



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:58 PM UTC

PDB ID : 6Y92 / pdb_00006y92
EMDB ID : EMD-10732
Title : Structure of full-length CD20 in complex with Ofatumumab Fab
Authors : Kumar, A.; Reyes, N.
Deposited on : 2020-03-06
Resolution : 4.73 Å(reported)
Based on initial model : 3GIZ

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:

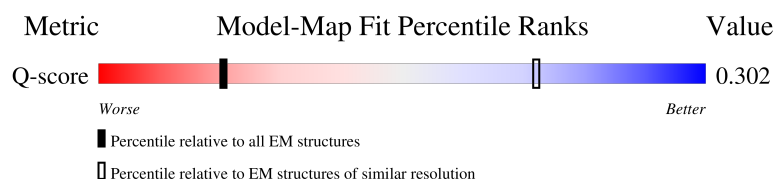
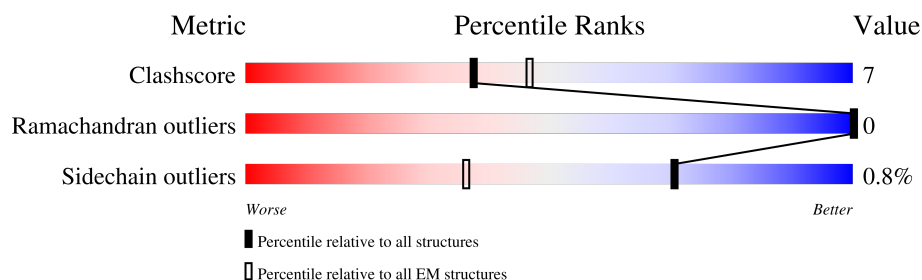
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

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

The reported resolution of this entry is 4.73 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	1643 (4.23 - 5.23)

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

Mol	Chain	Length	Quality of chain
1	A	178	
1	B	178	
2	D	211	
2	L	211	

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Mol	Chain	Length	Quality of chain
3	C	216	37% 81% 19%
3	H	216	36% 81% 19%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9497 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 B-lymphocyte antigen CD20.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	178	Total	C	N	O	S	0	0
			1394	916	223	241	14		
1	B	178	Total	C	N	O	S	0	0
			1394	916	223	241	14		

- Molecule 2 is a protein called Ofatumumab Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	211	Total	C	N	O	S	0	0
			1632	1021	279	328	4		
2	L	211	Total	C	N	O	S	0	0
			1632	1021	279	328	4		

- Molecule 3 is a protein called Ofatumumab Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	216	Total	C	N	O	S	0	0
			1629	1031	273	318	7		
3	H	216	Total	C	N	O	S	0	0
			1629	1031	273	318	7		

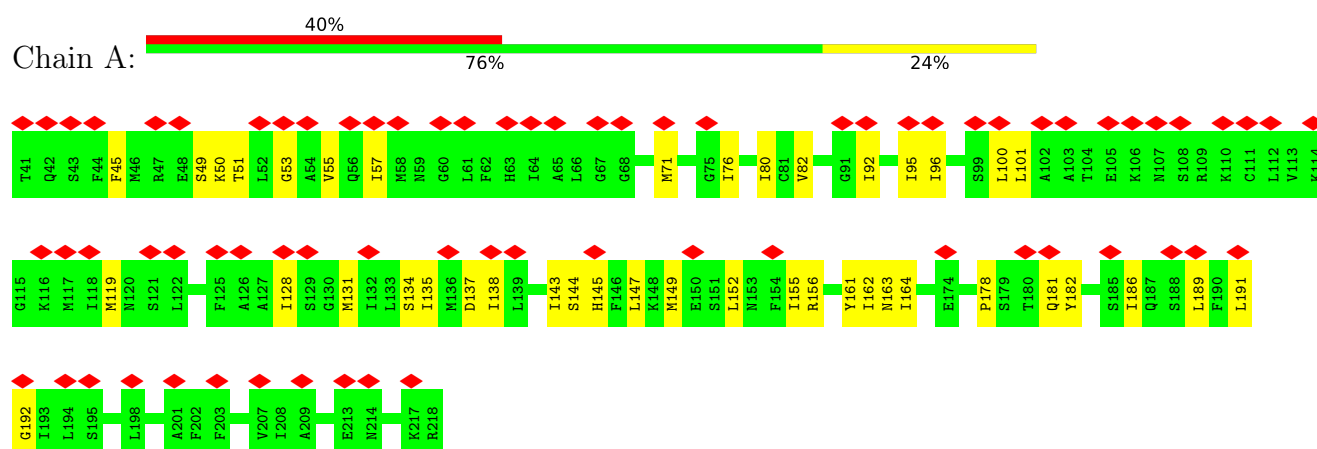
- Molecule 4 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: C₃₁H₅₀O₄).



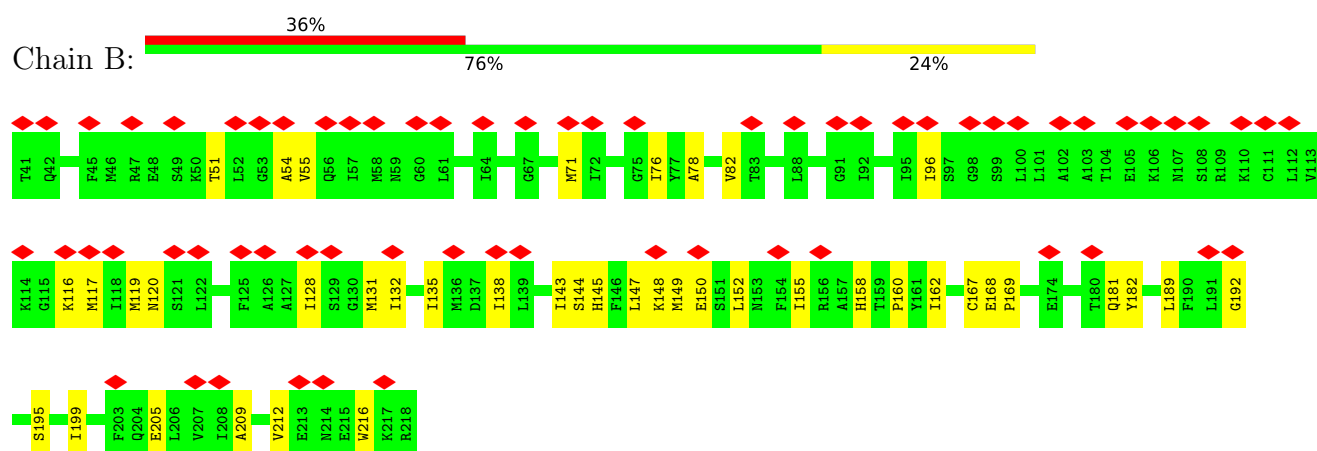
3 Residue-property plots

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.

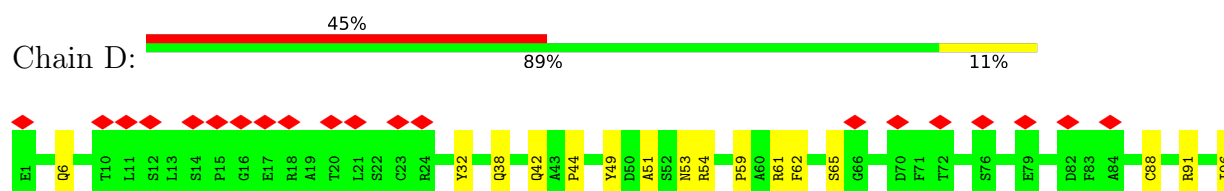
• Molecule 1: B-lymphocyte antigen CD20

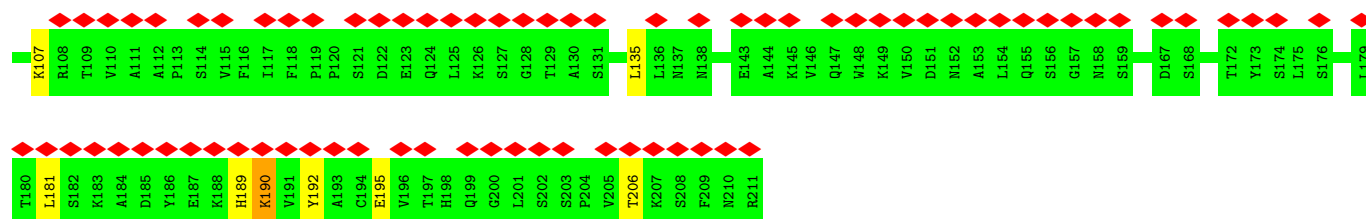


• Molecule 1: B-lymphocyte antigen CD20

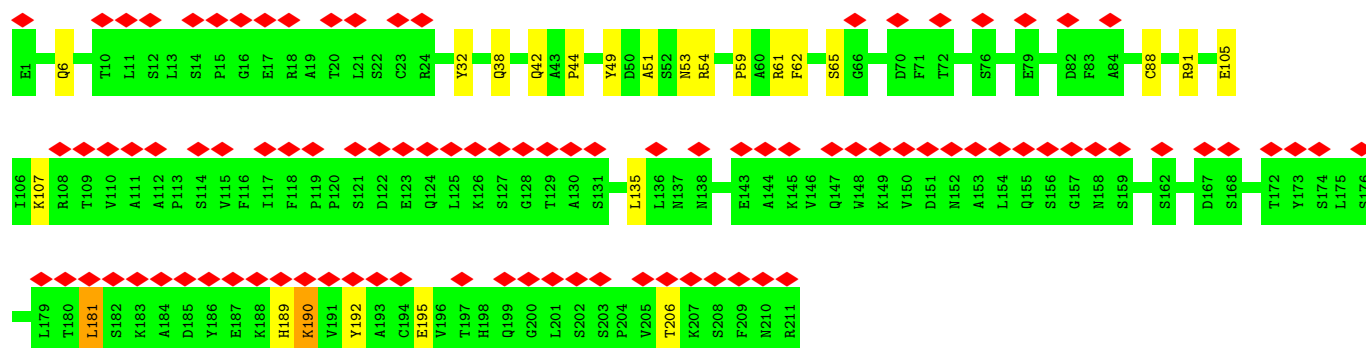
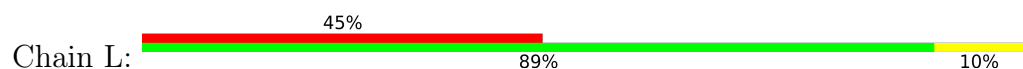


• Molecule 2: Ofatumumab Fab light chain

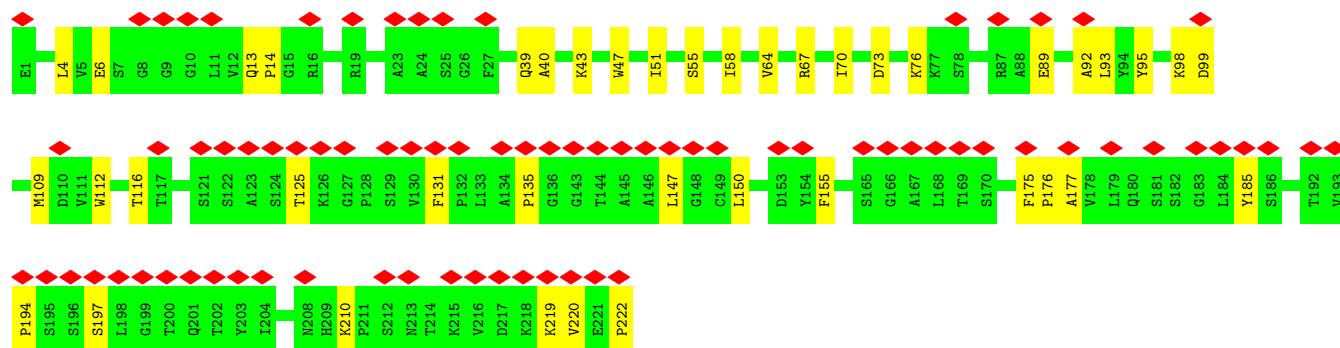
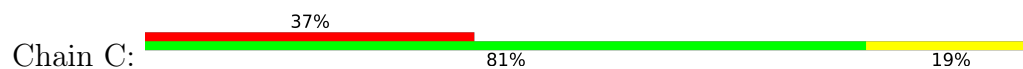




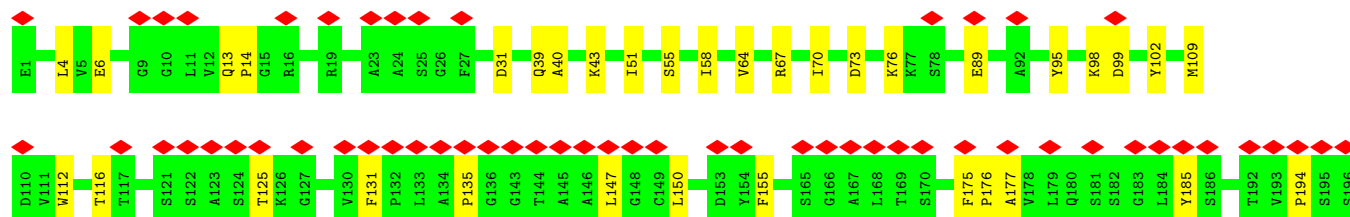
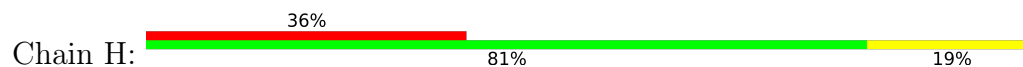
• Molecule 2: Ofatumumab Fab light chain



• Molecule 3: Ofatumumab Fab heavy chain



• Molecule 3: Ofatumumab Fab heavy chain



S197	L198	G199	T200	Q201	T202	Y203	I204	N208	H209	K210	P211	S212	N213	T214	K215	V216	D217	K218	K219	V220	E221	P222
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	99146	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.776	Depositor
Minimum map value	-1.906	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.091	Depositor
Recommended contour level	0.61	Depositor
Map size (Å)	270.0, 270.0, 270.0	wwPDB
Map dimensions	270, 270, 270	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	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: Y01

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	0.14	0/1426	0.40	0/1928
1	B	0.14	0/1426	0.39	0/1928
2	D	0.11	0/1668	0.32	1/2267 (0.0%)
2	L	0.11	0/1668	0.31	1/2267 (0.0%)
3	C	0.10	0/1669	0.29	0/2271
3	H	0.09	0/1669	0.28	0/2271
All	All	0.11	0/9526	0.33	2/12932 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	190	LYS	CB-CG-CD	5.32	123.54	111.30
2	D	190	LYS	CB-CG-CD	5.32	123.53	111.30

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	1394	0	1440	34	0
1	B	1394	0	1439	32	0
2	D	1632	0	1590	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	1632	0	1590	13	0
3	C	1629	0	1585	24	0
3	H	1629	0	1585	22	0
4	A	66	0	84	8	0
4	B	121	0	173	6	0
All	All	9497	0	9486	142	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 7.

All (142) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:PRO:O	1:A:182:TYR:HB3	1.72	0.90
1:A:76:ILE:HA	1:A:156:ARG:HH22	1.37	0.87
1:B:71:MET:HE1	1:B:82:VAL:HG22	1.66	0.78
1:A:96:ILE:HG23	1:A:119:MET:HE1	1.69	0.75
1:B:54:ALA:HB1	4:B:301:Y01:HAI	1.69	0.73
1:B:192:GLY:HA2	4:B:302:Y01:HAK1	1.74	0.70
1:B:131:MET:HE1	1:B:205:GLU:HG3	1.73	0.69
1:A:178:PRO:O	1:A:182:TYR:CB	2.41	0.67
1:A:156:ARG:HA	1:A:156:ARG:HE	1.60	0.67
1:A:76:ILE:HA	1:A:156:ARG:NH2	2.10	0.66
1:B:152:LEU:HD11	1:B:155:ILE:HG12	1.82	0.62
1:B:128:ILE:HA	1:B:131:MET:HE2	1.84	0.60
1:A:192:GLY:HA2	4:A:301:Y01:HAK1	1.84	0.59
1:B:145:HIS:NE2	1:B:147:LEU:O	2.37	0.57
1:B:116:LYS:O	1:B:120:ASN:ND2	2.37	0.57
3:H:135:PRO:HG2	3:H:222:PRO:HB3	1.88	0.55
1:B:148:LYS:HD3	1:B:150:GLU:HB2	1.89	0.55
1:A:128:ILE:HA	1:A:131:MET:SD	2.47	0.55
1:A:53:GLY:HA3	1:A:101:LEU:HD23	1.90	0.54
1:A:182:TYR:CE1	1:B:162:ILE:HG12	2.42	0.54
3:C:135:PRO:HG2	3:C:222:PRO:HB3	1.88	0.54
1:A:186:ILE:HD13	1:B:182:TYR:HE1	1.72	0.54
3:H:4:LEU:HD21	3:H:98:LYS:HE3	1.90	0.54
1:A:191:LEU:HD23	4:A:301:Y01:HAV2	1.89	0.53
2:D:6:GLN:NE2	2:D:88:CYS:SG	2.74	0.53
3:C:4:LEU:HD21	3:C:98:LYS:HE3	1.90	0.53
1:A:71:MET:HE1	1:A:82:VAL:HG22	1.90	0.53
2:D:54:ARG:NH2	2:D:62:PHE:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:38:GLN:HA	2:D:44:PRO:HB3	1.92	0.52
2:L:6:GLN:NE2	2:L:88:CYS:SG	2.74	0.52
1:A:145:HIS:NE2	1:A:147:LEU:O	2.43	0.52
3:H:219:LYS:NZ	3:H:220:VAL:O	2.37	0.52
1:B:143:ILE:HG22	1:B:144:SER:H	1.75	0.52
3:C:219:LYS:NZ	3:C:220:VAL:O	2.37	0.52
3:H:55:SER:HB2	3:H:58:ILE:HD11	1.92	0.52
2:L:38:GLN:HA	2:L:44:PRO:HB3	1.91	0.52
3:H:39:GLN:HE21	3:H:95:TYR:HE2	1.59	0.51
3:H:40:ALA:HB3	3:H:43:LYS:HB2	1.93	0.51
1:A:161:TYR:H	1:B:181:GLN:HE22	1.58	0.51
3:C:55:SER:HB2	3:C:58:ILE:HD11	1.92	0.51
1:A:181:GLN:NE2	1:B:158:HIS:O	2.44	0.50
1:A:51:THR:O	1:A:55:VAL:HG23	2.12	0.50
3:C:39:GLN:HE21	3:C:95:TYR:HE2	1.59	0.50
3:C:40:ALA:HB3	3:C:43:LYS:HB2	1.93	0.50
1:B:128:ILE:O	1:B:132:ILE:HG12	2.12	0.49
2:D:49:TYR:OH	2:D:53:ASN:ND2	2.45	0.49
1:A:143:ILE:HG22	1:A:144:SER:H	1.77	0.49
3:C:73:ASP:OD1	3:C:76:LYS:N	2.44	0.49
1:A:135:ILE:HA	1:A:138:ILE:HG22	1.94	0.49
2:L:49:TYR:OH	2:L:53:ASN:ND2	2.45	0.49
2:L:59:PRO:HB2	2:L:61:ARG:HH12	1.77	0.49
1:B:76:ILE:HD11	1:B:160:PRO:HA	1.95	0.49
1:A:45:PHE:O	1:A:49:SER:OG	2.27	0.48
3:C:6:GLU:OE2	3:C:116:THR:OG1	2.30	0.48
3:H:210:LYS:N	3:H:210:LYS:HD3	2.28	0.48
1:A:80:ILE:HA	1:A:149:MET:HG2	1.95	0.48
3:H:6:GLU:OE2	3:H:116:THR:OG1	2.30	0.48
2:L:51:ALA:HB1	2:L:65:SER:HA	1.96	0.48
1:A:76:ILE:HG12	1:A:163:ASN:HA	1.94	0.48
2:D:59:PRO:HB2	2:D:61:ARG:HH12	1.77	0.47
3:C:210:LYS:N	3:C:210:LYS:HD3	2.28	0.47
2:L:54:ARG:NH2	2:L:62:PHE:O	2.42	0.47
3:H:73:ASP:OD1	3:H:76:LYS:N	2.44	0.47
2:D:42:GLN:N	2:D:42:GLN:OE1	2.48	0.47
2:D:195:GLU:HG3	2:D:206:THR:HB	1.97	0.47
2:L:42:GLN:N	2:L:42:GLN:OE1	2.48	0.47
2:D:51:ALA:HB1	2:D:65:SER:HA	1.96	0.47
3:H:175:PHE:HD1	3:H:176:PRO:HD2	1.80	0.47
1:B:51:THR:O	1:B:55:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:LYS:HD2	1:B:150:GLU:H	1.80	0.46
1:B:168:GLU:HG3	1:B:169:PRO:HD2	1.96	0.46
3:H:125:THR:OG1	3:H:155:PHE:O	2.30	0.46
3:C:175:PHE:HD1	3:C:176:PRO:HD2	1.80	0.46
2:L:195:GLU:HG3	2:L:206:THR:HB	1.97	0.46
1:A:76:ILE:HG23	1:A:162:ILE:O	2.14	0.46
1:B:135:ILE:HA	1:B:138:ILE:HG22	1.97	0.46
1:A:152:LEU:HD11	1:A:155:ILE:HG12	1.97	0.46
3:H:64:VAL:HG13	3:H:67:ARG:HB2	1.98	0.45
2:D:96:ILE:HG12	3:C:47:TRP:CE3	2.51	0.45
3:H:109:MET:N	3:H:109:MET:SD	2.90	0.45
3:C:177:ALA:HB1	3:C:185:TYR:HB3	1.99	0.45
1:A:92:ILE:O	1:A:96:ILE:HG22	2.17	0.45
3:C:64:VAL:HG13	3:C:67:ARG:HB2	1.98	0.45
1:B:131:MET:CE	1:B:205:GLU:HG3	2.43	0.45
3:H:13:GLN:HG2	3:H:14:PRO:HD2	1.99	0.44
3:C:109:MET:SD	3:C:109:MET:N	2.90	0.44
1:A:149:MET:SD	1:A:149:MET:N	2.91	0.44
3:C:99:ASP:HA	3:C:109:MET:HA	2.00	0.44
3:C:13:GLN:HG2	3:C:14:PRO:HD2	1.99	0.44
3:C:109:MET:HG2	3:C:112:TRP:HE1	1.83	0.44
3:H:177:ALA:HB1	3:H:185:TYR:HB3	1.99	0.44
1:A:189:LEU:HD22	1:B:189:LEU:HD21	2.00	0.44
3:H:109:MET:HG2	3:H:112:TRP:HE1	1.83	0.44
3:C:194:PRO:HG2	3:C:197:SER:HB3	2.01	0.43
2:D:32:TYR:HE2	2:D:91:ARG:HB2	1.84	0.43
3:H:194:PRO:HG2	3:H:197:SER:HB3	2.00	0.43
3:H:99:ASP:HA	3:H:109:MET:HA	2.00	0.43
3:H:135:PRO:HB3	3:H:147:LEU:HB3	2.01	0.43
2:L:32:TYR:HE2	2:L:91:ARG:HB2	1.84	0.43
4:A:302:Y01:HAE1	4:A:302:Y01:HBD	1.90	0.43
4:B:304:Y01:HAE2	4:B:304:Y01:HBB	1.88	0.43
4:A:301:Y01:HBA	4:A:301:Y01:HAO1	1.86	0.43
1:B:117:MET:HE3	1:B:117:MET:HB3	1.90	0.42
1:B:148:LYS:HD2	1:B:150:GLU:N	2.34	0.42
2:D:189:HIS:HB3	2:D:192:TYR:HE1	1.84	0.42
4:B:304:Y01:HAA1	4:B:304:Y01:HAJ2	1.89	0.42
4:A:302:Y01:HAO2	4:A:302:Y01:HAP1	1.52	0.42
2:L:189:HIS:HB3	2:L:192:TYR:HE1	1.84	0.42
1:B:195:SER:O	1:B:199:ILE:HG12	2.20	0.42
1:A:92:ILE:HA	1:A:95:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:125:THR:OG1	3:C:155:PHE:O	2.30	0.42
1:A:100:LEU:HD22	1:A:119:MET:HG3	2.02	0.42
4:A:301:Y01:HAE2	4:A:301:Y01:HBB	1.90	0.42
3:C:131:PHE:HB2	3:C:150:LEU:HD23	2.02	0.42
3:C:135:PRO:HB3	3:C:147:LEU:HB3	2.01	0.42
3:H:131:PHE:HB2	3:H:150:LEU:HD23	2.02	0.42
1:A:156:ARG:HE	1:A:156:ARG:CA	2.29	0.41
2:D:44:PRO:HD2	3:C:112:TRP:CE3	2.55	0.41
1:B:209:ALA:HA	1:B:212:VAL:HG12	2.03	0.41
1:B:78:ALA:HB1	1:B:82:VAL:HG21	2.02	0.41
3:C:51:ILE:HB	3:C:70:ILE:HD12	2.02	0.41
3:C:92:ALA:O	3:C:93:LEU:HD22	2.20	0.41
2:L:105:GLU:OE1	2:L:107:LYS:N	2.31	0.41
1:A:57:ILE:HD12	1:A:95:ILE:HA	2.03	0.41
1:A:134:SER:HA	1:A:137:ASP:OD1	2.20	0.41
1:A:50:LYS:HD2	1:A:50:LYS:HA	1.88	0.41
1:B:117:MET:HG3	1:B:216:TRP:CZ2	2.56	0.41
1:B:167:CYS:SG	1:B:167:CYS:O	2.78	0.41
1:A:163:ASN:OD1	1:A:164:ILE:N	2.54	0.41
1:B:96:ILE:HG22	1:B:119:MET:HE1	2.03	0.41
1:B:149:MET:SD	1:B:149:MET:N	2.94	0.41
4:A:301:Y01:HAD2	4:A:301:Y01:HAS2	1.80	0.40
2:D:38:GLN:HG2	2:D:44:PRO:HG3	2.03	0.40
3:H:51:ILE:HB	3:H:70:ILE:HD12	2.02	0.40
2:L:38:GLN:HG2	2:L:44:PRO:HG3	2.03	0.40
2:L:181:LEU:HD13	2:L:181:LEU:HA	1.89	0.40
4:B:303:Y01:HAD2	4:B:303:Y01:HAS2	1.83	0.40
4:A:301:Y01:HAC2	4:A:301:Y01:HAJ2	1.72	0.40
2:D:107:LYS:HD2	2:D:107:LYS:HA	1.95	0.40
4:B:302:Y01:HAE2	4:B:302:Y01:HBB	1.91	0.40
3:H:31:ASP:HB3	3:H:102:TYR:HE1	1.86	0.40
1:B:143:ILE:HG22	1:B:144:SER:N	2.35	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	176/178 (99%)	171 (97%)	5 (3%)	0	100	100
1	B	176/178 (99%)	169 (96%)	7 (4%)	0	100	100
2	D	209/211 (99%)	200 (96%)	9 (4%)	0	100	100
2	L	209/211 (99%)	200 (96%)	9 (4%)	0	100	100
3	C	212/216 (98%)	205 (97%)	7 (3%)	0	100	100
3	H	212/216 (98%)	205 (97%)	7 (3%)	0	100	100
All	All	1194/1210 (99%)	1150 (96%)	44 (4%)	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	154/154 (100%)	154 (100%)	0	100	100
1	B	154/154 (100%)	154 (100%)	0	100	100
2	D	184/184 (100%)	181 (98%)	3 (2%)	55	69
2	L	184/184 (100%)	181 (98%)	3 (2%)	55	69
3	C	179/179 (100%)	178 (99%)	1 (1%)	78	81
3	H	179/179 (100%)	178 (99%)	1 (1%)	78	81
All	All	1034/1034 (100%)	1026 (99%)	8 (1%)	70	78

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	135	LEU
2	D	181	LEU
2	D	190	LYS

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Mol	Chain	Res	Type
3	C	89	GLU
3	H	89	GLU
2	L	135	LEU
2	L	181	LEU
2	L	190	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	ASN
2	D	100	GLN
2	D	147	GLN
3	H	35	HIS
3	H	39	GLN
2	L	100	GLN
2	L	158	ASN
1	B	171	ASN
1	B	181	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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
4	Y01	A	302	-	34,34,38	2.02	5 (14%)	52,52,57	2.09	13 (25%)
4	Y01	B	303	-	31,31,38	2.03	6 (19%)	48,48,57	1.82	12 (25%)
4	Y01	A	301	-	38,38,38	1.91	6 (15%)	57,57,57	1.85	14 (24%)
4	Y01	B	301	-	31,31,38	2.02	6 (19%)	48,48,57	1.82	12 (25%)
4	Y01	B	302	-	33,33,38	2.04	6 (18%)	51,51,57	1.91	12 (23%)
4	Y01	B	304	-	38,38,38	1.89	6 (15%)	57,57,57	1.79	14 (24%)

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
4	Y01	A	302	-	-	11/15/73/77	0/4/4/4
4	Y01	B	303	-	-	6/10/68/77	0/4/4/4
4	Y01	A	301	-	-	12/19/77/77	0/4/4/4
4	Y01	B	301	-	-	5/10/68/77	0/4/4/4
4	Y01	B	302	-	-	9/13/71/77	0/4/4/4
4	Y01	B	304	-	-	9/19/77/77	0/4/4/4

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	304	Y01	CBH-CAZ	-6.24	1.41	1.52
4	B	302	Y01	CBH-CAZ	-6.23	1.41	1.52
4	A	301	Y01	CBH-CAZ	-6.19	1.41	1.52
4	B	303	Y01	CBH-CAZ	-6.18	1.41	1.52
4	B	301	Y01	CBH-CAZ	-6.17	1.41	1.52
4	A	302	Y01	CBH-CAZ	-5.99	1.41	1.52
4	B	303	Y01	CAV-CAZ	-5.61	1.40	1.51
4	A	301	Y01	CAV-CAZ	-5.60	1.40	1.51
4	B	304	Y01	CAV-CAZ	-5.59	1.40	1.51
4	A	302	Y01	CAV-CAZ	-5.57	1.40	1.51
4	B	302	Y01	CAV-CAZ	-5.56	1.40	1.51
4	B	301	Y01	CAV-CAZ	-5.55	1.40	1.51
4	B	301	Y01	CAK-CAI	-5.16	1.39	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	302	Y01	CAK-CAI	-5.13	1.39	1.50
4	B	303	Y01	CAK-CAI	-5.12	1.39	1.50
4	A	301	Y01	CAK-CAI	-5.10	1.39	1.50
4	B	304	Y01	CAK-CAI	-5.03	1.39	1.50
4	A	302	Y01	CAK-CAI	-4.84	1.40	1.50
4	A	302	Y01	CAI-CAZ	3.70	1.40	1.33
4	B	303	Y01	CAI-CAZ	3.44	1.40	1.33
4	B	304	Y01	CAI-CAZ	3.42	1.40	1.33
4	A	301	Y01	CAI-CAZ	3.38	1.39	1.33
4	B	301	Y01	CAI-CAZ	3.36	1.39	1.33
4	B	302	Y01	CAI-CAZ	3.36	1.39	1.33
4	B	302	Y01	CBI-CBG	-2.65	1.50	1.55
4	A	301	Y01	CBI-CBG	-2.63	1.50	1.55
4	B	304	Y01	CBI-CBG	-2.51	1.50	1.55
4	B	301	Y01	CBI-CBG	-2.47	1.50	1.55
4	B	303	Y01	CBI-CBG	-2.47	1.50	1.55
4	B	304	Y01	CBH-CBF	-2.32	1.52	1.56
4	B	303	Y01	CBH-CBF	-2.26	1.52	1.56
4	A	301	Y01	CBH-CBF	-2.25	1.52	1.56
4	B	302	Y01	CBH-CBF	-2.17	1.52	1.56
4	B	301	Y01	CBH-CBF	-2.16	1.52	1.56
4	A	302	Y01	CBI-CBG	-2.12	1.51	1.55

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	302	Y01	CBI-CBG-CBD	-6.28	105.50	114.41
4	B	302	Y01	CBI-CBE-CBB	-5.49	112.46	119.51
4	A	301	Y01	CBI-CBE-CBB	-5.31	111.30	119.50
4	A	302	Y01	CBI-CBE-CBB	-5.05	111.69	119.50
4	B	304	Y01	CBI-CBE-CBB	-4.52	112.52	119.50
4	A	302	Y01	CBH-CBF-CBD	-4.35	106.36	112.71
4	B	301	Y01	CBI-CBE-CBB	-4.12	113.13	119.50
4	B	303	Y01	CBI-CBE-CBB	-4.06	113.22	119.50
4	B	301	Y01	CAV-CAZ-CBH	3.97	121.51	116.42
4	B	303	Y01	CAV-CAZ-CBH	3.95	121.49	116.42
4	A	301	Y01	CAV-CAZ-CBH	3.87	121.38	116.42
4	B	303	Y01	CAQ-CBG-CBD	-3.82	113.00	119.10
4	B	302	Y01	CAQ-CBG-CBD	-3.82	113.00	119.10
4	B	302	Y01	CAV-CAZ-CBH	3.81	121.30	116.42
4	B	304	Y01	CAQ-CBG-CBD	-3.79	113.06	119.10
4	A	301	Y01	CAQ-CBG-CBD	-3.79	113.06	119.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	301	Y01	CAQ-CBG-CBD	-3.77	113.09	119.10
4	B	304	Y01	CAV-CAZ-CBH	3.76	121.23	116.42
4	A	301	Y01	CAP-CBE-CBI	-3.75	99.43	103.84
4	A	302	Y01	CAV-CAZ-CBH	3.64	121.09	116.42
4	A	301	Y01	CBH-CBF-CBD	-3.64	107.40	112.71
4	B	302	Y01	CBH-CBF-CBD	-3.61	107.44	112.71
4	A	302	Y01	CAP-CBE-CBI	-3.57	99.64	103.84
4	B	304	Y01	CAS-CBF-CBH	-3.56	108.70	113.08
4	B	302	Y01	CAP-CBE-CBI	-3.49	99.73	103.84
4	B	304	Y01	CAP-CBE-CBI	-3.44	99.79	103.84
4	B	301	Y01	CAP-CBE-CBI	-3.42	99.81	103.84
4	B	303	Y01	CAP-CBE-CBI	-3.42	99.82	103.84
4	A	301	Y01	CAS-CBF-CBH	-3.40	108.89	113.08
4	B	304	Y01	CBH-CBF-CBD	-3.38	107.78	112.71
4	A	302	Y01	CAQ-CBG-CBI	-3.30	99.96	103.84
4	B	302	Y01	CAS-CBF-CBH	-3.29	109.03	113.08
4	B	303	Y01	CBH-CBF-CBD	-3.29	107.91	112.71
4	A	302	Y01	CAU-CBI-CBG	3.25	112.10	107.25
4	B	303	Y01	CAS-CBF-CBH	-3.24	109.09	113.08
4	B	303	Y01	CAT-CAR-CBC	-3.17	106.28	110.48
4	B	301	Y01	CBH-CBF-CBD	-3.17	108.09	112.71
4	B	301	Y01	CAS-CBF-CBH	-3.16	109.19	113.08
4	B	301	Y01	CAT-CAR-CBC	-3.16	106.30	110.48
4	A	302	Y01	CAK-CBD-CBF	-3.07	106.18	109.72
4	A	301	Y01	CBI-CBG-CBD	-3.05	110.08	114.41
4	B	302	Y01	CAD-CBH-CBF	-3.03	108.26	111.66
4	B	304	Y01	CBI-CBG-CBD	-3.01	110.14	114.41
4	A	302	Y01	CBG-CBI-CBE	-3.00	96.66	100.10
4	A	301	Y01	CAD-CBH-CBF	-2.96	108.33	111.66
4	B	304	Y01	CAD-CBH-CBF	-2.92	108.38	111.66
4	B	302	Y01	CBI-CBG-CBD	-2.89	110.31	114.41
4	B	301	Y01	CBG-CBI-CBE	-2.85	96.83	100.10
4	B	304	Y01	CBC-OAW-CAY	-2.84	110.99	117.80
4	B	303	Y01	CAD-CBH-CBF	-2.77	108.55	111.66
4	A	301	Y01	CAS-CAU-CBI	-2.74	108.11	112.74
4	B	303	Y01	CBI-CBG-CBD	-2.74	110.52	114.41
4	B	301	Y01	CAD-CBH-CBF	-2.72	108.61	111.66
4	B	303	Y01	CBG-CBI-CBE	-2.70	97.00	100.10
4	B	301	Y01	CBI-CBG-CBD	-2.70	110.58	114.41
4	A	301	Y01	CBC-OAW-CAY	-2.69	111.35	117.80
4	A	302	Y01	CBC-OAW-CAY	-2.68	111.39	117.80
4	A	302	Y01	CBD-CAK-CAI	-2.68	109.05	112.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	301	Y01	CAV-CAZ-CAI	-2.67	116.95	120.57
4	A	302	Y01	CAV-CAZ-CAI	-2.66	116.96	120.57
4	A	301	Y01	CAV-CAZ-CAI	-2.66	116.97	120.57
4	B	302	Y01	CAV-CAZ-CAI	-2.62	117.01	120.57
4	B	303	Y01	CAV-CAZ-CAI	-2.62	117.01	120.57
4	B	302	Y01	CAS-CAU-CBI	-2.61	108.34	112.74
4	B	302	Y01	CBG-CBI-CBE	-2.58	97.13	100.10
4	B	304	Y01	CAV-CAZ-CAI	-2.56	117.10	120.57
4	B	303	Y01	CAS-CAU-CBI	-2.53	108.48	112.74
4	B	304	Y01	CAS-CAU-CBI	-2.52	108.49	112.74
4	B	301	Y01	CAS-CAU-CBI	-2.51	108.51	112.74
4	A	302	Y01	CAQ-CBG-CBD	-2.46	115.18	119.10
4	B	304	Y01	CAT-CAR-CBC	-2.32	106.56	110.33
4	B	302	Y01	CBC-OAW-CAY	-2.30	112.30	117.80
4	A	301	Y01	CAT-CAR-CBC	-2.24	106.68	110.33
4	B	304	Y01	CBG-CBI-CBE	-2.24	97.53	100.10
4	A	301	Y01	CBG-CBI-CBE	-2.19	97.58	100.10
4	A	301	Y01	CAQ-CBG-CBI	-2.07	101.40	103.84
4	B	304	Y01	CAQ-CBG-CBI	-2.00	101.48	103.84

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	Y01	CAC-CBB-CBE-CBI
4	A	302	Y01	CAO-CBB-CBE-CBI
4	A	302	Y01	CAC-CBB-CBE-CBI
4	A	301	Y01	CAC-CBB-CBE-CAP
4	A	302	Y01	CAC-CBB-CBE-CAP
4	B	301	Y01	CAC-CBB-CBE-CBI
4	B	303	Y01	CAC-CBB-CBE-CBI
4	B	304	Y01	CAC-CBB-CBE-CBI
4	A	302	Y01	CAO-CBB-CBE-CAP
4	B	302	Y01	OAG-CAY-OAW-CBC
4	B	302	Y01	CAM-CAY-OAW-CBC
4	A	301	Y01	CAO-CBB-CBE-CBI
4	B	301	Y01	CAO-CBB-CBE-CBI
4	B	303	Y01	CAO-CBB-CBE-CBI
4	B	304	Y01	CAO-CBB-CBE-CBI
4	B	304	Y01	CAV-CBC-OAW-CAY
4	A	301	Y01	CAJ-CAO-CBB-CBE
4	A	301	Y01	CAJ-CAO-CBB-CAC

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Mol	Chain	Res	Type	Atoms
4	A	301	Y01	CAO-CBB-CBE-CAP
4	A	302	Y01	CAJ-CAO-CBB-CAC
4	B	302	Y01	CAC-CBB-CBE-CBI
4	A	302	Y01	CAM-CAY-OAW-CBC
4	B	304	Y01	CAR-CBC-OAW-CAY
4	A	302	Y01	OAG-CAY-OAW-CBC
4	B	301	Y01	CAN-CAJ-CAO-CBB
4	B	304	Y01	CAM-CAY-OAW-CBC
4	B	304	Y01	OAG-CAY-OAW-CBC
4	A	302	Y01	CAR-CBC-OAW-CAY
4	A	302	Y01	CAX-CAL-CAM-CAY
4	B	301	Y01	CAC-CBB-CBE-CAP
4	B	303	Y01	CAC-CBB-CBE-CAP
4	B	304	Y01	CAC-CBB-CBE-CAP
4	A	302	Y01	CAJ-CAO-CBB-CBE
4	B	302	Y01	CAO-CBB-CBE-CBI
4	B	302	Y01	CAC-CBB-CBE-CAP
4	A	302	Y01	CAV-CBC-OAW-CAY
4	B	304	Y01	CAO-CBB-CBE-CAP
4	B	301	Y01	CAO-CBB-CBE-CAP
4	B	303	Y01	CAO-CBB-CBE-CAP
4	A	301	Y01	CAM-CAY-OAW-CBC
4	A	301	Y01	OAG-CAY-OAW-CBC
4	B	302	Y01	CAO-CBB-CBE-CAP
4	B	303	Y01	CAN-CAJ-CAO-CBB
4	B	304	Y01	CAX-CAL-CAM-CAY
4	A	301	Y01	CAM-CAL-CAX-OAH
4	A	301	Y01	CAM-CAL-CAX-OAF
4	B	303	Y01	CAO-CAJ-CAN-CBA
4	A	301	Y01	CAL-CAM-CAY-OAW
4	B	302	Y01	CAL-CAM-CAY-OAW
4	B	302	Y01	CAM-CAL-CAX-OAH
4	A	301	Y01	CAL-CAM-CAY-OAG
4	B	302	Y01	CAL-CAM-CAY-OAG

There are no ring outliers.

6 monomers are involved in 14 short contacts:

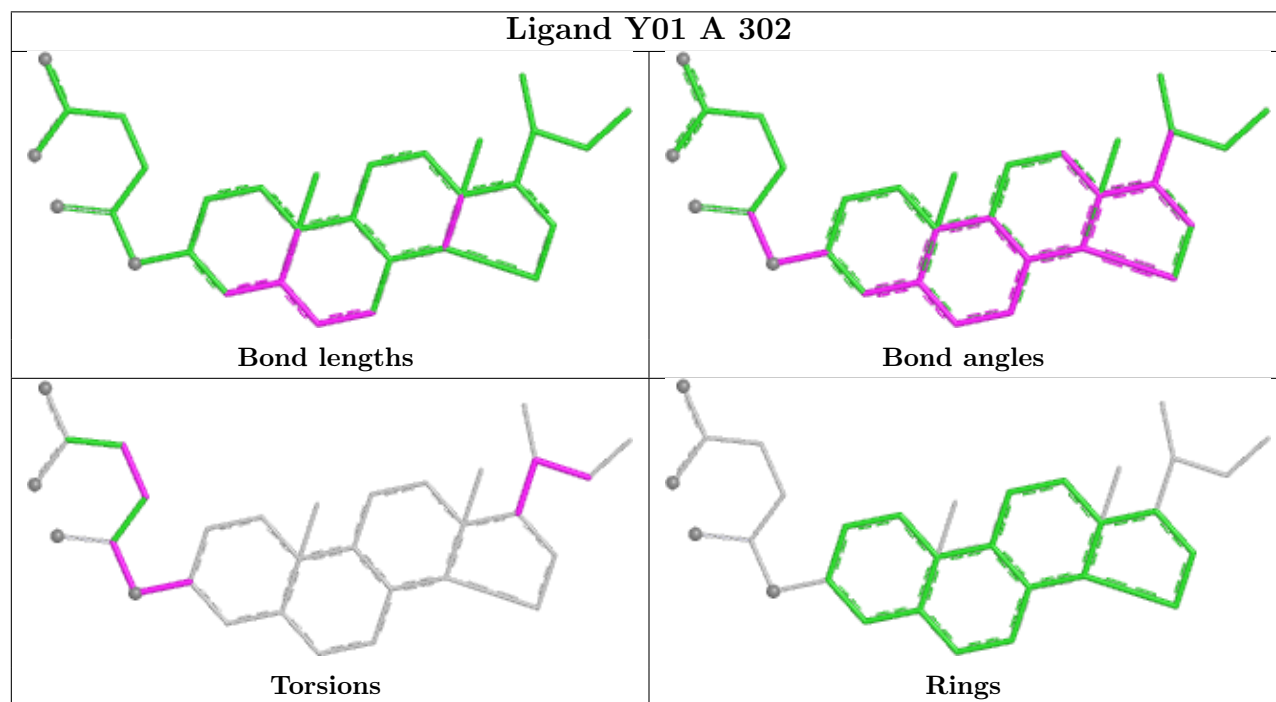
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	302	Y01	2	0
4	B	303	Y01	1	0
4	A	301	Y01	6	0

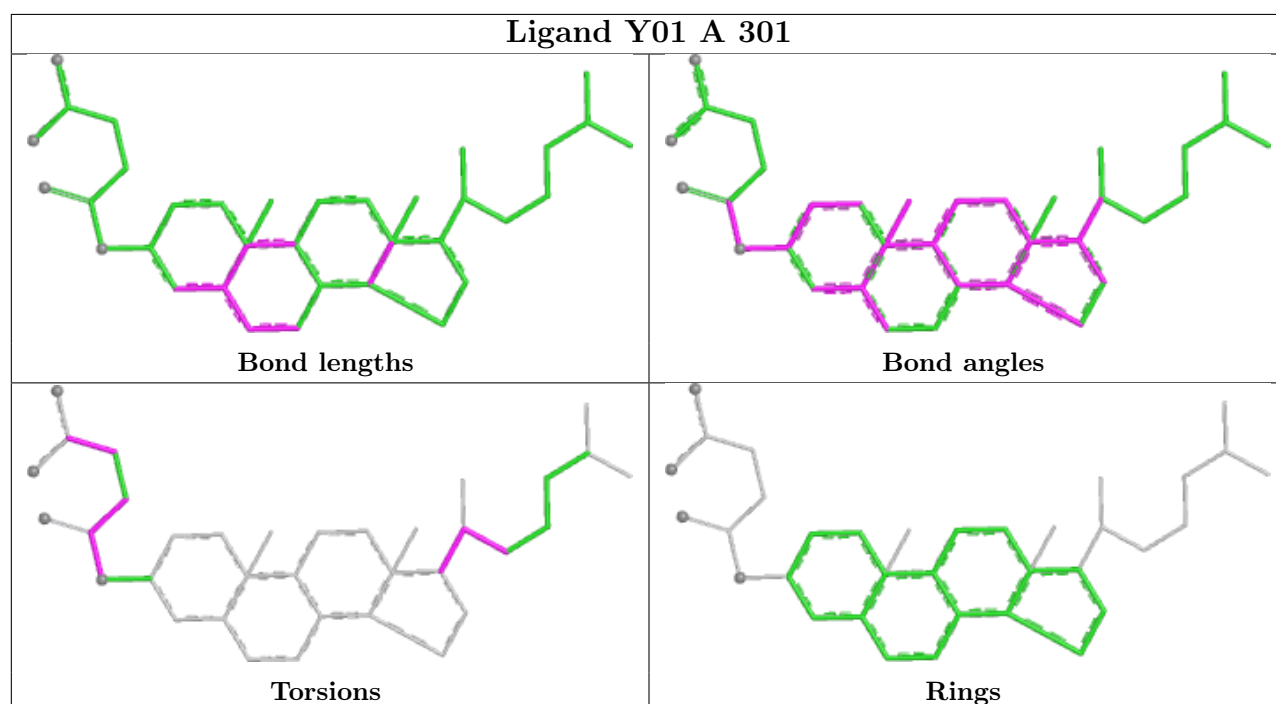
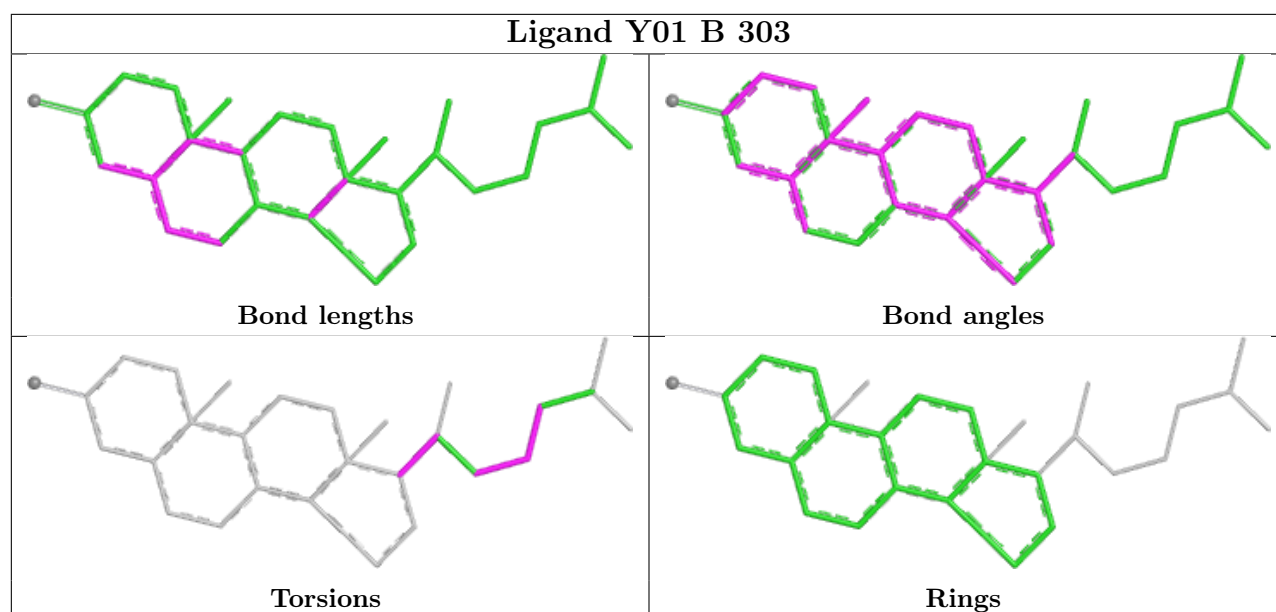
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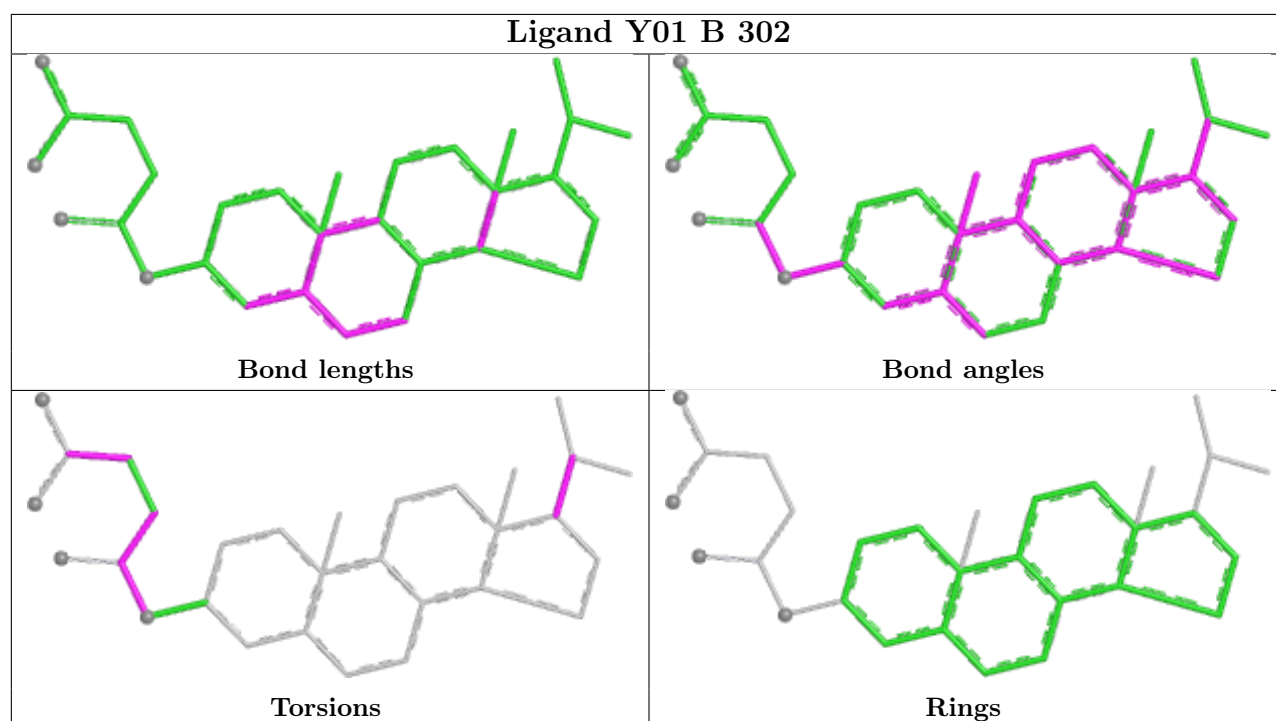
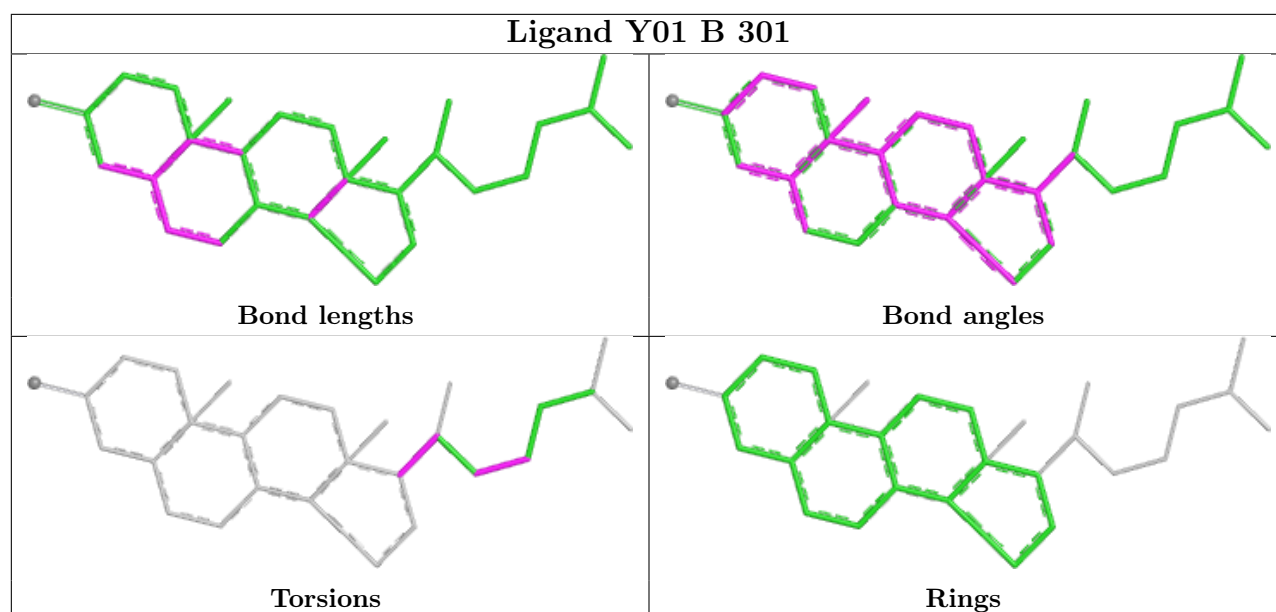
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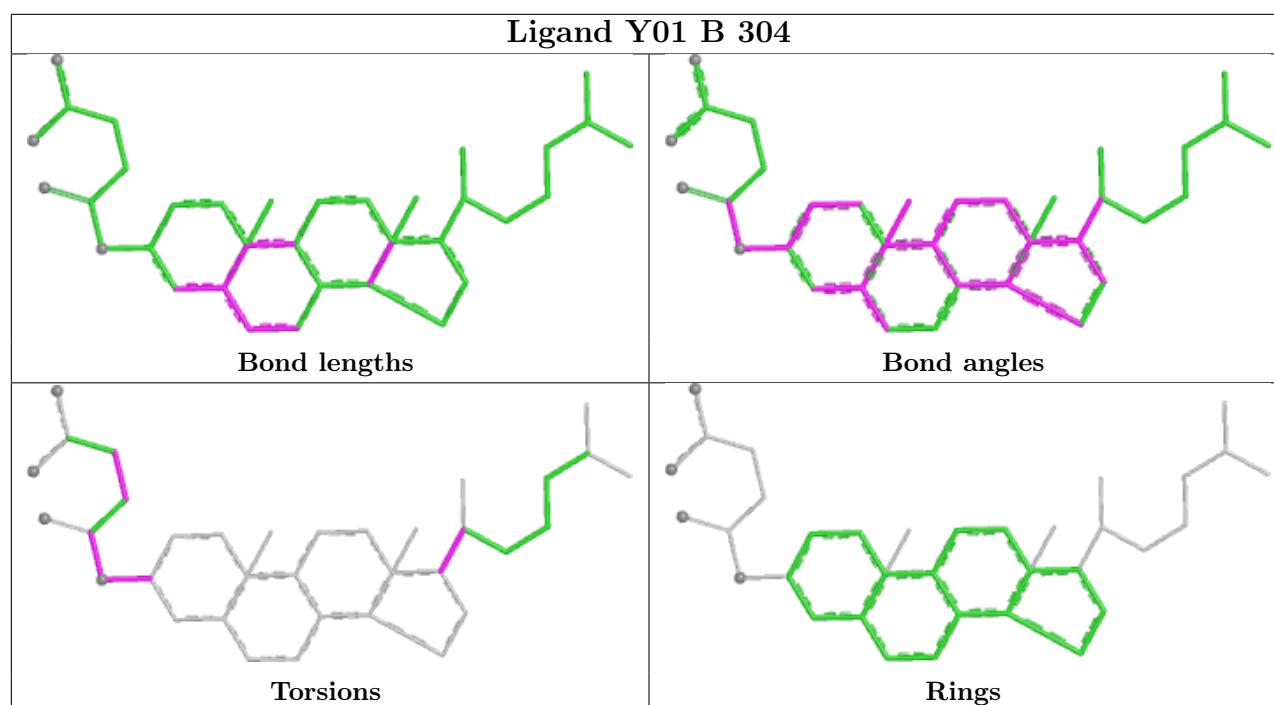
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	301	Y01	1	0
4	B	302	Y01	2	0
4	B	304	Y01	2	0

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	1
3	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	136:GLY	C	143:GLY	N	11.91
1	H	136:GLY	C	143:GLY	N	11.91

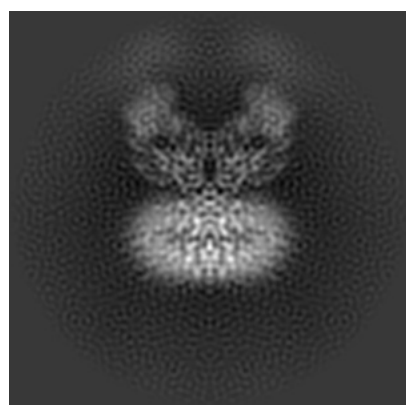
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10732. These allow visual inspection of the internal detail of the map and identification of artifacts.

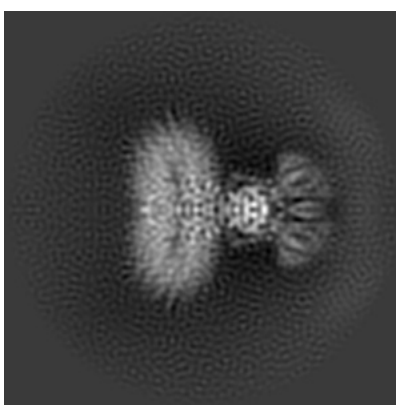
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

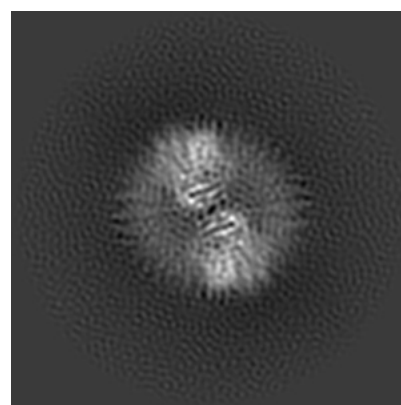
6.1.1 Primary map



X



Y

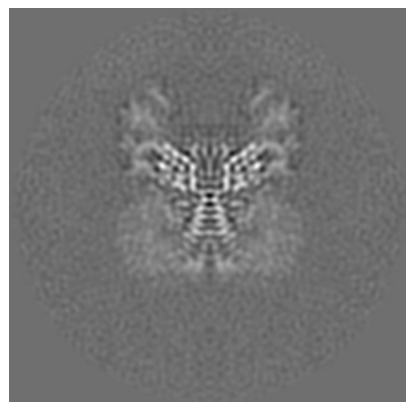


Z

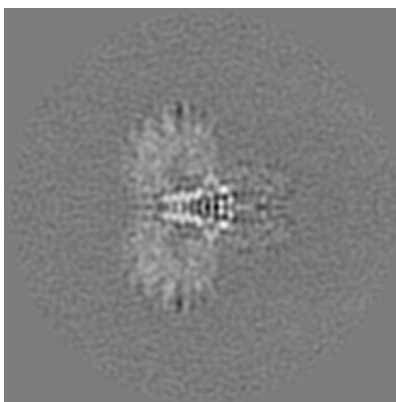
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

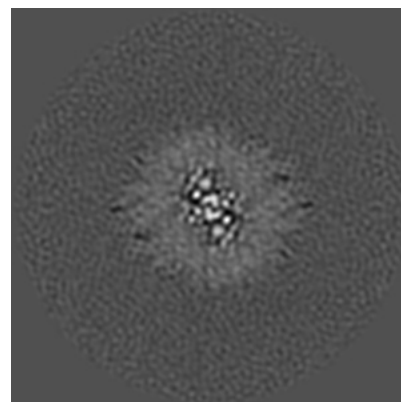
6.2.1 Primary map



X Index: 135



Y Index: 135

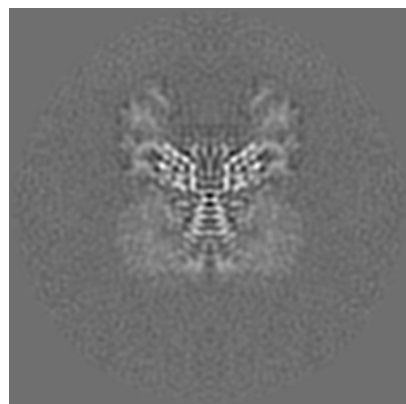


Z Index: 135

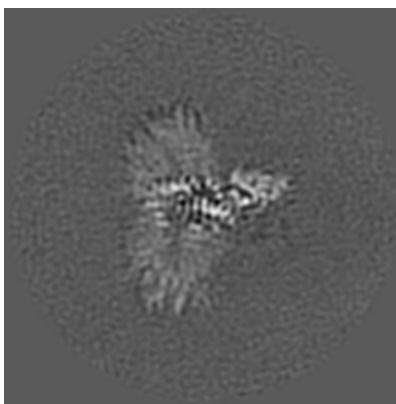
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

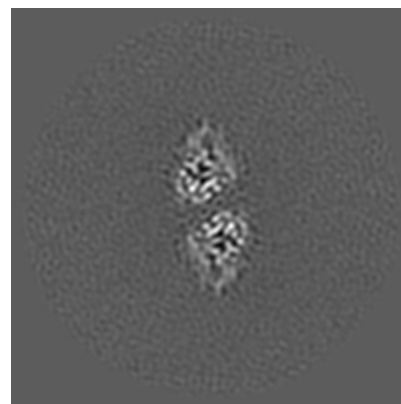
6.3.1 Primary map



X Index: 135



Y Index: 130

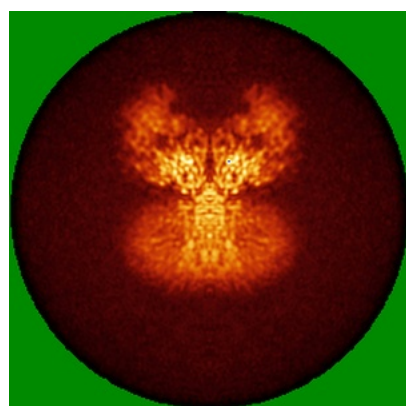


Z Index: 168

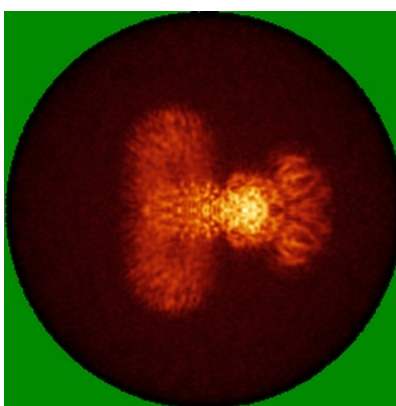
The images above show the largest variance slices of the map in three orthogonal directions.

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

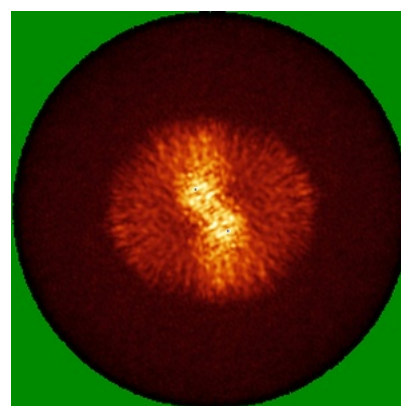
6.4.1 Primary map



X



Y

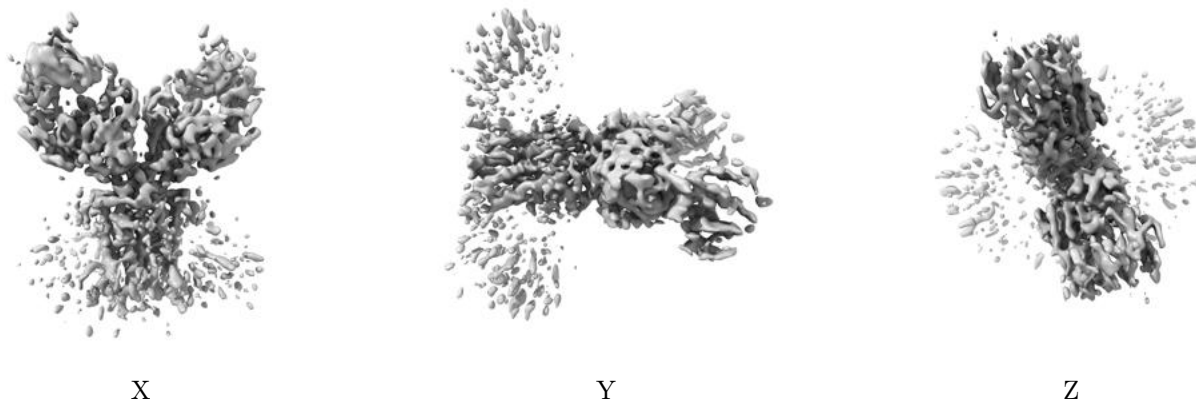


Z

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 0.61. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

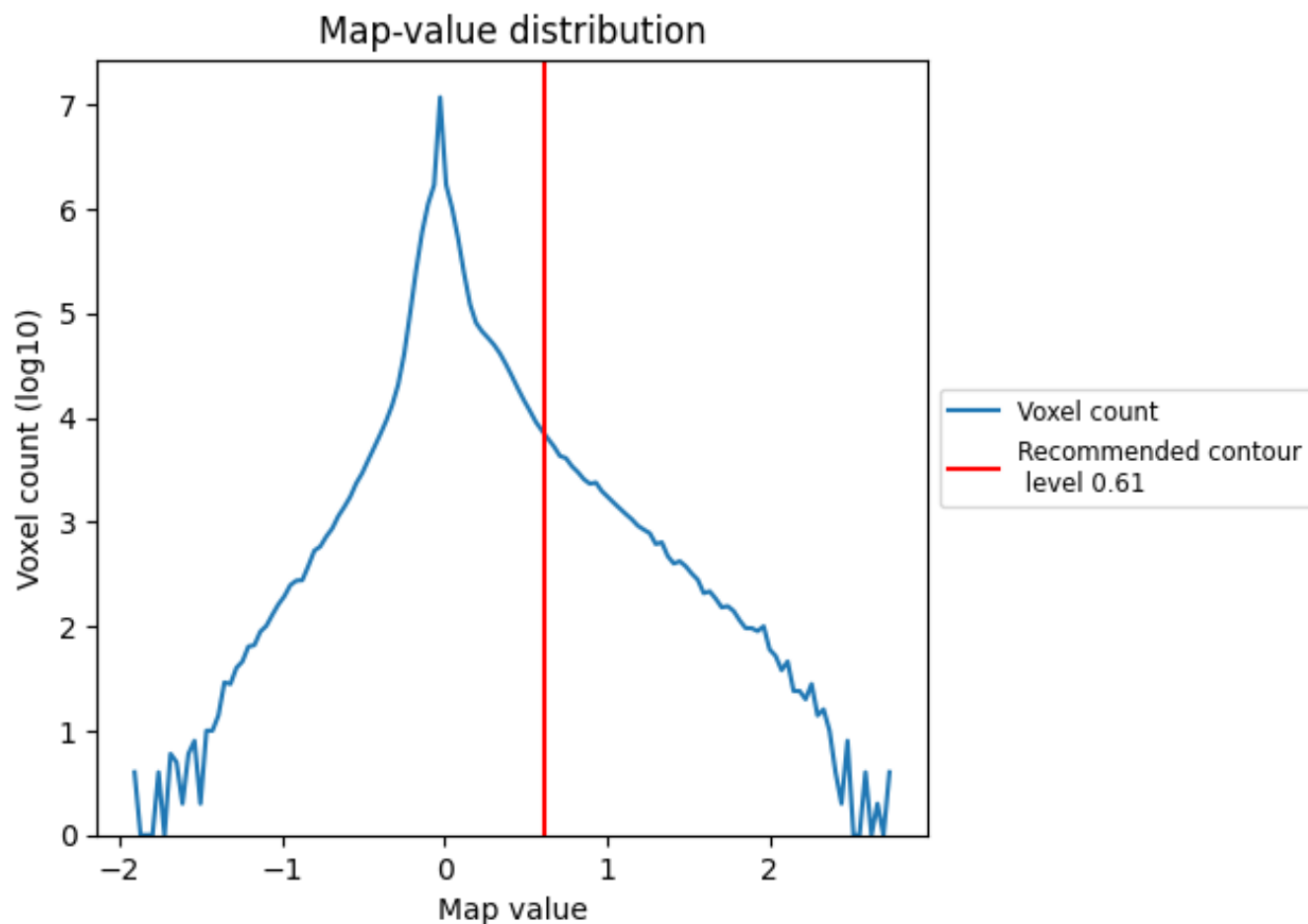
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

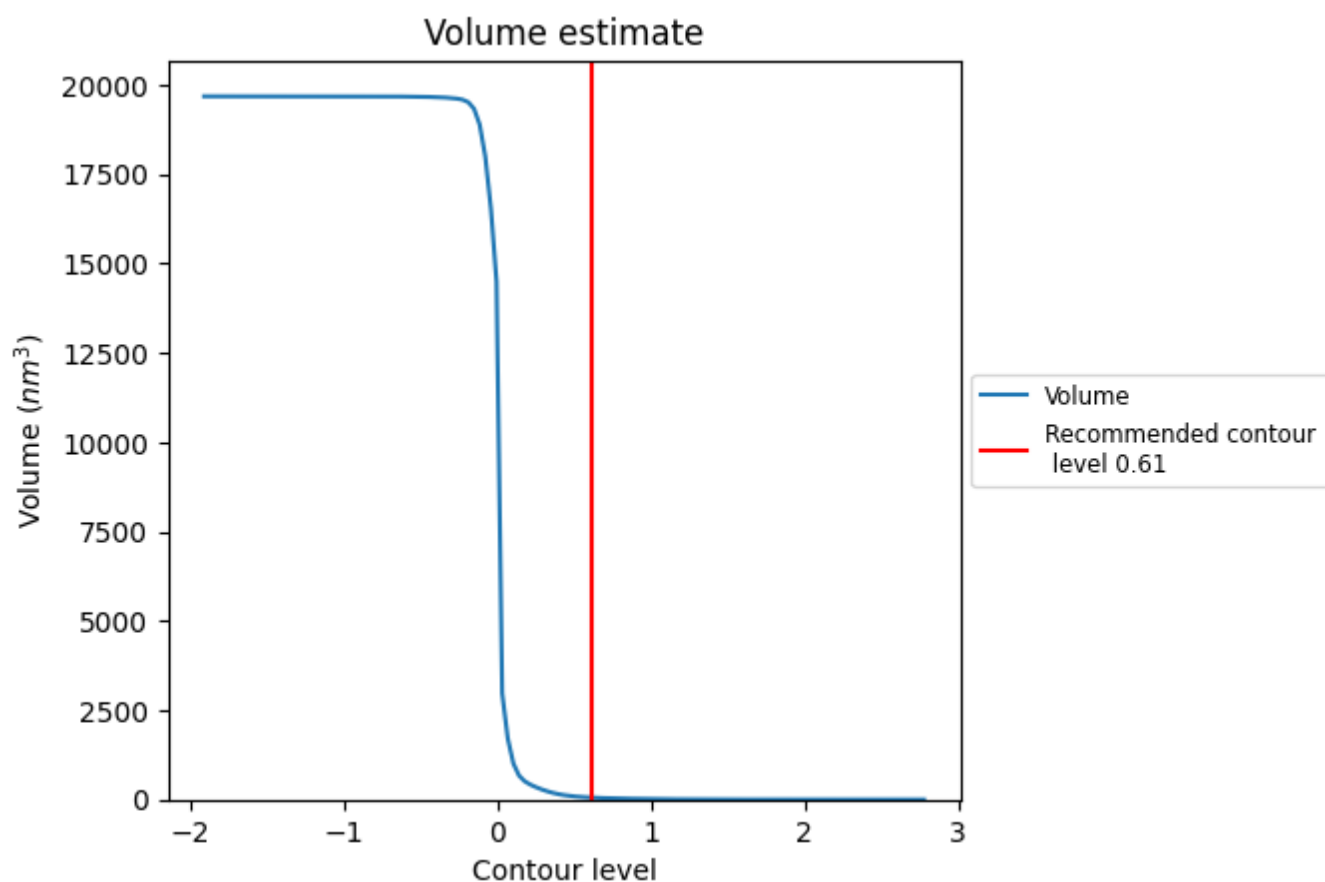
This section contains the results of statistical analysis of the map.

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.

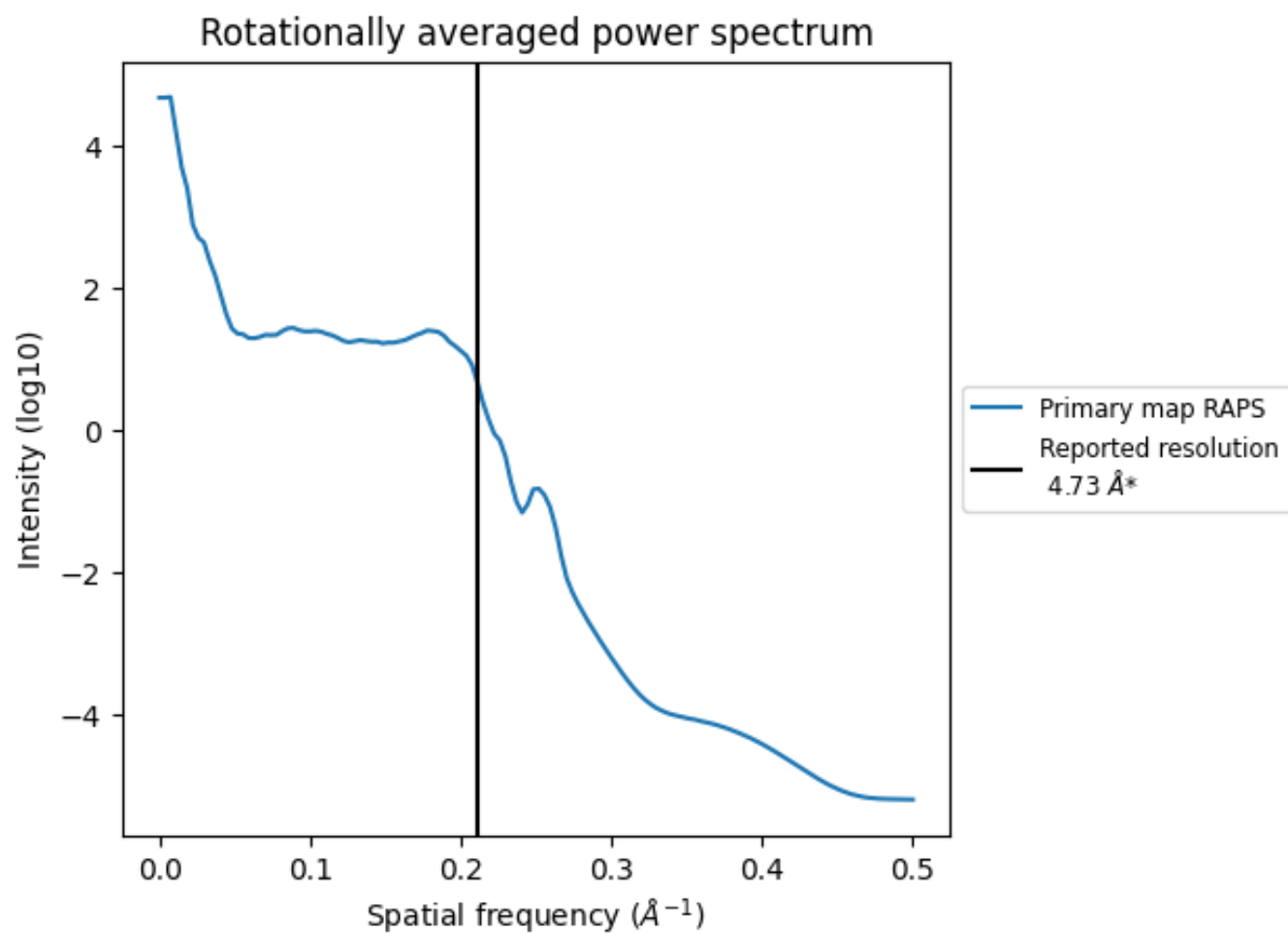
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 56 nm³; this corresponds to an approximate mass of 51 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 0.211 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

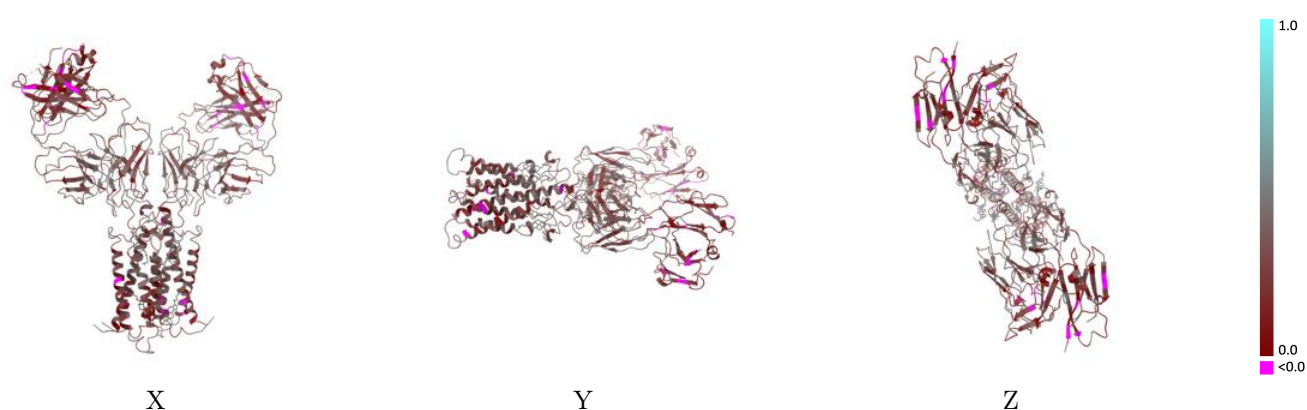
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10732 and PDB model 6Y92. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

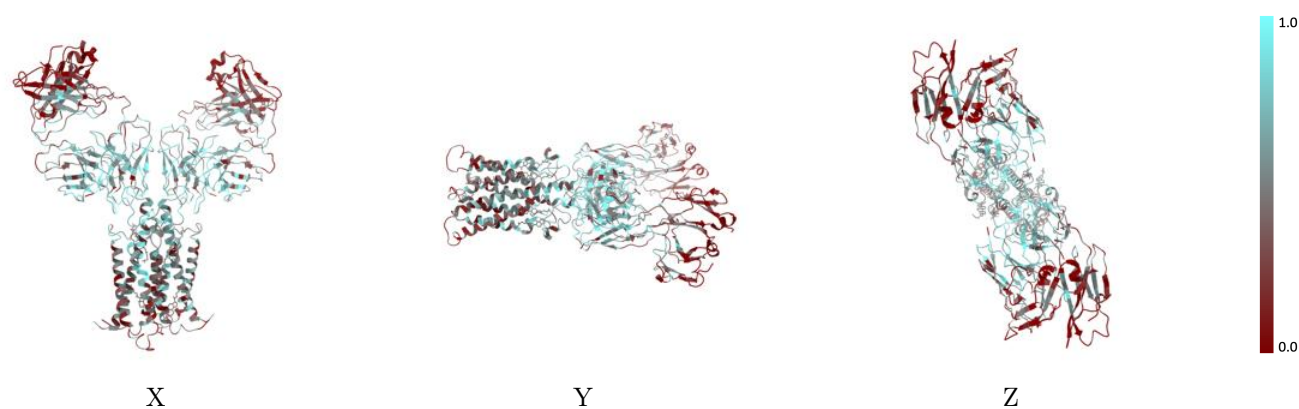
This section was not generated.

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



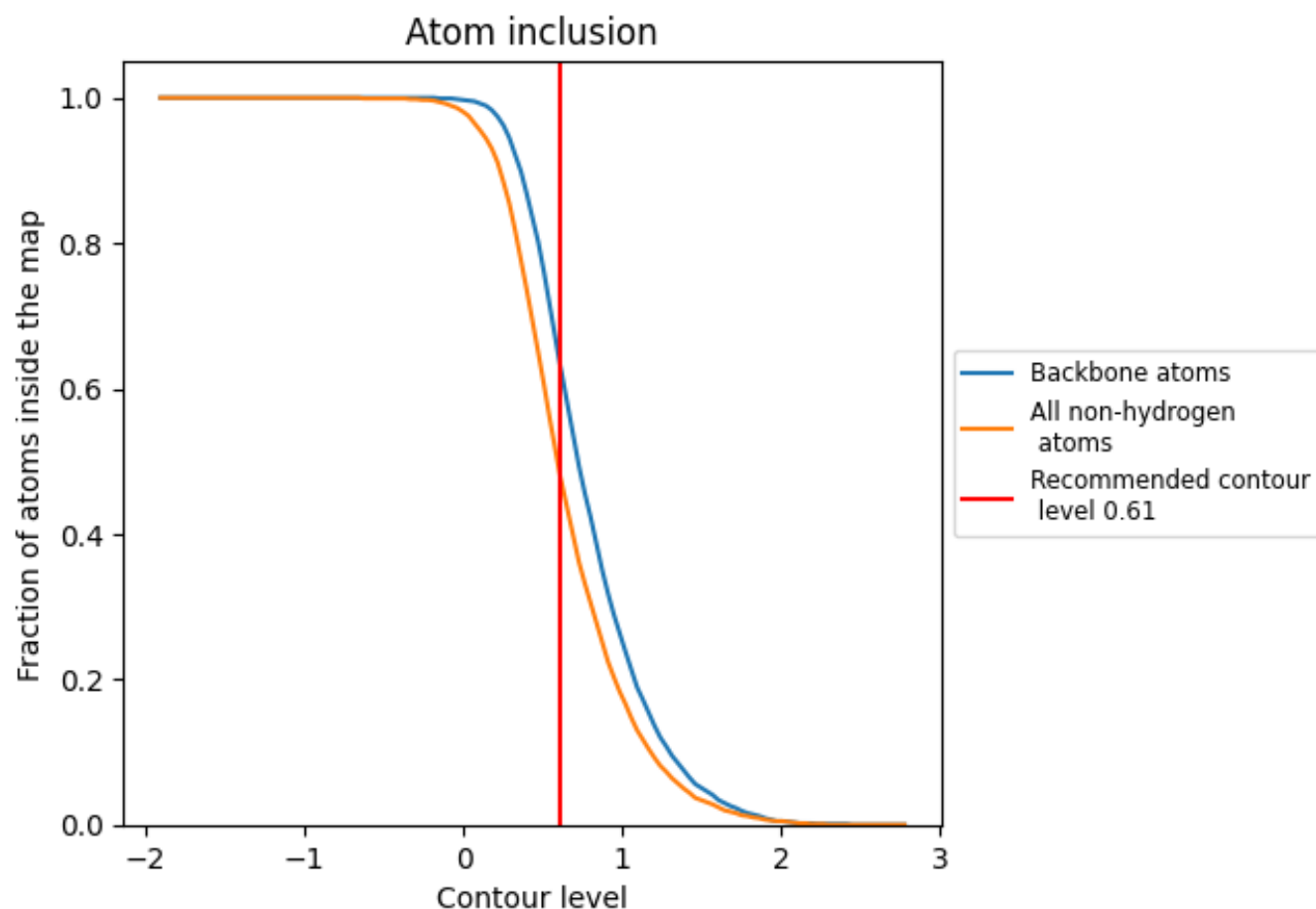
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.61).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 48% 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 (0.61) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4780	0.3020
A	0.4990	0.3130
B	0.4860	0.3060
C	0.5180	0.3090
D	0.4270	0.2880
H	0.5170	0.3090
L	0.4240	0.2880

1.0

0.0

<0.0