



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 01:28 PM UTC

PDB ID : 7OZ1 / pdb_00007oz1
EMDB ID : EMD-13118
Title : Cryo-EM structure of ABCG1 E242Q mutant with ATP and cholesterol hemisuccinate bound
Authors : Skarda, L.; Kowal, J.; Locher, K.P.
Deposited on : 2021-06-25
Resolution : 4.00 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.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

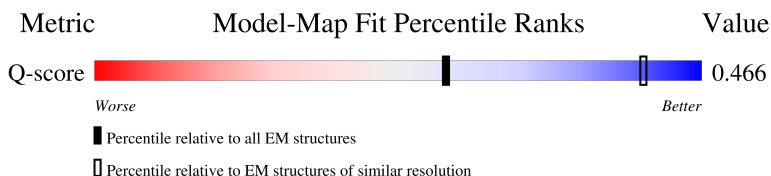
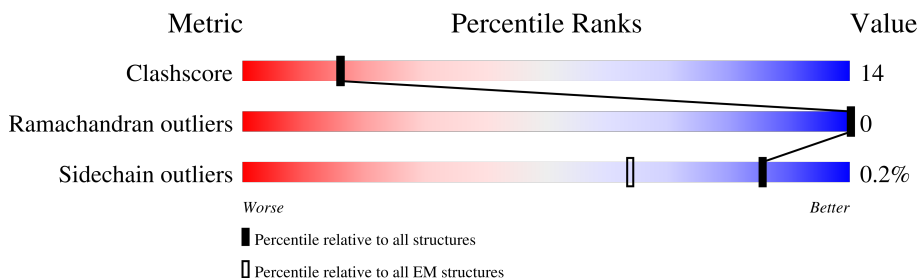
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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	7587 (3.50 - 4.50)

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	680	15% 59% 20% 20%
1	B	680	15% 60% 20% 20%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8942 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 Isoform 4 of ATP-binding cassette sub-family G member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	544	Total	C	N	O	S	0	0
			4257	2765	701	757	34		
1	B	544	Total	C	N	O	S	0	0
			4257	2765	701	757	34		

There are 30 discrepancies between the modelled and reference sequences:

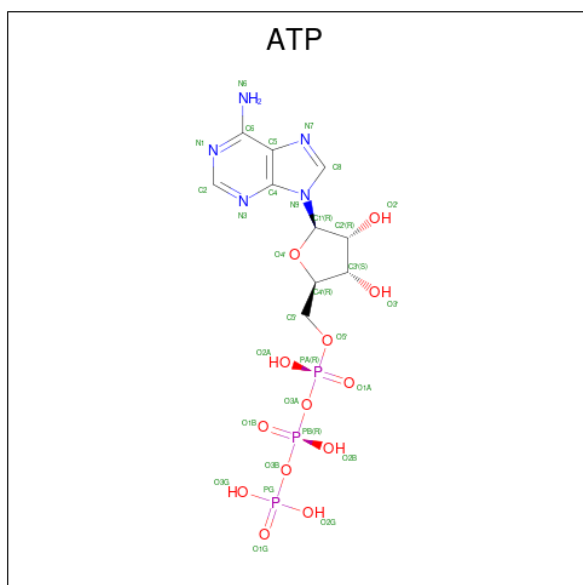
Chain	Residue	Modelled	Actual	Comment	Reference
A	242	GLN	GLU	engineered mutation	UNP P45844
A	667	SER	-	linker	UNP P45844
A	668	SER	-	linker	UNP P45844
A	669	ARG	-	linker	UNP P45844
A	670	VAL	-	linker	UNP P45844
A	671	ASP	-	linker	UNP P45844
A	672	THR	-	expression tag	UNP P45844
A	673	GLU	-	expression tag	UNP P45844
A	674	THR	-	expression tag	UNP P45844
A	675	SER	-	expression tag	UNP P45844
A	676	GLN	-	expression tag	UNP P45844
A	677	VAL	-	expression tag	UNP P45844
A	678	ALA	-	expression tag	UNP P45844
A	679	PRO	-	expression tag	UNP P45844
A	680	ALA	-	expression tag	UNP P45844
B	242	GLN	GLU	engineered mutation	UNP P45844
B	667	SER	-	linker	UNP P45844
B	668	SER	-	linker	UNP P45844
B	669	ARG	-	linker	UNP P45844
B	670	VAL	-	linker	UNP P45844
B	671	ASP	-	linker	UNP P45844
B	672	THR	-	expression tag	UNP P45844
B	673	GLU	-	expression tag	UNP P45844
B	674	THR	-	expression tag	UNP P45844
B	675	SER	-	expression tag	UNP P45844
B	676	GLN	-	expression tag	UNP P45844

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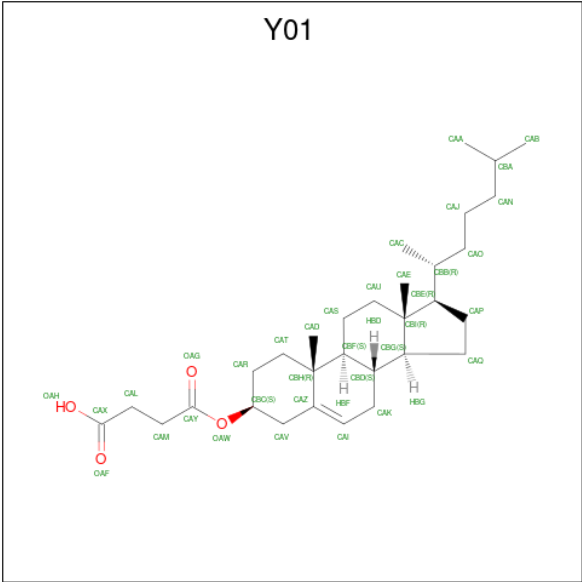
Chain	Residue	Modelled	Actual	Comment	Reference
B	677	VAL	-	expression tag	UNP P45844
B	678	ALA	-	expression tag	UNP P45844
B	679	PRO	-	expression tag	UNP P45844
B	680	ALA	-	expression tag	UNP P45844

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



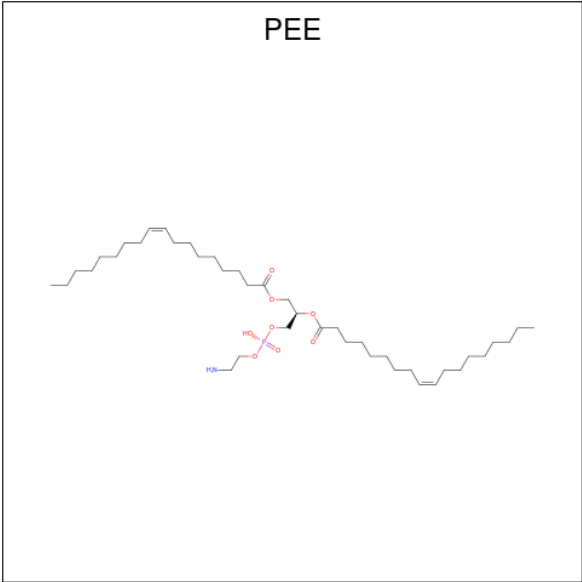
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 3 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: $C_{31}H_{50}O_4$).

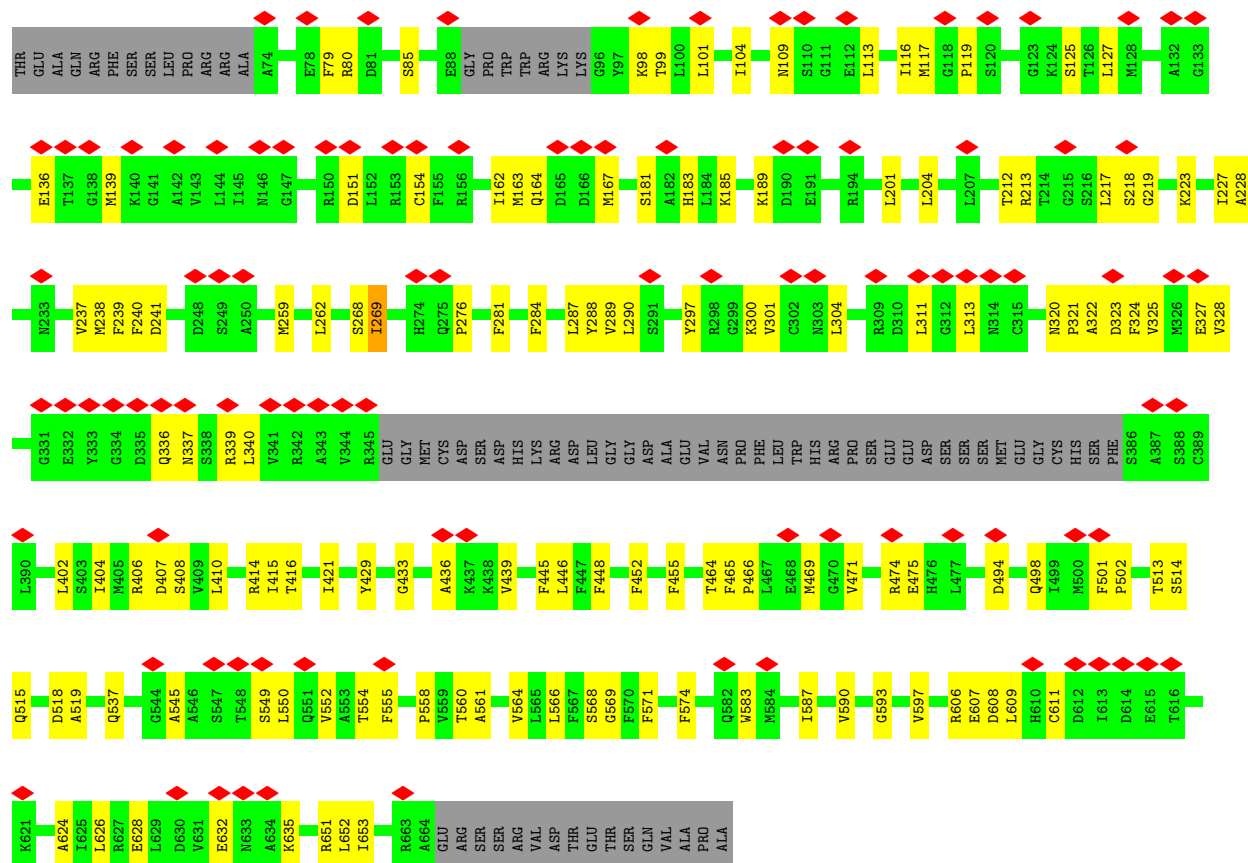


Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	
3	B	1	Total	C	O	0
			35	31	4	
3	B	1	Total	C	O	0
			35	31	4	
3	B	1	Total	C	O	0
			35	31	4	
3	B	1	Total	C	O	0
			35	31	4	

- Molecule 4 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: C₄₁H₇₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			43	33	1	8	1	
4	B	1	Total	C	N	O	P	0
			43	33	1	8	1	



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39791	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.76	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.059	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.016	Depositor
Map size ($\text{\AA}$)	253.44, 253.44, 253.44	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.66, 0.66, 0.66	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: PEE, ATP, 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	0.28	0/4346	0.46	1/5877 (0.0%)
1	B	0.28	0/4346	0.46	1/5877 (0.0%)
All	All	0.28	0/8692	0.46	2/11754 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	PRO	N-CA-C	-8.89	94.16	112.47
1	B	276	PRO	N-CA-C	-8.88	94.17	112.47

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	4257	0	4343	119	0
1	B	4257	0	4343	118	0
2	A	31	0	12	1	0
2	B	31	0	12	1	0
3	A	140	0	196	27	0
3	B	140	0	196	28	0
4	A	43	0	63	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	43	0	63	5	0
All	All	8942	0	9228	259	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 14.

All (259) 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:A:704:Y01:HAR2	3:A:704:Y01:CAL	1.60	1.32
3:B:705:Y01:CAL	3:B:705:Y01:HAR2	1.60	1.31
3:B:705:Y01:CAR	3:B:705:Y01:HAL2	1.78	1.13
3:A:704:Y01:CAR	3:A:704:Y01:HAL2	1.78	1.12
3:A:704:Y01:HAR2	3:A:704:Y01:HAL2	1.06	1.06
3:B:705:Y01:HAR2	3:B:705:Y01:HAL2	1.06	1.04
1:B:455:PHE:CZ	3:B:703:Y01:HAA2	1.94	1.02
1:A:455:PHE:CZ	3:A:702:Y01:HAA2	1.94	1.01
1:B:79:PHE:HE2	1:B:104:ILE:HG22	1.32	0.92
1:B:561:ALA:HB3	3:B:703:Y01:CAB	2.00	0.92
1:A:79:PHE:HE2	1:A:104:ILE:HG22	1.32	0.91
1:A:561:ALA:HB3	3:A:702:Y01:CAB	2.00	0.90
3:A:704:Y01:CAL	3:A:704:Y01:CAR	2.48	0.82
3:A:704:Y01:HAL2	3:A:704:Y01:CBC	2.12	0.80
1:A:561:ALA:HB3	3:A:702:Y01:HAB3	1.63	0.79
1:B:561:ALA:HB3	3:B:703:Y01:HAB3	1.63	0.79
3:B:705:Y01:HAL2	3:B:705:Y01:CBC	2.12	0.79
1:A:238:MET:SD	1:A:262:LEU:HD21	2.23	0.79
1:B:238:MET:SD	1:B:262:LEU:HD21	2.23	0.78
3:B:705:Y01:HAR2	3:B:705:Y01:HAL1	1.65	0.78
3:A:704:Y01:HAR2	3:A:704:Y01:HAL1	1.65	0.77
3:B:705:Y01:CAL	3:B:705:Y01:CAR	2.48	0.75
1:B:79:PHE:CE2	1:B:104:ILE:HG22	2.21	0.75
1:A:555:PHE:HA	3:A:702:Y01:CAD	2.18	0.74
1:A:320:ASN:ND2	1:B:320:ASN:HD21	1.86	0.74
1:B:561:ALA:HB3	3:B:703:Y01:HAB2	1.70	0.74
1:B:555:PHE:HA	3:B:703:Y01:CAD	2.18	0.73
1:A:320:ASN:HD21	1:B:320:ASN:ND2	1.86	0.73
1:A:561:ALA:HB3	3:A:702:Y01:HAB2	1.70	0.73
1:A:79:PHE:CE2	1:A:104:ILE:HG22	2.21	0.72
1:B:125:SER:OG	2:B:701:ATP:O1B	2.11	0.69
1:B:337:ASN:HA	1:B:340:LEU:HB2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:ASN:HA	1:A:340:LEU:HB2	1.75	0.69
1:B:455:PHE:CE2	3:B:703:Y01:HAA2	2.30	0.67
1:A:455:PHE:HZ	3:A:702:Y01:HAA2	1.58	0.66
1:A:421:ILE:HD12	1:A:452:PHE:CE1	2.30	0.66
1:B:237:VAL:HG12	1:B:239:PHE:CE1	2.31	0.66
1:A:237:VAL:HG12	1:A:239:PHE:CE1	2.31	0.66
1:A:455:PHE:CE2	3:A:702:Y01:HAA2	2.30	0.66
1:B:421:ILE:HD12	1:B:452:PHE:CE1	2.30	0.66
1:B:561:ALA:CB	3:B:703:Y01:HAB2	2.26	0.66
1:A:561:ALA:CB	3:A:702:Y01:HAB2	2.26	0.65
1:A:555:PHE:HA	3:A:702:Y01:HAD1	1.77	0.65
1:B:555:PHE:HA	3:B:703:Y01:HAD1	1.77	0.65
1:A:652:LEU:HD23	3:A:706:Y01:HAK2	1.77	0.65
1:A:125:SER:OG	2:A:701:ATP:O1B	2.13	0.64
1:B:652:LEU:HD23	3:B:702:Y01:HAK2	1.79	0.64
1:A:465:PHE:HE2	1:A:545:ALA:HB2	1.63	0.63
1:A:320:ASN:ND2	1:B:320:ASN:ND2	2.45	0.63
1:B:164:GLN:HG3	1:B:241:ASP:OD2	2.00	0.62
1:B:436:ALA:HB2	1:B:609:LEU:HB3	1.81	0.62
1:B:455:PHE:HZ	3:B:703:Y01:HAA2	1.58	0.62
1:B:465:PHE:HE2	1:B:545:ALA:HB2	1.63	0.62
1:A:164:GLN:HG3	1:A:241:ASP:OD2	1.99	0.62
1:B:455:PHE:CZ	3:B:703:Y01:CAA	2.79	0.62
1:A:436:ALA:HB2	1:A:609:LEU:HB3	1.81	0.62
1:B:181:SER:OG	1:B:185:LYS:NZ	2.32	0.62
1:A:583:TRP:HB2	3:A:704:Y01:HAU2	1.83	0.61
1:A:181:SER:OG	1:A:185:LYS:NZ	2.32	0.61
1:A:455:PHE:CZ	3:A:702:Y01:CAA	2.79	0.61
1:B:237:VAL:CG1	1:B:239:PHE:CE1	2.84	0.61
1:A:237:VAL:CG1	1:A:239:PHE:CE1	2.84	0.60
1:B:238:MET:SD	1:B:262:LEU:CD2	2.89	0.60
1:B:433:GLY:O	1:B:606:ARG:NH2	2.31	0.60
1:B:583:TRP:HB2	3:B:705:Y01:HAU2	1.83	0.60
1:A:238:MET:SD	1:A:262:LEU:CD2	2.89	0.59
1:A:466:PRO:HG2	1:A:550:LEU:HD13	1.85	0.59
1:B:466:PRO:HG2	1:B:550:LEU:HD13	1.85	0.59
1:B:410:LEU:HD11	1:B:464:THR:HG21	1.85	0.59
1:A:320:ASN:HD21	1:B:320:ASN:HD21	1.44	0.59
1:A:410:LEU:HD11	1:A:464:THR:HG21	1.85	0.59
1:A:433:GLY:O	1:A:606:ARG:NH2	2.31	0.58
1:A:414:ARG:NH2	1:A:498:GLN:OE1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ASP:OD1	1:A:408:SER:N	2.33	0.58
1:A:117:MET:HE1	1:A:322:ALA:HB1	1.86	0.57
1:B:304:LEU:HD22	1:B:321:PRO:HB3	1.85	0.57
1:B:297:TYR:OH	1:B:300:LYS:O	2.16	0.57
1:A:436:ALA:HB3	1:A:611:CYS:HB3	1.87	0.57
1:B:414:ARG:NH2	1:B:498:GLN:OE1	2.37	0.57
1:A:304:LEU:HD22	1:A:321:PRO:HB3	1.85	0.57
1:B:436:ALA:HB3	1:B:611:CYS:HB3	1.87	0.57
1:A:101:LEU:HD13	1:A:104:ILE:HD12	1.87	0.56
1:B:117:MET:HE1	1:B:322:ALA:HB1	1.86	0.56
1:B:101:LEU:HD13	1:B:104:ILE:HD12	1.87	0.56
1:A:79:PHE:HE2	1:A:104:ILE:CG2	2.12	0.55
1:B:79:PHE:HE2	1:B:104:ILE:CG2	2.12	0.55
3:B:705:Y01:HAL2	3:B:705:Y01:CAV	2.37	0.55
1:B:407:ASP:OD1	1:B:408:SER:N	2.33	0.55
1:B:558:PRO:HB2	3:B:703:Y01:HAE3	1.89	0.55
1:B:204:LEU:HD12	1:B:228:ALA:HB2	1.89	0.55
1:B:218:SER:OG	1:B:219:GLY:N	2.40	0.55
3:A:704:Y01:HAL2	3:A:704:Y01:CAV	2.37	0.55
1:A:204:LEU:HD12	1:A:228:ALA:HB2	1.89	0.54
1:A:241:ASP:OD1	1:A:241:ASP:O	2.26	0.54
1:A:259:MET:HG2	1:A:269:ILE:HG21	1.90	0.54
1:B:241:ASP:OD1	1:B:241:ASP:O	2.26	0.54
1:B:259:MET:HG2	1:B:269:ILE:HG21	1.90	0.54
1:A:558:PRO:HB2	3:A:702:Y01:HAE3	1.89	0.54
1:A:560:THR:HA	4:A:705:PEE:H63	1.90	0.54
1:A:404:ILE:HG13	1:A:410:LEU:HD13	1.90	0.53
1:A:518:ASP:OD1	1:A:519:ALA:N	2.35	0.53
1:B:518:ASP:OD1	1:B:519:ALA:N	2.35	0.53
1:A:163:MET:C	1:A:241:ASP:OD1	2.51	0.53
1:A:455:PHE:CE2	3:A:702:Y01:CAA	2.91	0.53
1:B:501:PHE:HB2	1:B:502:PRO:HD3	1.90	0.53
1:A:501:PHE:HB2	1:A:502:PRO:HD3	1.90	0.53
1:B:163:MET:C	1:B:241:ASP:OD1	2.51	0.53
1:A:218:SER:OG	1:A:219:GLY:N	2.40	0.53
1:B:136:GLU:HG2	1:B:139:MET:HE2	1.90	0.52
1:A:85:SER:HA	1:A:99:THR:HA	1.90	0.52
1:B:85:SER:HA	1:B:99:THR:HA	1.91	0.52
1:B:471:VAL:HG13	1:B:475:GLU:OE1	2.09	0.52
1:A:537:GLN:OE1	1:A:651:ARG:NH2	2.42	0.52
1:B:513:THR:OG1	1:B:515:GLN:NE2	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:537:GLN:OE1	1:B:651:ARG:NH2	2.42	0.52
1:B:560:THR:HA	4:B:706:PEE:H63	1.90	0.52
1:A:513:THR:OG1	1:A:515:GLN:NE2	2.30	0.52
1:B:287:LEU:HB2	1:B:301:VAL:HG22	1.92	0.52
1:B:455:PHE:CE2	3:B:703:Y01:CAA	2.91	0.52
1:A:287:LEU:HB2	1:A:301:VAL:HG22	1.92	0.52
1:B:404:ILE:HG13	1:B:410:LEU:HD13	1.90	0.51
1:A:136:GLU:HG2	1:A:139:MET:HE2	1.90	0.51
1:B:212:THR:HG21	1:B:217:LEU:HD21	1.92	0.51
1:B:164:GLN:N	1:B:241:ASP:OD2	2.43	0.51
1:A:471:VAL:HG13	1:A:475:GLU:OE1	2.09	0.51
1:A:164:GLN:N	1:A:241:ASP:OD2	2.43	0.51
1:B:313:LEU:HD23	1:B:336:GLN:HE22	1.76	0.51
3:A:704:Y01:HAL2	3:A:704:Y01:HAV1	1.93	0.51
1:A:429:TYR:CE2	1:A:445:PHE:HB2	2.47	0.50
1:B:421:ILE:CD1	1:B:452:PHE:CE1	2.94	0.50
1:A:593:GLY:O	1:A:597:VAL:HG23	2.11	0.50
1:A:421:ILE:CD1	1:A:452:PHE:CE1	2.94	0.50
1:A:212:THR:HG21	1:A:217:LEU:HD21	1.92	0.50
1:A:313:LEU:HD23	1:A:336:GLN:HE22	1.76	0.50
1:B:429:TYR:CE2	1:B:445:PHE:HB2	2.47	0.50
1:A:446:LEU:HD21	1:A:597:VAL:HG12	1.94	0.50
1:B:593:GLY:O	1:B:597:VAL:HG23	2.11	0.50
3:A:702:Y01:HAN2	3:B:703:Y01:HAN2	1.93	0.49
3:B:705:Y01:HAR2	3:B:705:Y01:CAM	2.33	0.49
1:B:151:ASP:HB3	1:B:154:CYS:SG	2.53	0.49
1:A:151:ASP:HB3	1:A:154:CYS:SG	2.53	0.49
1:A:324:PHE:HA	1:A:327:GLU:OE1	2.13	0.49
1:B:324:PHE:HA	1:B:327:GLU:OE1	2.13	0.49
1:A:323:ASP:O	1:A:327:GLU:HG3	2.13	0.48
1:B:162:ILE:HD12	1:B:240:PHE:CE2	2.48	0.48
3:B:705:Y01:HAL2	3:B:705:Y01:HAV1	1.93	0.48
1:A:167:MET:O	1:A:474:ARG:NH2	2.46	0.48
1:B:446:LEU:HD21	1:B:597:VAL:HG12	1.94	0.48
1:B:167:MET:O	1:B:474:ARG:NH2	2.46	0.48
1:B:139:MET:O	1:B:139:MET:HG3	2.14	0.48
1:B:550:LEU:O	1:B:554:THR:OG1	2.25	0.48
4:A:705:PEE:H68	4:A:705:PEE:H62	1.76	0.48
1:B:607:GLU:HG2	1:B:608:ASP:H	1.79	0.48
1:A:80:ARG:HE	1:A:80:ARG:HB2	1.55	0.48
1:A:139:MET:O	1:A:139:MET:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ILE:HD12	1:A:240:PHE:CE2	2.48	0.48
1:A:550:LEU:O	1:A:554:THR:OG1	2.25	0.48
1:B:304:LEU:HD11	1:B:325:VAL:HG21	1.96	0.47
1:A:181:SER:O	1:A:185:LYS:NZ	2.48	0.47
1:A:569:GLY:HA3	1:A:574:PHE:CZ	2.49	0.47
1:B:323:ASP:O	1:B:327:GLU:HG3	2.13	0.47
1:B:569:GLY:HA3	1:B:574:PHE:CZ	2.49	0.47
1:A:607:GLU:HG2	1:A:608:ASP:H	1.79	0.47
1:A:304:LEU:HD11	1:A:325:VAL:HG21	1.96	0.47
1:A:494:ASP:O	1:A:498:GLN:HG2	2.15	0.47
1:B:494:ASP:O	1:B:498:GLN:HG2	2.15	0.47
4:A:705:PEE:H19	4:A:705:PEE:H26	1.58	0.46
1:B:181:SER:O	1:B:185:LYS:NZ	2.48	0.46
1:A:237:VAL:HG22	1:A:268:SER:OG	2.15	0.46
1:A:297:TYR:OH	1:A:300:LYS:O	2.16	0.46
1:A:653:ILE:HD12	3:A:703:Y01:HAB3	1.98	0.46
1:B:653:ILE:HD12	3:B:704:Y01:HAB3	1.98	0.46
1:A:237:VAL:HG11	1:A:239:PHE:CZ	2.52	0.45
1:A:259:MET:HE3	1:A:259:MET:HB2	1.82	0.45
1:A:433:GLY:HA3	1:A:514:SER:O	2.16	0.45
1:B:237:VAL:HG22	1:B:268:SER:OG	2.15	0.45
1:B:109:ASN:OD1	1:B:109:ASN:N	2.49	0.45
1:A:325:VAL:HA	1:A:328:VAL:HG12	1.99	0.45
1:B:433:GLY:HA3	1:B:514:SER:O	2.17	0.45
1:B:609:LEU:HD12	1:B:609:LEU:HA	1.77	0.45
1:B:465:PHE:CE2	1:B:545:ALA:HB2	2.49	0.44
1:A:116:ILE:HD13	1:A:127:LEU:HD23	2.00	0.44
1:B:116:ILE:HD13	1:B:127:LEU:HD23	2.00	0.44
1:A:465:PHE:CE2	1:A:545:ALA:HB2	2.49	0.44
1:B:223:LYS:O	1:B:227:ILE:HG13	2.18	0.44
1:B:289:VAL:HG11	1:B:325:VAL:HG11	2.00	0.44
1:B:311:LEU:HB3	1:B:339:ARG:HH21	1.83	0.44
1:B:325:VAL:HA	1:B:328:VAL:HG12	1.99	0.44
1:A:237:VAL:HG11	1:A:239:PHE:CE1	2.53	0.44
1:B:237:VAL:HG11	1:B:239:PHE:CZ	2.52	0.44
3:B:705:Y01:CAR	3:B:705:Y01:CAM	2.88	0.44
4:B:706:PEE:H79	4:B:706:PEE:H73	1.60	0.44
1:A:238:MET:HE1	1:A:262:LEU:CD2	2.48	0.43
1:A:555:PHE:HD1	3:A:702:Y01:HAT2	1.83	0.43
1:B:183:HIS:ND1	1:B:189:LYS:HE2	2.33	0.43
1:B:549:SER:OG	1:B:552:VAL:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:706:PEE:H48	4:B:706:PEE:H54	1.74	0.43
1:A:289:VAL:HG11	1:A:325:VAL:HG11	2.00	0.43
1:A:549:SER:OG	1:A:552:VAL:HG22	2.18	0.43
1:B:237:VAL:HG11	1:B:239:PHE:CE1	2.52	0.43
1:A:109:ASN:OD1	1:A:109:ASN:N	2.49	0.43
1:A:223:LYS:O	1:A:227:ILE:HG13	2.18	0.43
1:A:311:LEU:HB3	1:A:339:ARG:HH21	1.83	0.43
1:B:439:VAL:HG22	1:B:439:VAL:O	2.19	0.43
1:B:415:ILE:HG13	1:B:416:THR:N	2.34	0.43
1:B:259:MET:HE3	1:B:259:MET:HB2	1.82	0.43
4:B:706:PEE:H68	4:B:706:PEE:H62	1.76	0.43
1:A:183:HIS:HA	1:A:189:LYS:NZ	2.34	0.42
1:A:183:HIS:ND1	1:A:189:LYS:HE2	2.33	0.42
1:A:281:PHE:HZ	1:A:287:LEU:HD22	1.85	0.42
1:A:415:ILE:HG13	1:A:416:THR:N	2.34	0.42
1:A:439:VAL:O	1:A:439:VAL:HG22	2.19	0.42
4:A:705:PEE:H73	4:A:705:PEE:H79	1.60	0.42
1:B:238:MET:HE1	1:B:262:LEU:CD2	2.48	0.42
1:A:648:ILE:HG12	3:A:706:Y01:CAC	2.49	0.42
1:A:98:LYS:HE2	1:A:98:LYS:HB3	1.78	0.42
1:A:448:PHE:HB2	1:B:571:PHE:CD2	2.53	0.42
1:B:281:PHE:HZ	1:B:287:LEU:HD22	1.85	0.42
1:A:571:PHE:CD2	1:B:448:PHE:HB2	2.55	0.42
1:B:183:HIS:HA	1:B:189:LYS:NZ	2.34	0.42
1:B:555:PHE:HD1	3:B:703:Y01:HAT2	1.83	0.42
1:A:213:ARG:NH2	1:A:406:ARG:HG2	2.35	0.42
4:A:705:PEE:H48	4:A:705:PEE:H54	1.74	0.42
1:A:402:LEU:HD21	1:A:406:ARG:NH2	2.35	0.41
1:B:213:ARG:HH21	1:B:406:ARG:HG2	1.85	0.41
1:B:626:LEU:HB3	1:B:632:GLU:HB3	2.02	0.41
1:B:635:LYS:H	1:B:635:LYS:HD2	1.84	0.41
1:A:429:TYR:CD2	1:A:445:PHE:HB2	2.55	0.41
1:B:98:LYS:HE2	1:B:98:LYS:HB3	1.78	0.41
1:A:116:ILE:HG12	1:A:288:TYR:HB3	2.02	0.41
1:A:528:LEU:O	1:A:532:THR:HG22	2.21	0.41
3:A:704:Y01:HAR2	3:A:704:Y01:CAM	2.33	0.41
1:B:213:ARG:NH2	1:B:406:ARG:HG2	2.35	0.41
1:B:119:PRO:HD2	1:B:290:LEU:O	2.20	0.41
1:B:402:LEU:HD21	1:B:406:ARG:NH2	2.35	0.41
4:B:706:PEE:H19	4:B:706:PEE:H26	1.58	0.41
1:A:213:ARG:HH21	1:A:406:ARG:HG2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:LEU:C	1:A:568:SER:H	2.28	0.41
1:A:635:LYS:H	1:A:635:LYS:HD2	1.84	0.41
1:B:566:LEU:C	1:B:568:SER:H	2.28	0.41
1:A:305:VAL:O	1:A:309:ARG:HG2	2.21	0.41
1:A:651:ARG:HD3	1:A:651:ARG:HA	1.85	0.41
1:B:429:TYR:CD2	1:B:445:PHE:HB2	2.55	0.41
1:A:119:PRO:HD2	1:A:290:LEU:O	2.20	0.41
1:A:604:LEU:HD23	1:A:604:LEU:HA	1.89	0.41
1:B:80:ARG:HE	1:B:80:ARG:HB2	1.55	0.41
1:B:116:ILE:HG12	1:B:288:TYR:HB3	2.02	0.41
1:B:469:MET:HE2	1:B:469:MET:HB3	1.89	0.41
1:A:626:LEU:HB3	1:A:632:GLU:HB3	2.02	0.41
1:B:117:MET:SD	1:B:287:LEU:HD11	2.61	0.41
1:A:425:ILE:HD11	1:A:448:PHE:CE2	2.56	0.40
1:B:201:LEU:HD23	1:B:201:LEU:HA	1.86	0.40
1:B:587:ILE:HG12	3:B:704:Y01:HAC3	2.03	0.40
1:B:624:ALA:O	1:B:628:GLU:HB2	2.22	0.40
1:A:113:LEU:HG	1:A:284:PHE:HD1	1.86	0.40
1:A:609:LEU:HD12	1:A:609:LEU:HA	1.77	0.40
1:B:564:VAL:HG13	1:B:590:VAL:HB	2.04	0.40
1:A:555:PHE:CE1	1:A:559:VAL:HG21	2.56	0.40
1:B:113:LEU:HG	1:B:284:PHE:HD1	1.86	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	538/680 (79%)	497 (92%)	41 (8%)	0	100	100
1	B	538/680 (79%)	497 (92%)	41 (8%)	0	100	100
All	All	1076/1360 (79%)	994 (92%)	82 (8%)	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	466/583 (80%)	465 (100%)	1 (0%)	87	87
1	B	466/583 (80%)	465 (100%)	1 (0%)	87	87
All	All	932/1166 (80%)	930 (100%)	2 (0%)	85	87

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	269	ILE
1	B	269	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	GLN
1	A	392	GLN
1	A	418	HIS
1	A	442	ASN
1	A	515	GLN
1	A	582	GLN
1	A	633	ASN
1	B	175	GLN
1	B	183	HIS
1	B	320	ASN
1	B	392	GLN
1	B	418	HIS
1	B	442	ASN
1	B	515	GLN
1	B	582	GLN
1	B	633	ASN

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](#)

12 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$
2	ATP	A	701	-	32,33,33	1.40	4 (12%)	48,52,52	1.76	8 (16%)
2	ATP	B	701	-	32,33,33	1.39	4 (12%)	48,52,52	1.76	8 (16%)
3	Y01	B	703	-	38,38,38	0.52	0	57,57,57	1.12	5 (8%)
4	PEE	B	706	-	42,42,50	0.81	2 (4%)	45,47,55	0.56	0
3	Y01	A	704	-	38,38,38	0.53	0	57,57,57	0.71	0
3	Y01	A	702	-	38,38,38	0.51	0	57,57,57	1.12	5 (8%)
3	Y01	A	703	-	38,38,38	0.54	0	57,57,57	0.82	0
3	Y01	B	705	-	38,38,38	0.53	0	57,57,57	0.71	0
3	Y01	B	702	-	38,38,38	0.52	0	57,57,57	0.96	2 (3%)
4	PEE	A	705	-	42,42,50	0.81	2 (4%)	45,47,55	0.56	0
3	Y01	A	706	-	38,38,38	0.52	0	57,57,57	0.96	2 (3%)
3	Y01	B	704	-	38,38,38	0.54	0	57,57,57	0.82	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
2	ATP	A	701	-	-	5/22/38/38	0/3/3/3
2	ATP	B	701	-	-	5/22/38/38	0/3/3/3
3	Y01	B	703	-	-	15/19/77/77	0/4/4/4
4	PEE	B	706	-	-	22/46/46/54	-
3	Y01	A	704	-	-	9/19/77/77	0/4/4/4
3	Y01	A	702	-	-	15/19/77/77	0/4/4/4
3	Y01	A	703	-	-	9/19/77/77	0/4/4/4
3	Y01	B	705	-	-	9/19/77/77	0/4/4/4
3	Y01	B	702	-	-	11/19/77/77	0/4/4/4
4	PEE	A	705	-	-	22/46/46/54	-
3	Y01	A	706	-	-	11/19/77/77	0/4/4/4
3	Y01	B	704	-	-	9/19/77/77	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	ATP	C5-C4	4.75	1.47	1.39
2	B	701	ATP	C5-C4	4.74	1.47	1.39
4	A	705	PEE	C19-C18	3.44	1.51	1.29
4	B	706	PEE	C19-C18	3.43	1.51	1.29
4	B	706	PEE	C39-C38	3.40	1.51	1.31
4	A	705	PEE	C39-C38	3.39	1.51	1.31
2	A	701	ATP	C5-C6	2.70	1.48	1.41
2	B	701	ATP	C5-C6	2.68	1.48	1.41
2	A	701	ATP	C8-N7	2.32	1.36	1.31
2	B	701	ATP	C8-N7	2.30	1.36	1.31
2	A	701	ATP	C5-N7	-2.28	1.34	1.39
2	B	701	ATP	C5-N7	-2.27	1.34	1.39

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	ATP	C5-C4-N3	-5.86	118.65	126.72
2	B	701	ATP	C5-C4-N3	-5.85	118.66	126.72
2	A	701	ATP	N3-C4-N9	4.68	135.13	127.17
2	B	701	ATP	N3-C4-N9	4.67	135.11	127.17
2	A	701	ATP	C2-N3-C4	3.67	120.79	111.83
2	B	701	ATP	C2-N3-C4	3.67	120.78	111.83
2	B	701	ATP	C4-C5-N7	-3.39	106.71	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	ATP	C4-C5-N7	-3.38	106.72	110.58
2	B	701	ATP	N3-C2-N1	-3.16	123.80	128.58
3	A	702	Y01	CAP-CBE-CBB	3.16	116.95	112.18
2	A	701	ATP	N3-C2-N1	-3.15	123.81	128.58
3	B	703	Y01	CAP-CBE-CBB	3.13	116.91	112.18
3	B	702	Y01	CAP-CBE-CBB	2.85	116.49	112.18
3	A	706	Y01	CAP-CBE-CBB	2.84	116.47	112.18
3	B	703	Y01	CAS-CBF-CBD	2.79	115.67	111.78
3	A	702	Y01	CAS-CBF-CBD	2.76	115.63	111.78
3	A	702	Y01	CAQ-CBG-CBI	2.62	106.92	103.84
3	B	703	Y01	CAQ-CBG-CBI	2.61	106.91	103.84
2	A	701	ATP	C4-N9-C8	2.61	108.48	105.74
2	B	701	ATP	C4-N9-C8	2.60	108.47	105.74
3	A	706	Y01	CAO-CBB-CBE	2.60	115.72	110.33
3	B	702	Y01	CAO-CBB-CBE	2.59	115.71	110.33
3	A	702	Y01	CAU-CAS-CBF	2.51	117.40	113.14
3	B	703	Y01	CAU-CAS-CBF	2.49	117.37	113.14
2	B	701	ATP	C5-N7-C8	2.49	107.36	103.45
2	A	701	ATP	C5-N7-C8	2.46	107.32	103.45
2	B	701	ATP	C3'-C2'-C1'	2.45	106.09	101.46
2	A	701	ATP	C3'-C2'-C1'	2.44	106.07	101.46
3	B	703	Y01	CAO-CBB-CBE	2.37	115.24	110.33
3	A	702	Y01	CAO-CBB-CBE	2.36	115.23	110.33

There are no chirality outliers.

All (142) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	ATP	C5'-O5'-PA-O2A
2	B	701	ATP	C5'-O5'-PA-O2A
3	A	702	Y01	CAM-CAY-OAW-CBC
3	A	703	Y01	CAV-CBC-OAW-CAY
3	A	703	Y01	CAM-CAY-OAW-CBC
3	A	704	Y01	CAR-CBC-OAW-CAY
3	A	704	Y01	CAM-CAY-OAW-CBC
3	A	706	Y01	CAM-CAY-OAW-CBC
3	B	702	Y01	CAM-CAY-OAW-CBC
3	B	703	Y01	CAM-CAY-OAW-CBC
3	B	704	Y01	CAV-CBC-OAW-CAY
3	B	704	Y01	CAM-CAY-OAW-CBC
3	B	705	Y01	CAR-CBC-OAW-CAY
3	B	705	Y01	CAM-CAY-OAW-CBC

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Mol	Chain	Res	Type	Atoms
4	A	705	PEE	O2-C2-C3-O3
4	A	705	PEE	C1-O3P-P-O1P
4	A	705	PEE	C4-O4P-P-O3P
4	A	705	PEE	C4-O4P-P-O2P
4	A	705	PEE	C4-O4P-P-O1P
4	A	705	PEE	O4P-C4-C5-N
4	B	706	PEE	O2-C2-C3-O3
4	B	706	PEE	C1-O3P-P-O1P
4	B	706	PEE	C4-O4P-P-O3P
4	B	706	PEE	C4-O4P-P-O2P
4	B	706	PEE	C4-O4P-P-O1P
4	B	706	PEE	O4P-C4-C5-N
3	A	703	Y01	OAG-CAY-OAW-CBC
3	A	704	Y01	OAG-CAY-OAW-CBC
3	A	706	Y01	OAG-CAY-OAW-CBC
3	B	702	Y01	OAG-CAY-OAW-CBC
3	B	704	Y01	OAG-CAY-OAW-CBC
3	B	705	Y01	OAG-CAY-OAW-CBC
3	A	702	Y01	OAG-CAY-OAW-CBC
3	B	703	Y01	OAG-CAY-OAW-CBC
4	A	705	PEE	C14-C15-C16-C17
4	B	706	PEE	C14-C15-C16-C17
4	A	705	PEE	C43-C44-C45-C46
4	B	706	PEE	C43-C44-C45-C46
4	A	705	PEE	C16-C17-C18-C19
4	B	706	PEE	C16-C17-C18-C19
3	A	702	Y01	CAC-CBB-CBE-CBI
3	B	703	Y01	CAC-CBB-CBE-CBI
3	A	706	Y01	CAO-CBB-CBE-CBI
3	B	702	Y01	CAO-CBB-CBE-CBI
3	A	702	Y01	CAO-CBB-CBE-CBI
3	B	703	Y01	CAO-CBB-CBE-CBI
4	A	705	PEE	C37-C38-C39-C40
4	B	706	PEE	C37-C38-C39-C40
3	A	702	Y01	CAC-CBB-CBE-CAP
3	A	706	Y01	CAC-CBB-CBE-CAP
3	B	702	Y01	CAC-CBB-CBE-CAP
3	B	703	Y01	CAC-CBB-CBE-CAP
3	A	706	Y01	CAC-CBB-CBE-CBI
3	B	702	Y01	CAC-CBB-CBE-CBI
3	A	706	Y01	CAN-CAJ-CAO-CBB
3	B	702	Y01	CAN-CAJ-CAO-CBB

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Mol	Chain	Res	Type	Atoms
3	A	704	Y01	CAX-CAL-CAM-CAY
3	B	705	Y01	CAX-CAL-CAM-CAY
3	A	702	Y01	CAJ-CAO-CBB-CBE
3	B	703	Y01	CAJ-CAO-CBB-CBE
3	A	704	Y01	CAO-CAJ-CAN-CBA
3	B	705	Y01	CAO-CAJ-CAN-CBA
3	A	702	Y01	CAX-CAL-CAM-CAY
3	B	703	Y01	CAX-CAL-CAM-CAY
4	A	705	PEE	C34-C35-C36-C37
4	B	706	PEE	C34-C35-C36-C37
4	B	706	PEE	C31-C32-C33-C34
4	A	705	PEE	C31-C32-C33-C34
4	A	705	PEE	C32-C33-C34-C35
4	B	706	PEE	C32-C33-C34-C35
4	A	705	PEE	C13-C14-C15-C16
4	B	706	PEE	C13-C14-C15-C16
4	A	705	PEE	C41-C42-C43-C44
4	B	706	PEE	C41-C42-C43-C44
4	A	705	PEE	C1-C2-C3-O3
4	B	706	PEE	C1-C2-C3-O3
3	A	704	Y01	CAJ-CAN-CBA-CAB
3	B	705	Y01	CAJ-CAN-CBA-CAB
2	B	701	ATP	O4'-C4'-C5'-O5'
3	A	704	Y01	CAJ-CAN-CBA-CAA
3	B	705	Y01	CAJ-CAN-CBA-CAA
4	A	705	PEE	O3P-C1-C2-C3
4	B	706	PEE	O3P-C1-C2-C3
3	A	702	Y01	CAN-CAJ-CAO-CBB
3	B	703	Y01	CAN-CAJ-CAO-CBB
2	A	701	ATP	O4'-C4'-C5'-O5'
3	A	702	Y01	CAO-CBB-CBE-CAP
3	B	703	Y01	CAO-CBB-CBE-CAP
3	A	706	Y01	CAJ-CAO-CBB-CBE
3	B	702	Y01	CAJ-CAO-CBB-CBE
4	B	706	PEE	C42-C43-C44-C45
4	A	705	PEE	C42-C43-C44-C45
2	A	701	ATP	C3'-C4'-C5'-O5'
2	B	701	ATP	C3'-C4'-C5'-O5'
4	A	705	PEE	O3P-C1-C2-O2
4	B	706	PEE	O3P-C1-C2-O2
4	B	706	PEE	C33-C34-C35-C36
4	A	705	PEE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
2	A	701	ATP	C5'-O5'-PA-O3A
2	B	701	ATP	C5'-O5'-PA-O3A
4	A	705	PEE	C38-C39-C40-C41
4	B	706	PEE	C38-C39-C40-C41
3	A	703	Y01	CAL-CAM-CAY-OAW
3	B	704	Y01	CAL-CAM-CAY-OAW
4	A	705	PEE	C35-C36-C37-C38
4	B	706	PEE	C35-C36-C37-C38
3	A	706	Y01	CAX-CAL-CAM-CAY
3	B	702	Y01	CAX-CAL-CAM-CAY
3	B	705	Y01	CAN-CAJ-CAO-CBB
3	A	704	Y01	CAN-CAJ-CAO-CBB
3	A	702	Y01	CAO-CAJ-CAN-CBA
3	B	703	Y01	CAO-CAJ-CAN-CBA
3	A	703	Y01	CAM-CAL-CAX-OAF
3	B	704	Y01	CAM-CAL-CAX-OAF
3	A	703	Y01	CAM-CAL-CAX-OAH
3	A	706	Y01	CAM-CAL-CAX-OAF
3	B	702	Y01	CAM-CAL-CAX-OAF
3	B	704	Y01	CAM-CAL-CAX-OAH
3	B	703	Y01	CAM-CAL-CAX-OAF
3	A	702	Y01	CAM-CAL-CAX-OAF
3	B	703	Y01	CAM-CAL-CAX-OAH
3	A	706	Y01	CAJ-CAO-CBB-CAC
3	B	702	Y01	CAJ-CAO-CBB-CAC
3	A	702	Y01	CAM-CAL-CAX-OAH
3	A	706	Y01	CAM-CAL-CAX-OAH
3	B	702	Y01	CAM-CAL-CAX-OAH
3	A	703	Y01	CAJ-CAN-CBA-CAB
3	B	704	Y01	CAJ-CAN-CBA-CAB
3	A	703	Y01	CAN-CAJ-CAO-CBB
3	B	704	Y01	CAN-CAJ-CAO-CBB
3	A	704	Y01	CAL-CAM-CAY-OAW
3	B	705	Y01	CAL-CAM-CAY-OAW
2	B	701	ATP	PG-O3B-PB-O2B
3	B	703	Y01	CAL-CAM-CAY-OAW
3	A	702	Y01	CAL-CAM-CAY-OAW
3	B	703	Y01	CAJ-CAN-CBA-CAA
3	A	702	Y01	CAJ-CAN-CBA-CAA
3	B	704	Y01	CAJ-CAN-CBA-CAA
3	A	702	Y01	CAL-CAM-CAY-OAG
3	B	703	Y01	CAL-CAM-CAY-OAG

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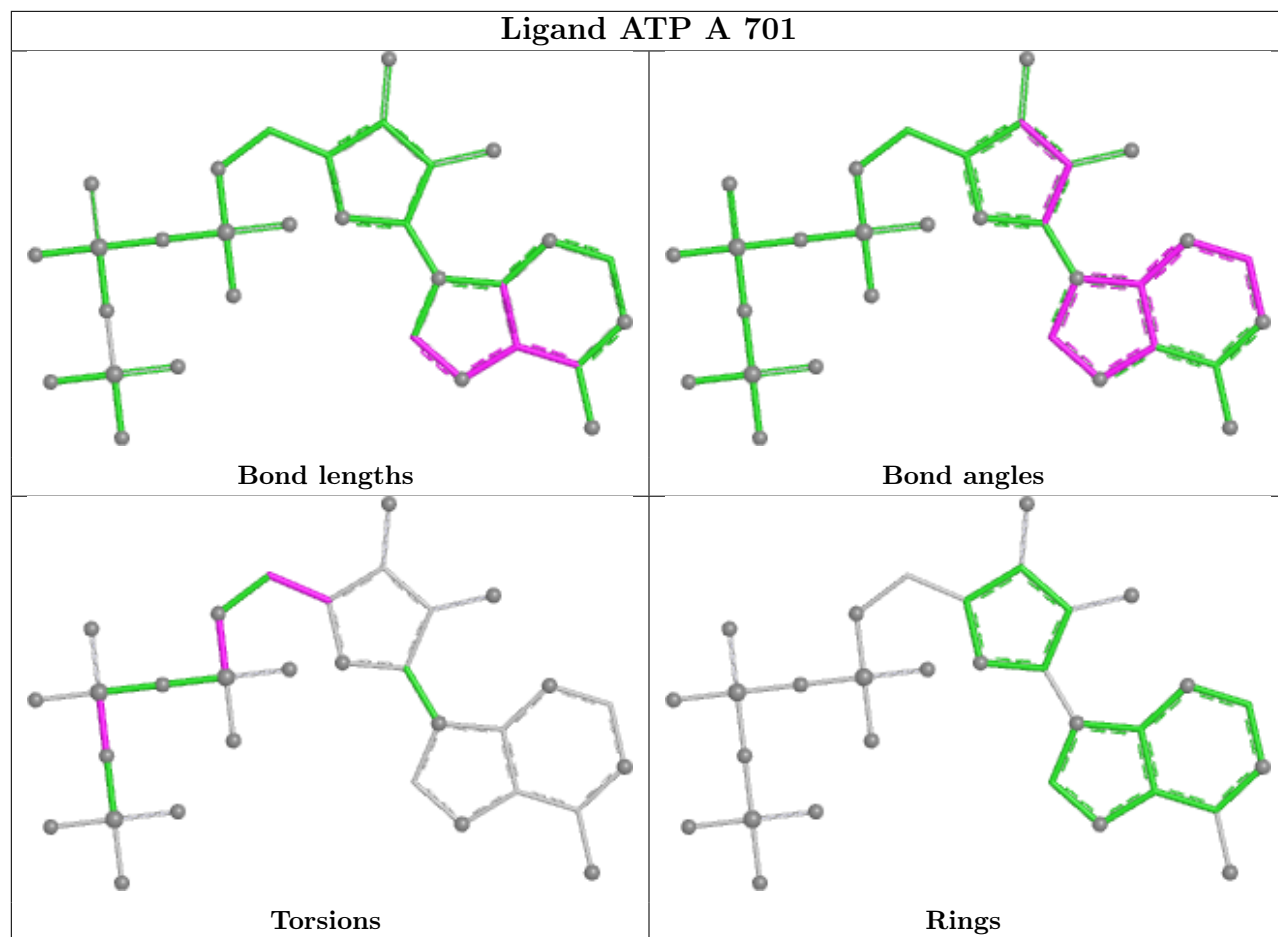
Mol	Chain	Res	Type	Atoms
3	A	703	Y01	CAJ-CAN-CBA-CAA
2	A	701	ATP	PG-O3B-PB-O2B

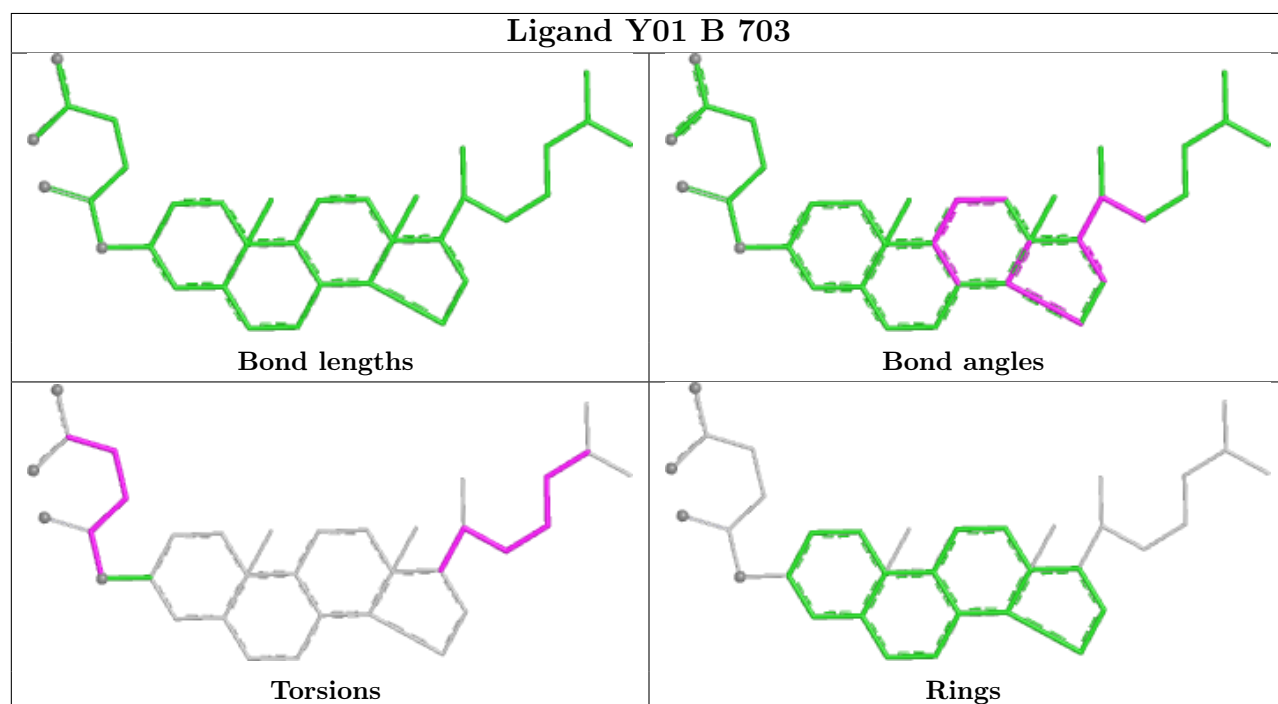
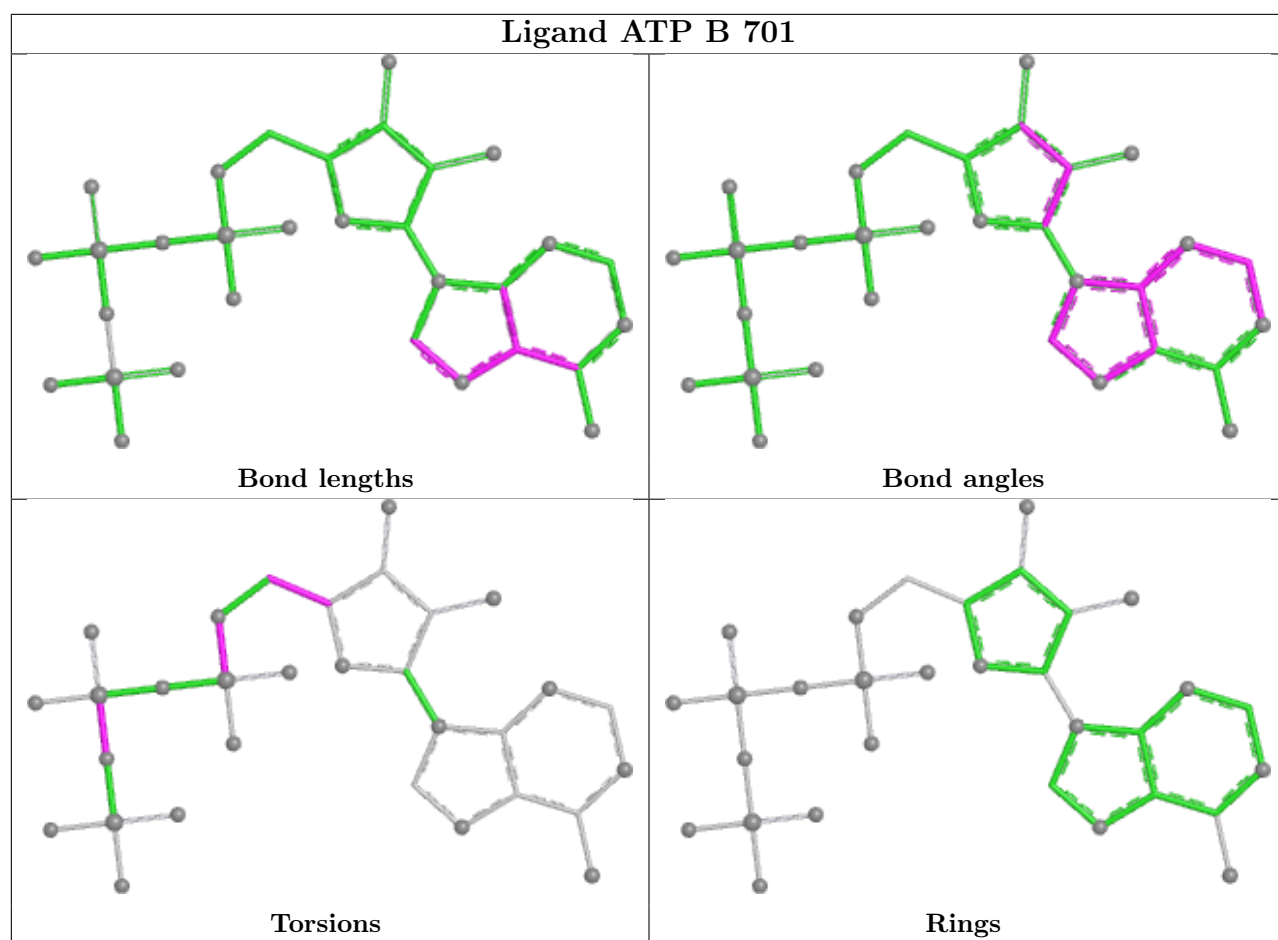
There are no ring outliers.

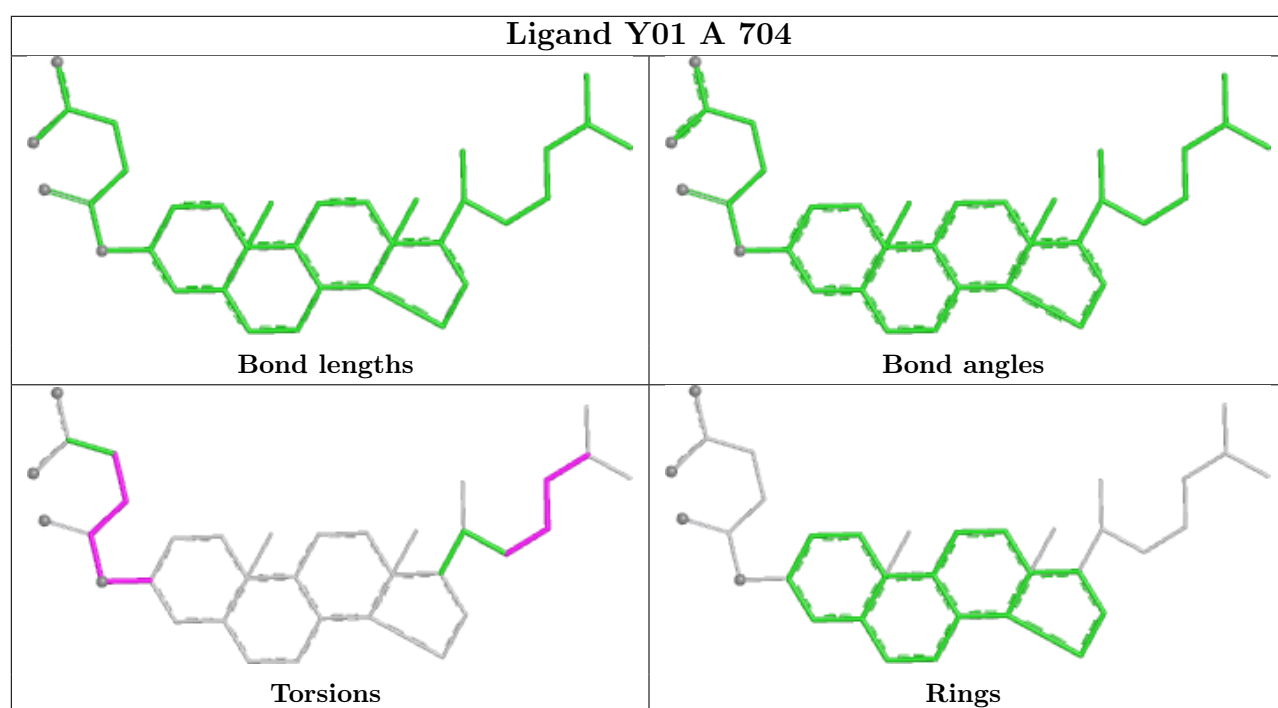
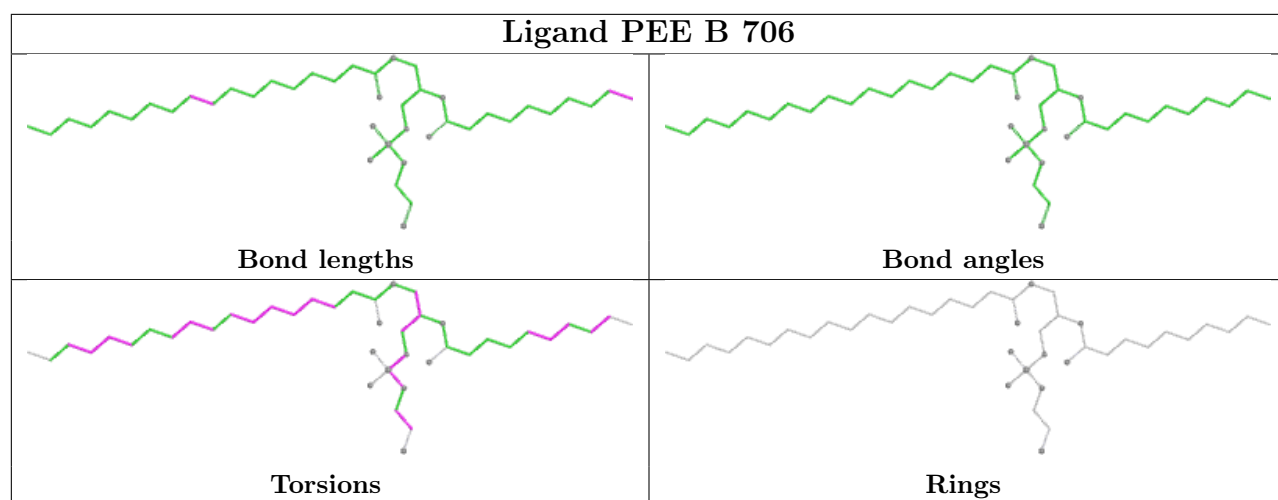
12 monomers are involved in 66 short contacts:

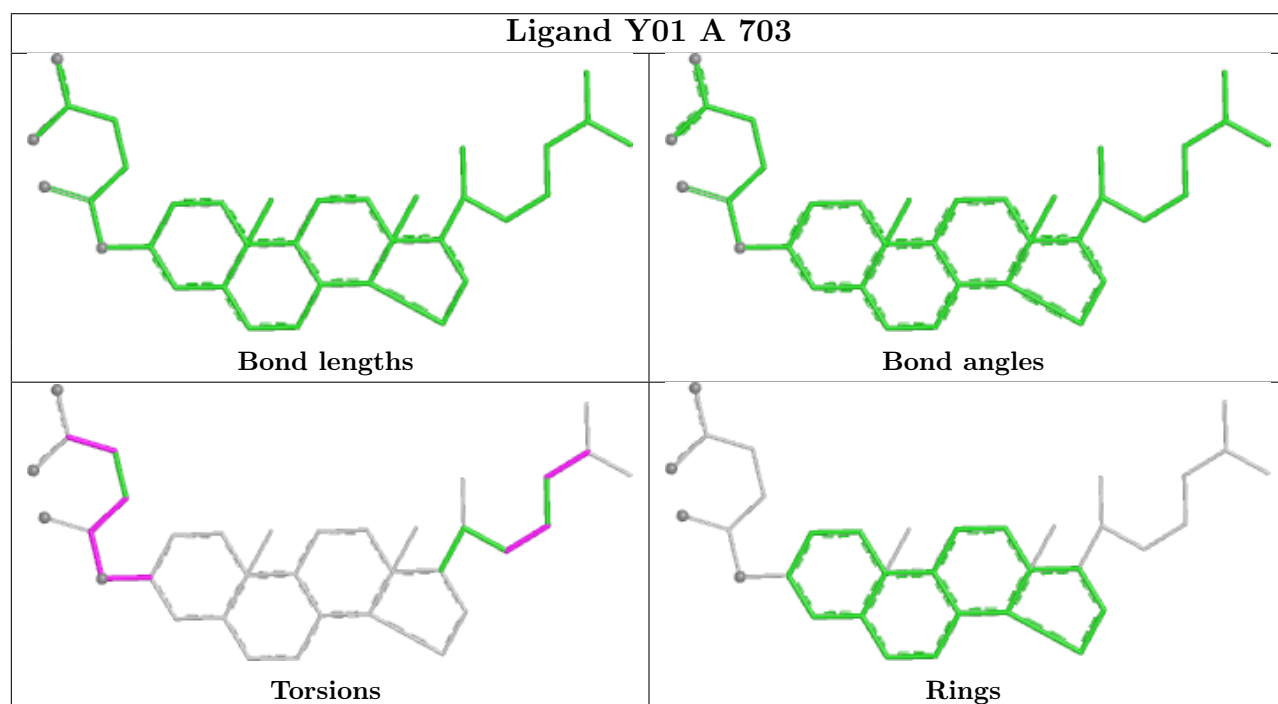
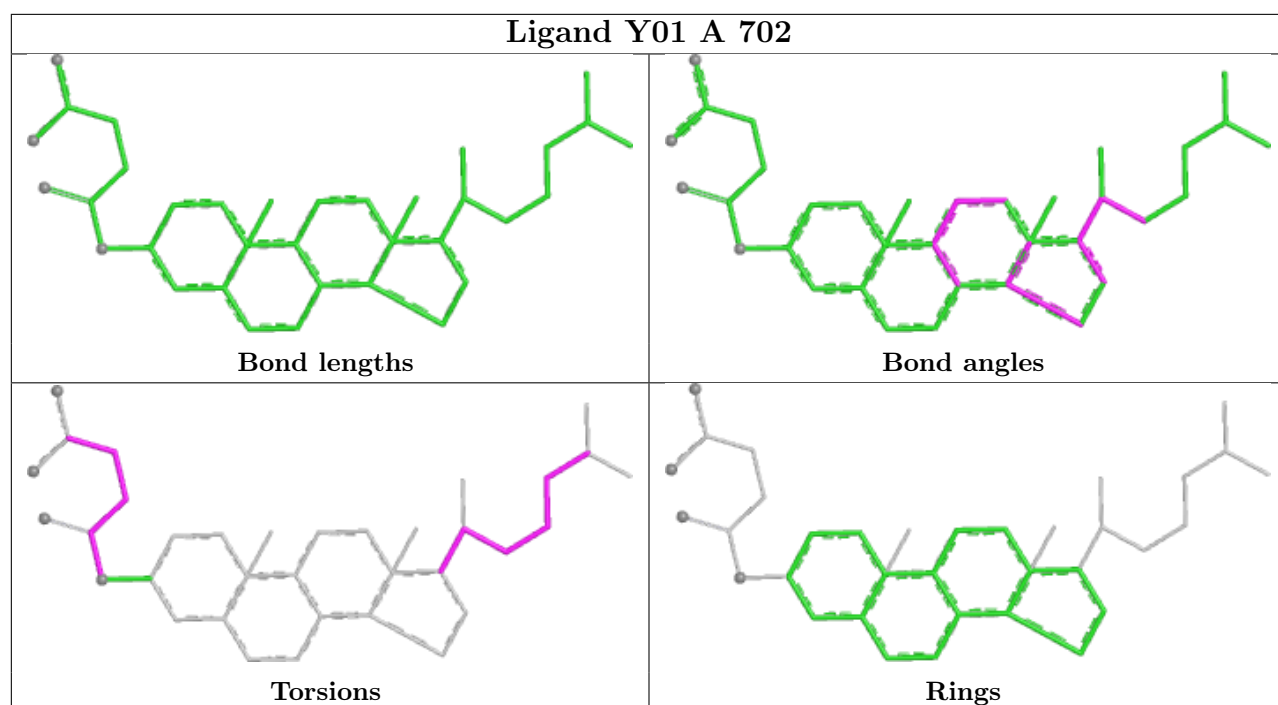
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	ATP	1	0
2	B	701	ATP	1	0
3	B	703	Y01	14	0
4	B	706	PEE	5	0
3	A	704	Y01	10	0
3	A	702	Y01	14	0
3	A	703	Y01	1	0
3	B	705	Y01	11	0
3	B	702	Y01	1	0
4	A	705	PEE	5	0
3	A	706	Y01	2	0
3	B	704	Y01	2	0

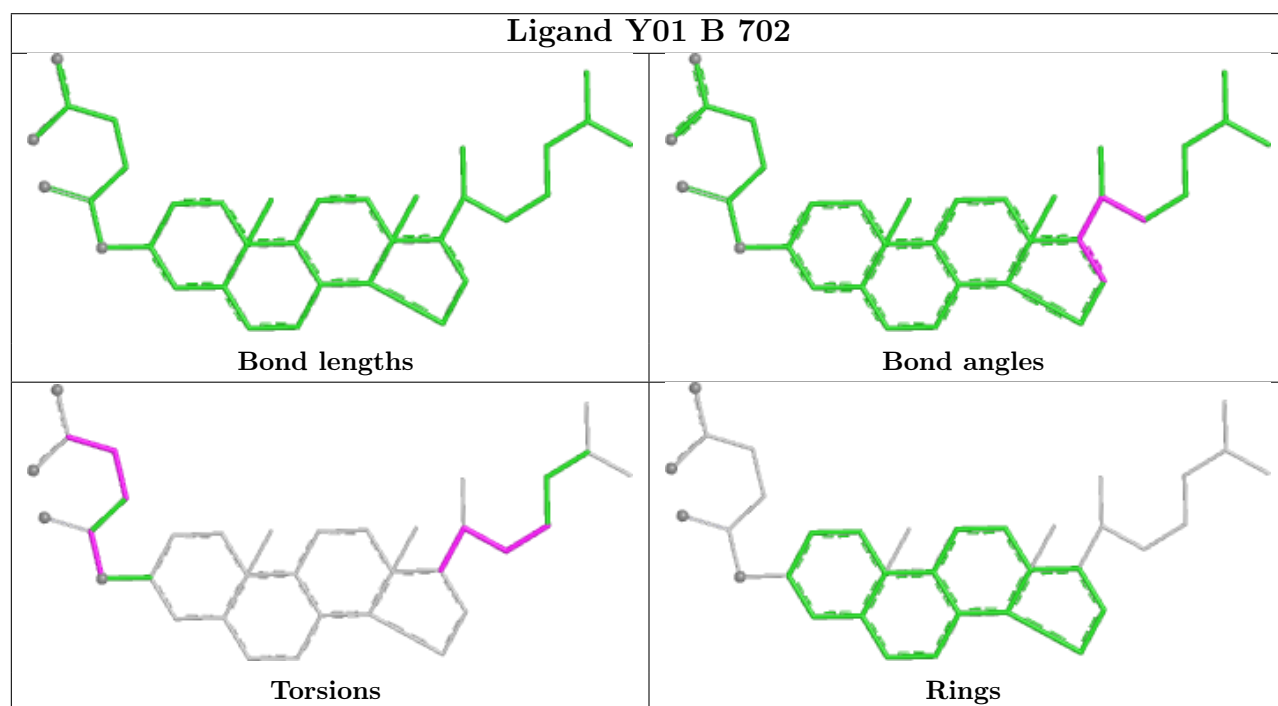
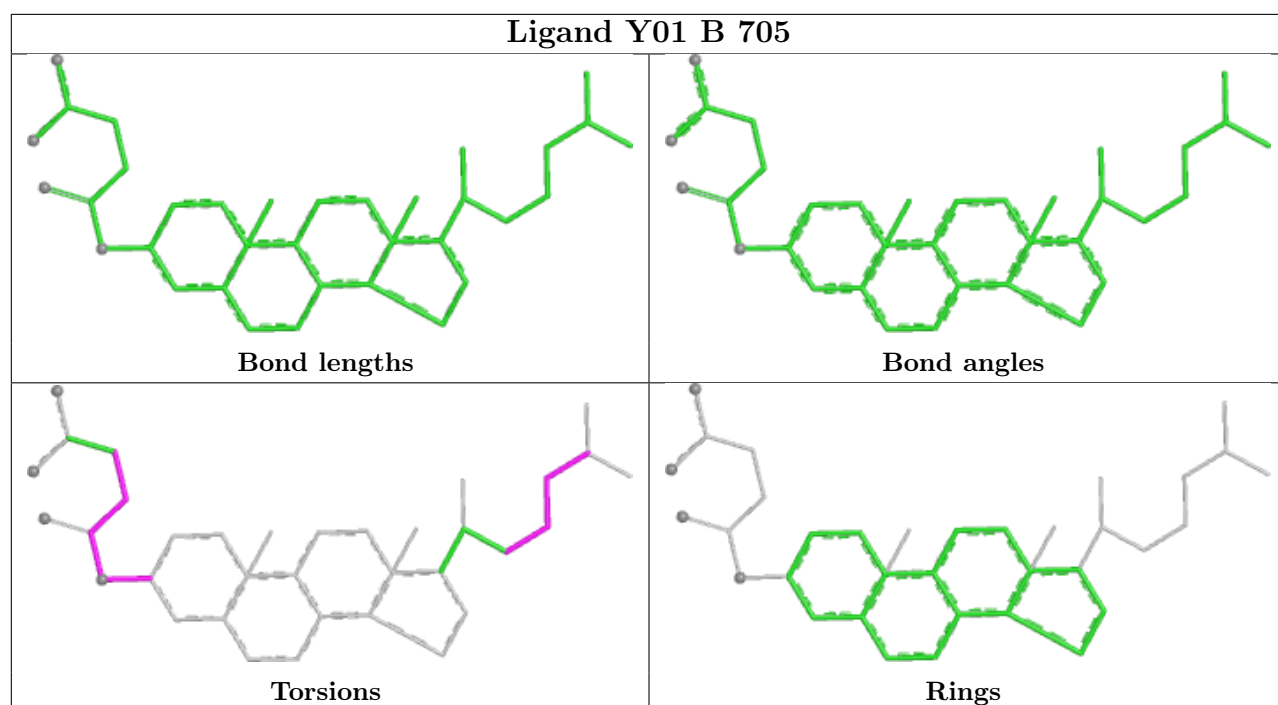
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

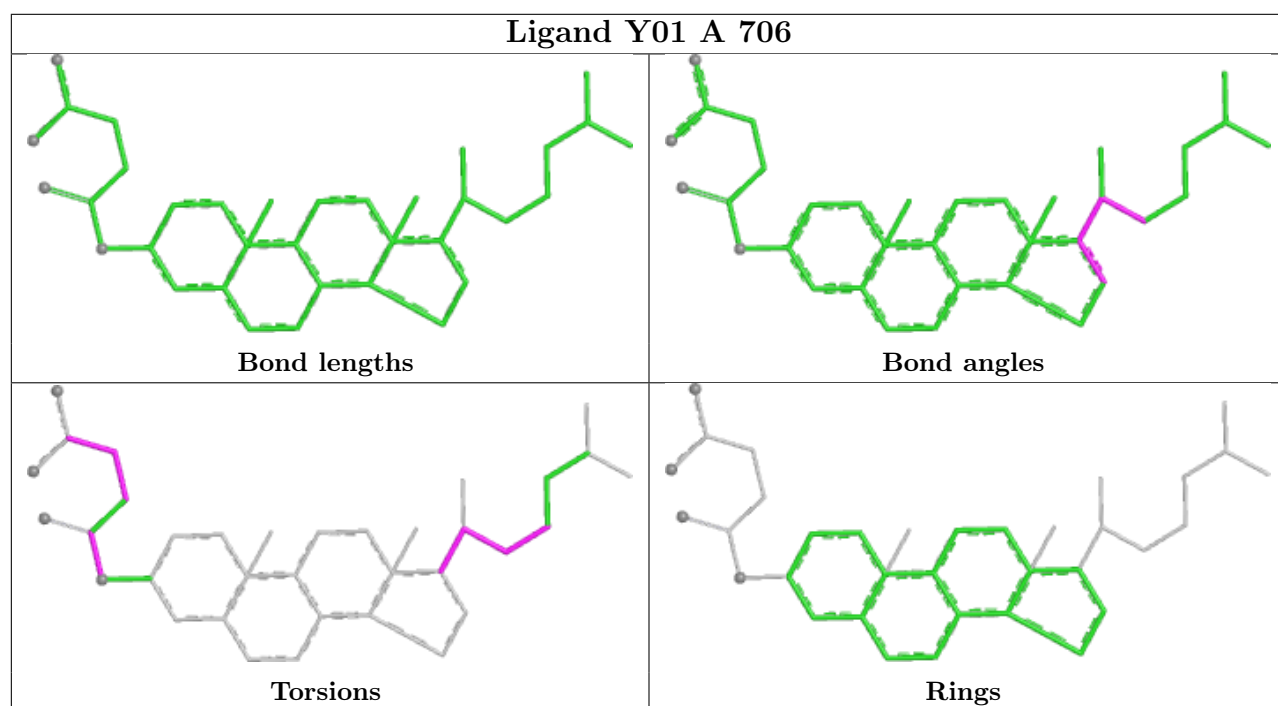
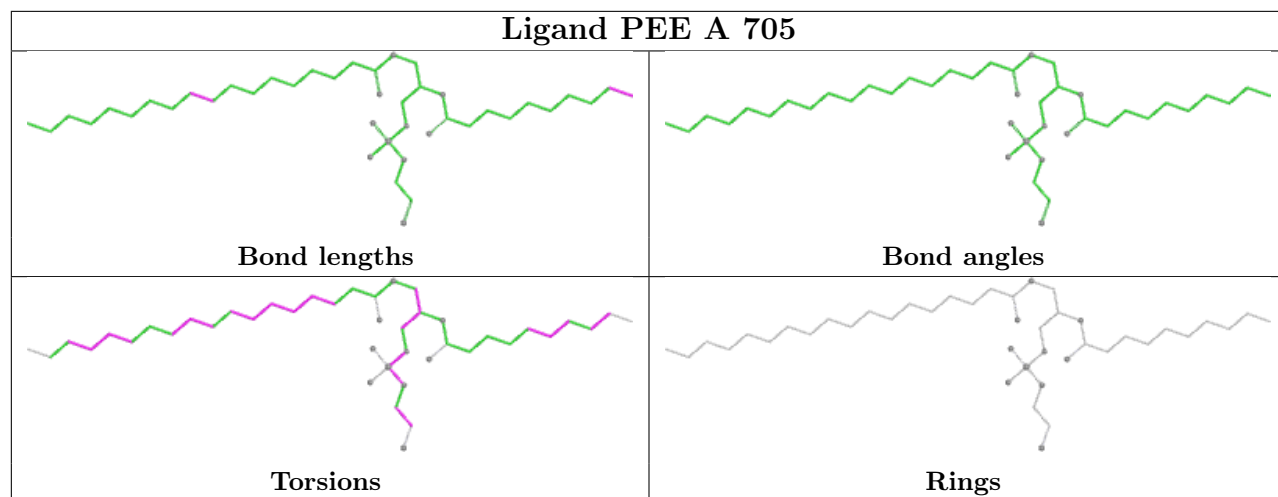


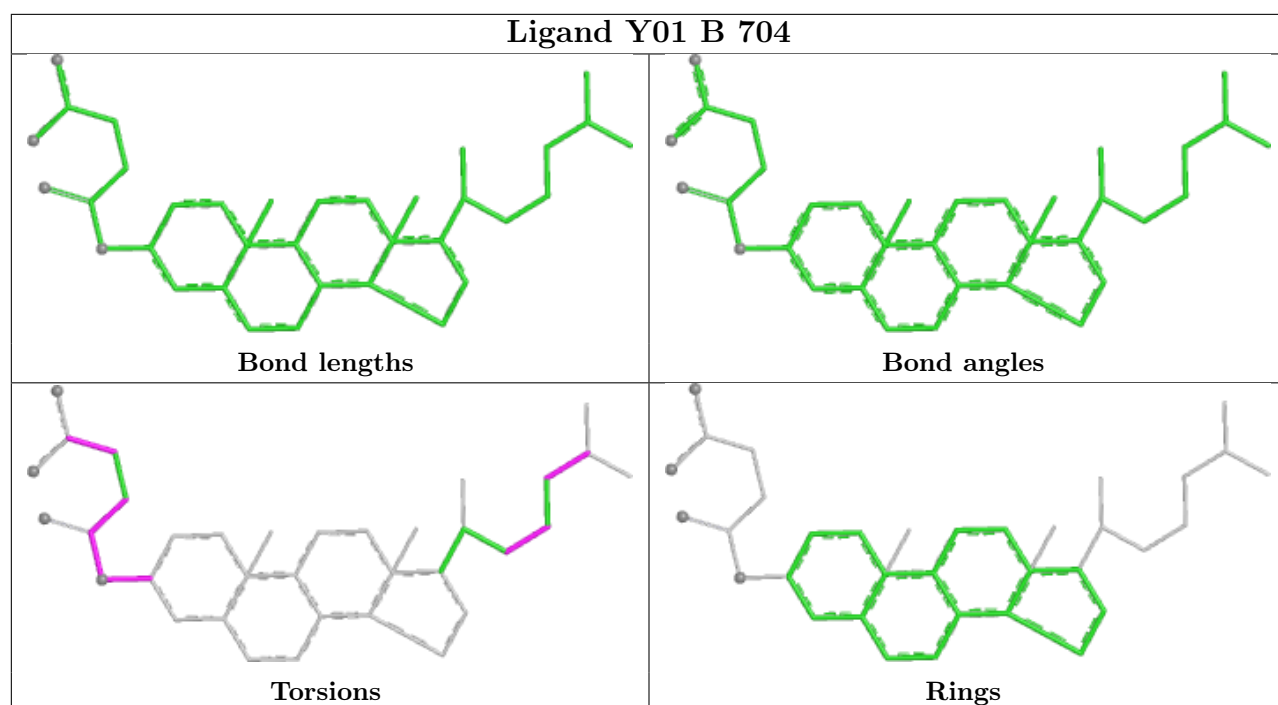












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

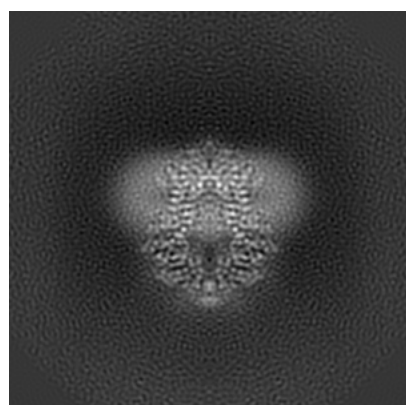
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13118. These allow visual inspection of the internal detail of the map and identification of artifacts.

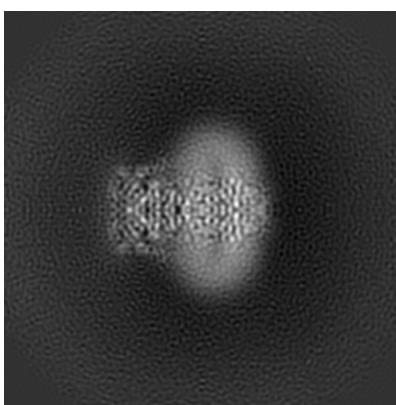
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

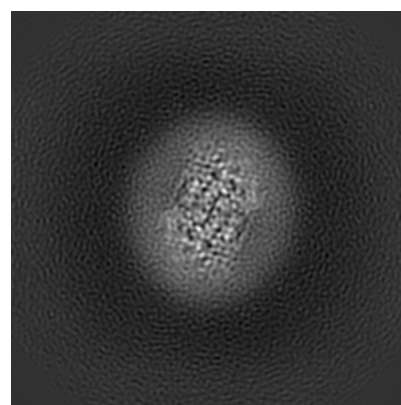
6.1.1 Primary map



X



Y

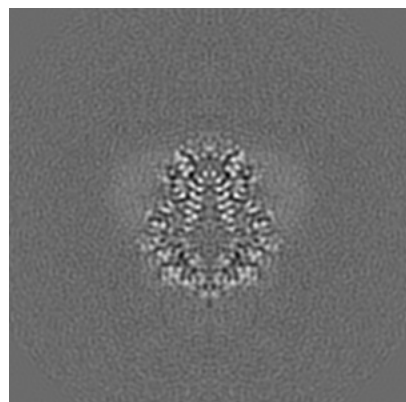


Z

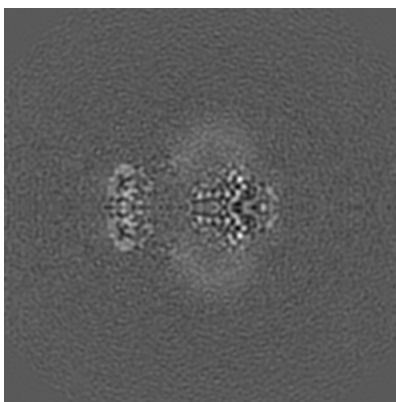
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

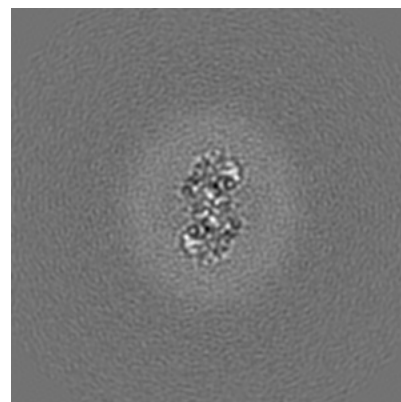
6.2.1 Primary map



X Index: 192



Y Index: 192

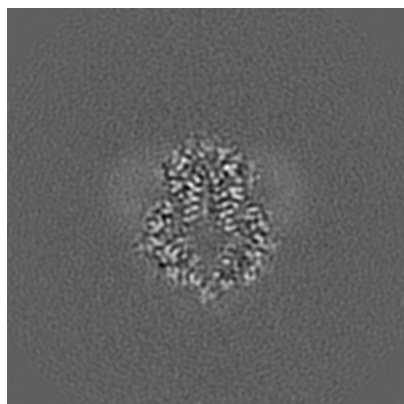


Z Index: 192

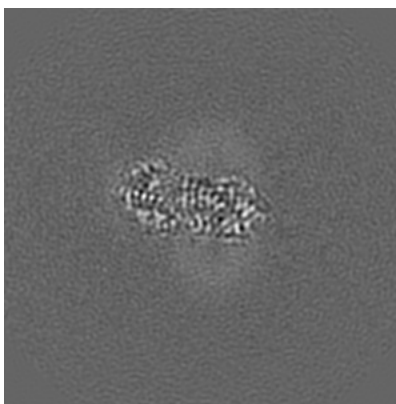
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

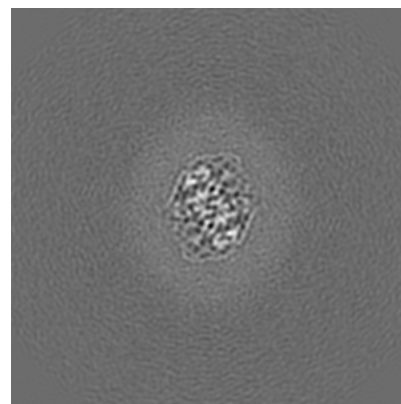
6.3.1 Primary map



X Index: 194



Y Index: 216

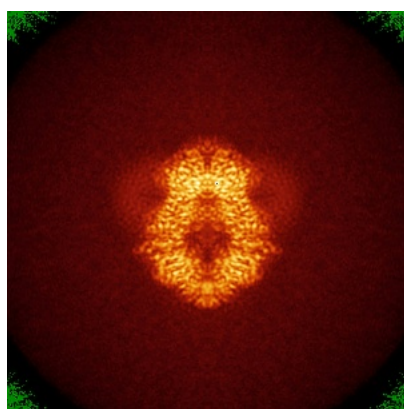


Z Index: 223

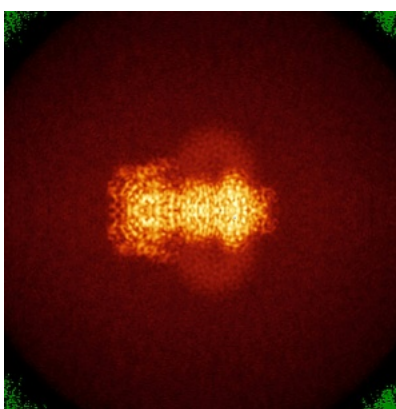
The images above show the largest variance slices of the map in three orthogonal directions.

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

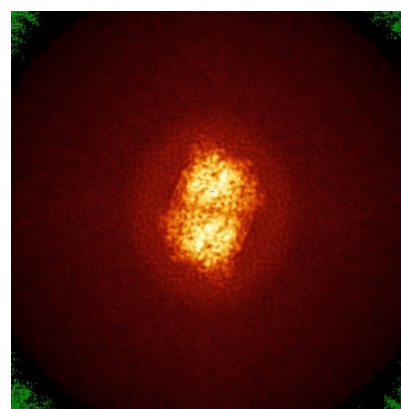
6.4.1 Primary map



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

This section was not generated.

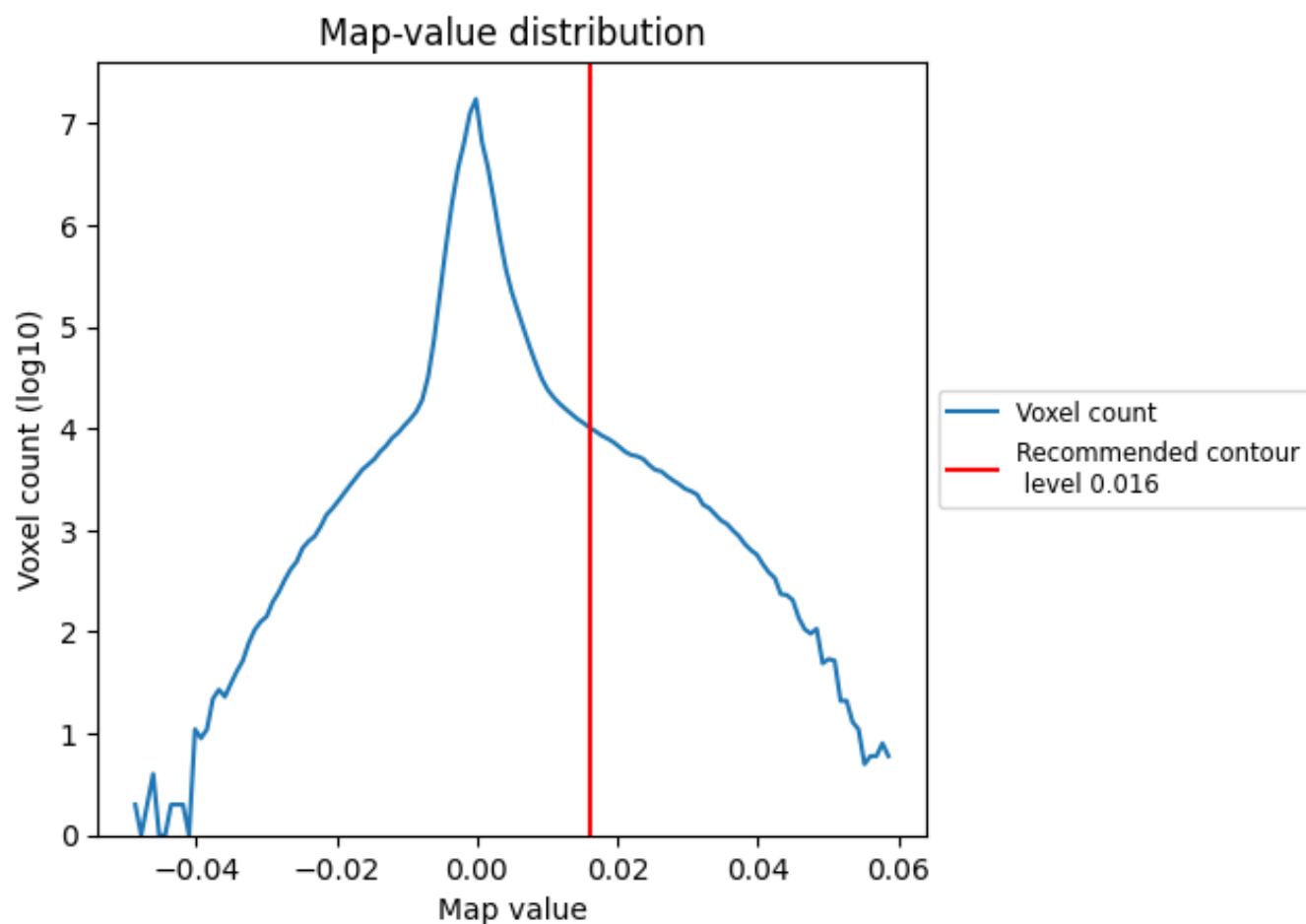
6.6 Mask visualisation

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

7 Map analysis [i](#)

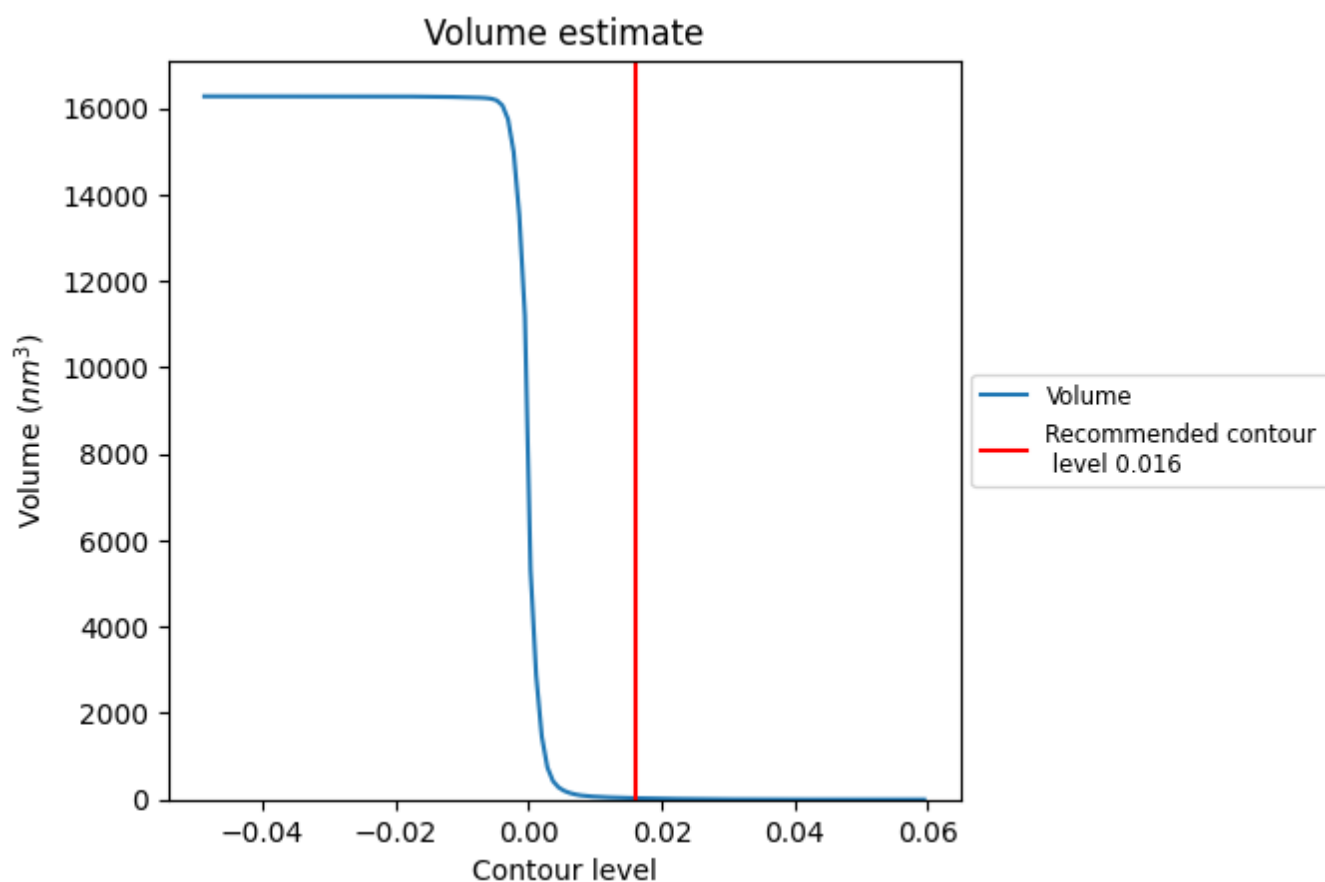
This section contains the results of statistical analysis of the map.

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.

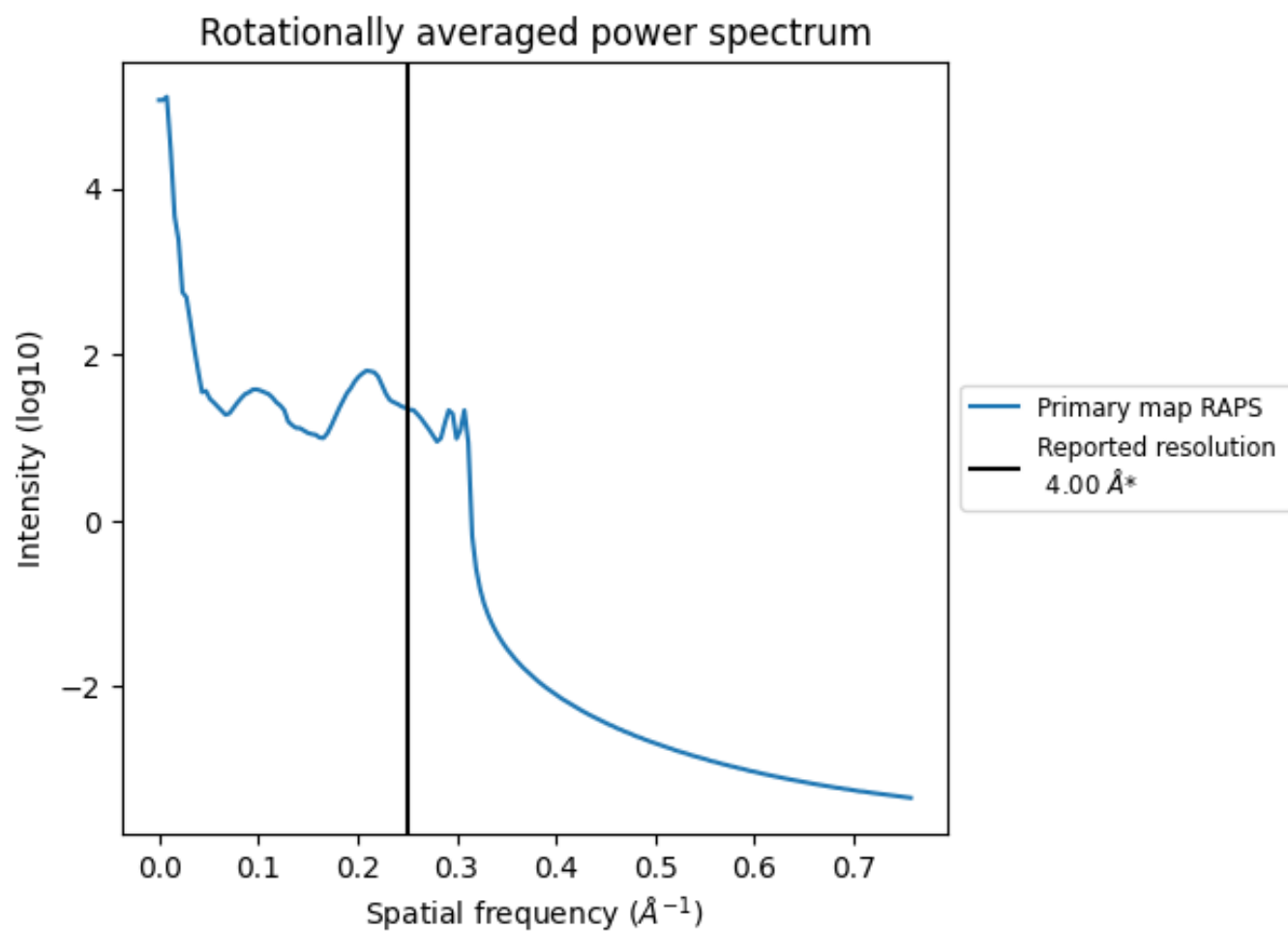
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 33 nm³; this corresponds to an approximate mass of 30 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 0.250 Å⁻¹

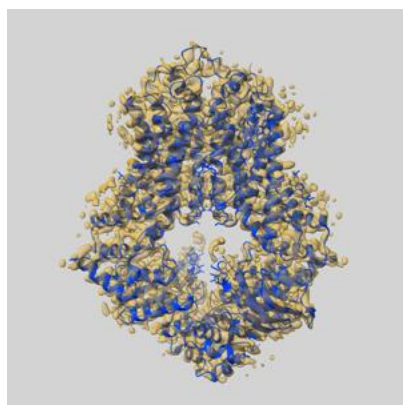
8 Fourier-Shell correlation ⓘ

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

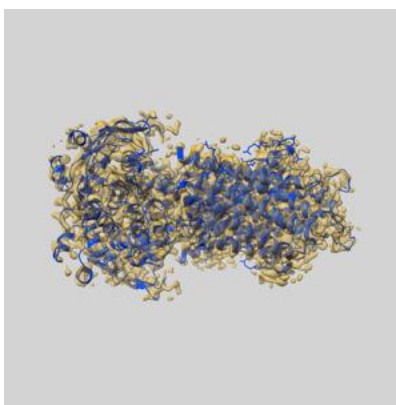
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13118 and PDB model 7OZ1. Per-residue inclusion information can be found in section [3](#) on page [7](#).

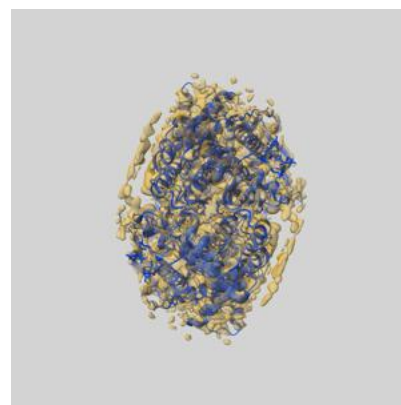
9.1 Map-model overlay [i](#)



X



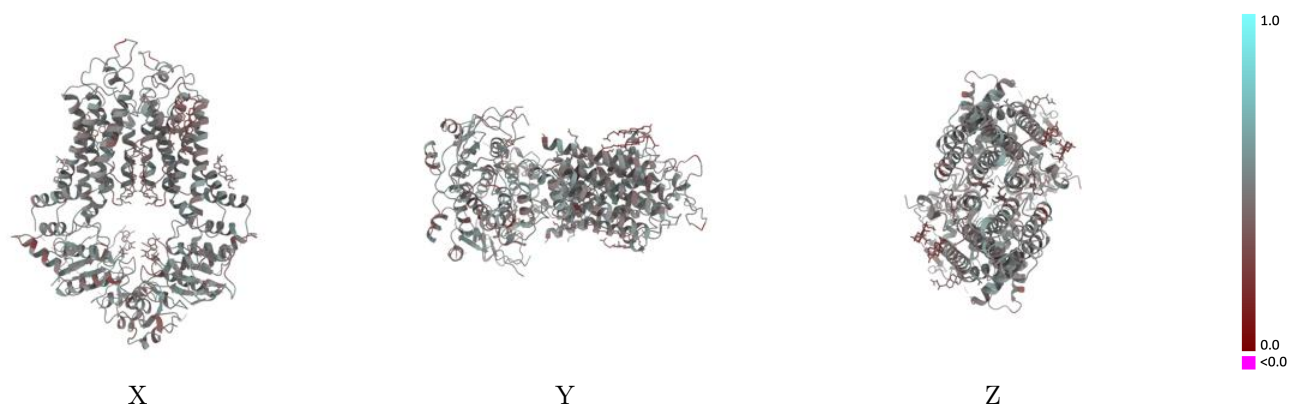
Y



Z

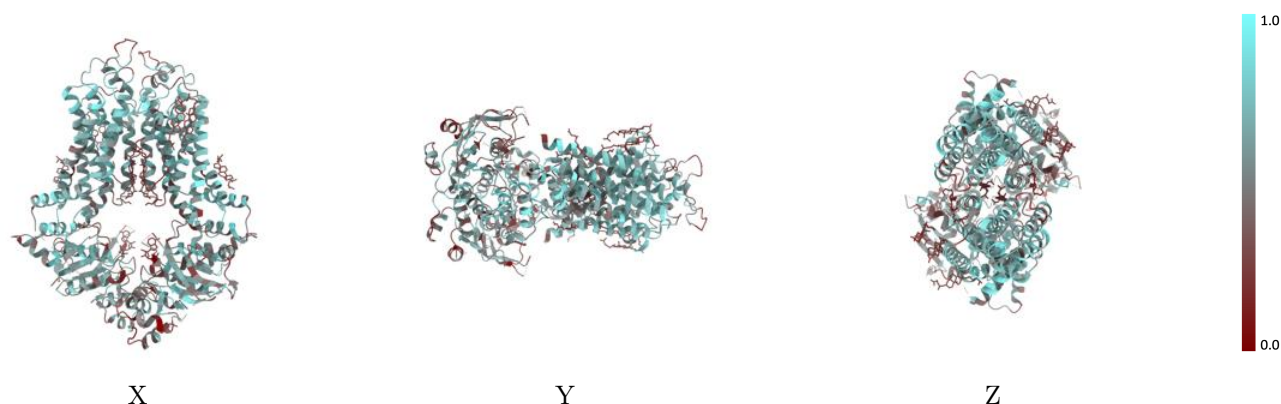
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



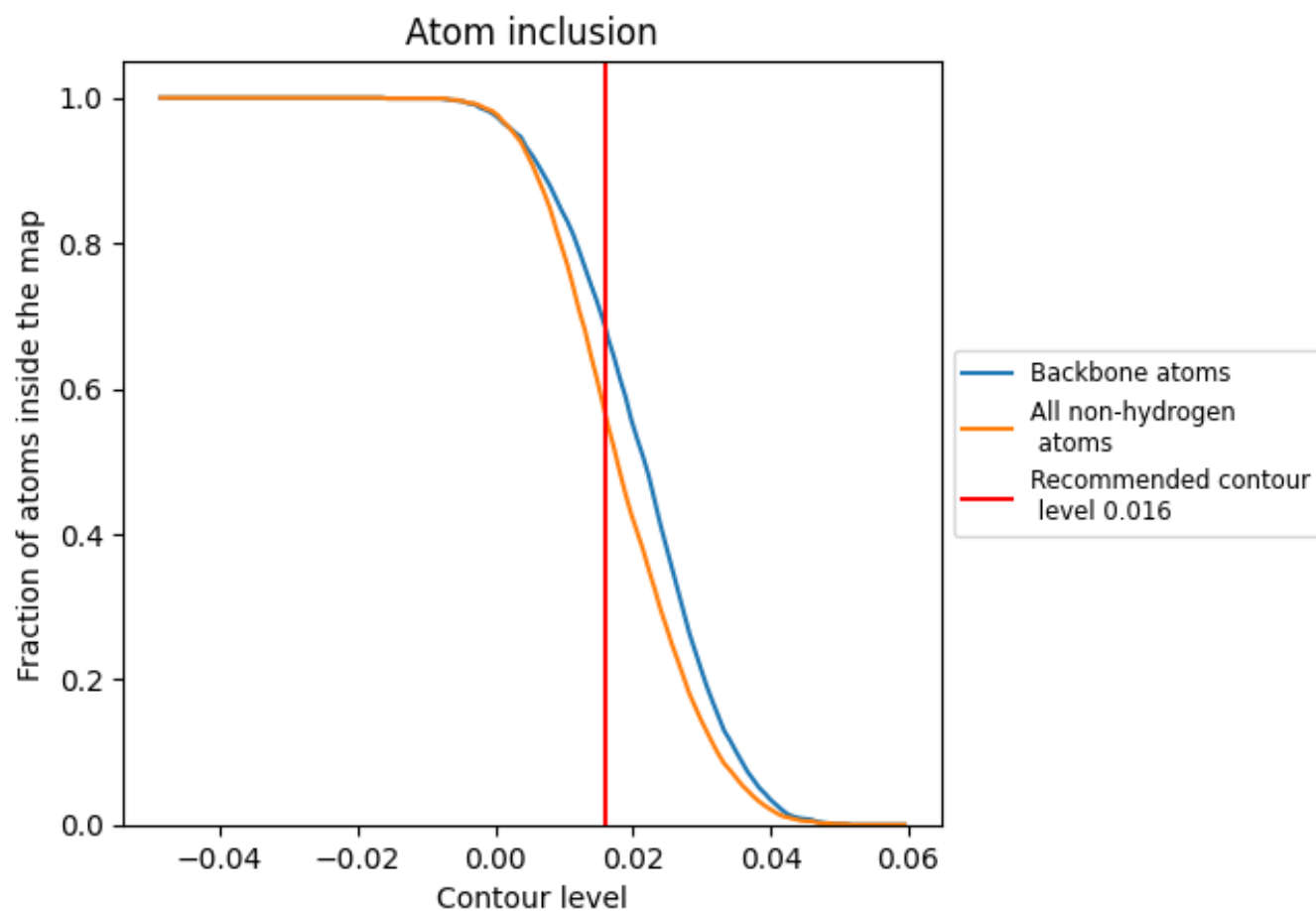
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.016).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 56% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5650	0.4660
A	0.5640	0.4660
B	0.5650	0.4660

