:PHE:HD2	1:B:162:LEU:HD11	1.77	0.49
3:D:90:GLU:O	3:D:95:ARG:NH2	2.46	0.49
4:E:32:GLU:OE1	4:G:34:ARG:NH2	2.46	0.49
1:B:71:PHE:O	1:B:79:GLY:N	2.46	0.48
2:C:288:ASP:CG	2:C:361:SER:HG	2.16	0.48
3:D:110:VAL:HG21	3:D:146:ALA:O	2.14	0.48
1:B:33:LEU:O	1:B:37:LEU:HD23	2.14	0.48
3:D:55:LEU:CD1	3:D:67:LEU:HD21	2.43	0.48
4:E:3:LYS:NZ	4:E:62:GLU:OE2	2.42	0.48
3:D:40:LEU:HD12	3:D:43:ILE:CD1	2.44	0.48
2:C:338:MET:N	2:C:339:PRO:CD	2.77	0.47
1:B:132:LEU:HD23	1:B:132:LEU:O	2.15	0.47
1:B:123:PHE:CD2	1:B:162:LEU:HD11	2.49	0.47
2:C:347:GLY:O	2:C:348:SER:OG	2.24	0.47
3:D:192:LEU:O	3:D:192:LEU:HD23	2.15	0.47
2:C:649:GLN:OE1	2:C:650:ILE:N	2.48	0.46
1:A:207:LEU:O	1:A:211:ILE:HG22	2.16	0.46
3:D:38:THR:O	3:D:38:THR:HG23	2.15	0.46
2:C:368:THR:HG22	2:C:448:TYR:HB2	1.97	0.46
4:F:58:LYS:NZ	5:F:201:ADP:O2'	2.46	0.46
2:C:398:LEU:N	2:C:427:SER:O	2.49	0.46
1:B:90:ARG:NH1	1:B:222:GLU:OE1	2.48	0.45
4:G:14:ASP:N	4:G:14:ASP:OD1	2.48	0.45
2:C:10:VAL:HG23	2:C:61:ALA:HB1	1.97	0.45
4:E:63:ILE:HG22	4:E:65:VAL:HG13	1.98	0.45
1:B:112:ASN:HB2	1:B:115:VAL:HG12	1.98	0.45
4:E:101:ARG:NH1	5:E:202:ADP:O3B	2.50	0.45
1:B:200:VAL:N	1:B:201:PRO:HD2	2.32	0.45
1:A:251:LEU:HD11	1:A:255:TYR:CZ	2.52	0.45
4:F:100:ILE:HG22	4:F:101:ARG:O	2.16	0.45
1:A:75:GLU:OE2	1:A:75:GLU:HA	2.17	0.45
3:D:215:ASP:OD1	3:D:216:GLU:N	2.49	0.45
2:C:192:CYS:SG	2:C:193:VAL:N	2.90	0.45
1:A:94:GLY:O	1:A:95:PHE:HB3	2.18	0.44
2:C:395:ILE:H	2:C:395:ILE:HD12	1.81	0.44
2:C:288:ASP:OD2	2:C:361:SER:OG	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:4:VAL:N	4:E:63:ILE:O	2.50	0.44
4:G:4:VAL:HG22	4:G:93:ILE:HD13	1.99	0.44
1:B:131:PRO:O	1:B:132:LEU:HB3	2.18	0.44
4:E:102:ILE:O	4:G:82:ARG:NH1	2.50	0.44
1:A:234:ILE:HG23	1:A:249:ILE:HG23	1.99	0.44
2:C:509:TYR:HE1	2:C:519:ILE:HD11	1.82	0.44
4:E:90:LYS:C	4:E:91:ILE:HD12	2.39	0.44
4:G:63:ILE:HG22	4:G:65:VAL:HG13	2.00	0.44
1:A:93:LEU:O	1:A:93:LEU:HD23	2.18	0.44
2:C:392:PRO:HB3	2:C:395:ILE:HD11	1.99	0.43
4:F:58:LYS:NZ	5:F:201:ADP:O3'	2.50	0.43
1:B:41:GLN:O	1:B:42:LEU:HB2	2.17	0.43
2:C:235:LEU:HD11	3:D:266:LEU:HB3	2.01	0.43
1:B:234:ILE:HG21	1:A:136:PRO:HG2	2.00	0.43
2:C:358:LEU:HD11	2:C:504:ILE:HG13	1.99	0.43
4:G:85:GLU:N	4:G:85:GLU:OE2	2.51	0.43
1:B:109:ILE:HG22	1:B:110:GLY:N	2.34	0.43
2:C:439:GLN:OE1	2:C:444:ASN:ND2	2.51	0.43
2:C:281:ILE:HG22	2:C:292:LEU:HD21	2.01	0.43
1:A:200:VAL:N	1:A:201:PRO:HD2	2.34	0.43
4:G:106:GLU:OE1	4:G:106:GLU:N	2.47	0.43
2:C:213:THR:HG1	2:C:219:HIS:H	1.67	0.42
4:F:106:GLU:OE1	4:F:107:LYS:N	2.52	0.42
2:C:360:LEU:HD12	2:C:360:LEU:O	2.19	0.42
2:C:563:LEU:O	2:C:566:THR:HG23	2.19	0.42
1:A:254:ILE:O	1:A:258:LEU:HD23	2.19	0.42
2:C:358:LEU:HG	2:C:358:LEU:O	2.18	0.42
3:D:52:PHE:CD2	3:D:207:VAL:HG11	2.53	0.42
1:B:95:PHE:O	1:B:95:PHE:CG	2.73	0.42
4:G:13:LEU:O	4:G:16:VAL:HG22	2.20	0.42
2:C:403:SER:O	2:C:408:ASN:ND2	2.49	0.42
2:C:571:ARG:HH22	2:C:603:THR:HG22	1.84	0.42
1:A:153:ILE:HD11	1:A:218:ILE:CD1	2.48	0.42
3:D:181:PHE:CZ	3:D:192:LEU:HD22	2.54	0.42
3:D:67:LEU:HA	3:D:70:ILE:HG12	2.01	0.42
3:D:226:MET:CE	3:D:239:LEU:HD13	2.49	0.41
2:C:571:ARG:HH11	2:C:571:ARG:HG3	1.85	0.41
4:E:91:ILE:HD11	4:F:102:ILE:CD1	2.50	0.41
4:G:10:PRO:HA	4:G:59:LEU:HD23	2.01	0.41
2:C:89:LEU:HD12	2:C:144:LYS:HG2	2.03	0.41
2:C:321:ALA:O	2:C:325:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:40:LEU:HD12	3:D:43:ILE:HD11	2.03	0.41
4:F:57:GLN:OE1	4:F:57:GLN:HA	2.20	0.41
4:F:74:VAL:CG2	4:G:100:ILE:HD11	2.51	0.41
1:B:243:GLU:HG2	1:B:244:THR:N	2.35	0.41
2:C:570:ASN:OD1	2:C:570:ASN:N	2.54	0.41
3:D:56:ILE:HG23	3:D:226:MET:HG2	2.03	0.41
1:B:132:LEU:CD1	1:B:220:ALA:HB1	2.51	0.41
1:A:123:PHE:O	1:A:127:ARG:N	2.49	0.41
1:A:218:ILE:HG23	1:A:219:VAL:N	2.35	0.41
2:C:306:LEU:HD11	2:C:495:THR:HG23	2.03	0.41
1:B:222:GLU:HA	1:B:222:GLU:OE2	2.21	0.40
4:F:26:VAL:O	4:F:26:VAL:HG23	2.22	0.40
1:B:73:ASN:HB2	1:B:77:ASP:OD1	2.21	0.40
3:D:164:ILE:O	3:D:168:LEU:N	2.53	0.40
1:B:125:VAL:HG22	1:A:261:LEU:HD22	2.02	0.40
2:C:73:ILE:O	2:C:73:ILE:HG13	2.21	0.40
2:C:440:LEU:HD12	2:C:448:TYR:HE1	1.87	0.40
3:D:56:ILE:HD11	3:D:212:HIS:O	2.22	0.40
3:D:175:LEU:O	3:D:207:VAL:HG23	2.21	0.40
1:A:33:LEU:O	1:A:37:LEU:HD13	2.22	0.40
4:F:3:LYS:NZ	4:F:62:GLU:OE2	2.47	0.40
4:G:5:GLU:O	4:G:5:GLU:HG2	2.21	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	251/279 (90%)	237 (94%)	14 (6%)	0	100	100
1	B	251/279 (90%)	238 (95%)	13 (5%)	0	100	100
2	C	656/682 (96%)	589 (90%)	67 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	255/277 (92%)	226 (89%)	29 (11%)	0	100	100
4	E	97/118 (82%)	90 (93%)	7 (7%)	0	100	100
4	F	89/118 (75%)	79 (89%)	10 (11%)	0	100	100
4	G	90/118 (76%)	86 (96%)	4 (4%)	0	100	100
All	All	1689/1871 (90%)	1545 (92%)	144 (8%)	0	100	100

There are no Ramachandran outliers to report.

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	212/233 (91%)	211 (100%)	1 (0%)	88	95
1	B	212/233 (91%)	210 (99%)	2 (1%)	78	90
2	C	556/579 (96%)	556 (100%)	0	100	100
3	D	224/243 (92%)	223 (100%)	1 (0%)	91	97
4	E	85/101 (84%)	85 (100%)	0	100	100
4	F	79/101 (78%)	78 (99%)	1 (1%)	69	87
4	G	80/101 (79%)	80 (100%)	0	100	100
All	All	1448/1591 (91%)	1443 (100%)	5 (0%)	92	98

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	25	LYS
1	B	127	ARG
1	A	127	ARG
3	D	95	ARG
4	F	82	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

5 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
5	ADP	E	201	-	24,29,29	0.93	1 (4%)	29,45,45	1.52	4 (13%)
5	ADP	D	301	-	24,29,29	0.94	1 (4%)	29,45,45	1.51	5 (17%)
5	ADP	E	202	-	24,29,29	0.93	1 (4%)	29,45,45	1.49	4 (13%)
5	ADP	C	701	-	24,29,29	0.95	1 (4%)	29,45,45	1.49	4 (13%)
5	ADP	F	201	-	24,29,29	0.95	1 (4%)	29,45,45	1.47	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ADP	E	201	-	-	5/12/32/32	0/3/3/3
5	ADP	D	301	-	-	2/12/32/32	0/3/3/3
5	ADP	E	202	-	-	2/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ADP	C	701	-	-	2/12/32/32	0/3/3/3
5	ADP	F	201	-	-	3/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	201	ADP	C5-C4	2.39	1.47	1.40
5	C	701	ADP	C5-C4	2.39	1.47	1.40
5	D	301	ADP	C5-C4	2.37	1.47	1.40
5	E	202	ADP	C5-C4	2.35	1.47	1.40
5	E	201	ADP	C5-C4	2.30	1.47	1.40

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	201	ADP	PA-O3A-PB	-3.84	119.63	132.83
5	D	301	ADP	PA-O3A-PB	-3.84	119.64	132.83
5	D	301	ADP	N3-C2-N1	-3.73	122.85	128.68
5	C	701	ADP	N3-C2-N1	-3.63	123.01	128.68
5	E	202	ADP	N3-C2-N1	-3.63	123.01	128.68
5	E	201	ADP	N3-C2-N1	-3.63	123.01	128.68
5	F	201	ADP	N3-C2-N1	-3.61	123.04	128.68
5	E	202	ADP	C3'-C2'-C1'	3.61	106.41	100.98
5	C	701	ADP	PA-O3A-PB	-3.53	120.73	132.83
5	F	201	ADP	PA-O3A-PB	-3.43	121.06	132.83
5	E	201	ADP	C3'-C2'-C1'	3.42	106.13	100.98
5	F	201	ADP	C3'-C2'-C1'	3.22	105.82	100.98
5	C	701	ADP	C3'-C2'-C1'	3.10	105.64	100.98
5	E	202	ADP	PA-O3A-PB	-3.02	122.47	132.83
5	D	301	ADP	C4-C5-N7	-2.88	106.40	109.40
5	D	301	ADP	C3'-C2'-C1'	2.83	105.25	100.98
5	C	701	ADP	C4-C5-N7	-2.77	106.51	109.40
5	F	201	ADP	C4-C5-N7	-2.55	106.74	109.40
5	E	201	ADP	C4-C5-N7	-2.50	106.79	109.40
5	E	202	ADP	C4-C5-N7	-2.50	106.80	109.40
5	D	301	ADP	C2-N1-C6	2.05	122.26	118.75

There are no chirality outliers.

All (14) torsion outliers are listed below:

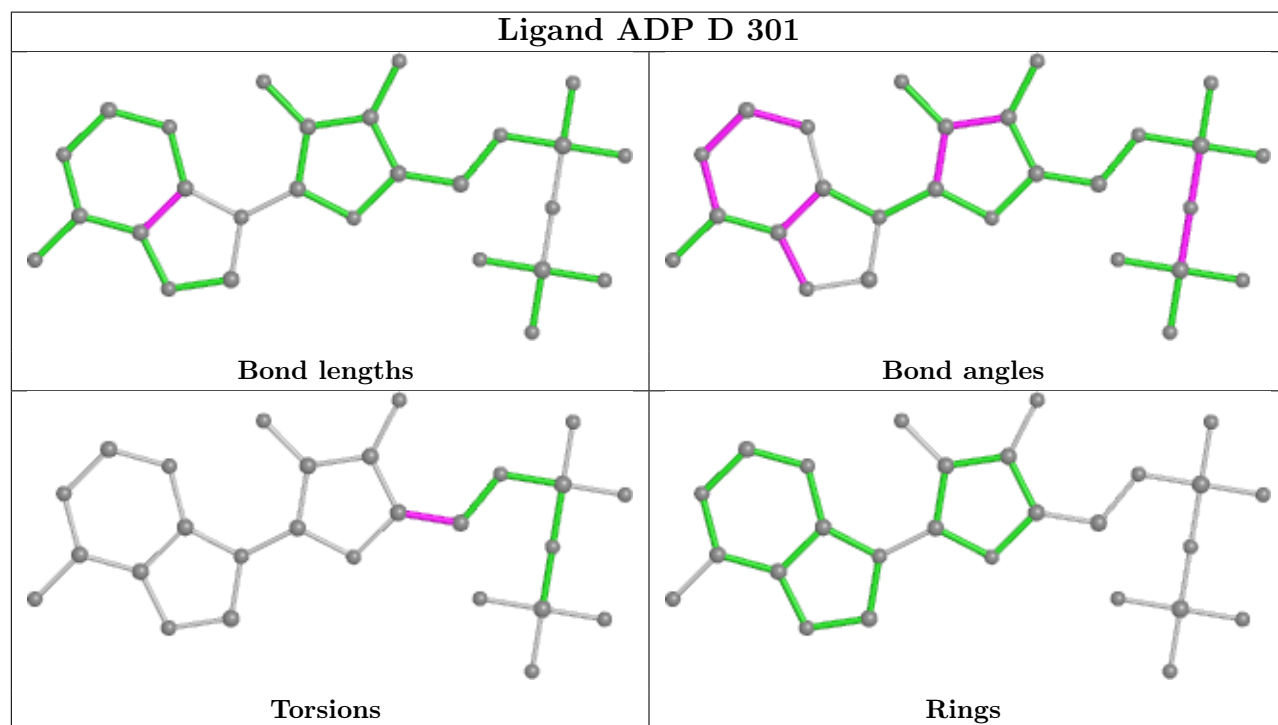
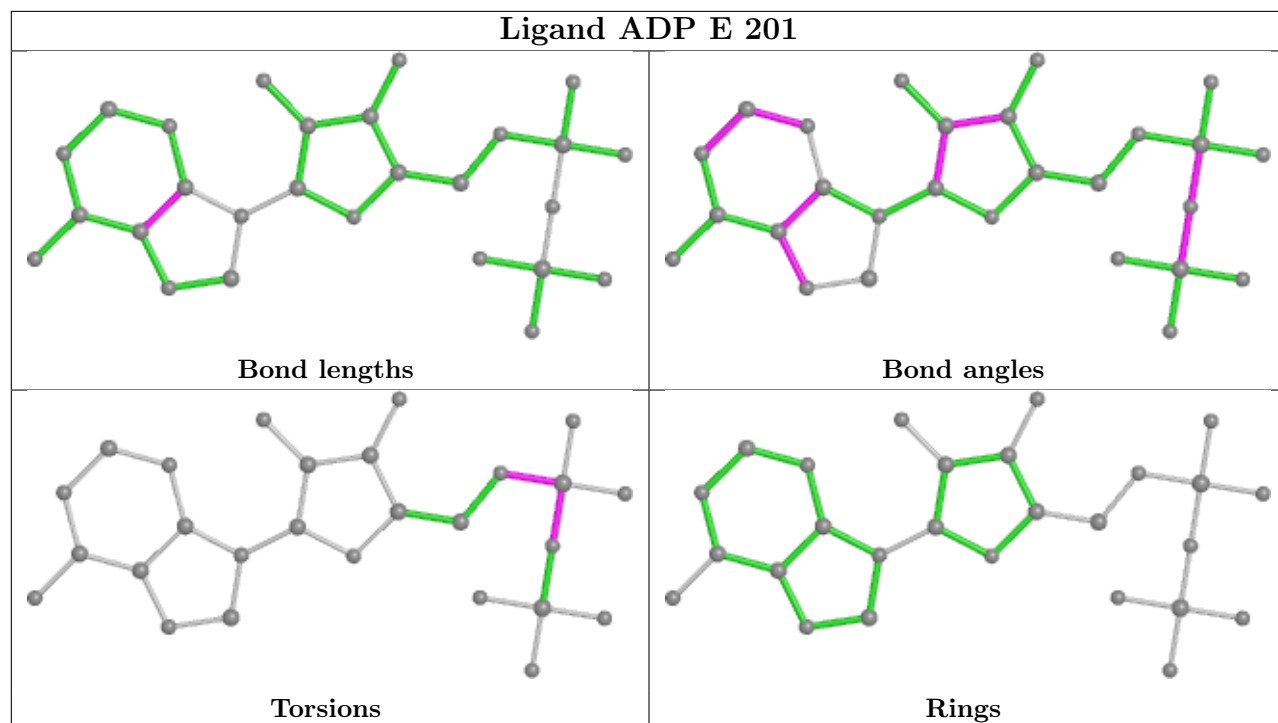
Mol	Chain	Res	Type	Atoms
5	E	201	ADP	C5'-O5'-PA-O1A
5	E	201	ADP	C5'-O5'-PA-O2A
5	E	201	ADP	C5'-O5'-PA-O3A
5	E	202	ADP	PB-O3A-PA-O5'
5	F	201	ADP	C3'-C4'-C5'-O5'
5	F	201	ADP	PB-O3A-PA-O1A
5	D	301	ADP	O4'-C4'-C5'-O5'
5	C	701	ADP	PB-O3A-PA-O1A
5	E	201	ADP	PB-O3A-PA-O1A
5	E	201	ADP	PB-O3A-PA-O2A
5	E	202	ADP	O4'-C4'-C5'-O5'
5	C	701	ADP	PB-O3A-PA-O2A
5	F	201	ADP	PB-O3A-PA-O2A
5	D	301	ADP	C3'-C4'-C5'-O5'

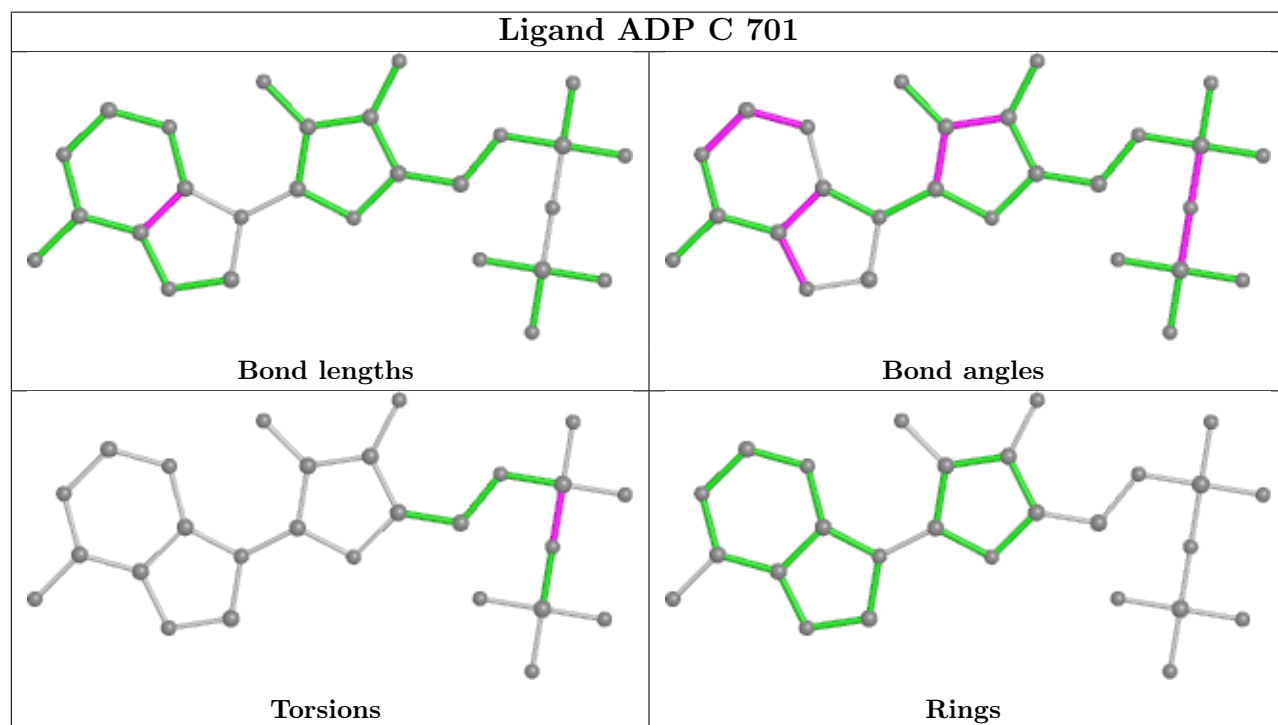
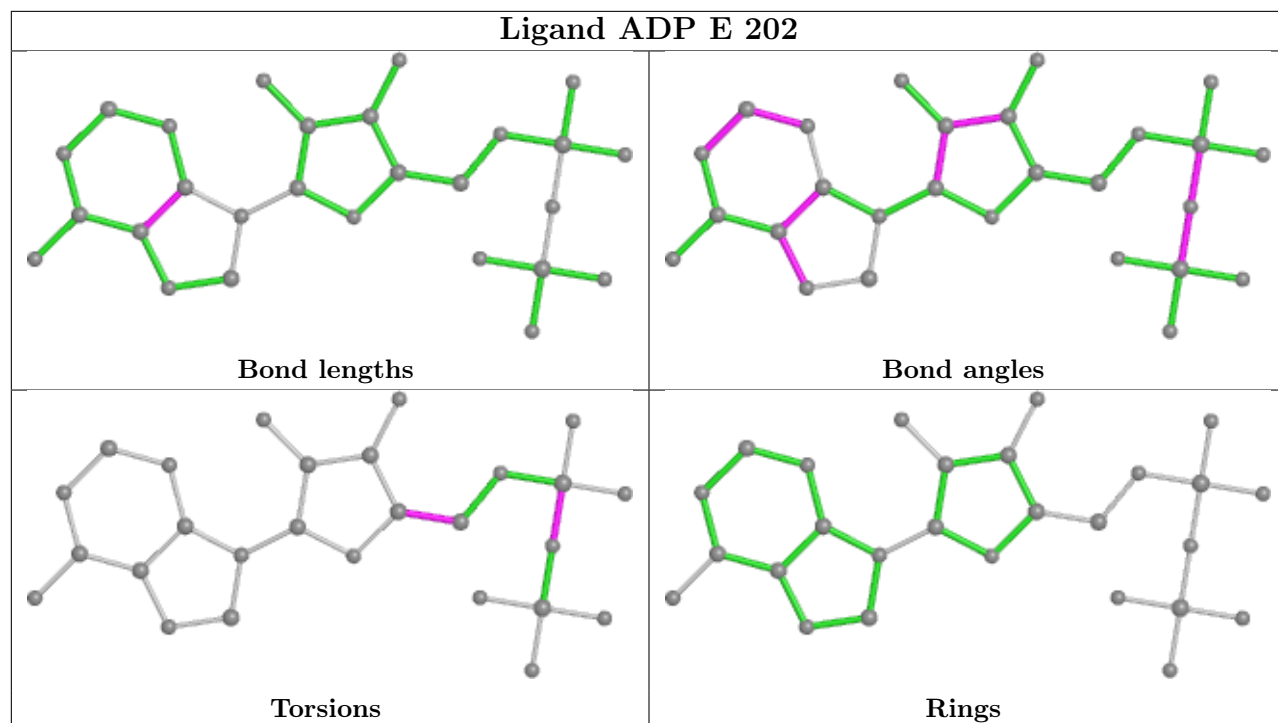
There are no ring outliers.

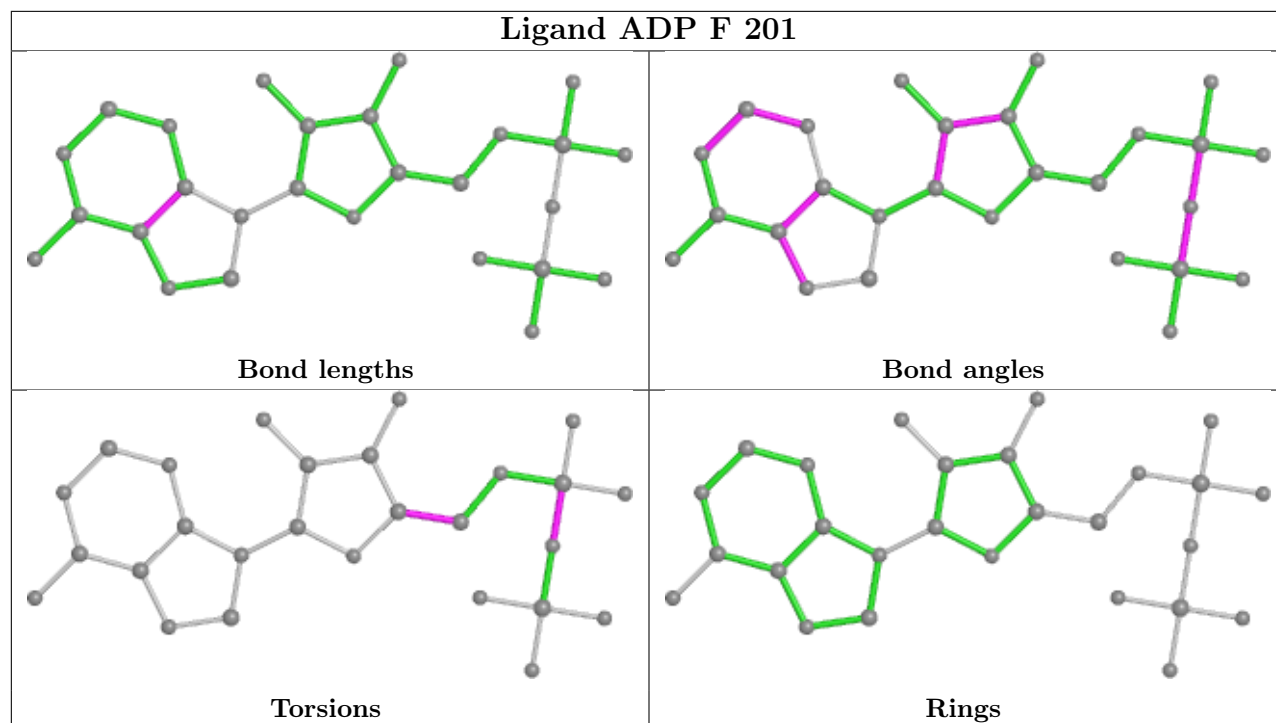
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	202	ADP	1	0
5	F	201	ADP	4	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.

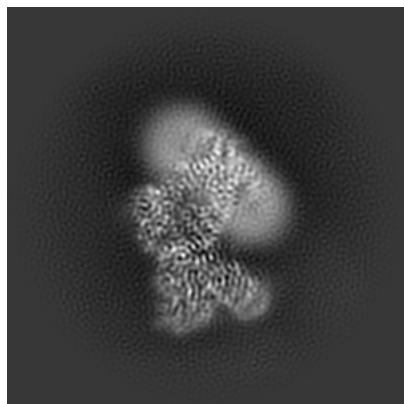
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37644. These allow visual inspection of the internal detail of the map and identification of artifacts.

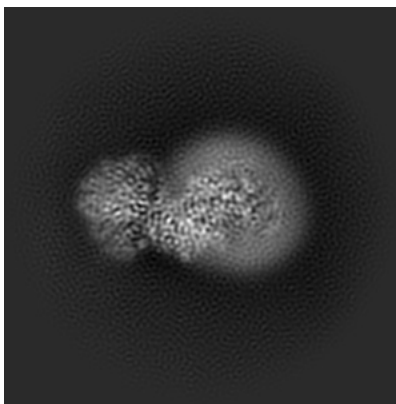
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

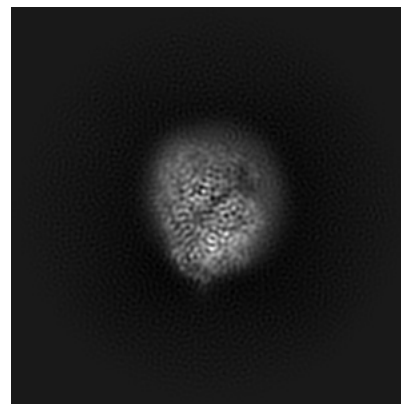
#### 6.1.1 Primary map



X

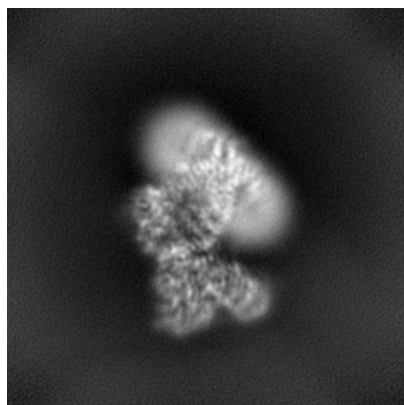


Y

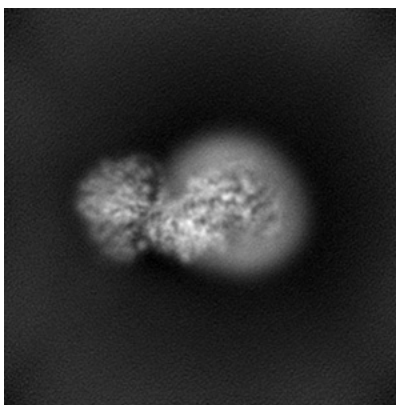


Z

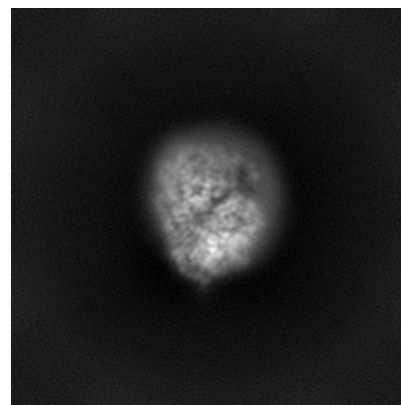
#### 6.1.2 Raw map



X



Y

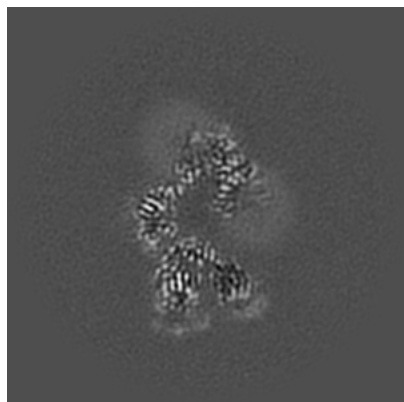


Z

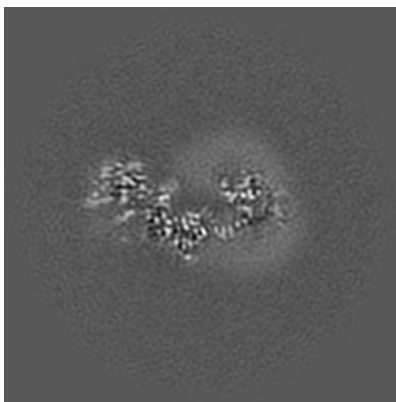
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

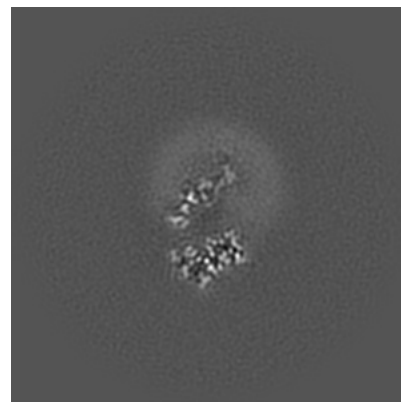
### 6.2.1 Primary map



X Index: 128

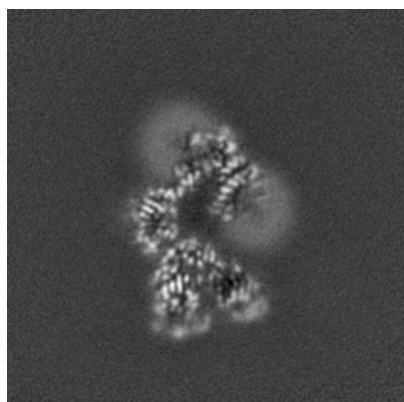


Y Index: 128

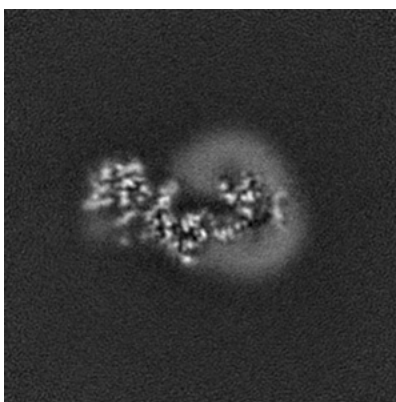


Z Index: 128

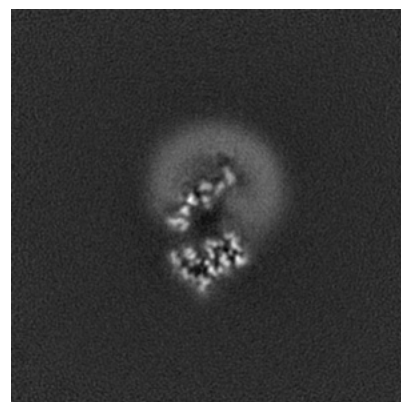
### 6.2.2 Raw map



X Index: 128



Y Index: 128

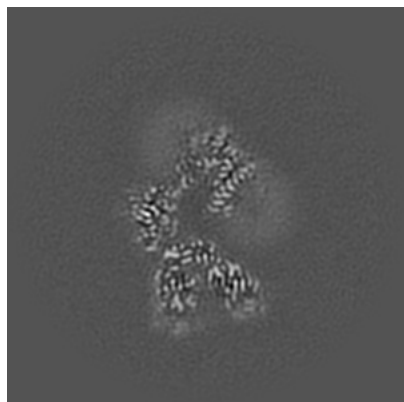


Z Index: 128

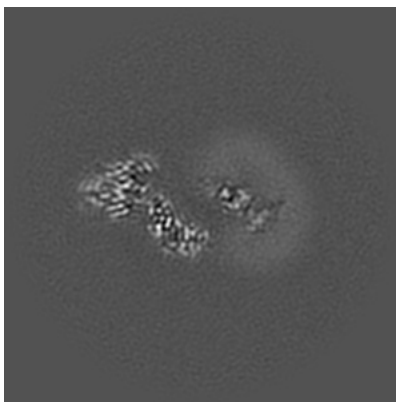
The images above show central slices of the map in three orthogonal directions.

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

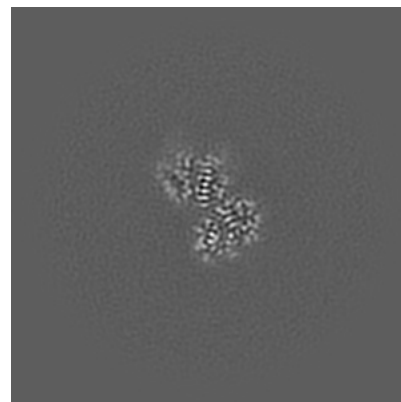
### 6.3.1 Primary map



X Index: 126

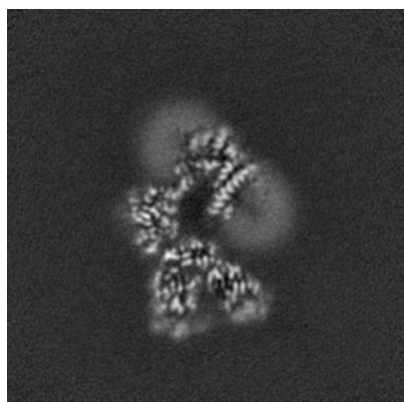


Y Index: 116

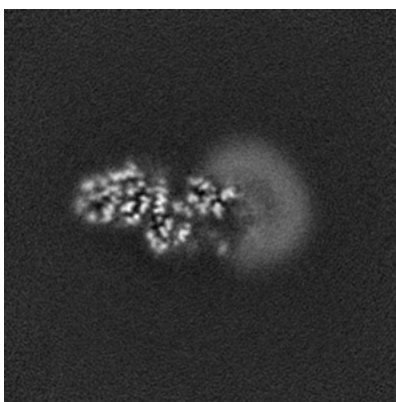


Z Index: 79

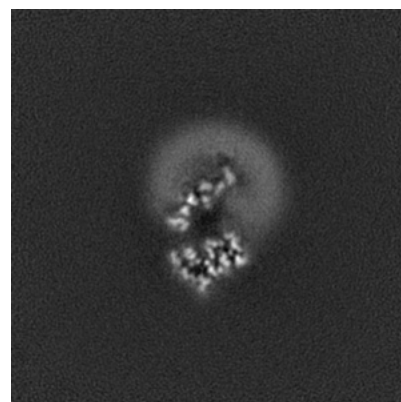
### 6.3.2 Raw map



X Index: 126



Y Index: 106



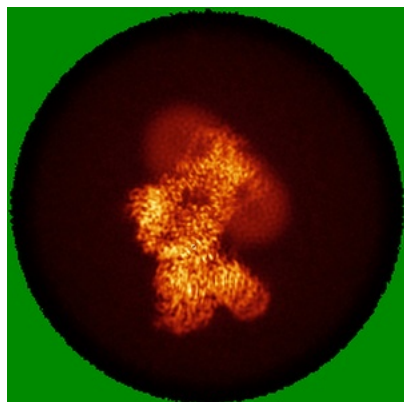
Z Index: 128

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

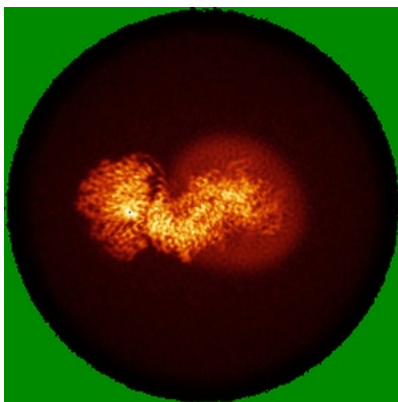


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

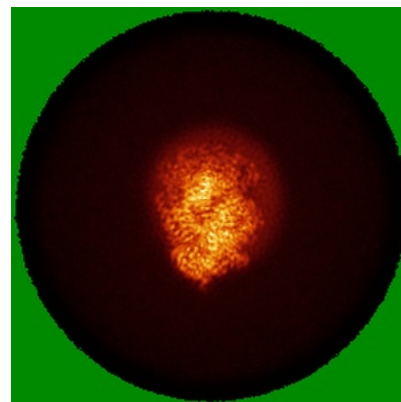
### 6.4.1 Primary map



X

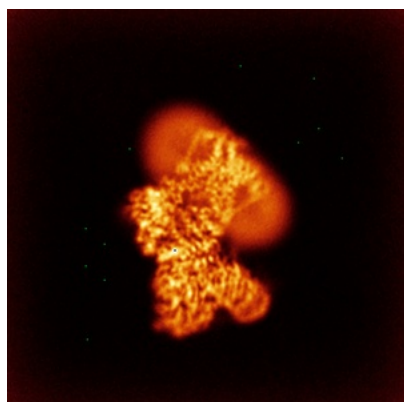


Y

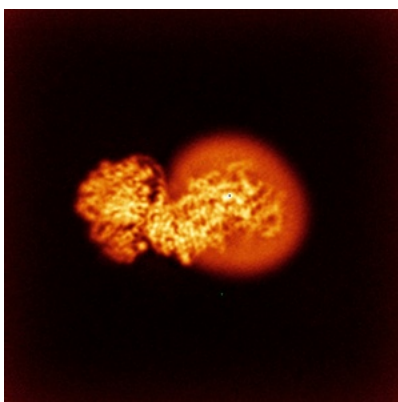


Z

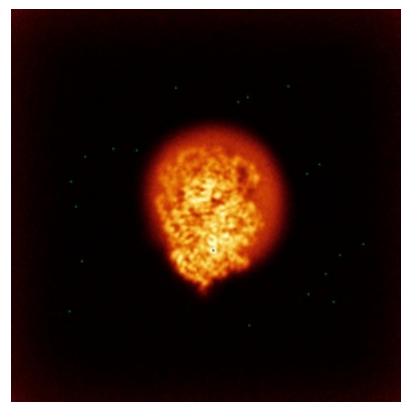
### 6.4.2 Raw map



X



Y

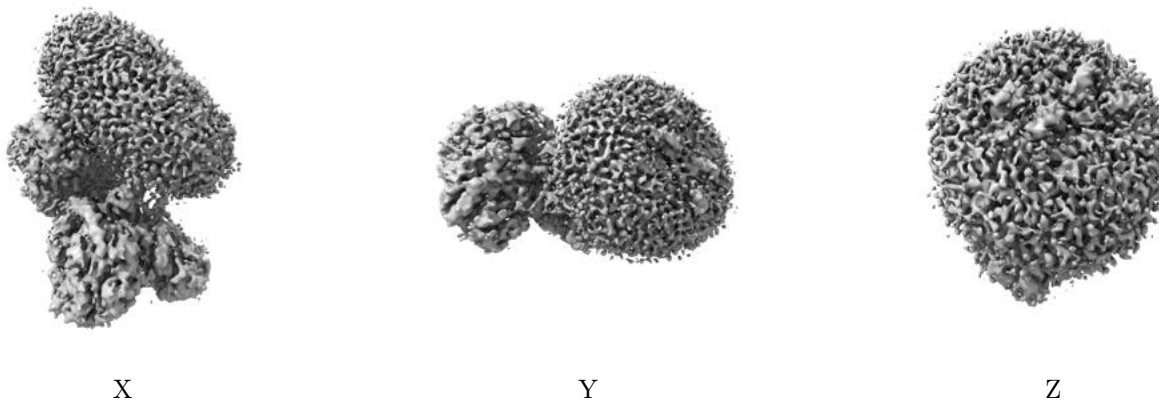


Z

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

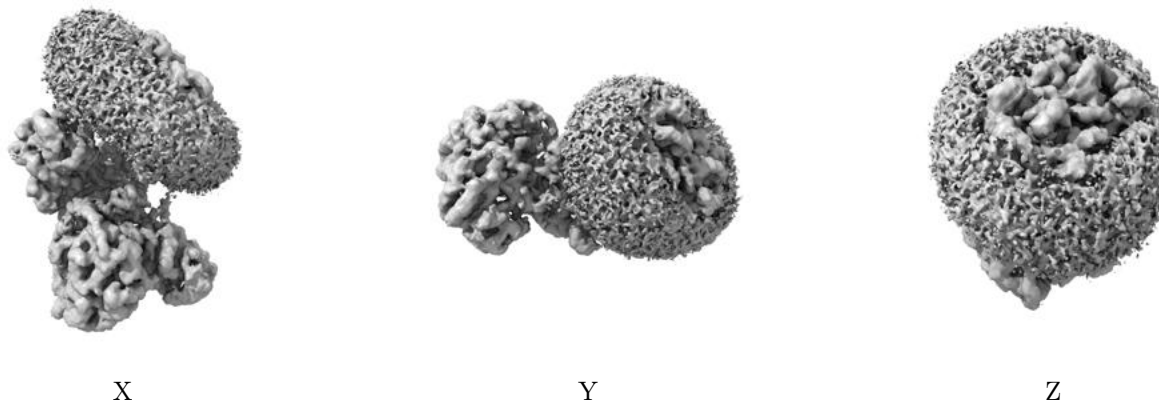
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.243. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

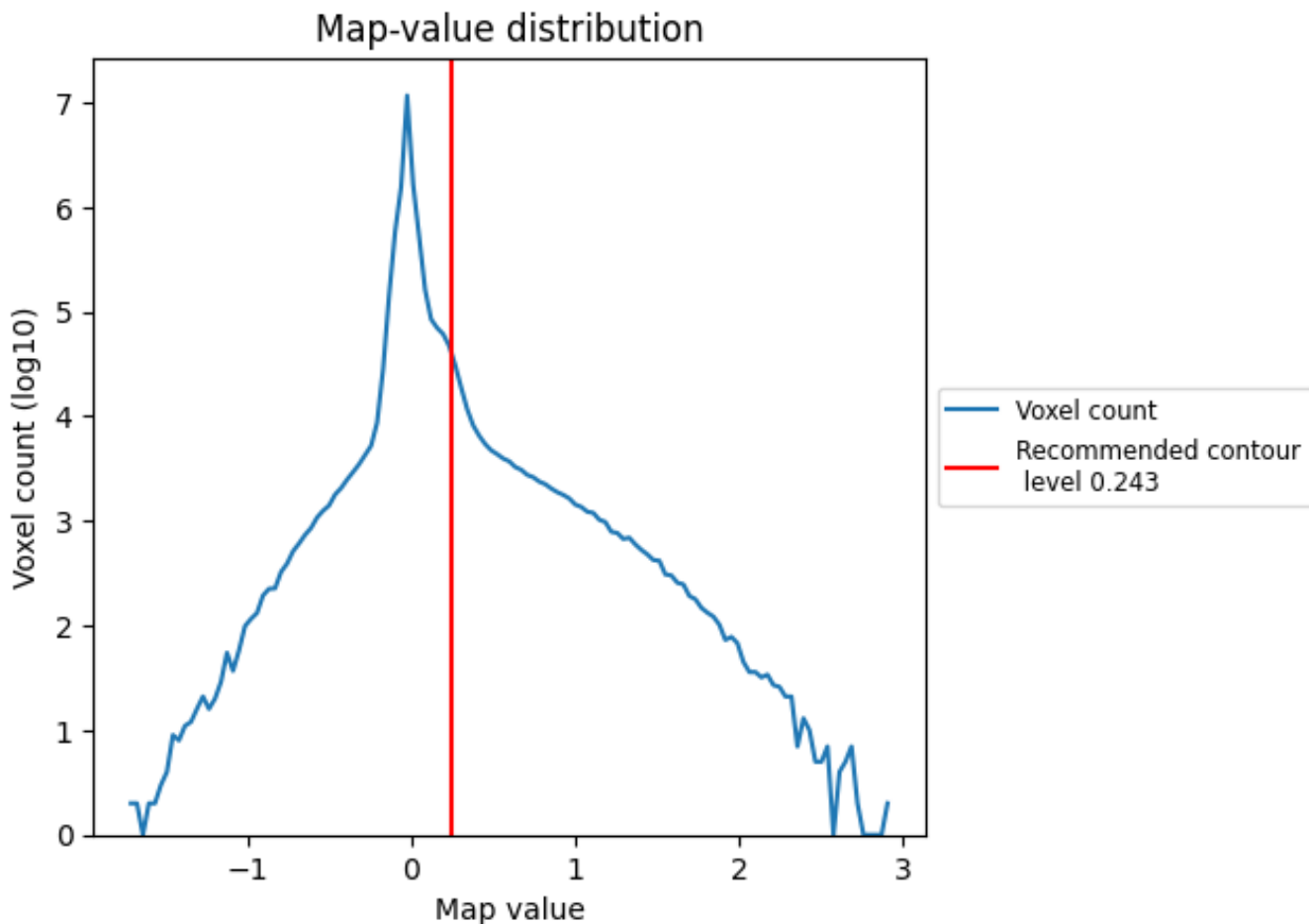
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

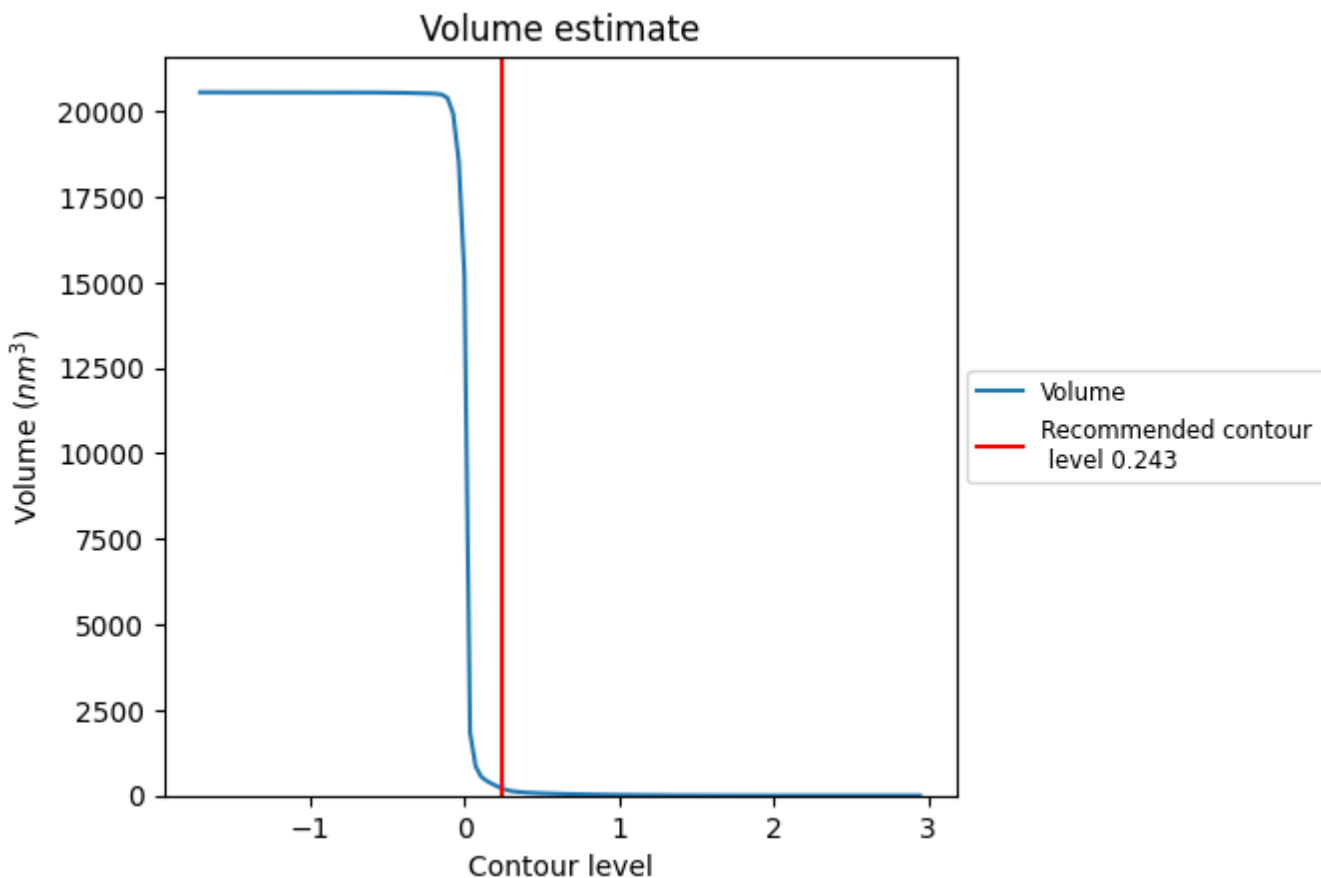
This section contains the results of statistical analysis of the map.

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



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

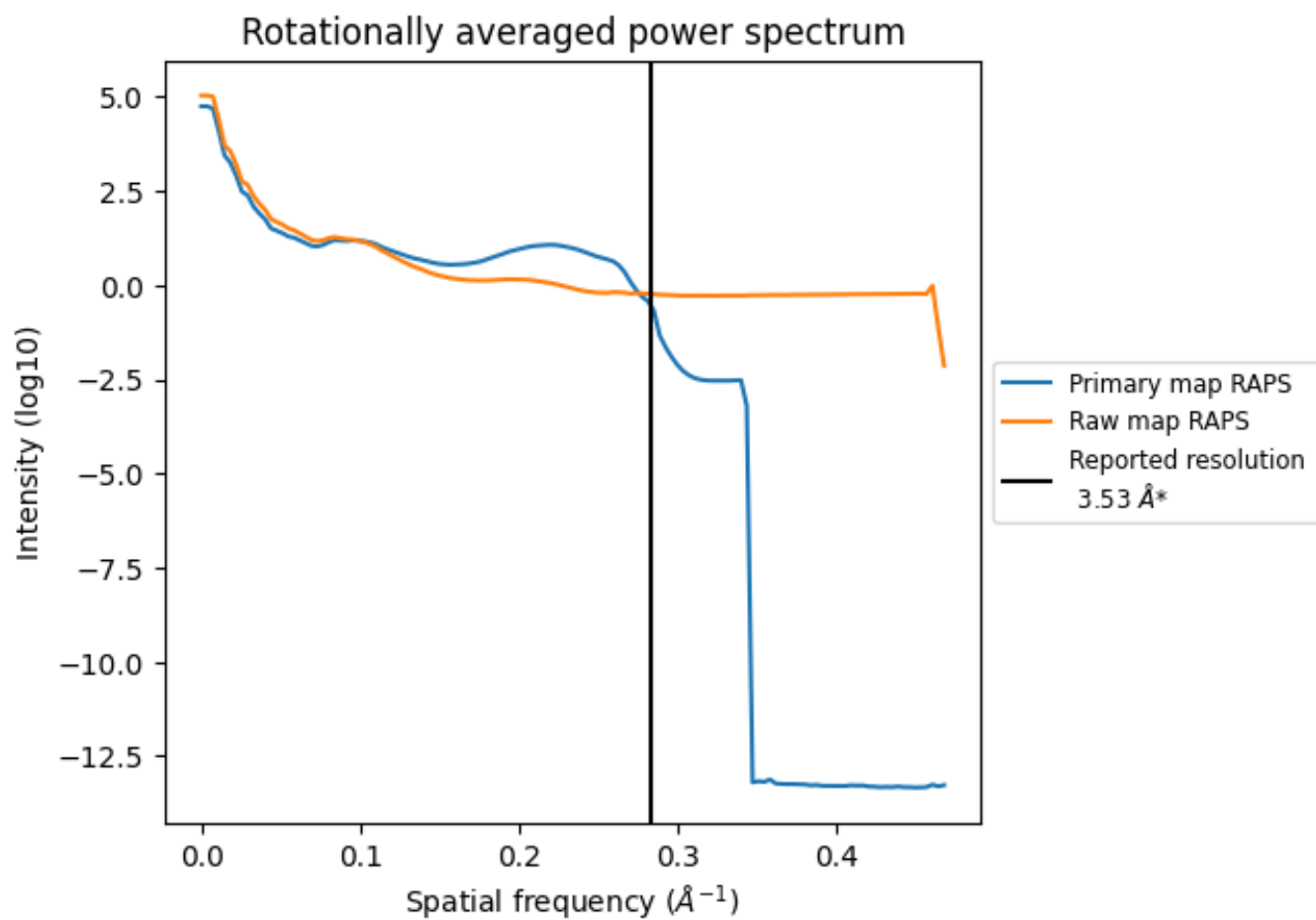
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 207 nm<sup>3</sup>; this corresponds to an approximate mass of 187 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)

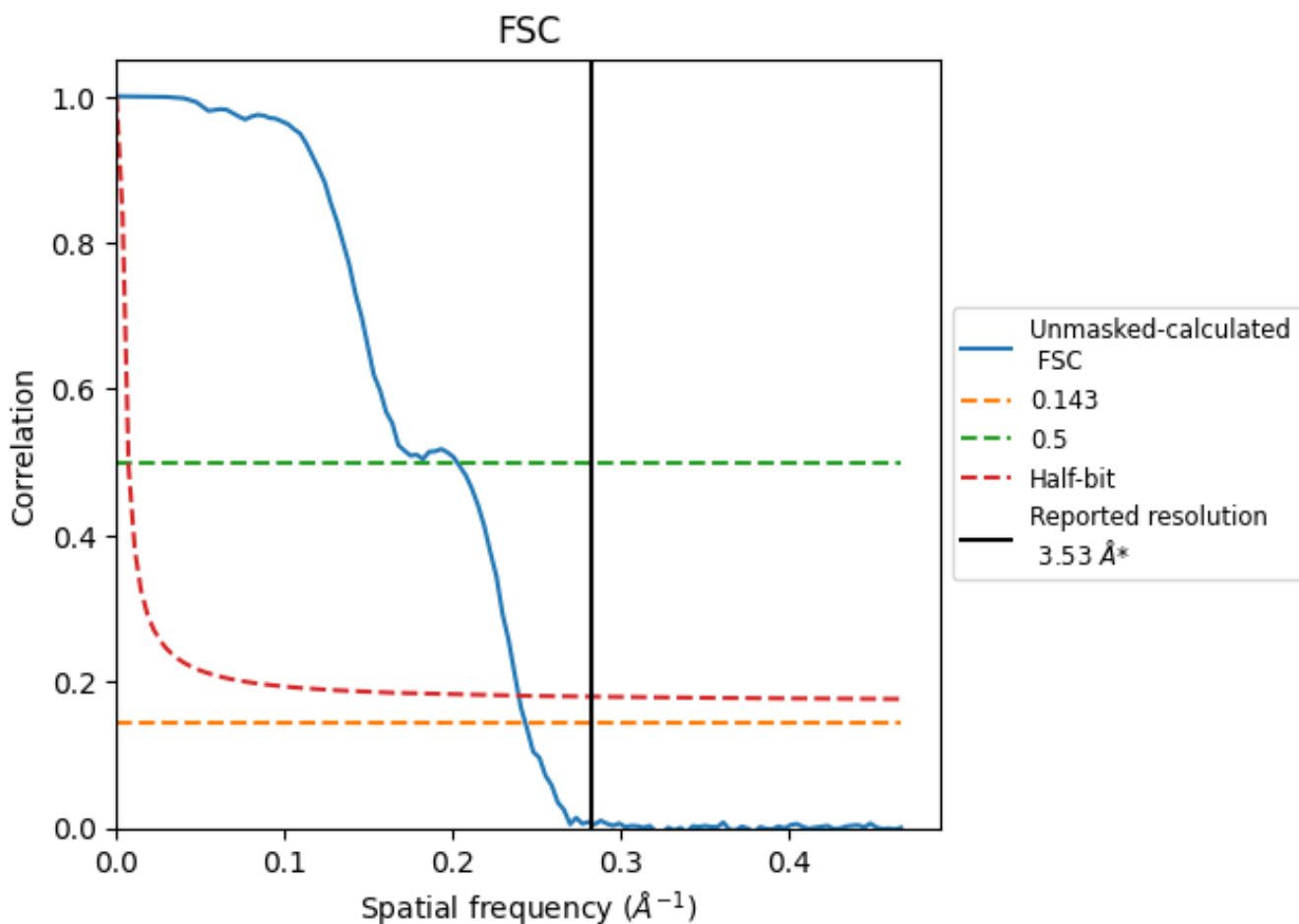


\*Reported resolution corresponds to spatial frequency of 0.283 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.283 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

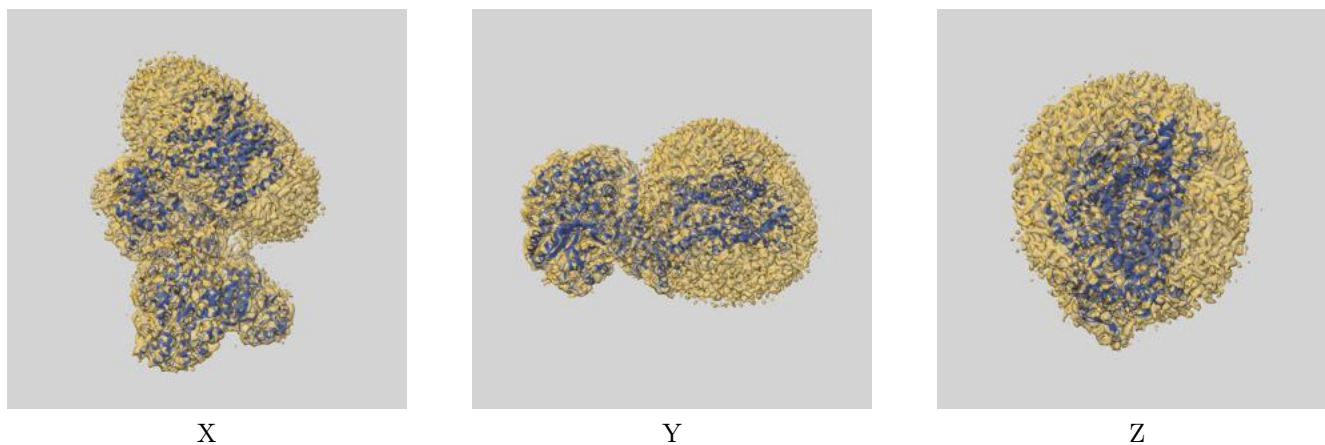
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.53	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.11	4.93	4.17

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.11 differs from the reported value 3.53 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-37644 and PDB model 8WM7. Per-residue inclusion information can be found in section [3](#) on page [6](#).

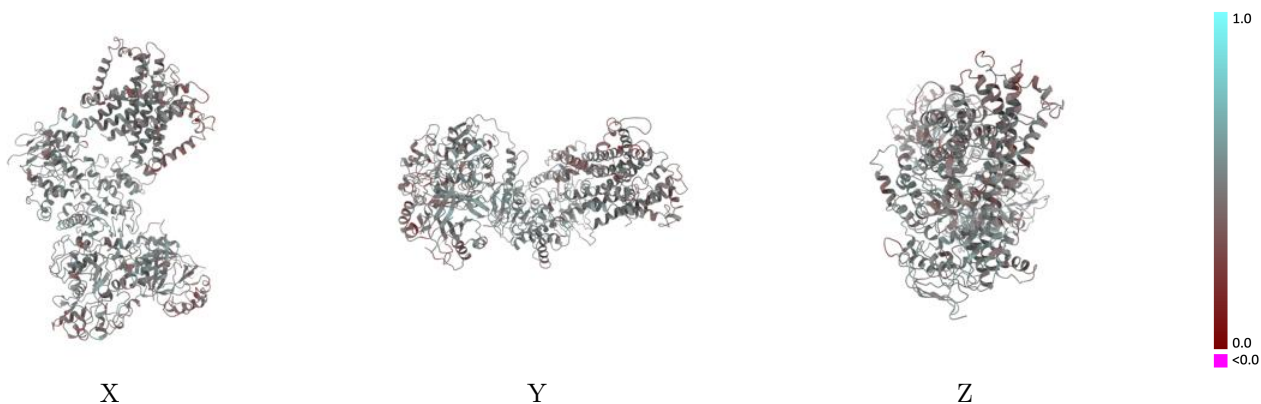
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.243 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.

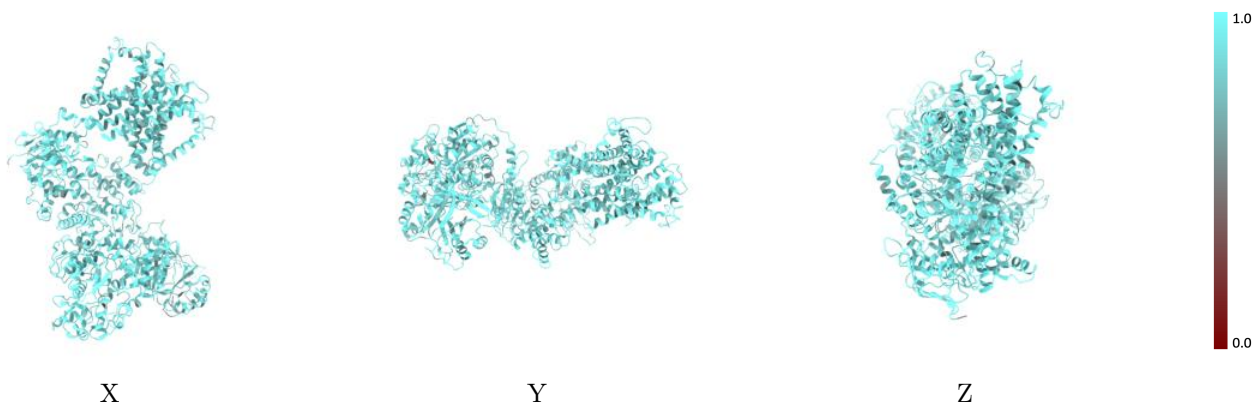


## 9.2 Q-score mapped to coordinate model [i](#)



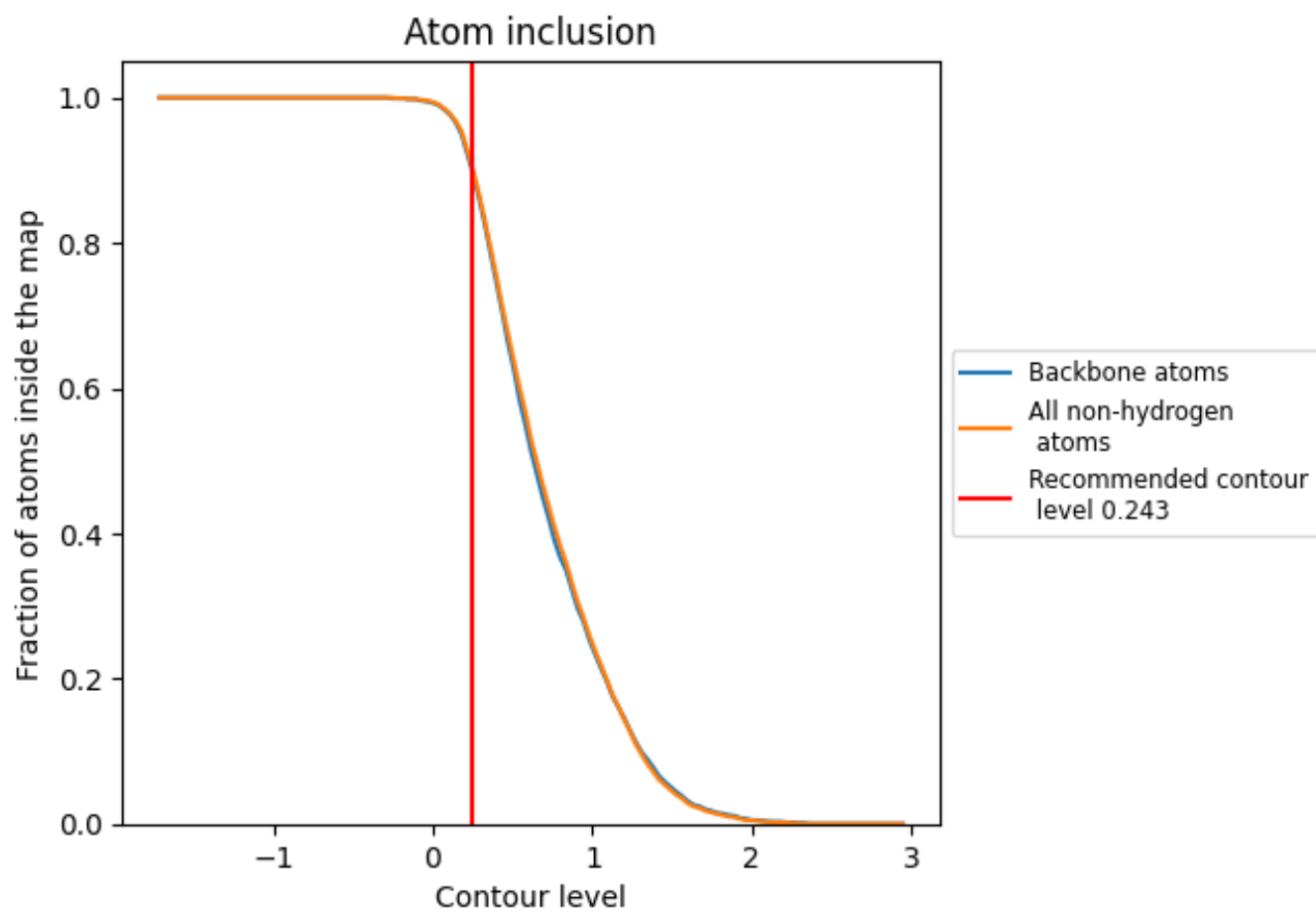
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.243).

















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 91% 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 (0.243) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9080	 0.4750
A	 0.9090	 0.4620
B	 0.9070	 0.4550
C	 0.9200	 0.4910
D	 0.9270	 0.4910
E	 0.8850	 0.4760
F	 0.8870	 0.4530
G	 0.8540	 0.4220

