



Full wwPDB EM Validation Report ⓘ

Nov 12, 2024 – 02:15 AM JST

PDB ID : 8IJL
EMDB ID : EMD-35488
Title : Cyo-EM structure of wildtype non-gastric proton pump in the presence of Na⁺, AlF and ADP
Authors : Abe, K.
Deposited on : 2023-02-27
Resolution : 2.62 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

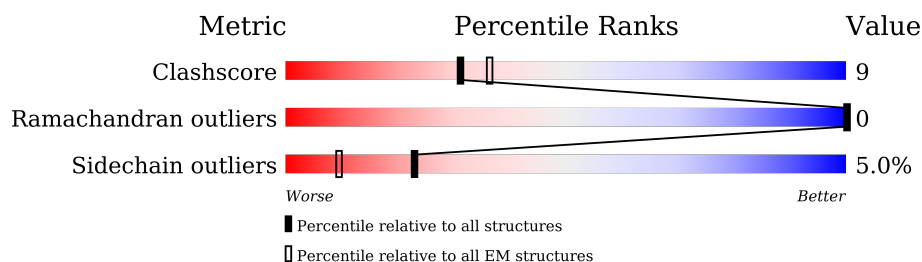
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.62 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	986	
2	B	324	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 10360 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 Sodium/potassium-transporting ATPase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	982	Total	C	N	O	S	0	0
			7638	4897	1277	1428	36		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	51	GLY	-	expression tag	UNP G3V8S4
A	52	MET	-	expression tag	UNP G3V8S4
A	512	ASN	ASP	engineered mutation	UNP G3V8S4

- Molecule 2 is a protein called Sodium/potassium-transporting ATPase subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	266	Total	C	N	O	S	0	0
			2165	1403	355	396	11		

There are 20 discrepancies between the modelled and reference sequences:

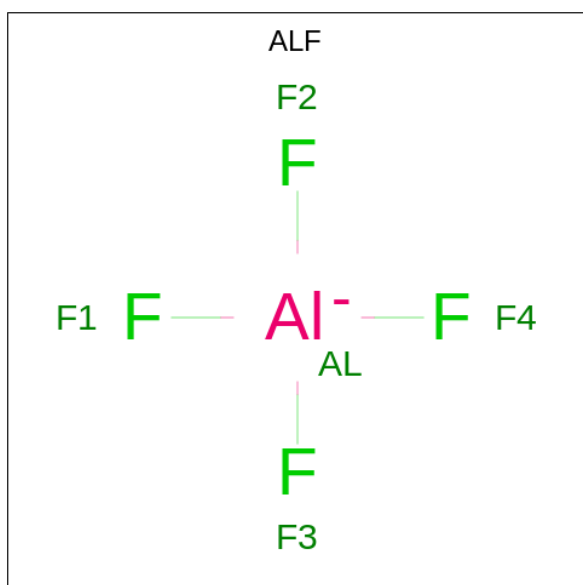
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP P07340
B	-18	GLY	-	expression tag	UNP P07340
B	-17	ASP	-	expression tag	UNP P07340
B	-16	TYR	-	expression tag	UNP P07340
B	-15	LYS	-	expression tag	UNP P07340
B	-14	ASP	-	expression tag	UNP P07340
B	-13	ASP	-	expression tag	UNP P07340
B	-12	ASP	-	expression tag	UNP P07340
B	-11	ASP	-	expression tag	UNP P07340
B	-10	LYS	-	expression tag	UNP P07340
B	-9	SER	-	expression tag	UNP P07340
B	-8	SER	-	expression tag	UNP P07340
B	-7	GLY	-	expression tag	UNP P07340
B	-6	GLU	-	expression tag	UNP P07340

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	ASN	-	expression tag	UNP P07340
B	-4	LEU	-	expression tag	UNP P07340
B	-3	TYR	-	expression tag	UNP P07340
B	-2	PHE	-	expression tag	UNP P07340
B	-1	GLN	-	expression tag	UNP P07340
B	0	GLY	-	expression tag	UNP P07340

- Molecule 3 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4) (labeled as "Ligand of Interest" by depositor).

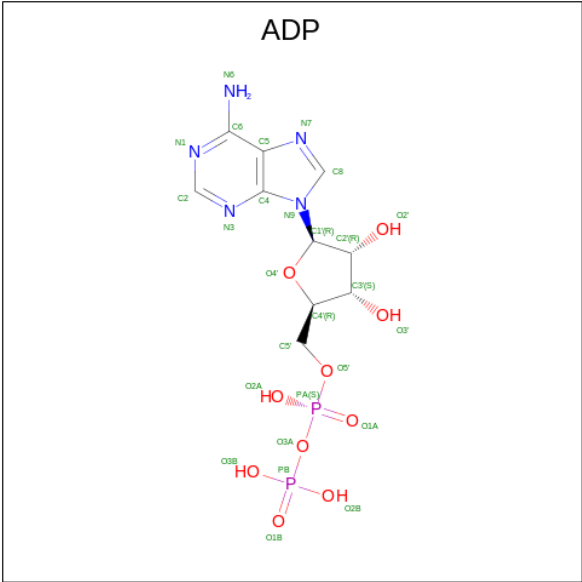


Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	Al	F	0
			5	1	4	

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

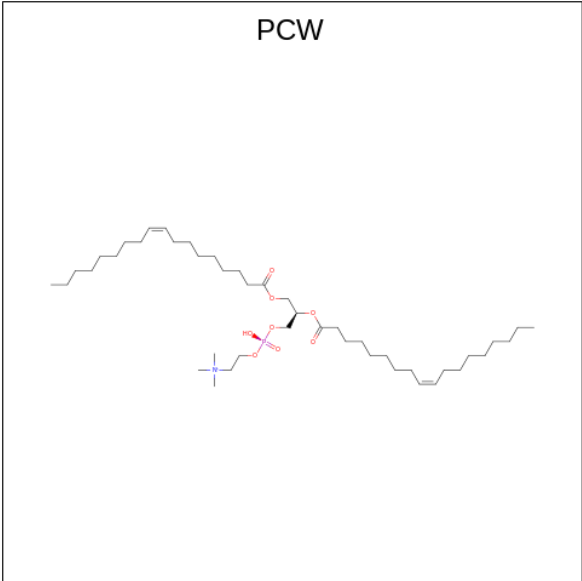
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 6 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: C₄₄H₈₅NO₈P).



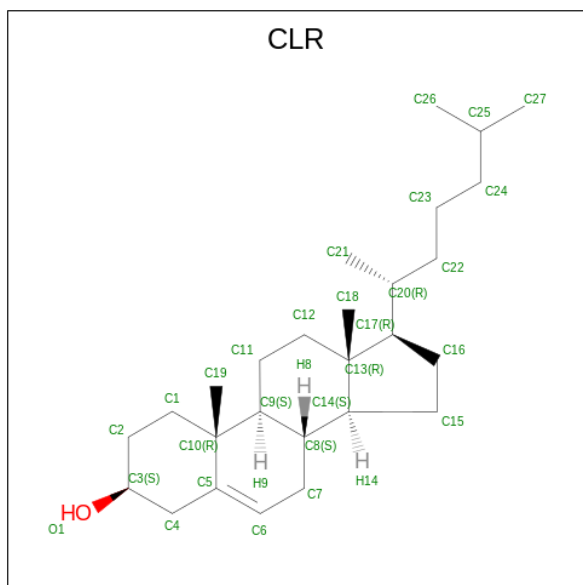
Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			49	39	1	8	1	
6	A	1	Total	C	N	O	P	0
			54	44	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
6	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
6	A	1	Total	C	N	O	P	0
			46	36	1	8	1	

- Molecule 7 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).

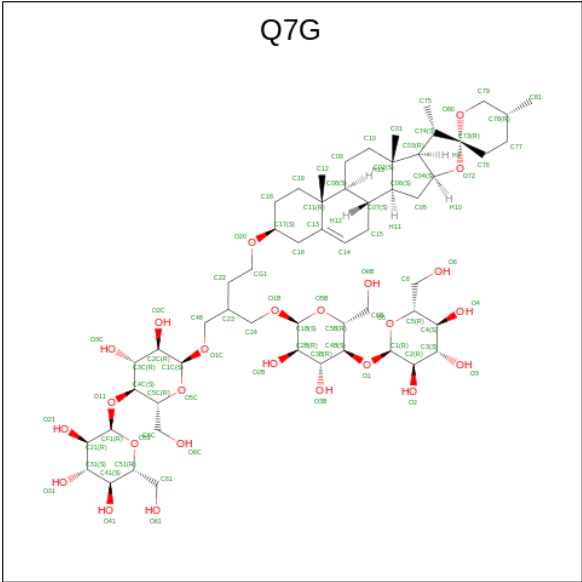


Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			28	27	1	
7	B	1	Total	C	O	0
			28	27	1	

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

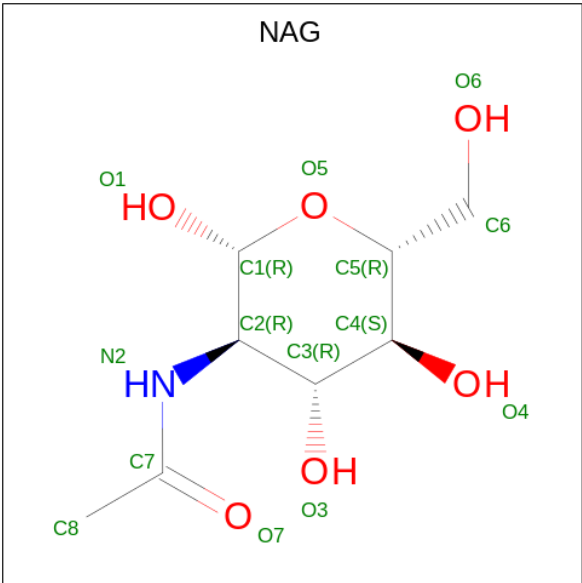
Mol	Chain	Residues	Atoms		AltConf
8	A	2	Total	Na	0
			2	2	

- Molecule 9 is 2-[[[4-O-alpha-D-glucopyranosyl-alpha-D-glucopyranosyl]oxy]methyl]-4-[[[(3b eta,9beta,14beta,17beta,25R)-spirost-5-en-3-yl]oxy]butyl 4-O-alpha-D-glucopyranosyl-alpha-D-glucopyranoside (three-letter code: Q7G) (formula: $C_{56}H_{92}O_{25}$).



Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	C	O	0
			39	34	5	
9	A	1	Total	C	O	0
			70	50	20	
9	B	1	Total	C	O	0
			39	34	5	
9	B	1	Total	C	O	0
			39	34	5	

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
10	B	1	Total	C	N	O	0
			14	8	1	5	

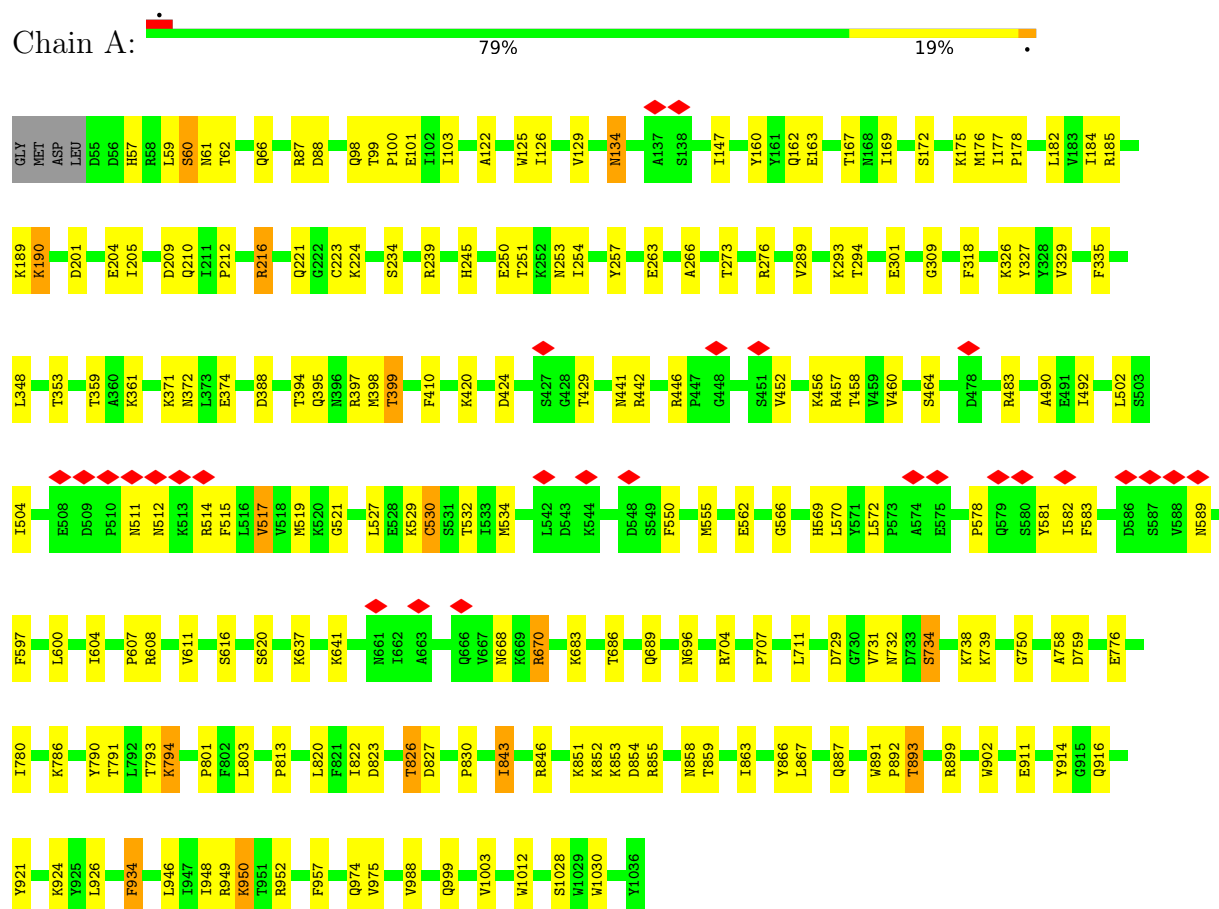
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		AltConf
11	A	8	Total	O	0
			8	8	

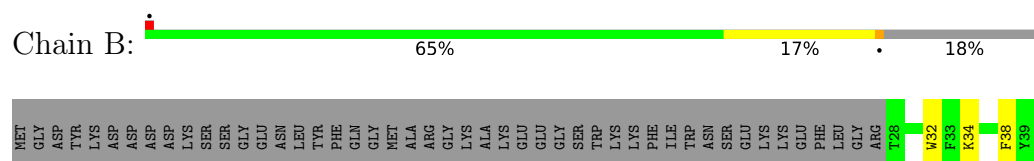
3 Residue-property plots

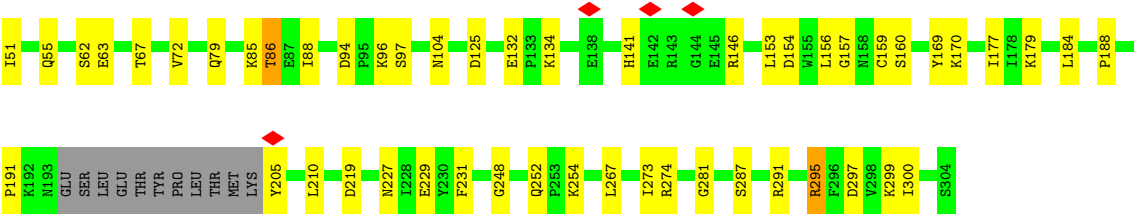
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Sodium/potassium-transporting ATPase subunit alpha



- Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	224740	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 ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.280	Depositor
Minimum map value	-1.480	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.227	Depositor
Map size (Å)	348.6, 348.6, 348.6	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83000004, 0.83000004, 0.83000004	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: NAG, MG, Q7G, ALF, PCW, NA, CLR, 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	0/7781	0.46	0/10561
2	B	0.27	0/2220	0.46	0/2991
All	All	0.26	0/10001	0.46	0/13552

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	7638	0	7784	132	0
2	B	2165	0	2148	32	0
3	A	5	0	0	1	0
4	A	1	0	0	0	0
5	A	27	0	12	2	0
6	A	257	0	389	37	0
7	A	28	0	46	3	0
7	B	28	0	46	16	0
8	A	2	0	0	0	0
9	A	109	0	0	0	0
9	B	78	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	14	0	13	0	0
11	A	8	0	0	0	0
All	All	10360	0	10438	178	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 9.

All (178) 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:863:ILE:HD11	7:B:402:CLR:H193	1.46	0.97
1:A:858:ASN:HB3	6:A:1106:PCW:H42	1.48	0.96
1:A:854:ASP:HA	6:A:1106:PCW:H72	1.49	0.92
1:A:863:ILE:CD1	7:B:402:CLR:H193	2.00	0.91
1:A:359:THR:HG21	1:A:780:ILE:HD11	1.59	0.83
1:A:858:ASN:HB3	6:A:1106:PCW:H62	1.60	0.82
1:A:863:ILE:HD13	7:B:402:CLR:H111	1.70	0.72
1:A:855:ARG:HG2	6:A:1106:PCW:H41	1.73	0.71
1:A:521:GLY:HA2	5:A:1103:ADP:H8	1.57	0.70
2:B:32:TRP:HZ3	7:B:402:CLR:H151	1.56	0.69
1:A:293:LYS:NZ	1:A:301:GLU:OE1	2.26	0.69
2:B:32:TRP:CZ3	7:B:402:CLR:H151	2.28	0.67
1:A:858:ASN:CB	6:A:1106:PCW:H42	2.24	0.67
1:A:887:GLN:HE22	1:A:999:GLN:HE21	1.41	0.66
1:A:452:VAL:O	1:A:457:ARG:NH1	2.28	0.66
2:B:227:ASN:ND2	2:B:229:GLU:OE2	2.28	0.66
1:A:855:ARG:H	6:A:1106:PCW:H51	1.62	0.65
1:A:859:THR:HG21	7:B:402:CLR:H192	1.79	0.64
1:A:578:PRO:HD2	1:A:581:TYR:HD2	1.62	0.63
1:A:245:HIS:HB3	1:A:250:GLU:O	1.98	0.63
6:A:1106:PCW:H262	7:B:402:CLR:H263	1.81	0.63
1:A:521:GLY:HA2	5:A:1103:ADP:C8	2.34	0.62
1:A:794:LYS:HE3	1:A:823:ASP:OD1	2.01	0.61
1:A:504:ILE:HG13	1:A:517:VAL:HB	1.84	0.60
1:A:169:ILE:O	1:A:172:SER:OG	2.17	0.60
1:A:855:ARG:CG	6:A:1106:PCW:H41	2.31	0.60
1:A:87:ARG:NH1	1:A:88:ASP:OD1	2.34	0.60
1:A:858:ASN:HD22	6:A:1106:PCW:C8	2.16	0.59
1:A:892:PRO:HB2	6:A:1107:PCW:H321	1.84	0.59
1:A:512:ASN:O	1:A:514:ARG:NH1	2.37	0.58
1:A:134:ASN:N	1:A:134:ASN:OD1	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ASN:ND2	1:A:759:ASP:OD1	2.38	0.56
1:A:801:PRO:HB3	1:A:813:PRO:HB2	1.87	0.56
2:B:291:ARG:O	2:B:295:ARG:NH1	2.38	0.56
1:A:863:ILE:CD1	7:B:402:CLR:H111	2.33	0.55
6:A:1106:PCW:H362	7:A:1109:CLR:H71	1.88	0.55
1:A:578:PRO:HD2	1:A:581:TYR:CD2	2.40	0.55
1:A:410:PHE:HE2	1:A:424:ASP:HB2	1.72	0.55
1:A:582:ILE:O	1:A:589:ASN:ND2	2.40	0.55
1:A:178:PRO:HB3	1:A:210:GLN:HB2	1.88	0.54
1:A:185:ARG:NH2	1:A:201:ASP:OD2	2.39	0.54
1:A:583:PHE:HA	1:A:589:ASN:HD22	1.71	0.54
2:B:267:LEU:HD22	2:B:273:ILE:HD13	1.90	0.54
1:A:184:ILE:HG12	1:A:189:LYS:HG2	1.91	0.53
2:B:287:SER:O	2:B:291:ARG:NH1	2.40	0.53
1:A:731:VAL:O	1:A:734:SER:OG	2.26	0.53
2:B:295:ARG:NH2	2:B:297:ASP:OD2	2.31	0.53
6:A:1106:PCW:H171	7:B:402:CLR:H182	1.90	0.53
1:A:707:PRO:HG3	1:A:732:ASN:HB2	1.89	0.53
1:A:122:ALA:O	1:A:126:ILE:HG13	2.09	0.53
1:A:318:PHE:HB3	1:A:335:PHE:HE2	1.75	0.52
1:A:515:PHE:HB2	1:A:572:LEU:HB2	1.92	0.52
1:A:858:ASN:HD22	6:A:1106:PCW:H81	1.74	0.52
1:A:562:GLU:HG2	1:A:604:ILE:HD12	1.91	0.52
1:A:490:ALA:HB3	1:A:504:ILE:HB	1.91	0.51
6:A:1105:PCW:H361	2:B:38:PHE:HB2	1.91	0.51
1:A:446:ARG:HH11	1:A:458:THR:HG22	1.76	0.51
1:A:182:LEU:HD23	1:A:204:GLU:HB2	1.92	0.50
1:A:398:MET:HE3	1:A:604:ILE:HA	1.93	0.50
1:A:999:GLN:O	1:A:1003:VAL:HG23	2.11	0.50
1:A:59:LEU:O	1:A:216:ARG:NH2	2.41	0.50
2:B:169:TYR:O	2:B:170:LYS:HB3	2.10	0.50
6:A:1107:PCW:H151	2:B:51:ILE:HG12	1.93	0.50
1:A:335:PHE:HZ	1:A:803:LEU:HD23	1.77	0.50
2:B:146:ARG:HB2	2:B:252:GLN:HG3	1.92	0.50
1:A:729:ASP:HB2	1:A:750:GLY:HA2	1.94	0.49
7:B:402:CLR:H183	7:B:402:CLR:H222	1.94	0.49
1:A:442:ARG:HH11	1:A:442:ARG:HG2	1.76	0.49
1:A:790:TYR:HE2	1:A:827:ASP:HB2	1.77	0.49
1:A:251:THR:HG23	1:A:253:ASN:H	1.77	0.49
1:A:668:ASN:OD1	1:A:668:ASN:N	2.46	0.49
2:B:188:PRO:HB3	2:B:210:LEU:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:VAL:HG13	1:A:570:LEU:HB3	1.94	0.49
1:A:294:THR:OG1	1:A:374:GLU:OE2	2.29	0.49
2:B:191:PRO:HD3	2:B:281:GLY:HA2	1.94	0.48
1:A:62:THR:O	1:A:66:GLN:HG3	2.12	0.48
1:A:185:ARG:HB2	1:A:190:LYS:HE3	1.94	0.48
6:A:1105:PCW:H342	2:B:34:LYS:HG2	1.96	0.48
2:B:43:TYR:HE2	7:B:402:CLR:H25	1.79	0.48
1:A:125:TRP:O	1:A:129:VAL:HG13	2.12	0.48
1:A:348:LEU:HD13	1:A:791:THR:HG21	1.96	0.48
1:A:863:ILE:HD13	7:B:402:CLR:C11	2.40	0.48
7:B:402:CLR:H241	7:B:402:CLR:C21	2.44	0.48
2:B:184:LEU:HD11	2:B:248:GLY:HA2	1.94	0.48
1:A:309:GLY:HA3	7:A:1109:CLR:H112	1.97	0.47
1:A:527:LEU:HD22	1:A:550:PHE:CD1	2.49	0.47
1:A:866:TYR:HD2	6:A:1106:PCW:H411	1.80	0.47
1:A:169:ILE:HD11	1:A:738:LYS:HD3	1.95	0.47
1:A:289:VAL:HG11	1:A:711:LEU:HD11	1.97	0.47
2:B:156:LEU:O	2:B:231:PHE:HB2	2.14	0.47
1:A:57:HIS:HB3	1:A:254:ILE:HD11	1.97	0.47
1:A:327:TYR:HE2	1:A:899:ARG:HH22	1.62	0.47
2:B:88:ILE:HB	2:B:300:ILE:HG12	1.97	0.47
1:A:975:VAL:HG21	6:A:1104:PCW:H232	1.97	0.47
2:B:51:ILE:O	2:B:55:GLN:HG2	2.16	0.46
1:A:793:THR:HG1	1:A:949:ARG:HH12	1.57	0.46
2:B:86:THR:HG22	2:B:299:LYS:HE2	1.97	0.46
1:A:793:THR:OG1	1:A:949:ARG:NH1	2.33	0.46
1:A:822:ILE:HA	1:A:826:THR:HB	1.98	0.46
1:A:178:PRO:HG3	1:A:212:PRO:HA	1.98	0.45
7:A:1109:CLR:H232	7:A:1109:CLR:H211	1.68	0.45
6:A:1107:PCW:H382	6:A:1107:PCW:H411	1.62	0.45
1:A:429:THR:HG23	1:A:534:MET:HG2	1.98	0.45
1:A:492:ILE:HD12	1:A:502:LEU:HD23	1.99	0.45
1:A:289:VAL:HB	1:A:739:LYS:HD3	1.97	0.45
6:A:1105:PCW:H442	2:B:42:PHE:HA	1.99	0.45
1:A:530:CYS:SG	1:A:597:PHE:N	2.90	0.45
1:A:395:GLN:OE1	1:A:397:ARG:NH2	2.47	0.45
1:A:397:ARG:HH21	1:A:399:THR:HG21	1.82	0.45
1:A:843:ILE:HG12	1:A:846:ARG:NH2	2.32	0.45
1:A:843:ILE:HG12	1:A:846:ARG:HH21	1.82	0.45
1:A:641:LYS:HE3	1:A:641:LYS:HB3	1.75	0.44
1:A:858:ASN:CB	6:A:1106:PCW:H62	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:CYS:HB3	1:A:239:ARG:HB2	1.99	0.44
1:A:827:ASP:HA	1:A:830:PRO:HD2	1.99	0.44
1:A:830:PRO:HB3	1:A:946:LEU:HD22	1.99	0.44
1:A:891:TRP:HB3	6:A:1107:PCW:O1P	2.17	0.44
2:B:156:LEU:HD23	2:B:156:LEU:HA	1.80	0.44
2:B:63:GLU:OE2	2:B:141:HIS:NE2	2.37	0.44
2:B:157:GLY:C	2:B:159:CYS:H	2.21	0.44
1:A:683:LYS:HB3	1:A:683:LYS:HE3	1.82	0.43
6:A:1108:PCW:H83	2:B:67:THR:HG23	2.00	0.43
1:A:176:MET:O	1:A:210:GLN:NE2	2.46	0.43
1:A:441:ASN:HB3	1:A:483:ARG:NH2	2.34	0.43
1:A:893:THR:OG1	6:A:1107:PCW:O2P	2.36	0.43
1:A:637:LYS:O	1:A:641:LYS:HG3	2.18	0.43
1:A:948:ILE:HG21	1:A:1012:TRP:HA	1.99	0.43
1:A:388:ASP:OD2	3:A:1101:ALF:F3	2.26	0.42
6:A:1107:PCW:H332	6:A:1107:PCW:H172	2.01	0.42
1:A:911:GLU:HA	1:A:916:GLN:O	2.19	0.42
2:B:153:LEU:HD12	2:B:153:LEU:HA	1.87	0.42
1:A:442:ARG:HG2	1:A:442:ARG:NH1	2.33	0.42
1:A:529:LYS:NZ	1:A:529:LYS:HB2	2.34	0.42
1:A:686:THR:HB	1:A:689:GLN:HG3	2.01	0.42
1:A:1030:TRP:HB2	6:A:1105:PCW:H142	2.01	0.42
1:A:527:LEU:HD12	1:A:527:LEU:HA	1.84	0.42
1:A:100:PRO:HB2	1:A:103:ILE:HG12	2.02	0.42
2:B:132:GLU:CD	2:B:132:GLU:H	2.22	0.42
1:A:914:TYR:OH	2:B:62:SER:O	2.20	0.42
1:A:921:TYR:HA	1:A:924:LYS:HE3	2.01	0.42
2:B:274:ARG:HG2	2:B:299:LYS:HG2	2.01	0.42
1:A:160:TYR:O	1:A:163:GLU:HG2	2.20	0.42
1:A:162:GLN:HB2	1:A:353:THR:HG23	2.01	0.42
1:A:177:ILE:HD12	1:A:257:TYR:CZ	2.55	0.42
1:A:776:GLU:O	1:A:780:ILE:HG13	2.19	0.42
1:A:851:LYS:HG3	1:A:852:LYS:HG2	2.02	0.42
1:A:853:LYS:O	6:A:1106:PCW:C5	2.67	0.42
1:A:704:ARG:HD2	1:A:704:ARG:HA	1.91	0.42
1:A:502:LEU:HD13	1:A:519:MET:HB2	2.02	0.42
2:B:254:LYS:HB3	2:B:254:LYS:HE3	1.67	0.42
7:B:402:CLR:H162	7:B:402:CLR:H221	1.87	0.42
1:A:826:THR:O	1:A:974:GLN:HG2	2.18	0.41
6:A:1105:PCW:H472	6:A:1105:PCW:H261	2.01	0.41
1:A:608:ARG:HB2	1:A:611:VAL:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:786:LYS:HE2	1:A:952:ARG:HG3	2.01	0.41
1:A:855:ARG:HG2	6:A:1106:PCW:H51	2.03	0.41
1:A:205:ILE:HD11	1:A:266:ALA:HB3	2.02	0.41
1:A:394:THR:HA	1:A:607:PRO:HA	2.02	0.41
1:A:801:PRO:HG3	1:A:934:PHE:CZ	2.55	0.41
1:A:1028:SER:HB2	6:A:1105:PCW:H32	2.02	0.41
2:B:94:ASP:O	2:B:97:SER:OG	2.38	0.41
7:B:402:CLR:H222	7:B:402:CLR:C18	2.50	0.41
1:A:902:TRP:HH2	1:A:926:LEU:HD23	1.84	0.41
1:A:957:PHE:HB3	6:A:1104:PCW:H83	2.01	0.41
1:A:867:LEU:HD21	6:A:1106:PCW:H431	2.02	0.41
1:A:60:SER:OG	1:A:61:ASN:N	2.53	0.41
6:A:1106:PCW:H152	7:B:402:CLR:C19	2.50	0.41
1:A:147:ILE:HG21	1:A:820:LEU:HD13	2.03	0.41
1:A:371:LYS:NZ	1:A:758:ALA:O	2.48	0.41
1:A:950:LYS:HB2	1:A:950:LYS:HE2	1.84	0.41
6:A:1107:PCW:H132	6:A:1107:PCW:H161	1.89	0.41
6:A:1107:PCW:H211	6:A:1107:PCW:H182	1.68	0.41
1:A:224:LYS:HB2	1:A:263:GLU:HG2	2.03	0.40
1:A:670:ARG:NH1	1:A:696:ASN:HB3	2.36	0.40
2:B:134:LYS:HE2	2:B:134:LYS:HB3	1.74	0.40
6:A:1105:PCW:H182	6:A:1105:PCW:H211	1.95	0.40
1:A:566:GLY:HA2	1:A:600:LEU:HD23	2.03	0.40
1:A:853:LYS:O	6:A:1106:PCW:H52	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	980/986 (99%)	960 (98%)	20 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	262/324 (81%)	256 (98%)	6 (2%)	0	100	100
All	All	1242/1310 (95%)	1216 (98%)	26 (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	838/841 (100%)	799 (95%)	39 (5%)	22	43
2	B	236/286 (82%)	221 (94%)	15 (6%)	14	30
All	All	1074/1127 (95%)	1020 (95%)	54 (5%)	23	41

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	SER
1	A	98	GLN
1	A	99	THR
1	A	101	GLU
1	A	134	ASN
1	A	167	THR
1	A	175	LYS
1	A	190	LYS
1	A	209	ASP
1	A	216	ARG
1	A	221	GLN
1	A	234	SER
1	A	273	THR
1	A	276	ARG
1	A	326	LYS
1	A	329	VAL
1	A	361	LYS
1	A	399	THR

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Mol	Chain	Res	Type
1	A	420	LYS
1	A	456	LYS
1	A	460	VAL
1	A	464	SER
1	A	511	ASN
1	A	517	VAL
1	A	530	CYS
1	A	532	THR
1	A	555	MET
1	A	569	HIS
1	A	616	SER
1	A	620	SER
1	A	670	ARG
1	A	734	SER
1	A	794	LYS
1	A	826	THR
1	A	843	ILE
1	A	893	THR
1	A	934	PHE
1	A	950	LYS
1	A	988	VAL
2	B	40	VAL
2	B	72	VAL
2	B	79	GLN
2	B	85	LYS
2	B	86	THR
2	B	96	LYS
2	B	104	ASN
2	B	125	ASP
2	B	154	ASP
2	B	160	SER
2	B	177	ILE
2	B	179	LYS
2	B	205	TYR
2	B	219	ASP
2	B	295	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	538	GLN
1	A	540	GLN

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Mol	Chain	Res	Type
1	A	551	HIS
1	A	589	ASN
1	A	887	GLN
2	B	84	GLN
2	B	242	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](#)

Of 17 ligands modelled in this entry, 3 are monoatomic - leaving 14 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	Q7G	B	403	-	44,44,90	0.30	0	66,68,138	0.55	1 (1%)
6	PCW	A	1107	-	53,53,53	0.91	2 (3%)	59,61,61	2.17	9 (15%)
5	ADP	A	1103	-	24,29,29	0.65	0	29,45,45	0.85	1 (3%)
3	ALF	A	1101	-	0,4,4	-	-	-	-	-
10	NAG	B	401	2	14,14,15	0.31	0	17,19,21	0.55	0
6	PCW	A	1108	-	45,45,53	1.01	2 (4%)	51,53,61	1.06	3 (5%)
7	CLR	B	402	-	31,31,31	0.28	0	48,48,48	0.77	0
6	PCW	A	1105	-	53,53,53	0.93	2 (3%)	59,61,61	0.98	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PCW	A	1104	-	48,48,53	0.98	2 (4%)	54,56,61	0.99	3 (5%)
7	CLR	A	1109	-	31,31,31	0.72	0	48,48,48	1.11	2 (4%)
9	Q7G	B	404	-	44,44,90	0.34	0	66,68,138	0.63	2 (3%)
6	PCW	A	1106	-	53,53,53	0.40	0	59,61,61	0.37	0
9	Q7G	A	1112	-	44,44,90	0.24	0	66,68,138	0.30	0
9	Q7G	A	1113	-	78,78,90	0.16	0	118,120,138	0.40	0

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	Q7G	B	403	-	-	4/12/100/200	0/6/6/10
6	PCW	A	1107	-	-	16/57/57/57	-
5	ADP	A	1103	-	-	1/12/32/32	0/3/3/3
10	NAG	B	401	2	-	3/6/23/26	0/1/1/1
6	PCW	A	1108	-	-	13/49/49/57	-
7	CLR	B	402	-	-	6/10/68/68	0/4/4/4
6	PCW	A	1105	-	-	17/57/57/57	-
6	PCW	A	1104	-	-	18/52/52/57	-
7	CLR	A	1109	-	-	5/10/68/68	0/4/4/4
9	Q7G	B	404	-	-	4/12/100/200	0/6/6/10
6	PCW	A	1106	-	-	14/57/57/57	-
9	Q7G	A	1112	-	-	2/12/100/200	0/6/6/10
9	Q7G	A	1113	-	-	10/26/174/200	0/9/9/10

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1105	PCW	O3-C11	4.26	1.45	1.33
6	A	1104	PCW	O3-C11	4.23	1.45	1.33
6	A	1108	PCW	O3-C11	4.23	1.45	1.33
6	A	1107	PCW	O3-C11	4.17	1.45	1.33
6	A	1104	PCW	O2-C31	4.14	1.46	1.34
6	A	1108	PCW	O2-C31	4.07	1.45	1.34
6	A	1107	PCW	O2-C31	4.05	1.45	1.34
6	A	1105	PCW	O2-C31	4.04	1.45	1.34

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1107	PCW	C8-N-C6	-8.99	85.86	108.97
6	A	1107	PCW	C8-N-C7	-8.57	86.95	108.97
6	A	1107	PCW	C8-N-C5	-5.74	86.42	109.92
6	A	1108	PCW	O2-C31-C32	4.25	120.66	111.50
6	A	1107	PCW	O2-C31-C32	4.14	120.42	111.50
6	A	1104	PCW	O2-C31-C32	4.04	120.21	111.50
6	A	1107	PCW	C7-N-C6	3.96	119.16	108.97
6	A	1105	PCW	O2-C31-C32	3.81	119.71	111.50
7	A	1109	CLR	C13-C17-C20	-3.34	114.25	119.49
6	A	1107	PCW	C2-O2-C31	-2.97	110.47	117.79
6	A	1105	PCW	O3-C11-C12	2.71	120.42	111.91
6	A	1104	PCW	O3-C11-C12	2.63	120.17	111.91
6	A	1107	PCW	C6-N-C5	2.58	120.48	109.92
6	A	1108	PCW	O3-C11-C12	2.56	119.95	111.91
9	B	404	Q7G	C79-O80-C73	2.53	118.50	113.72
6	A	1105	PCW	C2-O2-C31	-2.46	111.74	117.79
9	B	403	Q7G	C79-O80-C73	2.45	118.37	113.72
6	A	1107	PCW	C7-N-C5	2.27	119.19	109.92
5	A	1103	ADP	C5-C6-N6	2.24	123.76	120.35
6	A	1108	PCW	C2-O2-C31	-2.24	112.28	117.79
6	A	1107	PCW	C13-C12-C11	-2.21	105.58	113.62
6	A	1104	PCW	C2-O2-C31	-2.11	112.58	117.79
9	B	404	Q7G	O80-C73-C76	2.07	112.70	110.77
7	A	1109	CLR	C8-C7-C6	-2.04	109.81	112.73

There are no chirality outliers.

All (113) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1104	PCW	C32-C31-O2-C2
6	A	1104	PCW	C4-O4P-P-O2P
6	A	1105	PCW	C1-O3P-P-O4P
6	A	1107	PCW	O4P-C4-C5-N
6	A	1107	PCW	C4-O4P-P-O1P
6	A	1108	PCW	C4-O4P-P-O2P
9	A	1112	Q7G	C22-CG1-O20-C17
9	A	1113	Q7G	C2B-C1B-O1B-C24
9	A	1113	Q7G	O5B-C1B-O1B-C24
9	B	404	Q7G	C22-CG1-O20-C17
6	A	1105	PCW	O11-C11-O3-C3
6	A	1104	PCW	O31-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
6	A	1105	PCW	C12-C11-O3-C3
7	A	1109	CLR	C13-C17-C20-C21
7	A	1109	CLR	C13-C17-C20-C22
9	A	1113	Q7G	C3C-C4C-O11-CF1
7	A	1109	CLR	C16-C17-C20-C21
7	B	402	CLR	C16-C17-C20-C21
6	A	1104	PCW	C11-C12-C13-C14
10	B	401	NAG	C8-C7-N2-C2
7	B	402	CLR	C13-C17-C20-C22
6	A	1104	PCW	C21-C22-C23-C24
6	A	1108	PCW	C31-C32-C33-C34
7	B	402	CLR	C13-C17-C20-C21
7	A	1109	CLR	C16-C17-C20-C22
6	A	1106	PCW	C4-O4P-P-O3P
6	A	1107	PCW	C4-O4P-P-O3P
10	B	401	NAG	O7-C7-N2-C2
6	A	1107	PCW	C4-C5-N-C7
6	A	1107	PCW	C12-C11-O3-C3
6	A	1105	PCW	C21-C22-C23-C24
7	B	402	CLR	C23-C24-C25-C26
6	A	1108	PCW	C21-C22-C23-C24
6	A	1108	PCW	C23-C24-C25-C26
6	A	1106	PCW	C31-C32-C33-C34
9	B	404	Q7G	C16-C17-O20-CG1
9	B	404	Q7G	C18-C17-O20-CG1
9	A	1113	Q7G	C22-CG1-O20-C17
9	B	403	Q7G	C22-CG1-O20-C17
6	A	1107	PCW	O11-C11-O3-C3
9	A	1112	Q7G	C23-C24-O1B-C1B
6	A	1107	PCW	C32-C31-O2-C2
7	B	402	CLR	C23-C24-C25-C27
6	A	1107	PCW	O31-C31-O2-C2
7	A	1109	CLR	C20-C22-C23-C24
6	A	1104	PCW	C22-C23-C24-C25
6	A	1105	PCW	C32-C31-O2-C2
6	A	1104	PCW	C4-O4P-P-O3P
9	A	1113	Q7G	O5B-C5B-C6B-O6B
10	B	401	NAG	O5-C5-C6-O6
6	A	1104	PCW	O3P-C1-C2-O2
6	A	1107	PCW	C4-C5-N-C8
6	A	1108	PCW	C16-C17-C18-C19
9	A	1113	Q7G	C2C-C1C-O1C-C48

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Mol	Chain	Res	Type	Atoms
6	A	1106	PCW	C32-C33-C34-C35
6	A	1104	PCW	C23-C24-C25-C26
9	B	403	Q7G	C23-C48-O1C-C1C
9	B	404	Q7G	C23-C24-O1B-C1B
6	A	1107	PCW	C15-C16-C17-C18
6	A	1105	PCW	O31-C31-O2-C2
6	A	1106	PCW	C1-O3P-P-O4P
6	A	1104	PCW	O2-C2-C3-O3
9	A	1113	Q7G	O5C-C1C-O1C-C48
7	B	402	CLR	C20-C22-C23-C24
9	A	1113	Q7G	C5C-C4C-O11-CF1
6	A	1106	PCW	C2-C1-O3P-P
6	A	1108	PCW	C32-C33-C34-C35
9	A	1113	Q7G	C23-C22-CG1-O20
5	A	1103	ADP	PB-O3A-PA-O5'
6	A	1104	PCW	C15-C16-C17-C18
9	B	403	Q7G	C23-C22-CG1-O20
9	A	1113	Q7G	C16-C17-O20-CG1
6	A	1105	PCW	C4-O4P-P-O3P
6	A	1108	PCW	C1-O3P-P-O4P
6	A	1108	PCW	C4-O4P-P-O3P
6	A	1104	PCW	C4-O4P-P-O1P
6	A	1105	PCW	C1-O3P-P-O1P
6	A	1106	PCW	C4-O4P-P-O2P
6	A	1104	PCW	O3P-C1-C2-C3
6	A	1107	PCW	C12-C13-C14-C15
6	A	1105	PCW	O3P-C1-C2-O2
6	A	1108	PCW	C11-C12-C13-C14
6	A	1105	PCW	O4P-C4-C5-N
6	A	1106	PCW	C3-C2-O2-C31
6	A	1104	PCW	C19-C20-C21-C22
6	A	1104	PCW	C17-C18-C19-C20
6	A	1107	PCW	C1-O3P-P-O4P
6	A	1108	PCW	C12-C13-C14-C15
6	A	1104	PCW	C1-C2-C3-O3
6	A	1106	PCW	O31-C31-O2-C2
6	A	1105	PCW	O3P-C1-C2-C3
6	A	1106	PCW	C33-C34-C35-C36
6	A	1106	PCW	C18-C19-C20-C21
6	A	1105	PCW	C35-C36-C37-C38
6	A	1105	PCW	C37-C38-C39-C40
6	A	1105	PCW	C39-C40-C41-C42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	A	1105	PCW	C17-C18-C19-C20
6	A	1106	PCW	C1-C2-O2-C31
6	A	1107	PCW	O2-C31-C32-C33
6	A	1106	PCW	C20-C21-C22-C23
6	A	1107	PCW	C43-C44-C45-C46
6	A	1105	PCW	O3-C11-C12-C13
6	A	1107	PCW	C33-C34-C35-C36
6	A	1106	PCW	C21-C22-C23-C24
6	A	1108	PCW	O3-C11-C12-C13
6	A	1106	PCW	C32-C31-O2-C2
6	A	1107	PCW	O31-C31-C32-C33
6	A	1104	PCW	C1-O3P-P-O2P
6	A	1105	PCW	O11-C11-C12-C13
6	A	1108	PCW	O11-C11-C12-C13
6	A	1104	PCW	O11-C11-O3-C3
9	B	403	Q7G	C23-C24-O1B-C1B
6	A	1108	PCW	C15-C16-C17-C18

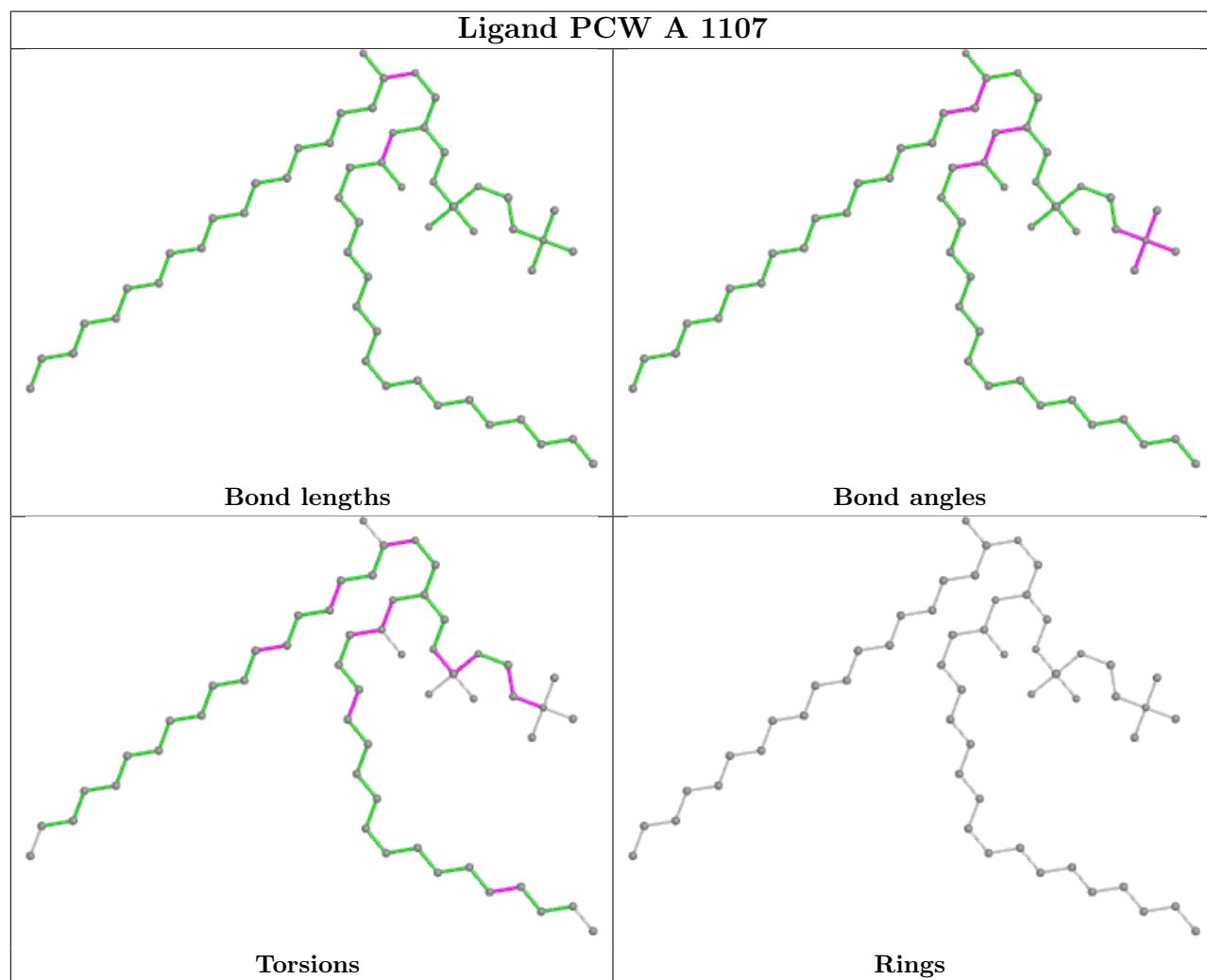
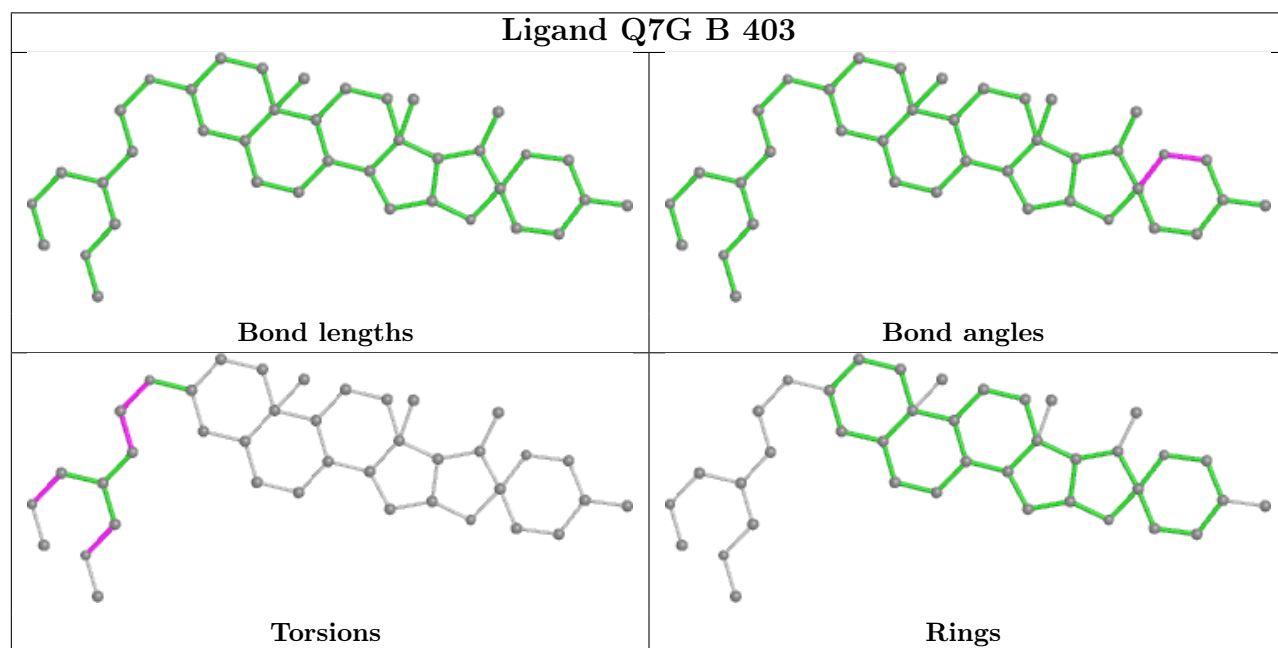
There are no ring outliers.

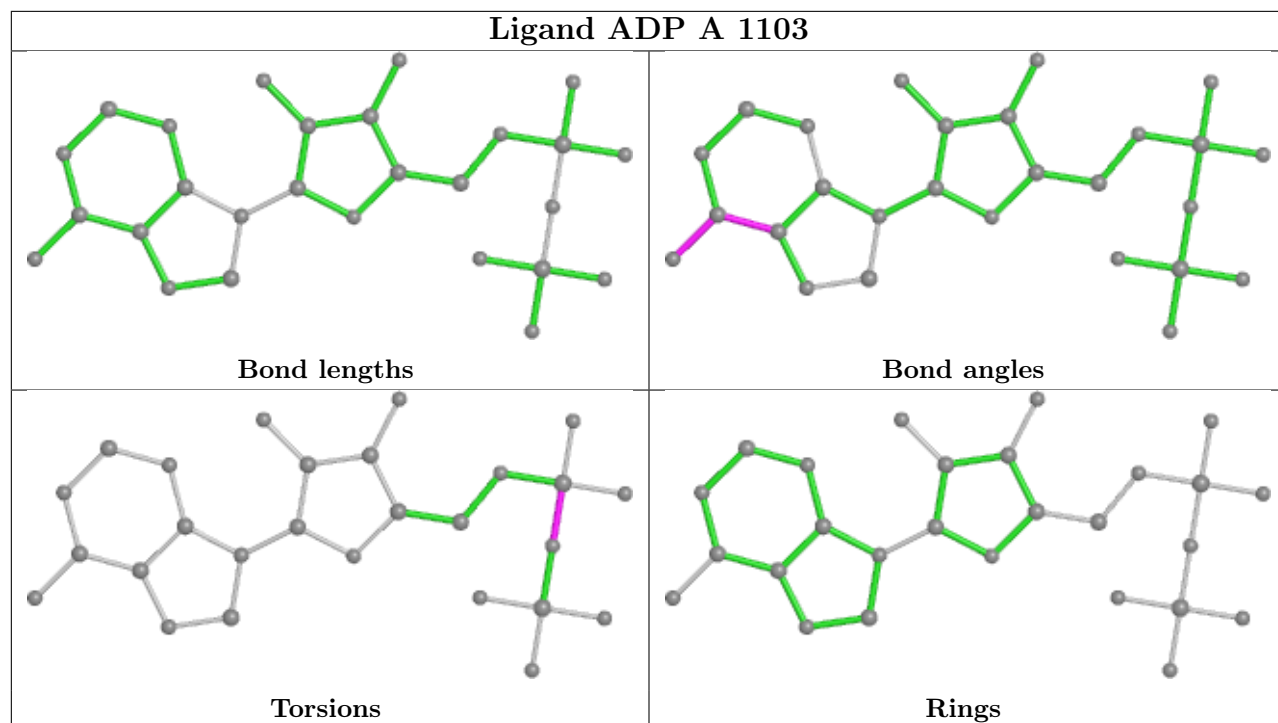
9 monomers are involved in 55 short contacts:

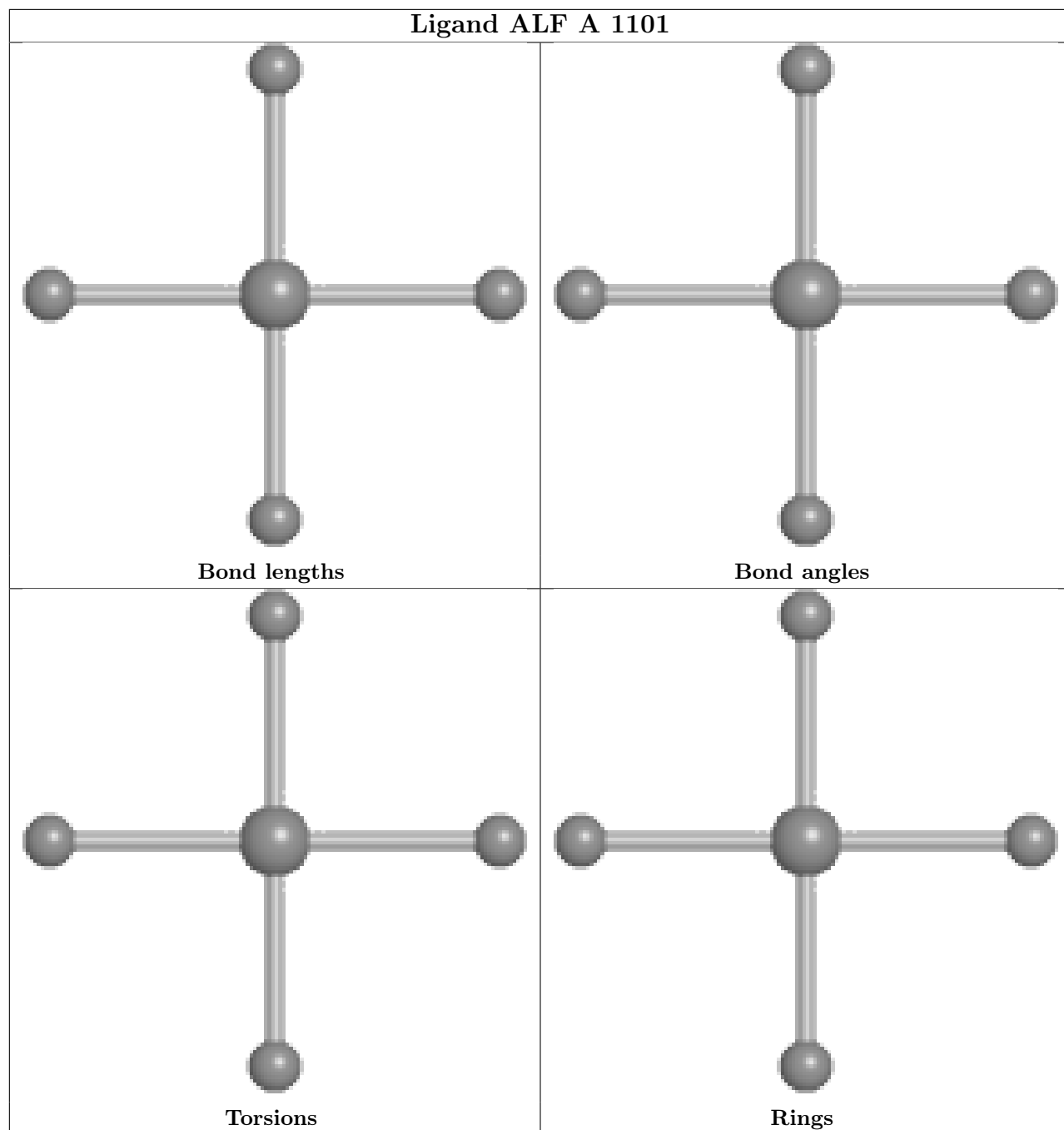
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1107	PCW	8	0
5	A	1103	ADP	2	0
3	A	1101	ALF	1	0
6	A	1108	PCW	1	0
7	B	402	CLR	16	0
6	A	1105	PCW	7	0
6	A	1104	PCW	2	0
7	A	1109	CLR	3	0
6	A	1106	PCW	19	0

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.

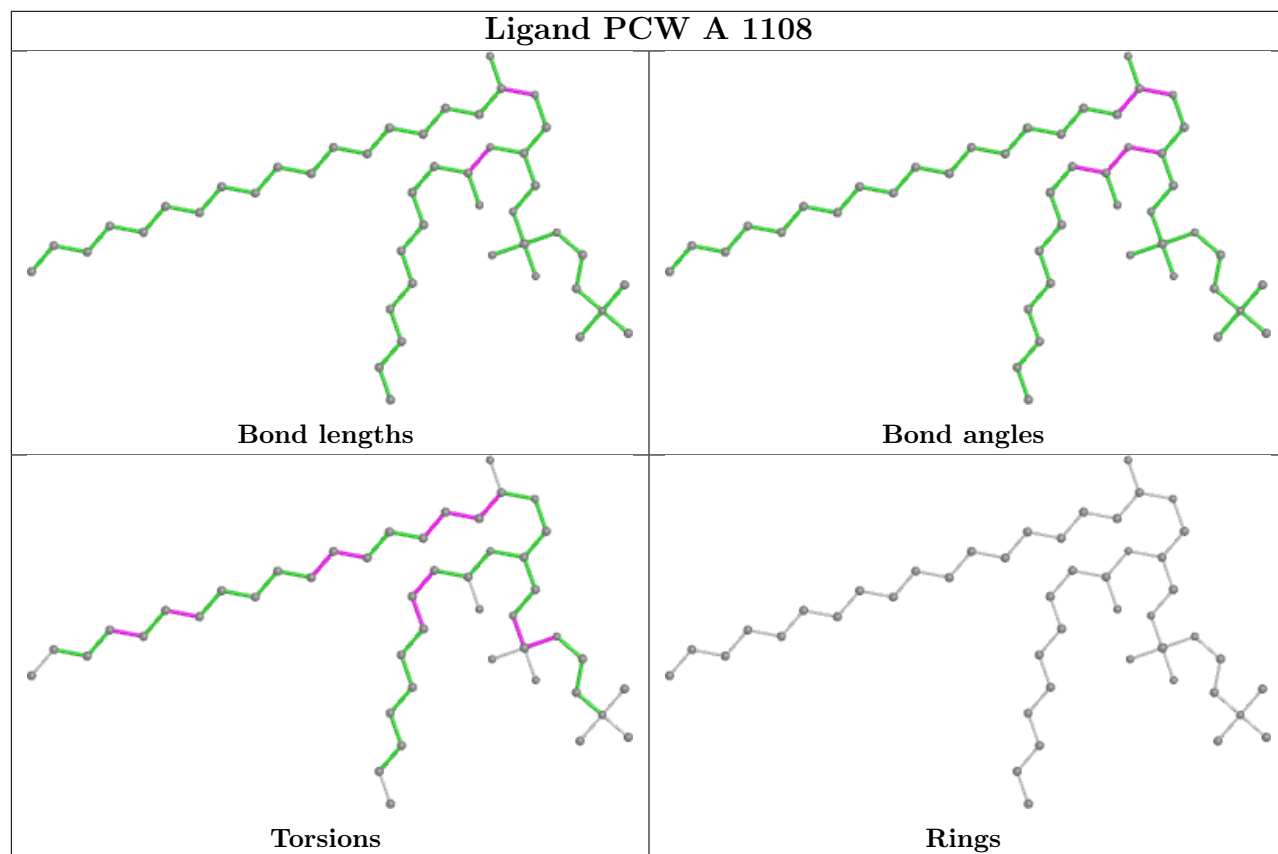
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



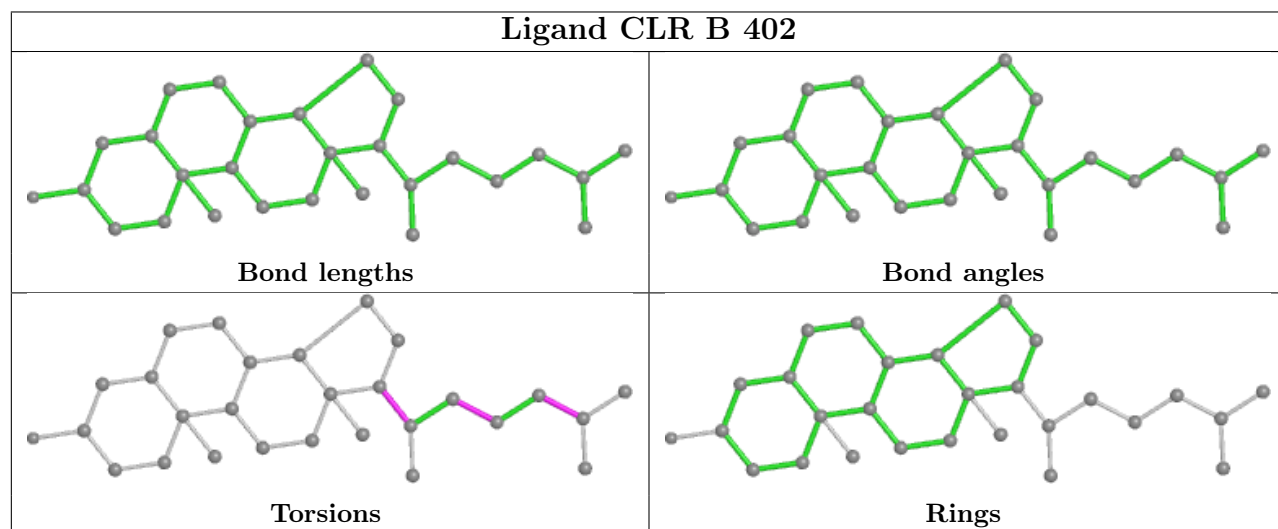


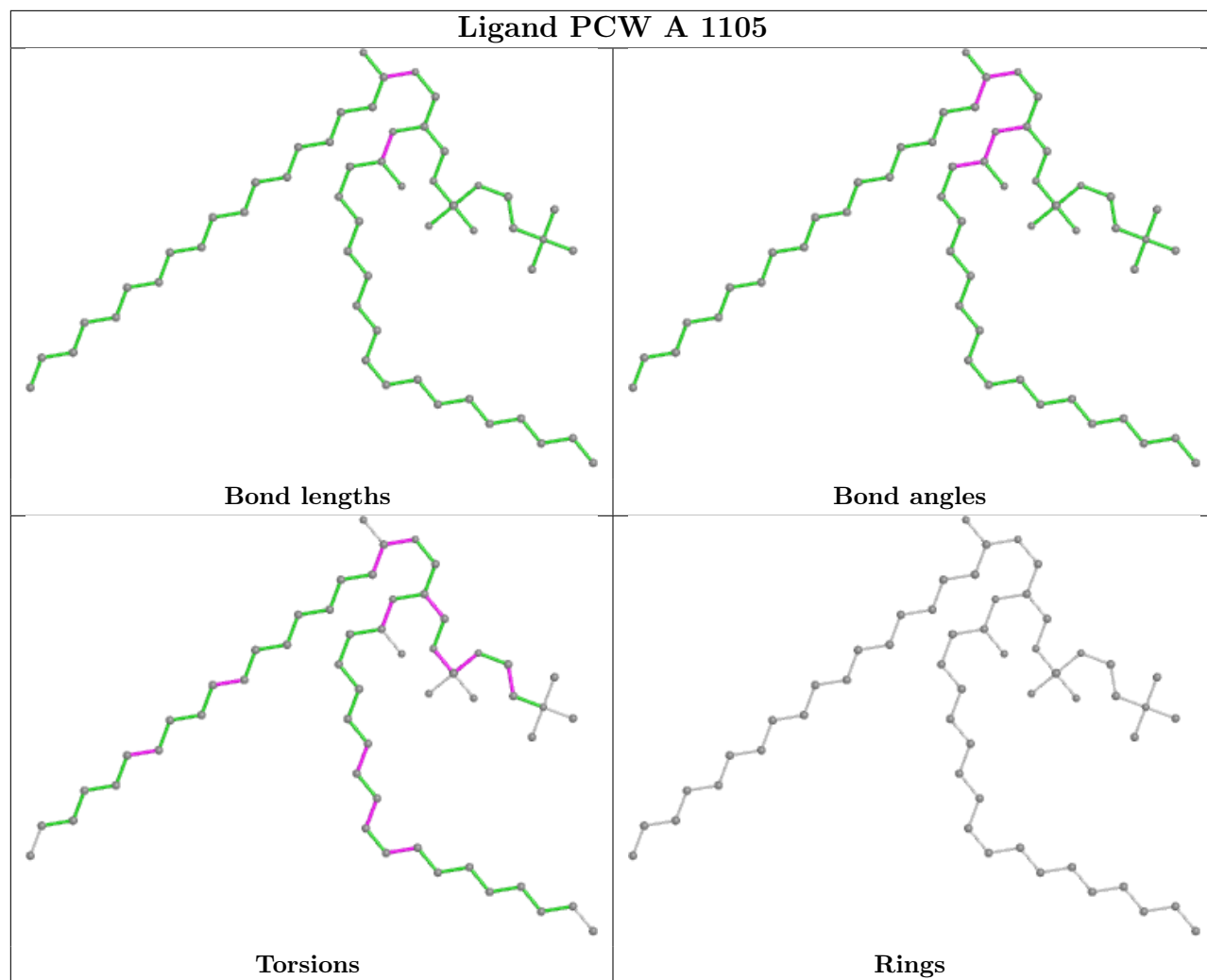


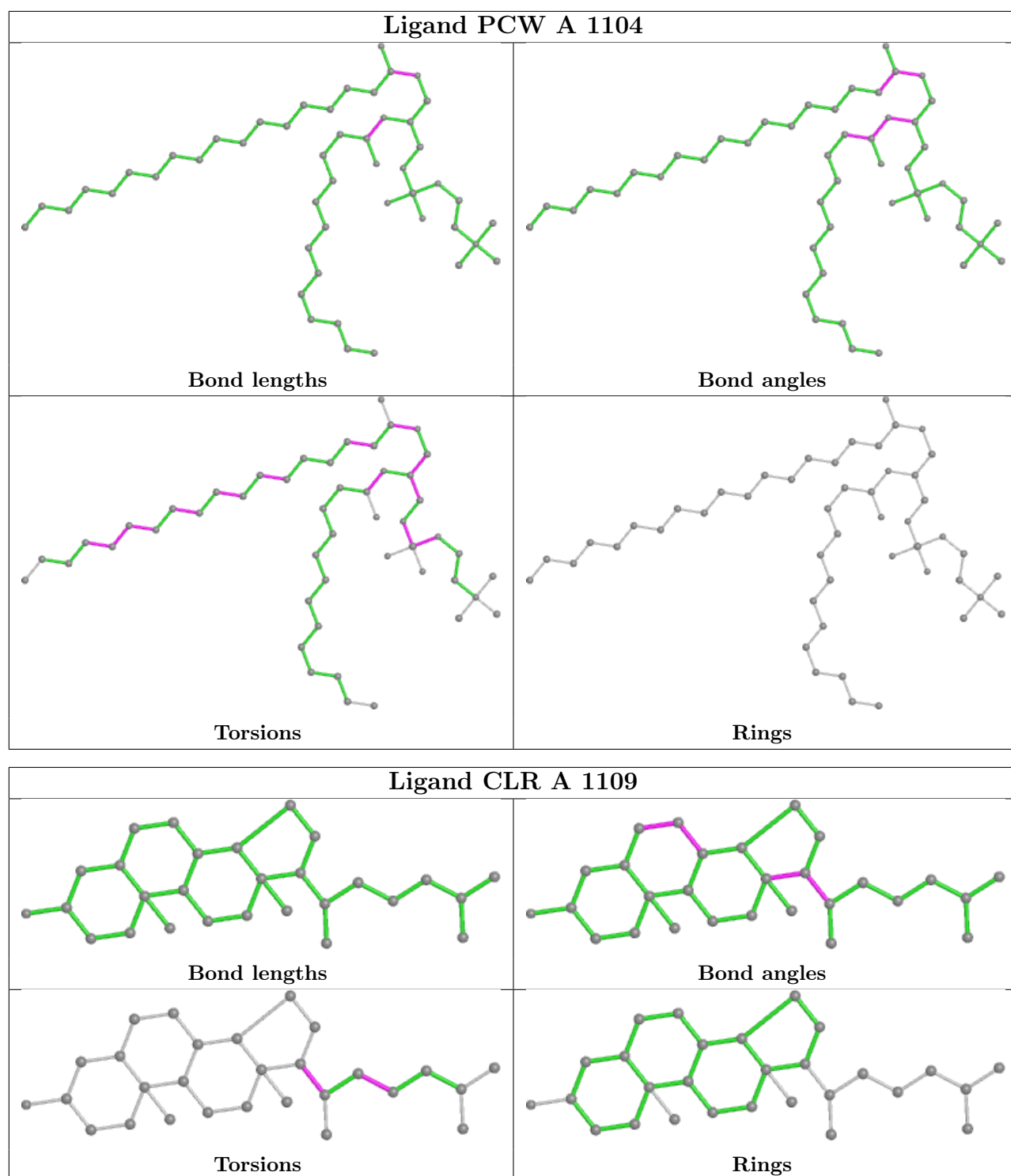
Ligand PCW A 1108

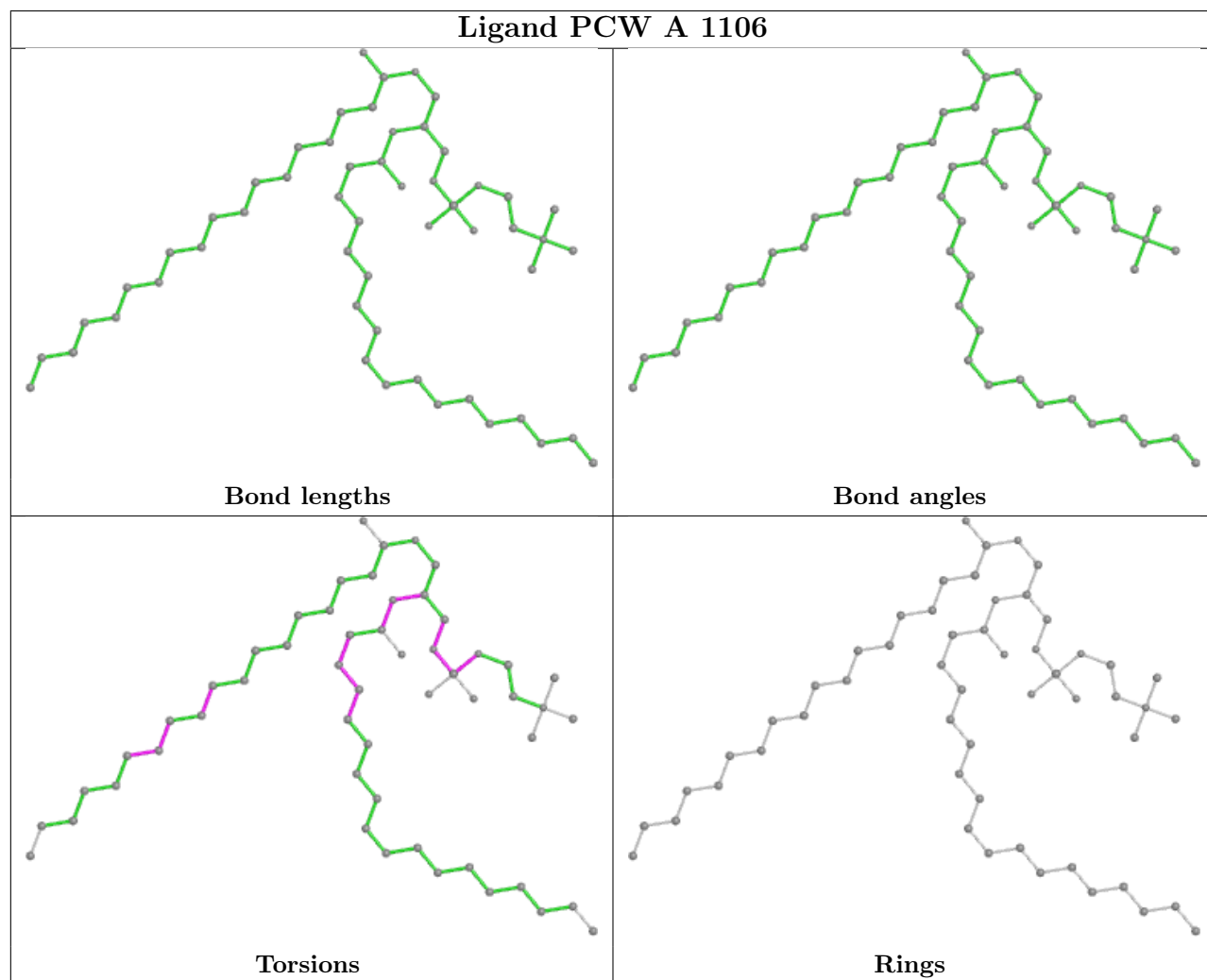
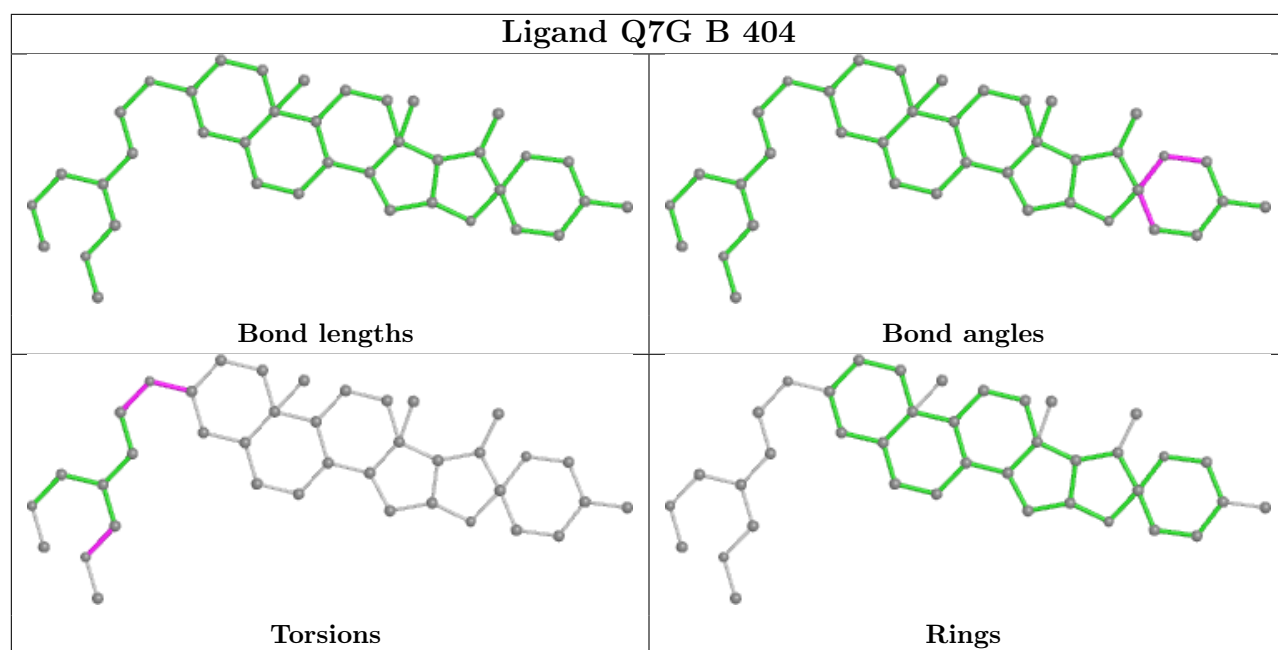


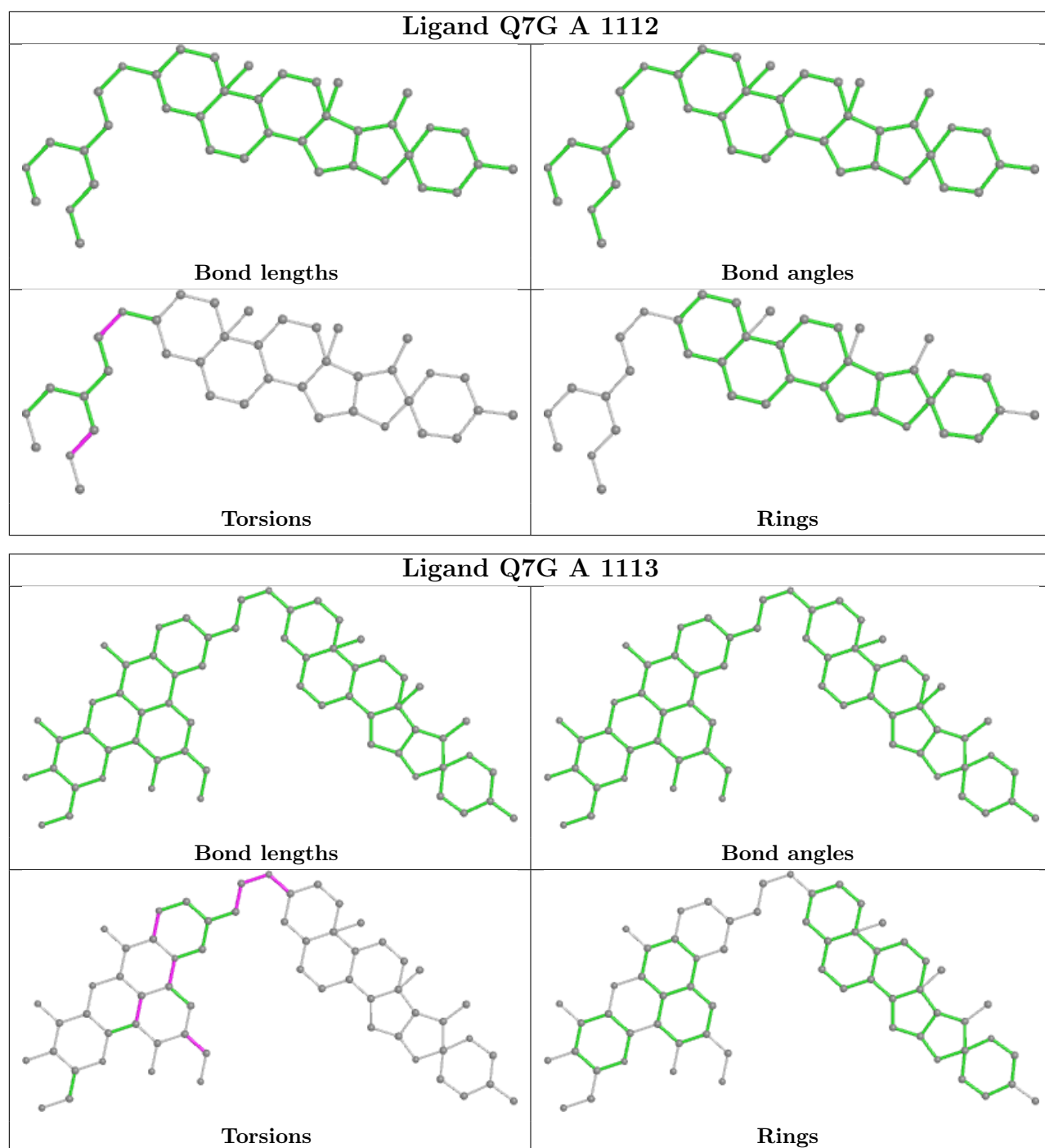
Ligand CLR B 402











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.

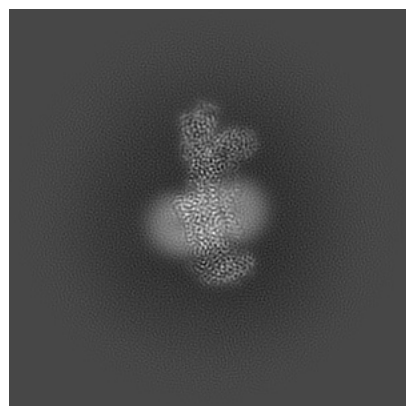
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35488. These allow visual inspection of the internal detail of the map and identification of artifacts.

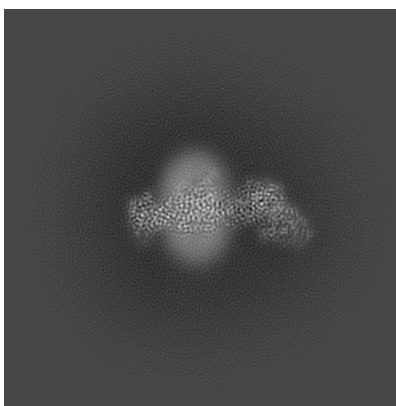
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

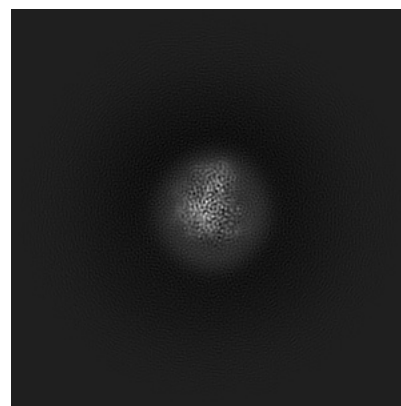
6.1.1 Primary map



X

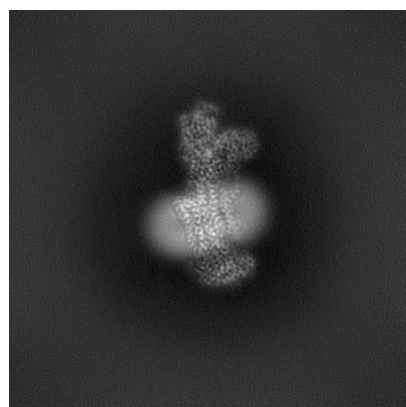


Y

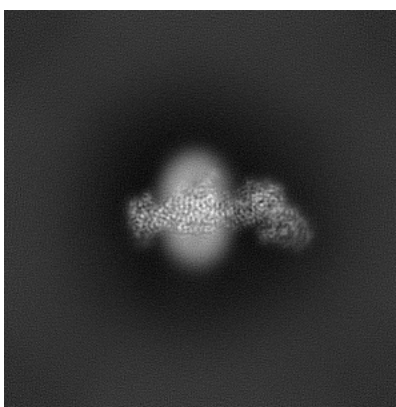


Z

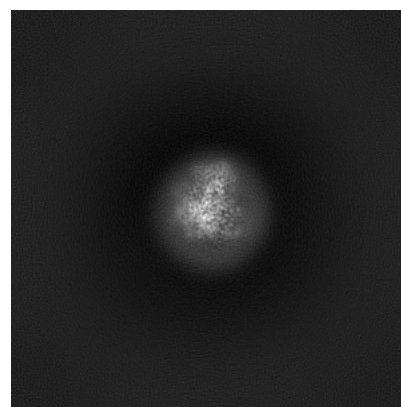
6.1.2 Raw map



X



Y

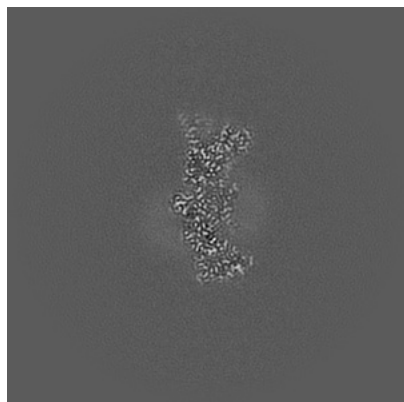


Z

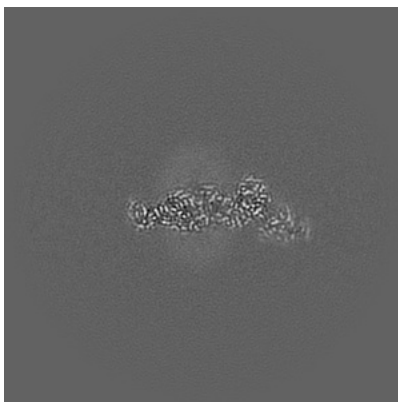
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

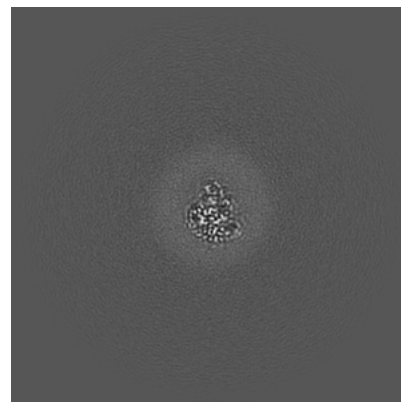
6.2.1 Primary map



X Index: 210

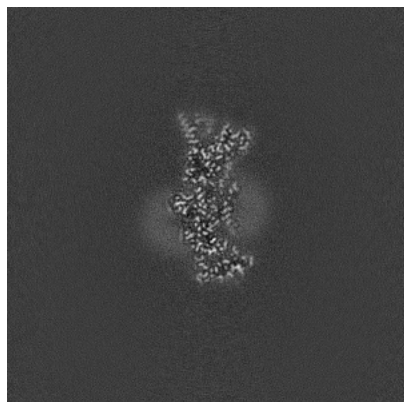


Y Index: 210

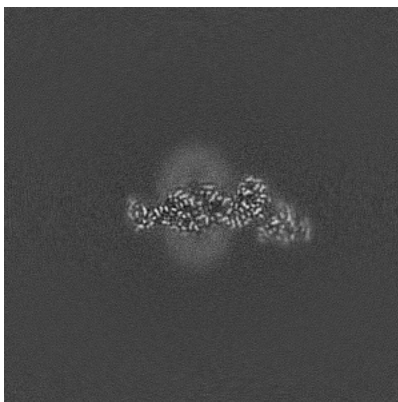


Z Index: 210

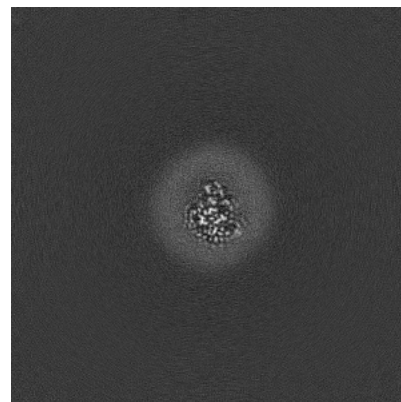
6.2.2 Raw map



X Index: 210



Y Index: 210

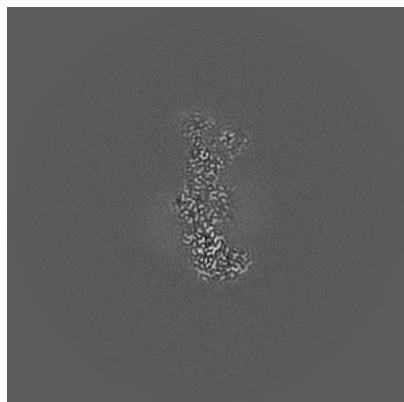


Z Index: 210

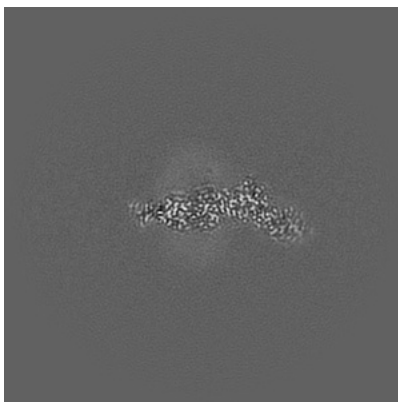
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

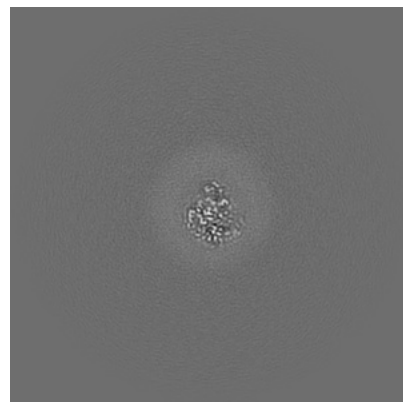
6.3.1 Primary map



X Index: 204

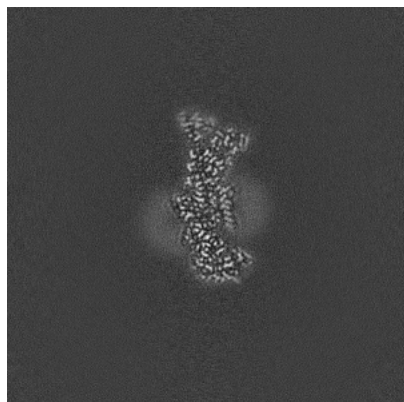


Y Index: 202

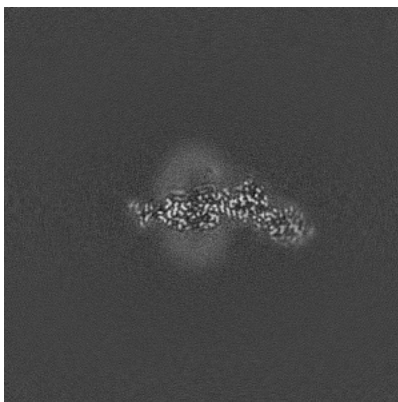


Z Index: 211

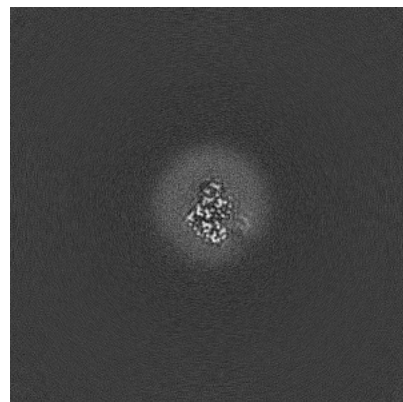
6.3.2 Raw map



X Index: 207



Y Index: 202

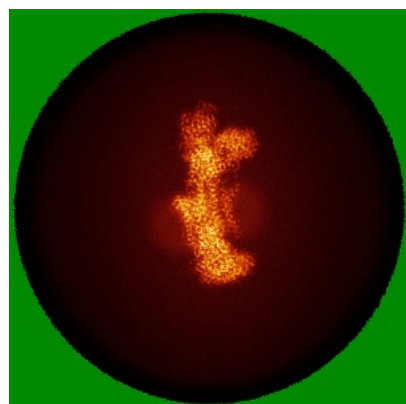


Z Index: 218

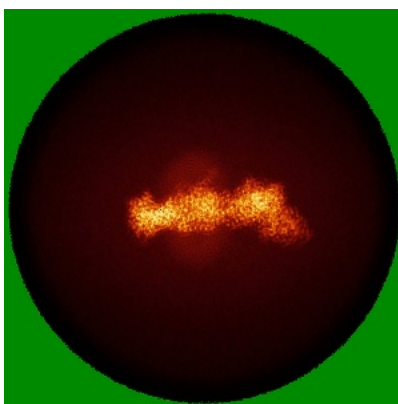
The images above show the largest variance slices of the map in three orthogonal directions.

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

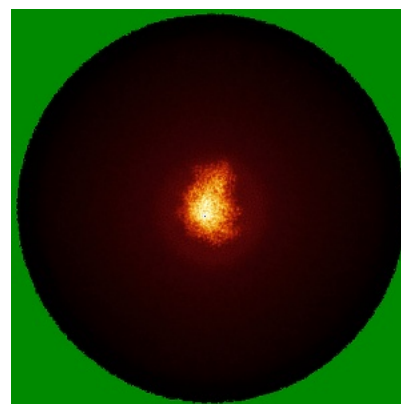
6.4.1 Primary map



X

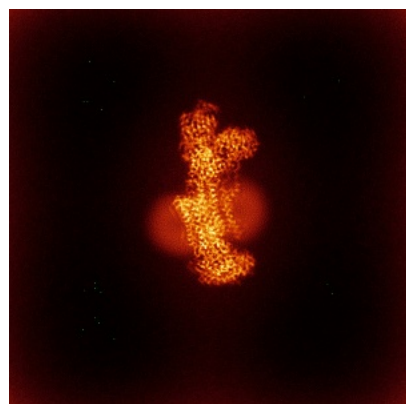


Y

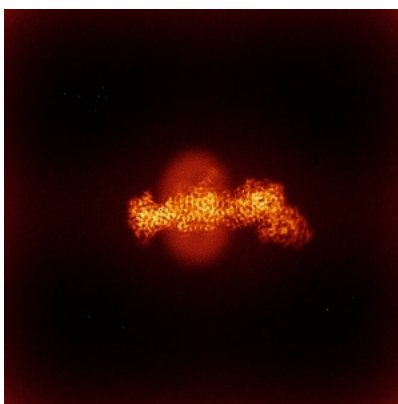


Z

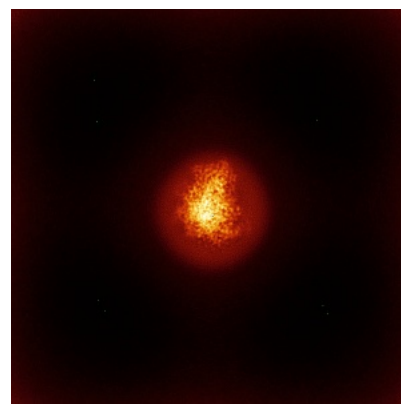
6.4.2 Raw map



X



Y

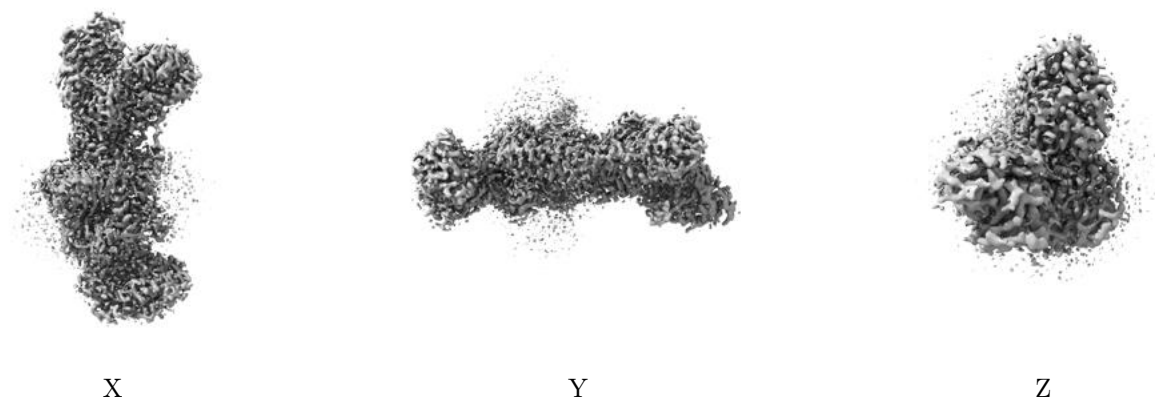


Z

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.

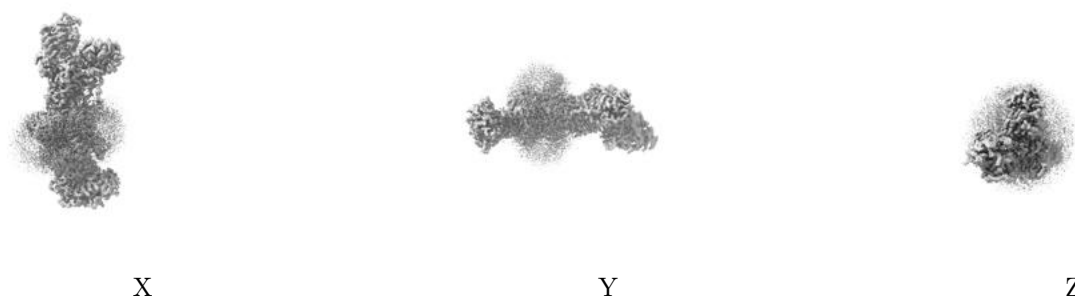
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.227. 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.

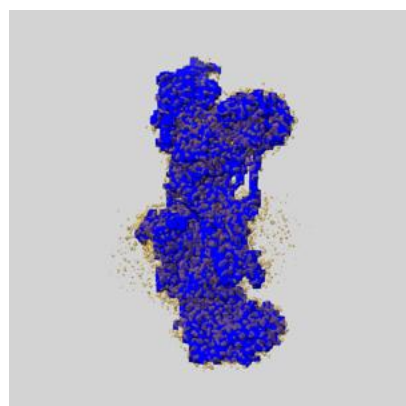
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

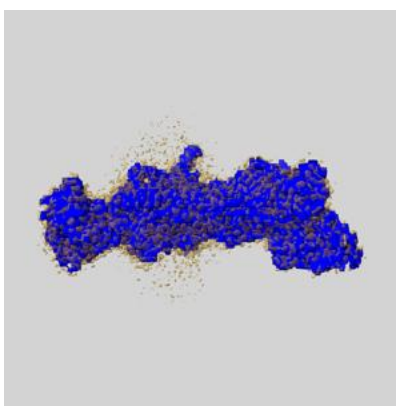
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

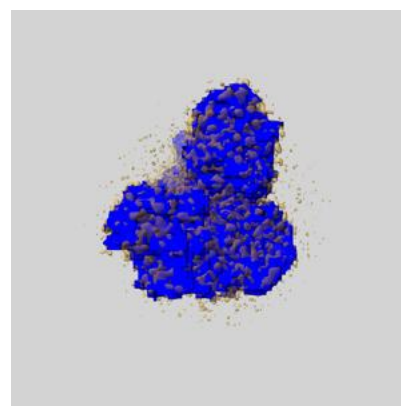
6.6.1 emd_35488_msk_1.map [i](#)



X



Y

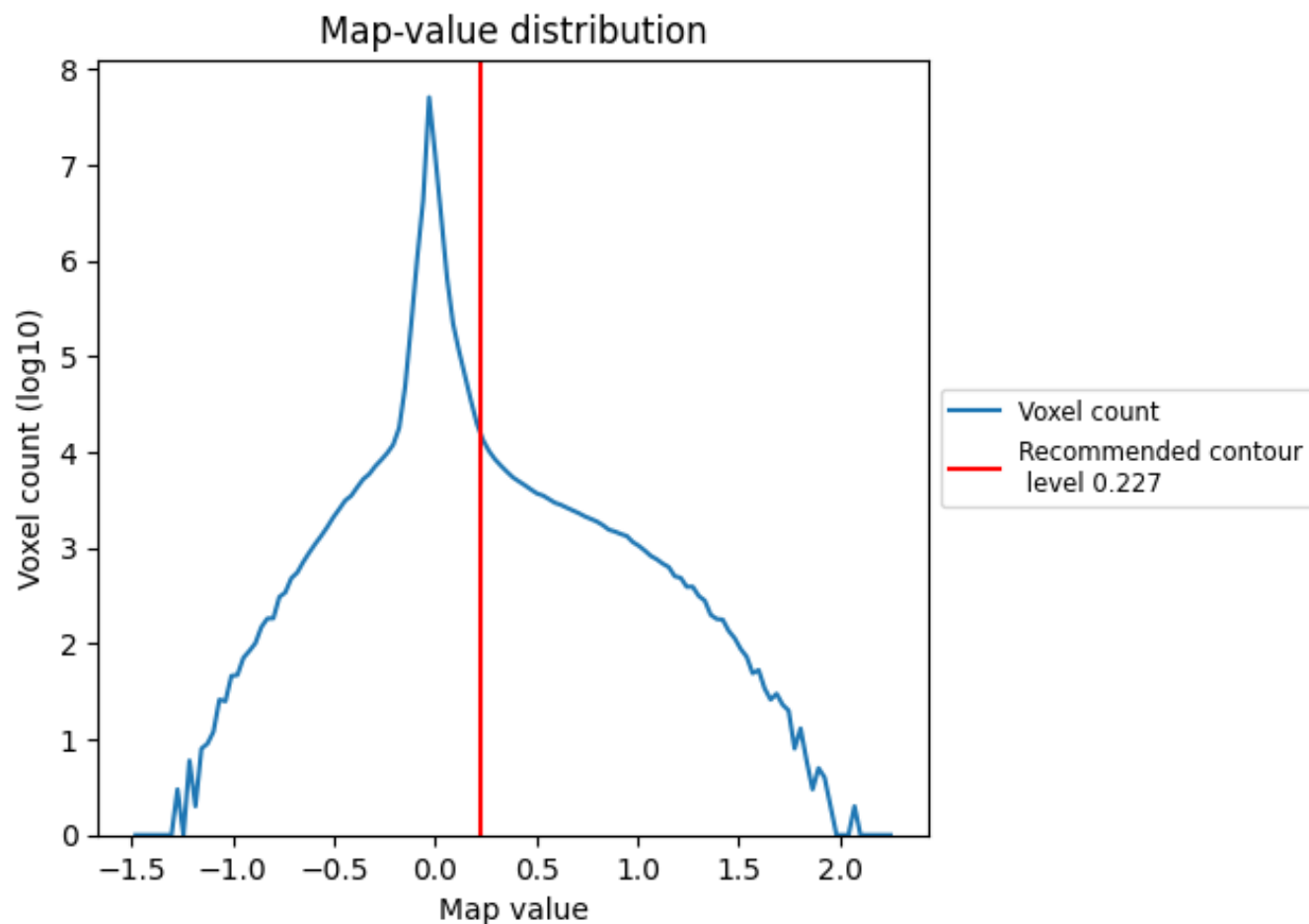


Z

7 Map analysis [i](#)

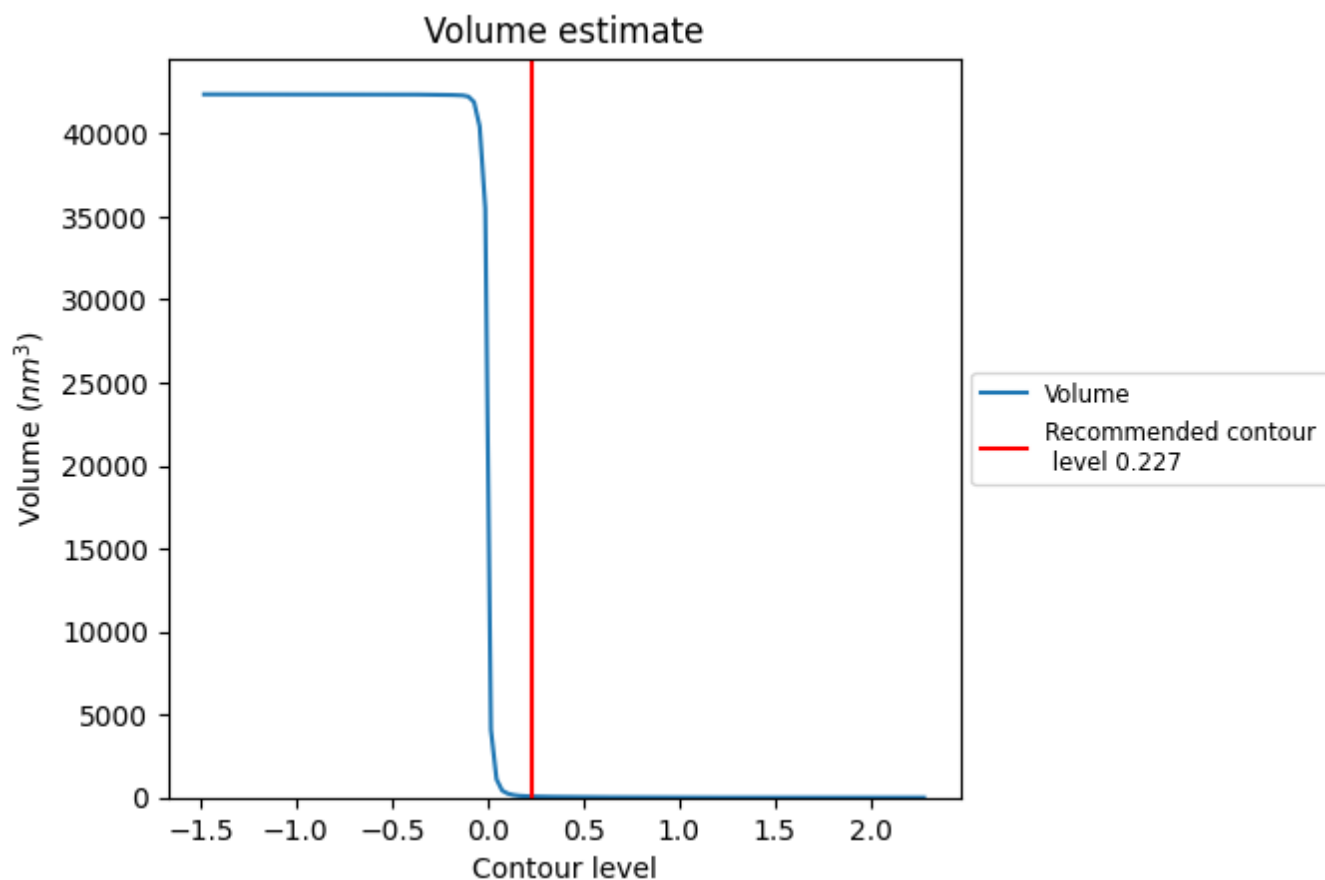
This section contains the results of statistical analysis of the map.

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.

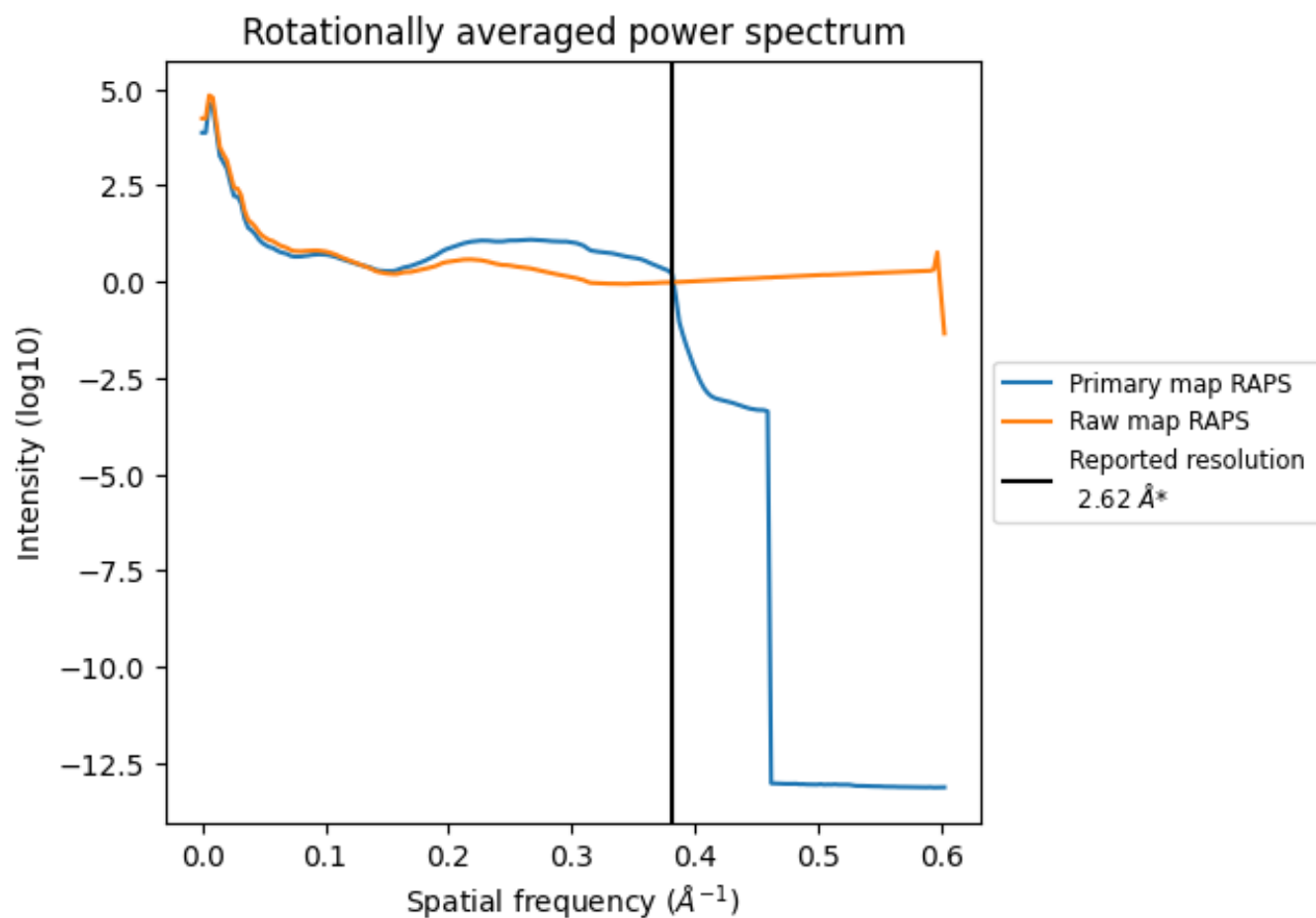
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 67 nm³; this corresponds to an approximate mass of 61 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 ⓘ

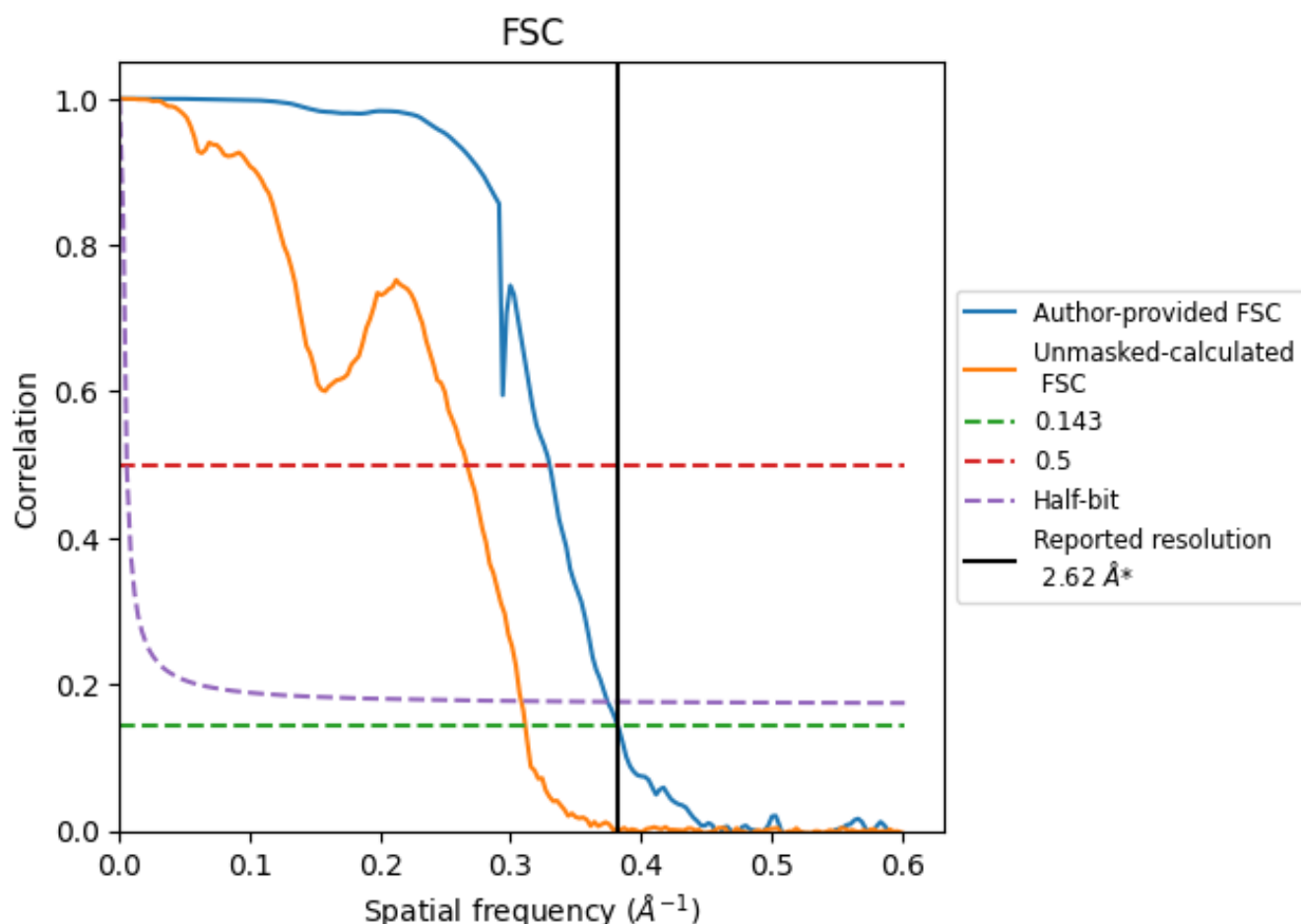


*Reported resolution corresponds to spatial frequency of 0.382 Å⁻¹

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 0.382 \AA^{-1}

8.2 Resolution estimates [i](#)

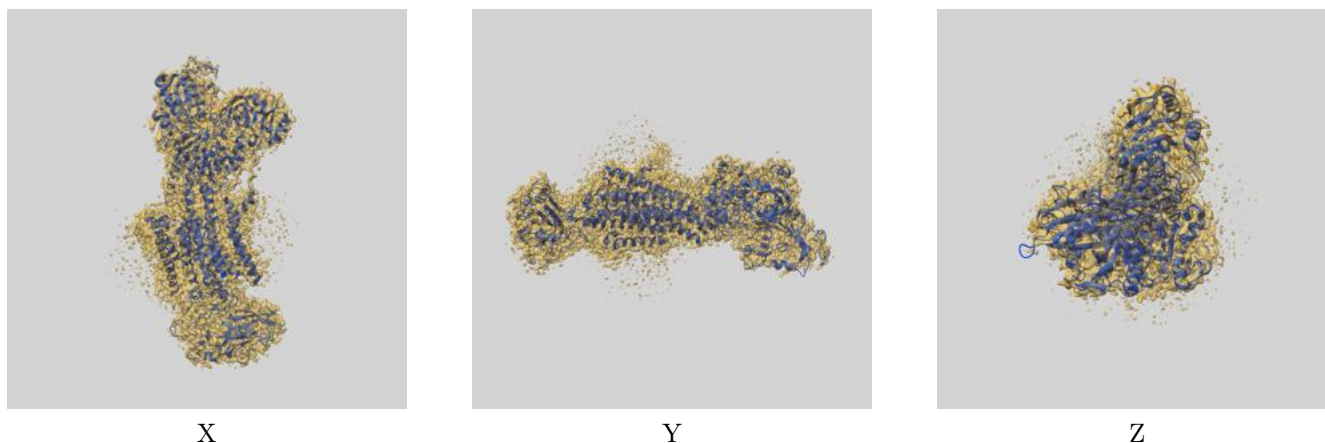
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.62	-	-
Author-provided FSC curve	2.62	3.03	2.67
Unmasked-calculated*	3.21	3.75	3.24

*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 3.21 differs from the reported value 2.62 by more than 10 %

9 Map-model fit [i](#)

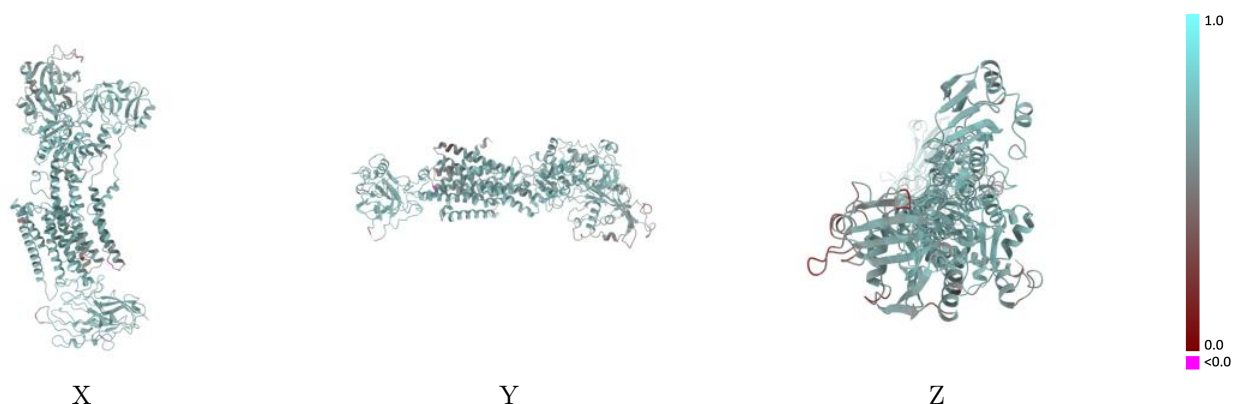
This section contains information regarding the fit between EMDB map EMD-35488 and PDB model 8IJL. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



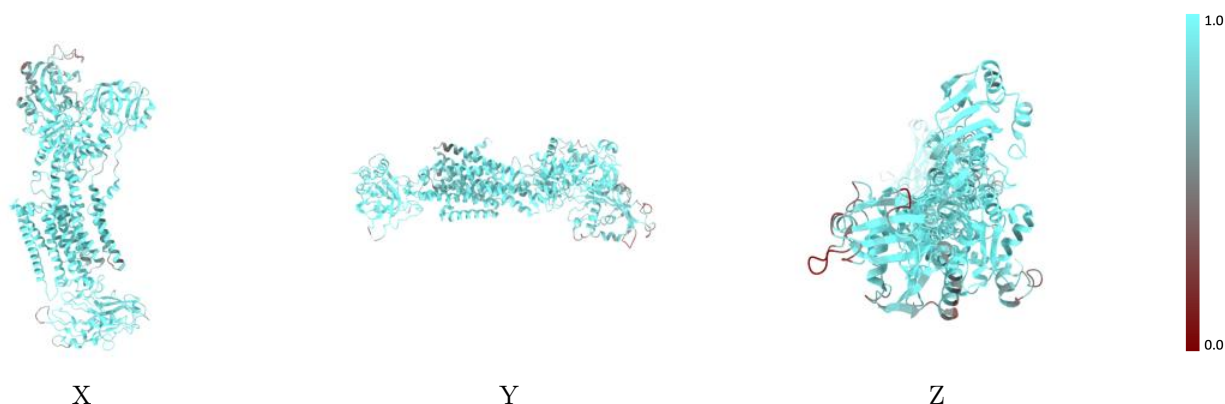
The images above show the 3D surface view of the map at the recommended contour level 0.227 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



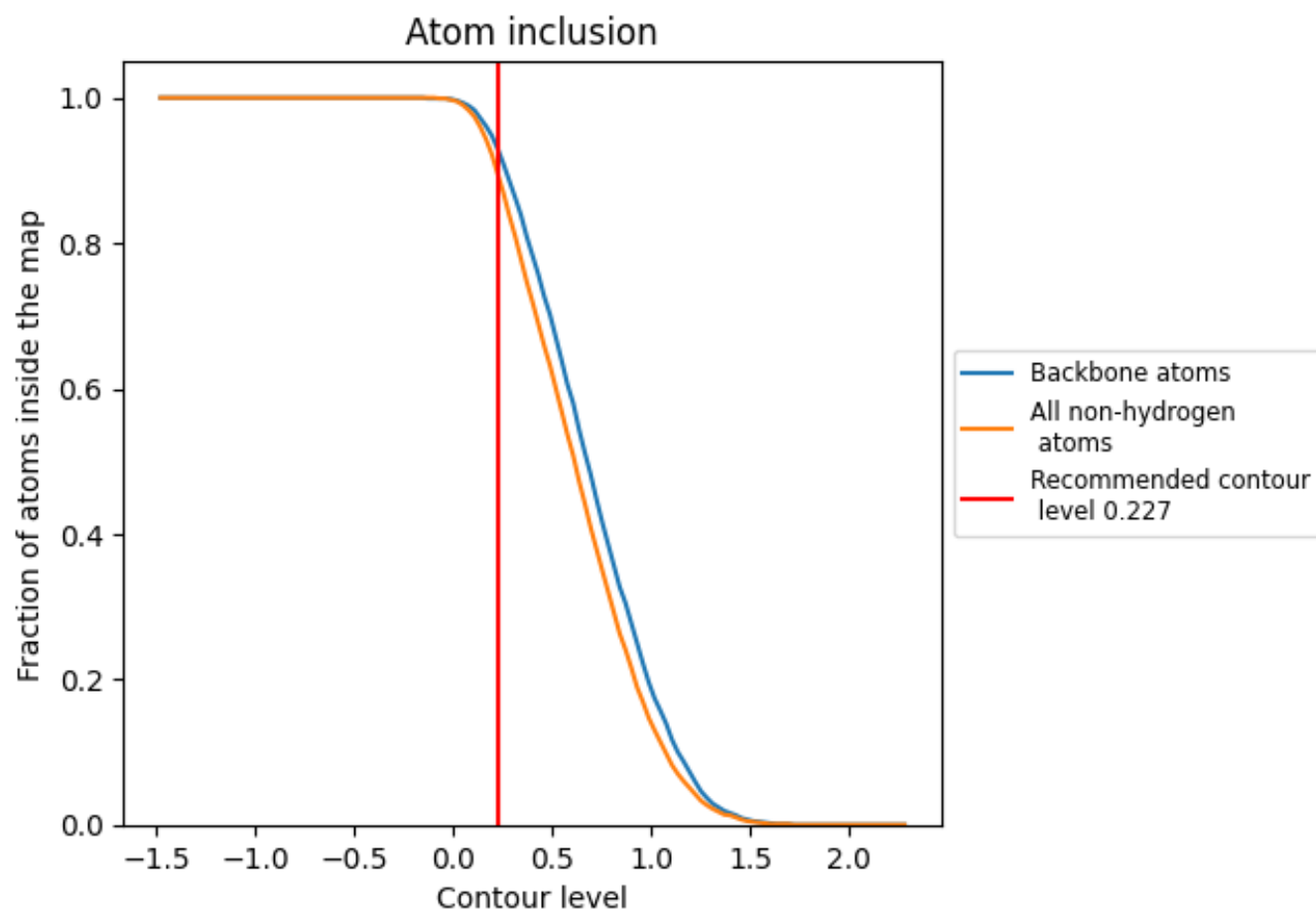
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.227).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 89% 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 (0.227) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8930	<div></div> 0.6120
A	<div></div> 0.8940	<div></div> 0.6120
B	<div></div> 0.8920	<div></div> 0.6120

