Full wwPDB EM Validation Report ⓘ

Aug 27, 2026 – 08:44 am BST

PDB ID	:	9S2C / pdb_00009s2c
EMDB ID	:	EMD-54488
Title	:	CgCdr1 in complex with ATP, ADP-VO4
Authors	:	Pata, J.; Zarkadas, E.; Schoehn, G.; Chaptal, V.; Falson, P.
Deposited on	:	2025-07-21
Resolution	:	2.90 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:

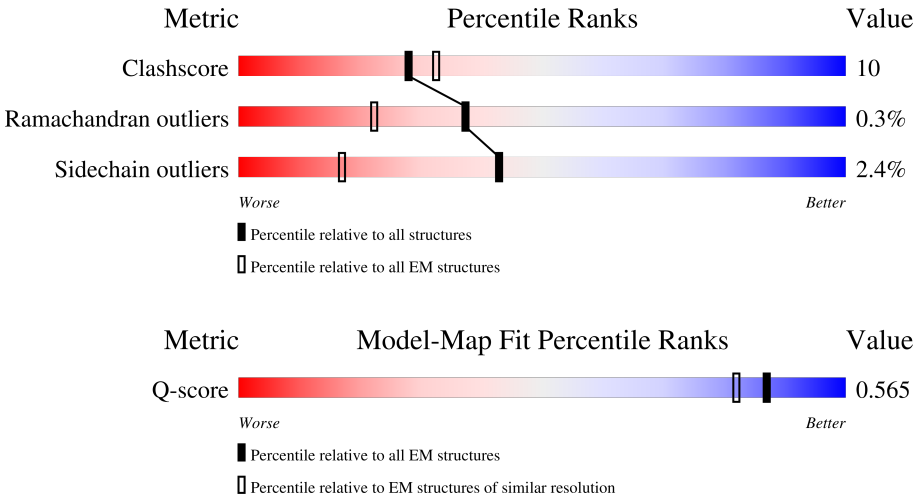
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.50

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 2.90 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	13054 (2.40 - 3.40)

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 <=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	1508	70% 21% 8%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11410 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.

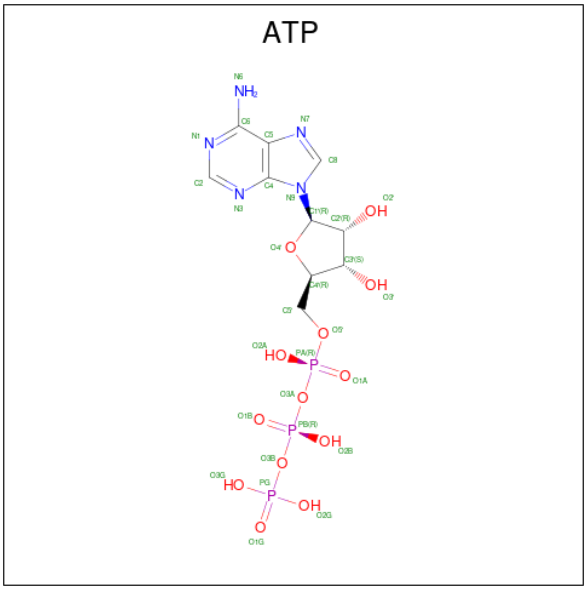
- Molecule 1 is a protein called Pleiotropic ABC efflux transporter of multiple drugs CDR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1388	11092	7158	1854	2020	60	0	0

There are 9 discrepancies between the modelled and reference sequences:

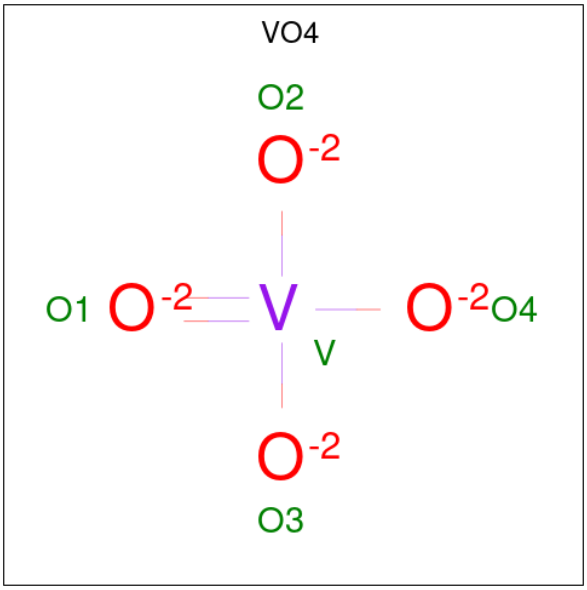
Chain	Residue	Modelled	Actual	Comment	Reference
A	1500	GLY	-	expression tag	UNP Q6FK23
A	1501	GLY	-	expression tag	UNP Q6FK23
A	1502	ARG	-	expression tag	UNP Q6FK23
A	1503	HIS	-	expression tag	UNP Q6FK23
A	1504	HIS	-	expression tag	UNP Q6FK23
A	1505	HIS	-	expression tag	UNP Q6FK23
A	1506	HIS	-	expression tag	UNP Q6FK23
A	1507	HIS	-	expression tag	UNP Q6FK23
A	1508	HIS	-	expression tag	UNP Q6FK23

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is VANADATE ION (CCD ID: VO4) (formula: O_4V) (labeled as "Ligand of Interest" by depositor).

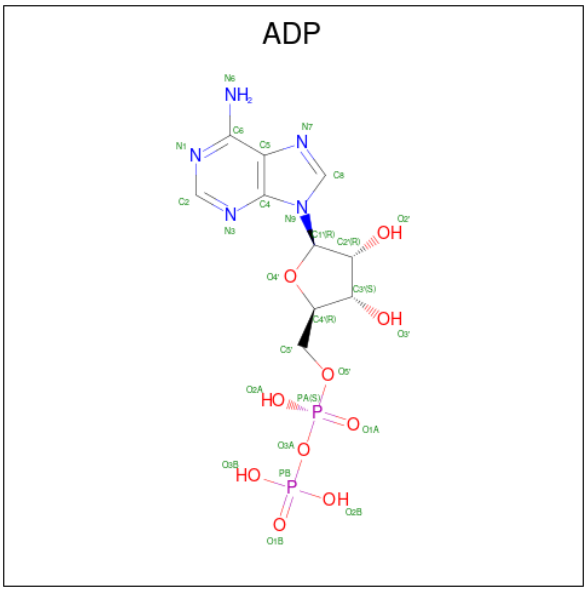


Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	O	V	0
			5	4	1	

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

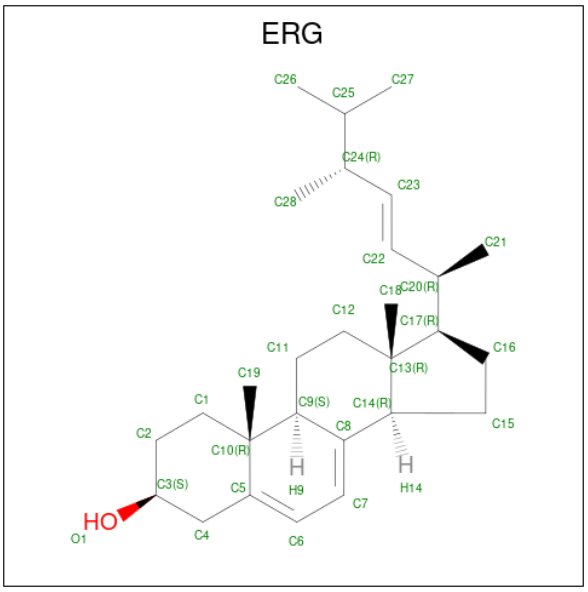
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	

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



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

- Molecule 6 is ERGOSTEROL (CCD ID: ERG) (formula: $C_{28}H_{44}O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			29	28	1	
6	A	1	Total	C	O	0
			29	28	1	

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Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total 29	C 28	O 1	0
6	A	1	Total 29	C 28	O 1	0
6	A	1	Total 29	C 28	O 1	0
6	A	1	Total 29	C 28	O 1	0
6	A	1	Total 29	C 28	O 1	0
6	A	1	Total 29	C 28	O 1	0

- Molecule 7 is water.

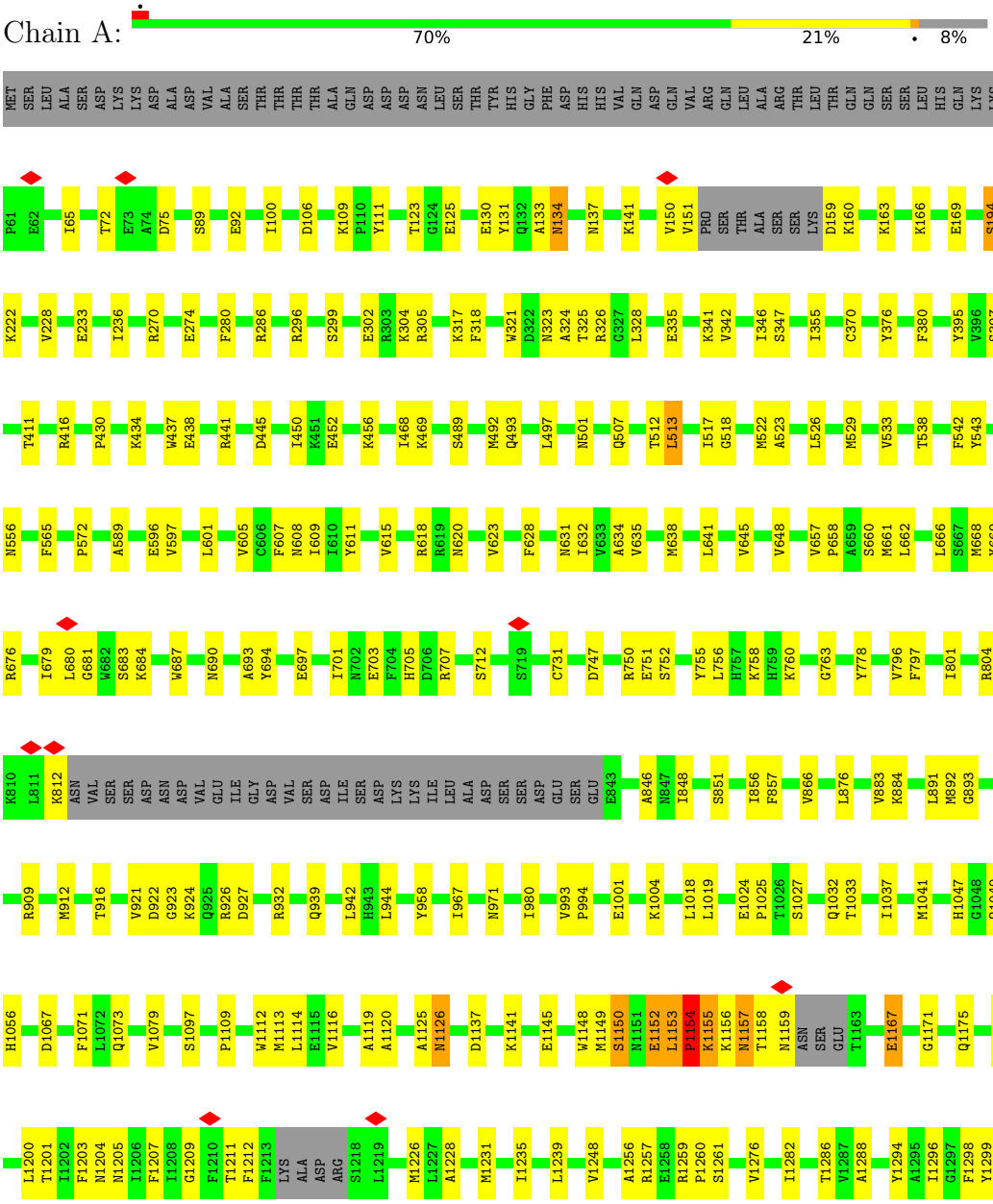
Mol	Chain	Residues	Atoms		AltConf
7	A	22	Total 22	O 22	0

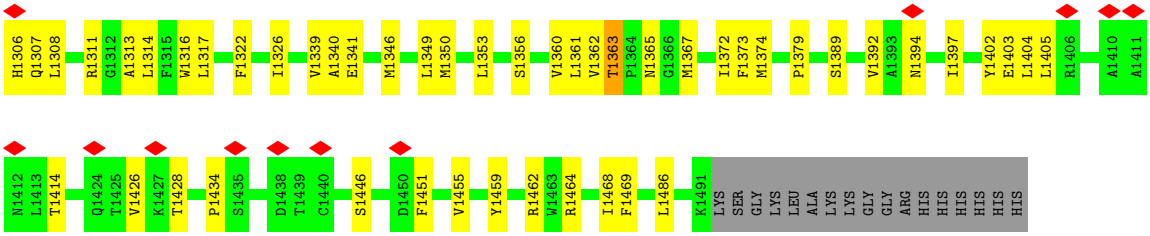
3 Residue-property plots (i)

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: Pleiotropic ABC efflux transporter of multiple drugs CDR1

Chain A:




H1306 Q1307 L1308 R1311 G1312 A1313 L1314 F1315 W1316 L1317 F1322 I1326 V1339 A1340 E1341 M1346 L1349 M1350 L1353 S1356 V1360 L1361 V1362 T1363 P1364 N1365 G1366 M1367 I1372 F1373 M1374 P1379 S1389 V1392 A1393 N1394 I1397 Y1402 E1403 L1404 L1405 R1406 A1410 A1411
N1412 L1413 T1414 Q1424 T1425 V1426 K1427 T1428 P1434 S1435 D1438 T1439 C1440 S1446 D1450 F1451 V1455 Y1459 R1462 W1463 R1464 I1468 F1469 L1486 K1491 LYS SER GLY LYS LEU ALA LYS LYS GLY GLY ARG HIS HIS HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	191450	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 ($e^-/Å^2$)	40.12	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	4.258	Depositor
Minimum map value	-2.085	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.063	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	322.176, 322.176, 322.176	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.839, 0.839, 0.839	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: VO4, ERG, ATP, ADP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.24	1/11375 (0.0%)	0.41	5/15421 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1154	PRO	C-O	8.28	1.34	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1157	ASN	CA-C-N	-7.47	107.27	121.54
1	A	1157	ASN	C-N-CA	-7.47	107.27	121.54
1	A	1154	PRO	CB-CA-C	-6.14	101.42	111.56
1	A	1152	GLU	CA-C-O	-5.68	114.47	120.55
1	A	1150	SER	N-CA-C	-5.57	107.73	114.75

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	11092	0	10932	209	0
2	A	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	5	0	0	1	0
4	A	1	0	0	0	0
5	A	27	0	12	2	0
6	A	232	0	350	14	0
7	A	22	0	0	2	0
All	All	11410	0	11306	217	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 10.

All (217) 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:522:MET:HE3	1:A:1349:LEU:HD22	1.63	0.80
1:A:1001:GLU:HG3	1:A:1033:THR:HG21	1.66	0.77
1:A:1353:LEU:HD13	1:A:1374:MET:HE1	1.69	0.75
1:A:1018:LEU:HG	1:A:1019:LEU:HD23	1.69	0.74
1:A:893:GLY:H	1:A:899:LYS:HD3	1.53	0.74
1:A:1153:LEU:O	1:A:1154:PRO:C	2.30	0.73
1:A:641:LEU:HB3	1:A:662:LEU:HD21	1.69	0.72
1:A:133:ALA:HB2	1:A:141:LYS:HE2	1.71	0.72
1:A:134:ASN:OD1	1:A:137:ASN:ND2	2.22	0.72
1:A:701:ILE:HD11	1:A:755:TYR:HB3	1.71	0.72
1:A:923:GLY:HA3	1:A:1154:PRO:HD3	1.73	0.69
1:A:1350:MET:HE2	6:A:1605:ERG:H193	1.73	0.69
1:A:1125:ALA:O	1:A:1126:ASN:ND2	2.26	0.68
1:A:1183:LEU:HB3	1:A:1276:VAL:HG21	1.75	0.68
1:A:883:VAL:HG12	1:A:1050:ALA:HB1	1.77	0.67
1:A:134:ASN:ND2	7:A:1701:HOH:O	2.27	0.66
1:A:620:ASN:HB3	1:A:623:VAL:HG22	1.80	0.63
1:A:1201:THR:HG22	1:A:1288:ALA:HB2	1.80	0.63
1:A:150:VAL:HG13	1:A:151:VAL:HG23	1.81	0.62
1:A:1073:GLN:HG2	1:A:1079:VAL:HG23	1.81	0.61
1:A:513:LEU:O	1:A:517:ILE:HG12	2.00	0.61
1:A:1154:PRO:O	1:A:1155:LYS:C	2.42	0.61
1:A:967:ILE:O	1:A:971:ASN:ND2	2.33	0.61
1:A:756:LEU:HD23	1:A:758:LYS:HZ3	1.66	0.60
1:A:1145:GLU:HG2	1:A:1149:MET:HE3	1.83	0.60
1:A:634:ALA:O	1:A:638:MET:HG3	2.01	0.60
1:A:801:ILE:O	1:A:805:MET:HG3	2.02	0.60
1:A:750:ARG:NH1	1:A:751:GLU:OE2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:851:SER:HB2	1:A:1049:GLN:HE21	1.67	0.60
1:A:549:MET:HE1	1:A:703:GLU:HB2	1.83	0.59
1:A:395:TYR:OH	1:A:430:PRO:O	2.18	0.59
1:A:645:VAL:HG13	1:A:658:PRO:HB2	1.83	0.59
1:A:809:ARG:HA	1:A:812:LYS:HG3	1.84	0.59
6:A:1606:ERG:H24	6:A:1608:ERG:H183	1.85	0.59
1:A:1314:LEU:HD21	1:A:1462:ARG:HB2	1.86	0.58
1:A:1156:LYS:O	1:A:1157:ASN:C	2.47	0.57
1:A:1282:ILE:HD11	6:A:1607:ERG:H6	1.86	0.57
1:A:523:ALA:HB2	1:A:607:PHE:CD2	2.39	0.57
1:A:684:LYS:O	1:A:687:TRP:HB3	2.04	0.57
1:A:899:LYS:NZ	3:A:1602:VO4:O3	2.36	0.57
1:A:1067:ASP:OD1	1:A:1067:ASP:N	2.36	0.57
1:A:669:TYR:OH	1:A:1211:THR:OG1	2.10	0.57
1:A:703:GLU:OE1	1:A:707:ARG:NH1	2.38	0.57
1:A:756:LEU:HD23	1:A:758:LYS:NZ	2.20	0.56
1:A:891:LEU:HD13	1:A:899:LYS:HB3	1.88	0.56
1:A:1426:VAL:HG12	1:A:1428:THR:HG22	1.87	0.56
1:A:1311:ARG:HH22	1:A:1394:ASN:HB2	1.70	0.56
1:A:299:SER:OG	1:A:302:GLU:HG3	2.05	0.56
1:A:618:ARG:HB3	1:A:623:VAL:HG21	1.88	0.56
1:A:687:TRP:CD1	1:A:687:TRP:C	2.83	0.56
1:A:123:THR:HG22	1:A:163:LYS:HG2	1.88	0.55
1:A:909:ARG:HG2	1:A:1260:PRO:HB3	1.87	0.55
1:A:1257:ARG:O	1:A:1261:SER:OG	2.21	0.55
1:A:1302:ALA:HB1	1:A:1308:LEU:HA	1.89	0.55
1:A:674:ILE:HD11	1:A:1212:PHE:CZ	2.42	0.55
1:A:325:THR:O	1:A:328:LEU:HG	2.08	0.54
1:A:218:ASN:O	1:A:222:LYS:HG2	2.09	0.53
1:A:1226:MET:HE3	1:A:1360:VAL:HG13	1.90	0.53
1:A:1171:GLY:O	1:A:1175:GLN:HG3	2.09	0.53
1:A:130:GLU:HB2	1:A:796:VAL:HG22	1.91	0.53
1:A:608:ASN:HD22	1:A:628:PHE:HD1	1.56	0.53
1:A:1200:LEU:HD22	1:A:1235:ILE:HD11	1.89	0.53
1:A:669:TYR:O	1:A:690:ASN:ND2	2.42	0.52
1:A:701:ILE:HG21	1:A:760:LYS:HB2	1.91	0.52
1:A:538:THR:HB	1:A:712:SER:HB3	1.90	0.52
1:A:565:PHE:HB3	1:A:1341:GLU:HG3	1.90	0.52
1:A:1109:PRO:O	1:A:1113:MET:HG3	2.10	0.52
1:A:657:VAL:HB	1:A:658:PRO:HD3	1.91	0.52
1:A:694:TYR:HB3	1:A:763:GLY:HA2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1204:ASN:HB2	1:A:1235:ILE:HD13	1.92	0.52
1:A:1414:THR:OG1	1:A:1434:PRO:O	2.27	0.52
1:A:856:ILE:HD13	1:A:1153:LEU:HD21	1.92	0.52
1:A:111:TYR:O	1:A:317:LYS:NZ	2.42	0.51
1:A:1486:LEU:HG	6:A:1606:ERG:H151	1.92	0.51
1:A:807:LYS:O	1:A:807:LYS:NZ	2.39	0.51
1:A:408:THR:O	1:A:411:THR:HG22	2.11	0.51
1:A:668:MET:SD	1:A:1211:THR:HG21	2.51	0.51
1:A:1153:LEU:O	1:A:1154:PRO:O	2.28	0.51
1:A:923:GLY:HA3	1:A:1154:PRO:HG3	1.93	0.51
1:A:924:LYS:NZ	1:A:1158:THR:HG21	2.26	0.50
1:A:1306:HIS:O	1:A:1307:GLN:NE2	2.44	0.50
1:A:233:GLU:HG3	1:A:323:ASN:HB3	1.92	0.50
1:A:611:TYR:O	1:A:615:VAL:HG22	2.11	0.50
1:A:857:PHE:HD1	1:A:921:VAL:HG22	1.77	0.50
1:A:194:SER:HA	1:A:199:THR:HG22	1.93	0.50
1:A:556:ASN:ND2	1:A:631:ASN:OD1	2.45	0.50
1:A:618:ARG:HD2	1:A:707:ARG:HD2	1.94	0.49
1:A:668:MET:HG3	1:A:1231:MET:HG3	1.94	0.49
1:A:856:ILE:HD13	1:A:1153:LEU:HD11	1.95	0.49
1:A:1114:LEU:HB3	1:A:1119:ALA:HB3	1.94	0.49
1:A:1313:ALA:O	1:A:1317:LEU:HG	2.13	0.49
1:A:892:MET:HG2	1:A:1055:ILE:HG23	1.94	0.49
1:A:899:LYS:HD2	1:A:1054:THR:HG23	1.95	0.49
1:A:1389:SER:OG	1:A:1459:TYR:HA	2.12	0.49
1:A:529:MET:HE2	1:A:1362:VAL:HB	1.94	0.48
1:A:1158:THR:OG1	1:A:1159:ASN:N	2.38	0.48
1:A:804:ARG:HG2	1:A:804:ARG:HH11	1.78	0.48
1:A:1209:GLY:HA2	1:A:1296:ILE:HB	1.94	0.48
1:A:1373:PHE:HZ	6:A:1605:ERG:H282	1.78	0.48
1:A:697:GLU:O	1:A:701:ILE:HG12	2.14	0.48
1:A:296:ARG:HB3	1:A:912:MET:HE1	1.95	0.48
1:A:1205:ASN:CG	1:A:1288:ALA:HB1	2.39	0.48
1:A:1154:PRO:HB2	1:A:1155:LYS:H	1.33	0.48
1:A:529:MET:HE3	1:A:1367:MET:HE2	1.95	0.48
1:A:679:ILE:HG22	1:A:684:LYS:HG2	1.96	0.48
1:A:1148:TRP:NE1	1:A:1152:GLU:HG3	2.29	0.47
1:A:668:MET:HE1	1:A:1207:PHE:HD2	1.78	0.47
1:A:923:GLY:HA3	1:A:1154:PRO:CD	2.42	0.47
1:A:236:ILE:HG21	1:A:572:PRO:HB2	1.97	0.47
1:A:876:LEU:HD11	1:A:902:LEU:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:VAL:O	1:A:609:ILE:HD12	2.15	0.47
1:A:618:ARG:NH1	1:A:705:HIS:O	2.48	0.47
6:A:1611:ERG:H193	6:A:1611:ERG:H111	1.80	0.47
1:A:927:ASP:OD2	1:A:927:ASP:N	2.42	0.46
1:A:317:LYS:HD3	1:A:317:LYS:HA	1.73	0.46
1:A:932:ARG:NE	1:A:1167:GLU:O	2.49	0.46
1:A:1112:TRP:O	1:A:1116:VAL:HG13	2.16	0.46
1:A:228:VAL:HG13	1:A:318:PHE:HD2	1.80	0.46
1:A:866:VAL:HG21	5:A:1604:ADP:C6	2.50	0.45
1:A:912:MET:SD	5:A:1604:ADP:N6	2.89	0.45
1:A:1148:TRP:CD1	1:A:1152:GLU:HG3	2.51	0.45
1:A:1402:TYR:CD2	1:A:1403:GLU:HG3	2.52	0.45
1:A:529:MET:HE1	1:A:1356:SER:O	2.16	0.45
1:A:660:SER:CB	1:A:1200:LEU:HD21	2.47	0.45
1:A:993:VAL:HG22	1:A:994:PRO:HD2	1.98	0.45
1:A:1259:ARG:HB3	1:A:1260:PRO:HD3	1.98	0.45
1:A:1363:THR:HG22	1:A:1365:ASN:H	1.82	0.45
1:A:922:ASP:HA	1:A:1153:LEU:HD13	1.97	0.45
1:A:1004:LYS:HD2	1:A:1025:PRO:HA	1.99	0.45
1:A:1464:ARG:O	1:A:1468:ILE:HG12	2.16	0.45
1:A:628:PHE:CZ	1:A:632:ILE:HD11	2.52	0.45
1:A:1353:LEU:HD23	1:A:1353:LEU:HA	1.75	0.45
1:A:522:MET:O	1:A:526:LEU:HG	2.16	0.45
1:A:1137:ASP:OD2	1:A:1141:LYS:NZ	2.50	0.44
1:A:169:GLU:HG2	1:A:450:ILE:HD11	1.99	0.44
1:A:1205:ASN:ND2	1:A:1288:ALA:HB1	2.32	0.44
1:A:1154:PRO:O	1:A:1155:LYS:O	2.35	0.44
1:A:270:ARG:O	1:A:274:GLU:HG2	2.17	0.44
1:A:884:LYS:HE2	1:A:1149:MET:HE2	1.99	0.44
1:A:280:PHE:HB3	1:A:305:ARG:HD2	2.00	0.44
1:A:662:LEU:O	1:A:666:LEU:HG	2.18	0.44
1:A:1294:TYR:HA	1:A:1299:TYR:HE2	1.83	0.44
1:A:1322:PHE:O	1:A:1326:ILE:HG13	2.18	0.44
6:A:1612:ERG:H183	6:A:1612:ERG:H20	1.89	0.44
1:A:676:ARG:O	1:A:676:ARG:NH1	2.51	0.43
1:A:542:PHE:O	1:A:543:TYR:HB3	2.17	0.43
1:A:680:LEU:O	1:A:683:SER:OG	2.35	0.43
1:A:452:GLU:O	1:A:456:LYS:HG2	2.18	0.43
1:A:1024:GLU:HB3	1:A:1027:SER:HB2	2.00	0.43
1:A:1379:PRO:HB2	1:A:1469:PHE:HE1	1.83	0.43
1:A:1037:ILE:HG22	1:A:1041:MET:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1152:GLU:O	1:A:1153:LEU:O	2.37	0.43
1:A:747:ASP:OD1	1:A:750:ARG:NH2	2.52	0.43
6:A:1609:ERG:H272	6:A:1609:ERG:H23	1.87	0.43
1:A:1194:LEU:HD23	1:A:1194:LEU:HA	1.93	0.43
1:A:166:LYS:HG3	1:A:376:TYR:CE1	2.53	0.43
1:A:304:LYS:HA	1:A:304:LYS:HD3	1.78	0.43
1:A:397:SER:HB2	1:A:406:PHE:CD1	2.54	0.43
1:A:848:ILE:HD13	1:A:980:ILE:HD12	1.99	0.43
1:A:1200:LEU:HD23	1:A:1200:LEU:HA	1.70	0.43
1:A:1298:PHE:HA	1:A:1301:ASN:HD22	1.84	0.43
1:A:65:ILE:O	1:A:100:ILE:HD11	2.19	0.42
1:A:321:TRP:HB3	1:A:324:ALA:HB2	2.00	0.42
1:A:846:ALA:HB1	1:A:1047:HIS:HE1	1.83	0.42
1:A:939:GLN:NE2	7:A:1702:HOH:O	2.51	0.42
1:A:408:THR:HG22	1:A:1032:GLN:HG2	2.00	0.42
1:A:492:MET:HE2	1:A:492:MET:HB3	1.90	0.42
1:A:1405:LEU:HD22	1:A:1405:LEU:H	1.84	0.42
1:A:518:GLY:HA2	6:A:1609:ERG:H211	2.02	0.42
1:A:160:LYS:HA	1:A:160:LYS:HD3	1.76	0.42
1:A:341:LYS:HE2	1:A:341:LYS:HB2	1.85	0.42
1:A:434:LYS:O	1:A:438:GLU:HG3	2.19	0.42
1:A:489:SER:O	1:A:493:GLN:HG3	2.20	0.42
1:A:445:ASP:OD2	1:A:445:ASP:N	2.52	0.42
1:A:661:MET:HA	1:A:1203:PHE:CE2	2.54	0.42
1:A:1404:LEU:O	1:A:1405:LEU:C	2.62	0.42
1:A:342:VAL:HG13	1:A:346:ILE:HD12	2.00	0.42
1:A:589:ALA:HB1	1:A:778:TYR:CE2	2.55	0.42
1:A:1071:PHE:CZ	1:A:1113:MET:HB3	2.54	0.42
1:A:1286:THR:HA	1:A:1316:TRP:HE1	1.85	0.42
1:A:958:TYR:OH	1:A:971:ASN:OD1	2.33	0.42
1:A:1148:TRP:C	1:A:1150:SER:H	2.28	0.42
1:A:1397:ILE:HB	1:A:1446:SER:C	2.45	0.42
1:A:681:GLY:O	1:A:684:LYS:HB2	2.20	0.42
1:A:1451:PHE:O	1:A:1455:VAL:HG22	2.20	0.42
1:A:942:LEU:HD13	1:A:1256:ALA:HB1	2.02	0.41
1:A:370:CYS:HB2	1:A:380:PHE:CD2	2.55	0.41
6:A:1605:ERG:H262	6:A:1609:ERG:H271	2.02	0.41
1:A:75:ASP:OD1	1:A:75:ASP:N	2.53	0.41
1:A:906:LEU:O	1:A:926:ARG:NH1	2.54	0.41
1:A:1226:MET:SD	1:A:1455:VAL:HG11	2.60	0.41
1:A:497:LEU:O	1:A:501:ASN:ND2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1226:MET:HE3	1:A:1226:MET:HB3	1.95	0.41
1:A:1282:ILE:HD11	6:A:1607:ERG:H41	2.03	0.41
1:A:1372:ILE:HD12	1:A:1372:ILE:HA	1.94	0.41
6:A:1606:ERG:H263	6:A:1606:ERG:H23	1.82	0.41
1:A:89:SER:OG	1:A:92:GLU:HG3	2.21	0.41
1:A:335:GLU:HG3	1:A:1120:ALA:HB1	2.02	0.41
1:A:1156:LYS:C	1:A:1158:THR:N	2.72	0.41
1:A:1346:MET:HE2	1:A:1350:MET:HE3	2.02	0.41
1:A:106:ASP:O	1:A:109:LYS:NZ	2.38	0.41
1:A:676:ARG:CZ	1:A:687:TRP:CZ3	3.03	0.41
1:A:701:ILE:CD1	1:A:755:TYR:HB3	2.48	0.41
1:A:892:MET:CG	1:A:1055:ILE:HG23	2.51	0.41
1:A:111:TYR:CD2	1:A:468:ILE:HG12	2.55	0.41
1:A:131:TYR:HA	1:A:797:PHE:O	2.21	0.41
1:A:274:GLU:OE1	1:A:286:ARG:NH2	2.48	0.41
1:A:632:ILE:O	1:A:635:VAL:HG12	2.21	0.41
6:A:1609:ERG:H193	6:A:1609:ERG:H111	1.81	0.41
1:A:437:TRP:O	1:A:441:ARG:HG3	2.20	0.41
1:A:670:SER:O	1:A:693:ALA:HA	2.21	0.41
1:A:701:ILE:N	1:A:701:ILE:HD13	2.36	0.41
1:A:469:LYS:HB3	1:A:469:LYS:HE3	1.87	0.40
1:A:551:PHE:HD2	1:A:1361:LEU:HD11	1.85	0.40
6:A:1610:ERG:H193	6:A:1610:ERG:H111	1.83	0.40
1:A:1212:PHE:CD2	1:A:1228:ALA:HB2	2.57	0.40
1:A:1248:VAL:HG21	1:A:1340:ALA:HB2	2.04	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	1378/1508 (91%)	1310 (95%)	64 (5%)	4 (0%)	36 65

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1155	LYS
1	A	1167	GLU
1	A	1154	PRO
1	A	1153	LEU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1197/1303 (92%)	1168 (98%)	29 (2%)	43 75

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	THR
1	A	125	GLU
1	A	134	ASN
1	A	159	ASP
1	A	194	SER
1	A	326	ARG
1	A	347	SER
1	A	355	ILE
1	A	416	ARG
1	A	507	GLN
1	A	512	THR
1	A	513	LEU
1	A	533	VAL
1	A	596	GLU
1	A	597	VAL
1	A	601	LEU
1	A	648	VAL
1	A	731	CYS
1	A	752	SER
1	A	916	THR
1	A	944	LEU

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Mol	Chain	Res	Type
1	A	1056	HIS
1	A	1097	SER
1	A	1126	ASN
1	A	1178	LEU
1	A	1239	LEU
1	A	1339	VAL
1	A	1363	THR
1	A	1392	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	A	203	ASN
1	A	556	ASN
1	A	847	ASN
1	A	939	GLN
1	A	1039	GLN
1	A	1049	GLN
1	A	1140	GLN
1	A	1157	ASN
1	A	1204	ASN
1	A	1205	ASN
1	A	1412	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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	$\#\|Z\| > 2$
6	ERG	A	1612	-	31,32,32	0.47	0	47,50,50	0.99	2 (4%)
6	ERG	A	1609	1	31,32,32	0.55	0	47,50,50	1.23	5 (10%)
5	ADP	A	1604	4	27,29,29	1.38	4 (14%)	42,45,45	1.81	8 (19%)
6	ERG	A	1605	-	31,32,32	0.51	0	47,50,50	0.89	2 (4%)
6	ERG	A	1610	-	31,32,32	0.49	0	47,50,50	0.90	1 (2%)
6	ERG	A	1611	-	31,32,32	0.49	0	47,50,50	0.79	0
6	ERG	A	1608	-	31,32,32	0.51	0	47,50,50	0.96	1 (2%)
6	ERG	A	1606	-	31,32,32	0.53	0	47,50,50	1.05	5 (10%)
2	ATP	A	1601	-	29,33,33	0.37	0	44,52,52	0.58	1 (2%)
3	VO4	A	1602	4	0,4,4	-	-	-		
6	ERG	A	1607	-	31,32,32	0.50	0	47,50,50	0.91	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ERG	A	1612	-	-	9/13/71/71	0/4/4/4
6	ERG	A	1609	1	-	5/13/71/71	0/4/4/4
5	ADP	A	1604	4	-	9/16/32/32	0/3/3/3
6	ERG	A	1605	-	-	2/13/71/71	0/4/4/4
6	ERG	A	1610	-	-	2/13/71/71	0/4/4/4
6	ERG	A	1611	-	-	8/13/71/71	0/4/4/4
6	ERG	A	1608	-	-	5/13/71/71	0/4/4/4
6	ERG	A	1606	-	-	7/13/71/71	0/4/4/4
2	ATP	A	1601	-	-	2/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ERG	A	1607	-	-	2/13/71/71	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1604	ADP	C5-C4	4.48	1.47	1.39
5	A	1604	ADP	C5-C6	2.46	1.47	1.41
5	A	1604	ADP	C5-N7	-2.37	1.34	1.39
5	A	1604	ADP	C8-N7	2.31	1.36	1.31

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1604	ADP	C5-C4-N3	-5.75	119.24	126.75
5	A	1604	ADP	N3-C4-N9	4.59	134.64	127.08
5	A	1604	ADP	C2-N3-C4	3.73	120.56	111.75
6	A	1609	ERG	C12-C11-C9	3.29	120.87	112.60
6	A	1606	ERG	C20-C22-C23	3.26	135.79	125.67
5	A	1604	ADP	N3-C2-N1	-3.22	123.56	128.60
5	A	1604	ADP	C4-C5-N7	-2.94	107.03	110.62
6	A	1605	ERG	C19-C10-C5	-2.78	103.85	108.34
6	A	1609	ERG	C20-C22-C23	2.68	134.00	125.67
5	A	1604	ADP	C4-N9-C8	2.57	108.51	105.73
6	A	1612	ERG	C13-C17-C20	-2.53	116.16	119.43
6	A	1609	ERG	C24-C23-C22	2.53	133.52	125.67
5	A	1604	ADP	C5-N7-C8	2.45	107.00	103.51
6	A	1609	ERG	C21-C20-C22	-2.44	104.10	109.99
6	A	1605	ERG	C10-C5-C6	-2.34	118.46	122.58
6	A	1612	ERG	C14-C8-C9	2.31	118.14	114.66
6	A	1608	ERG	C13-C17-C20	2.25	122.33	119.43
6	A	1607	ERG	C19-C10-C5	-2.23	104.73	108.34
6	A	1609	ERG	C16-C15-C14	-2.23	101.63	105.30
6	A	1606	ERG	C24-C23-C22	2.20	132.49	125.67
6	A	1606	ERG	C21-C20-C22	2.19	115.29	109.99
6	A	1606	ERG	C16-C15-C14	-2.14	101.78	105.30
6	A	1606	ERG	C4-C5-C10	2.11	119.23	116.42
5	A	1604	ADP	C6-C5-N7	2.10	135.94	132.02
2	A	1601	ATP	PB-O3B-PG	2.05	139.88	132.83
6	A	1610	ERG	C17-C20-C22	-2.03	106.41	110.27

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1601	ATP	PB-O3B-PG-O3G
5	A	1604	ADP	C5'-O5'-PA-O1A
6	A	1606	ERG	C13-C17-C20-C21
6	A	1606	ERG	C13-C17-C20-C22
6	A	1606	ERG	C16-C17-C20-C21
6	A	1606	ERG	C16-C17-C20-C22
6	A	1611	ERG	C16-C17-C20-C21
6	A	1612	ERG	C13-C17-C20-C21
6	A	1612	ERG	C16-C17-C20-C21
6	A	1612	ERG	C16-C17-C20-C22
6	A	1607	ERG	C22-C23-C24-C28
5	A	1604	ADP	O4'-C4'-C5'-O5'
6	A	1607	ERG	C22-C23-C24-C25
6	A	1609	ERG	C22-C23-C24-C25
6	A	1612	ERG	C17-C20-C22-C23
5	A	1604	ADP	C3'-C4'-C5'-O5'
6	A	1611	ERG	C13-C17-C20-C21
6	A	1611	ERG	C13-C17-C20-C22
6	A	1611	ERG	C16-C17-C20-C22
6	A	1612	ERG	C13-C17-C20-C22
6	A	1612	ERG	C21-C20-C22-C23
6	A	1609	ERG	C22-C23-C24-C28
6	A	1606	ERG	C22-C23-C24-C25
5	A	1604	ADP	O4'-C1'-N9-C4
5	A	1604	ADP	O4'-C1'-N9-C8
6	A	1612	ERG	C23-C24-C25-C27
6	A	1606	ERG	C21-C20-C22-C23
5	A	1604	ADP	C5'-O5'-PA-O3A
5	A	1604	ADP	C5'-O5'-PA-O2A
6	A	1608	ERG	C23-C24-C25-C26
6	A	1609	ERG	C21-C20-C22-C23
6	A	1606	ERG	C20-C22-C23-C24
6	A	1608	ERG	C20-C22-C23-C24
6	A	1609	ERG	C20-C22-C23-C24
6	A	1608	ERG	C28-C24-C25-C26
6	A	1608	ERG	C28-C24-C25-C27
6	A	1611	ERG	C28-C24-C25-C26
5	A	1604	ADP	PB-O3A-PA-O2A
6	A	1605	ERG	C21-C20-C22-C23
6	A	1611	ERG	C22-C23-C24-C28
6	A	1611	ERG	C23-C24-C25-C26
6	A	1612	ERG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
6	A	1610	ERG	C21-C20-C22-C23
6	A	1609	ERG	C17-C20-C22-C23
6	A	1608	ERG	C16-C17-C20-C22
2	A	1601	ATP	PB-O3B-PG-O1G
6	A	1610	ERG	C22-C23-C24-C28
5	A	1604	ADP	PB-O3A-PA-O1A
6	A	1611	ERG	C21-C20-C22-C23
6	A	1612	ERG	C22-C23-C24-C28
6	A	1605	ERG	C22-C23-C24-C28

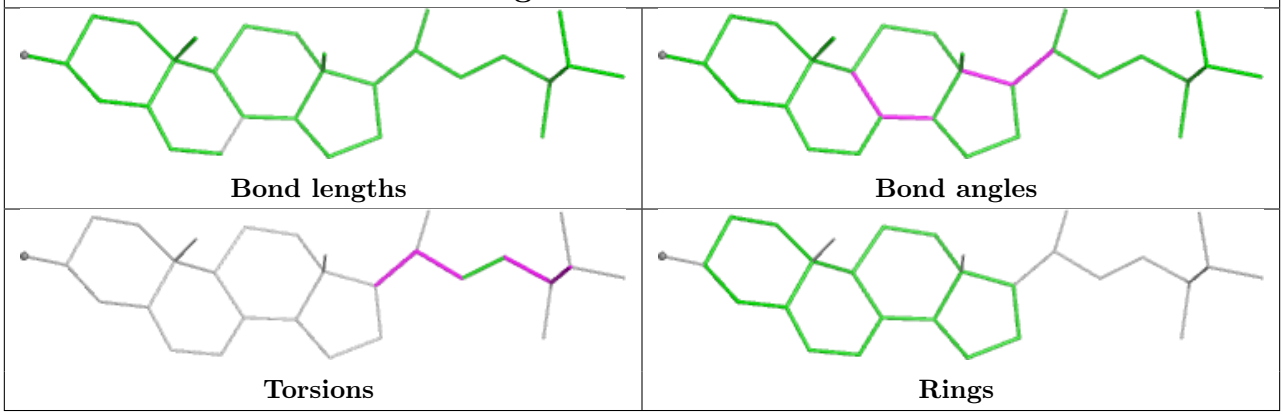
There are no ring outliers.

10 monomers are involved in 17 short contacts:

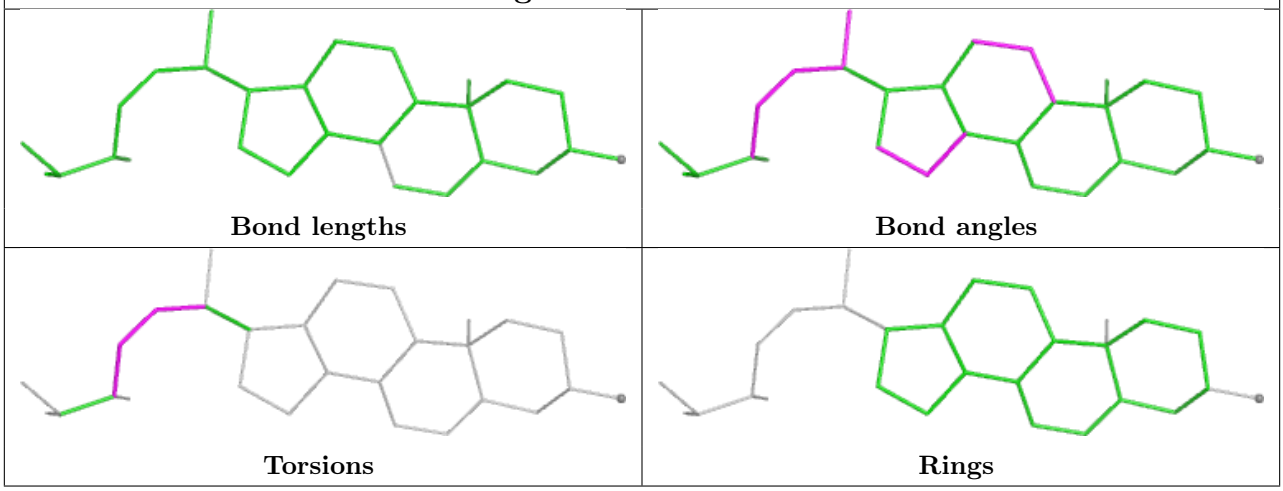
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1612	ERG	1	0
6	A	1609	ERG	4	0
5	A	1604	ADP	2	0
6	A	1605	ERG	3	0
6	A	1610	ERG	1	0
6	A	1611	ERG	1	0
6	A	1608	ERG	1	0
6	A	1606	ERG	3	0
3	A	1602	VO4	1	0
6	A	1607	ERG	2	0

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 then 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.

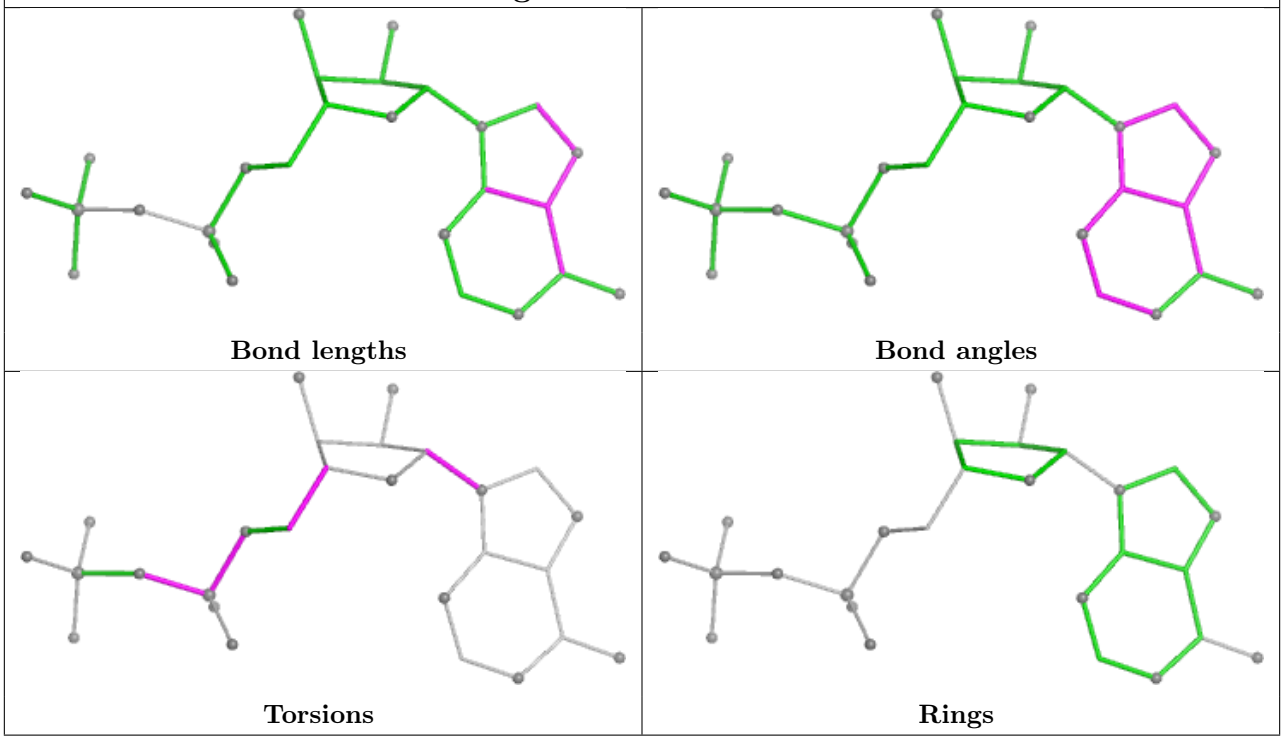
Ligand ERG A 1612



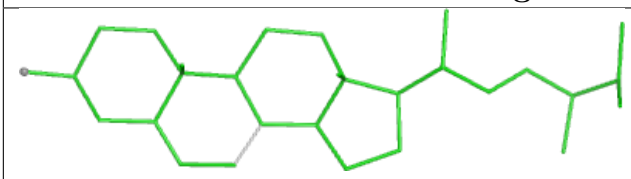
Ligand ERG A 1609



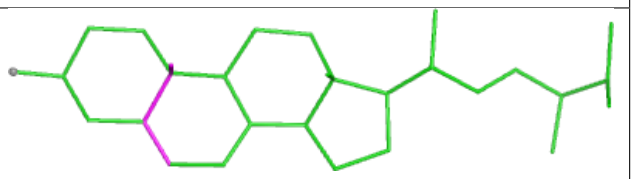
Ligand ADP A 1604



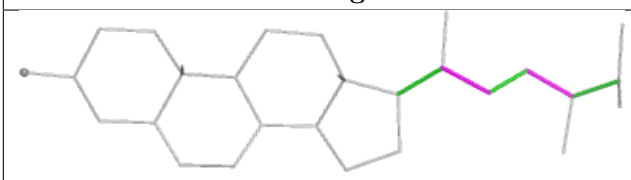
Ligand ERG A 1605



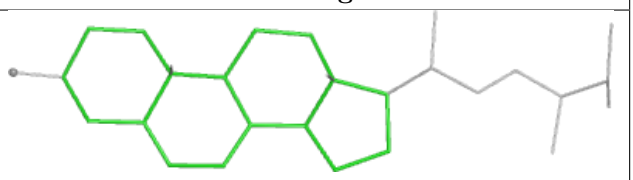
Bond lengths



Bond angles

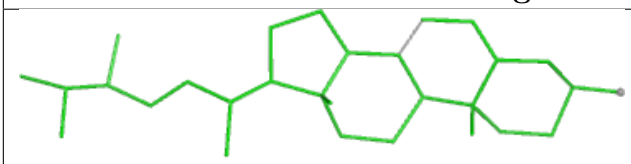


Torsions

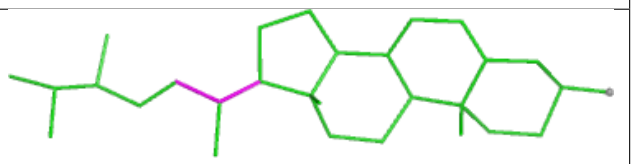


Rings

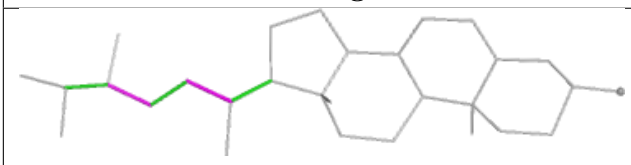
Ligand ERG A 1610



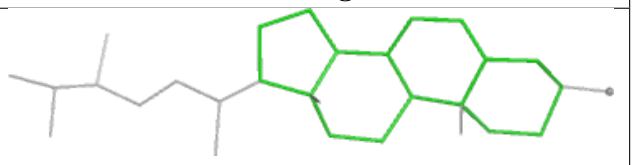
Bond lengths



Bond angles

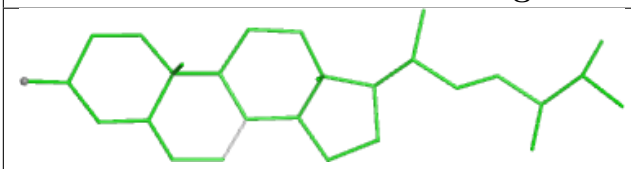


Torsions

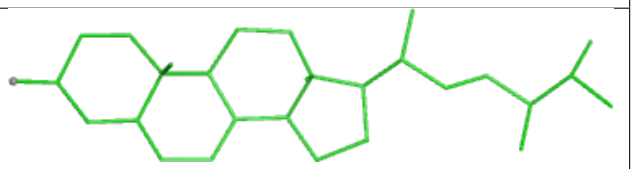


Rings

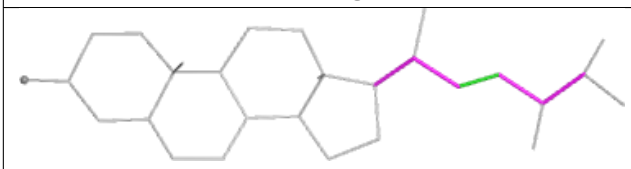
Ligand ERG A 1611



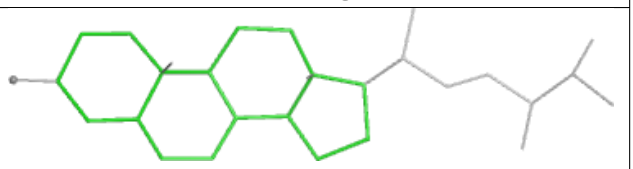
Bond lengths



Bond angles

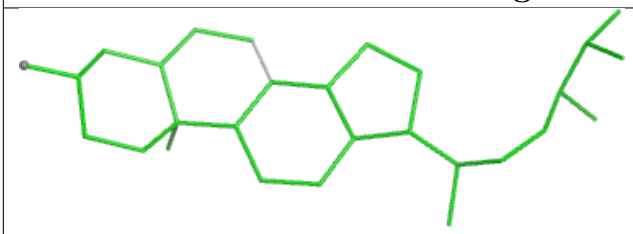


Torsions

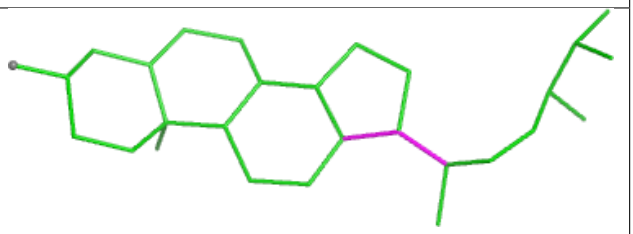


Rings

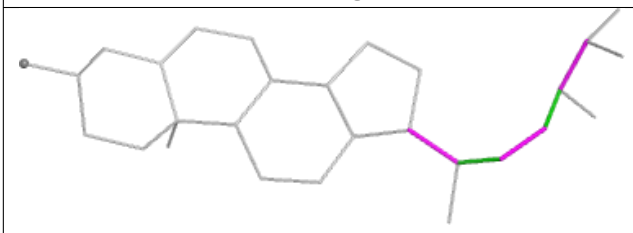
Ligand ERG A 1608



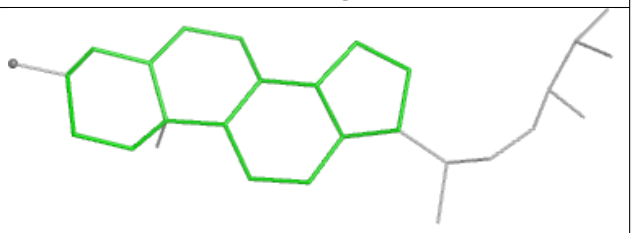
Bond lengths



Bond angles

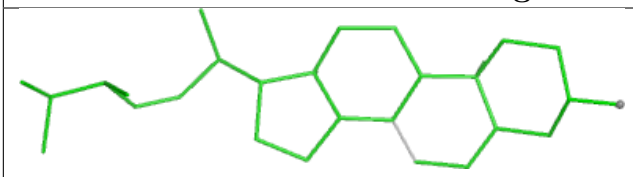


Torsions

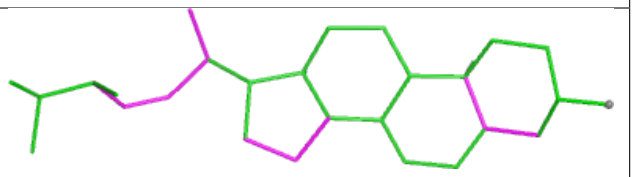


Rings

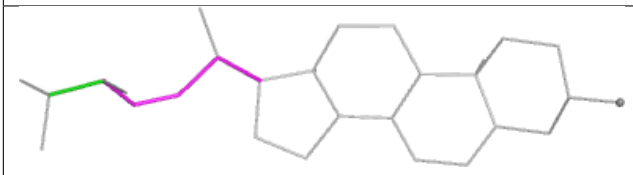
Ligand ERG A 1606



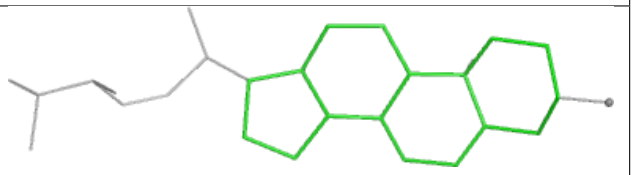
Bond lengths



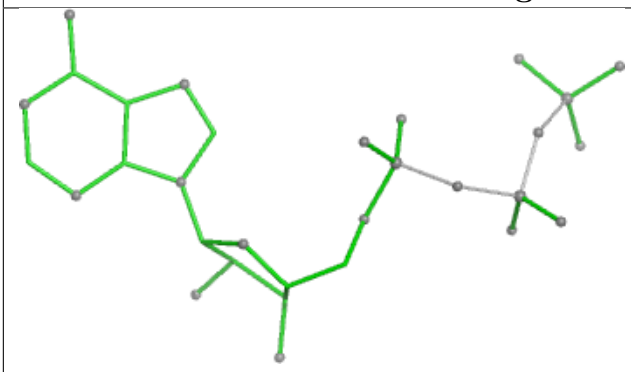
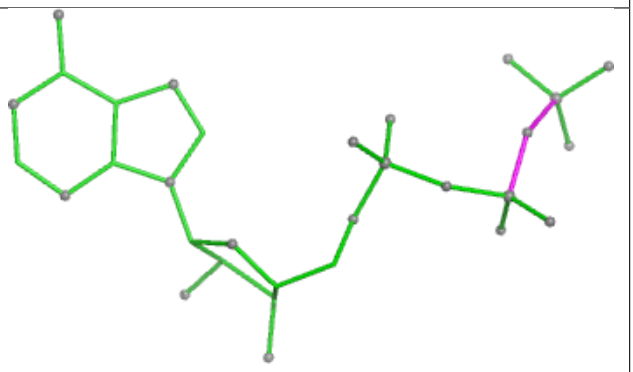
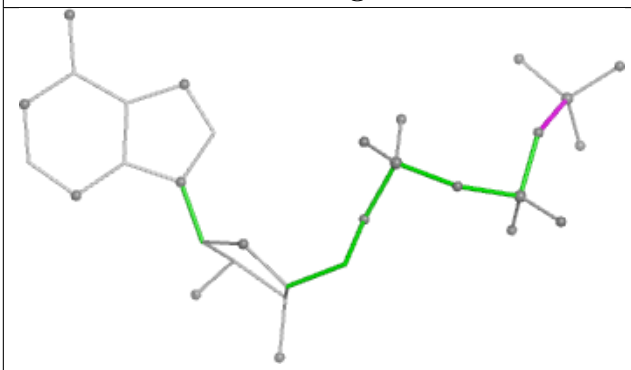
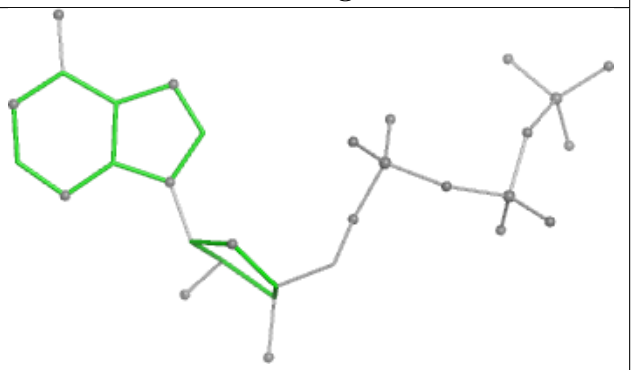
Bond angles



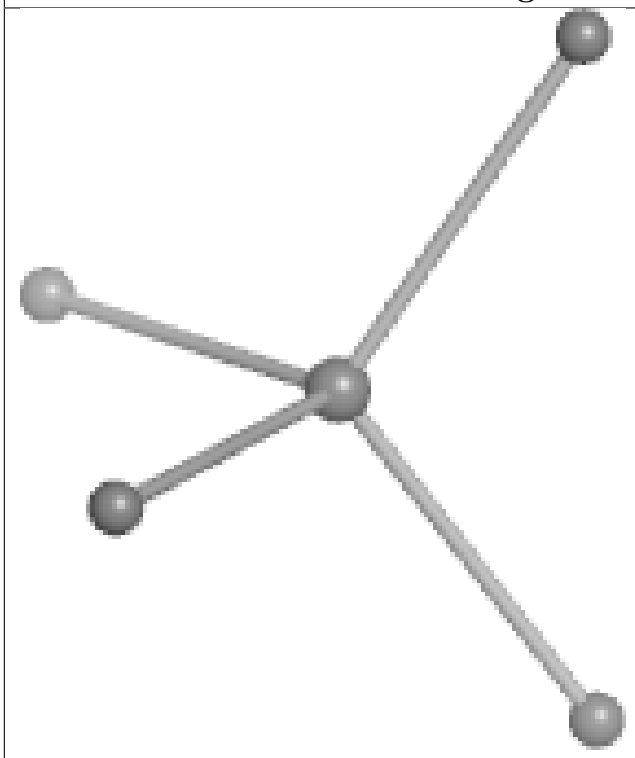
Torsions



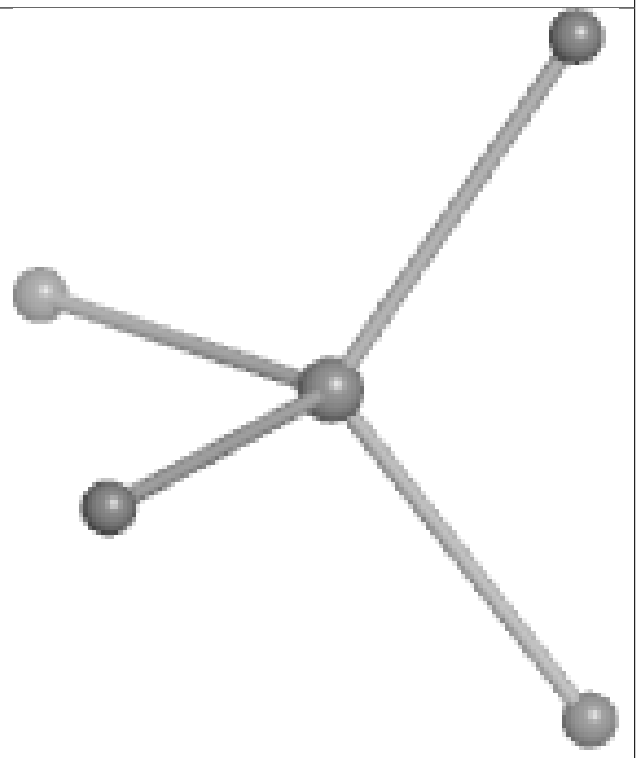
Rings

Ligand ATP A 1601	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

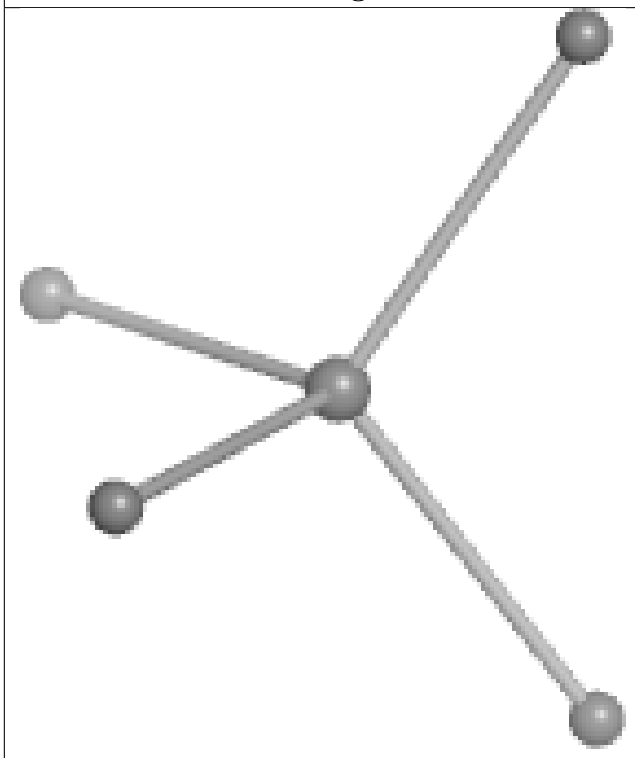
Ligand VO4 A 1602



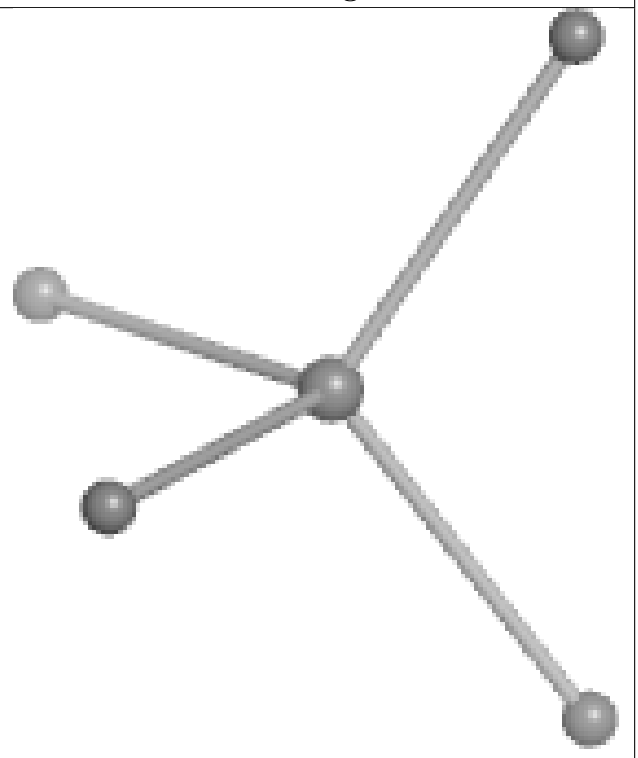
Bond lengths



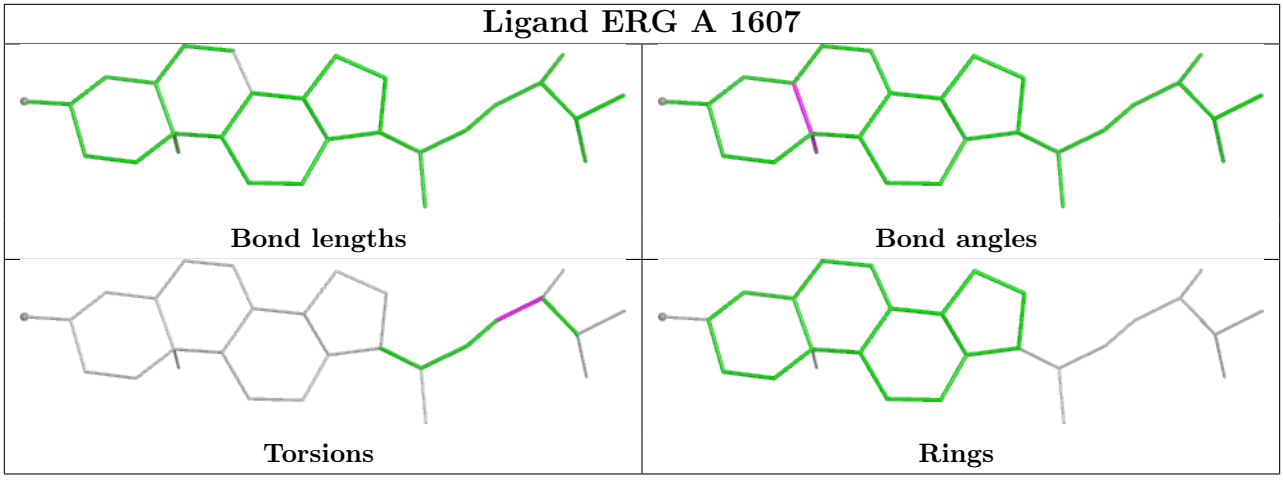
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

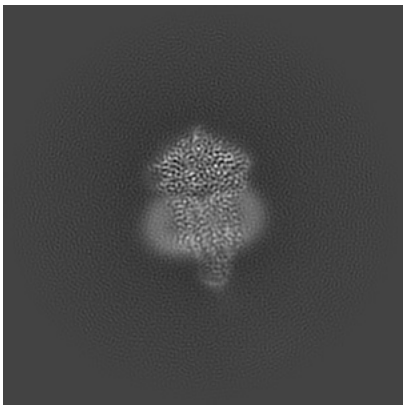
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-54488. These allow visual inspection of the internal detail of the map and identification of artifacts.

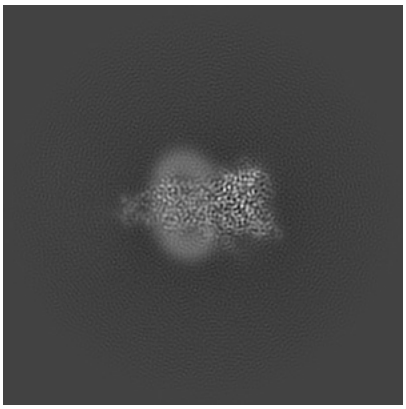
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

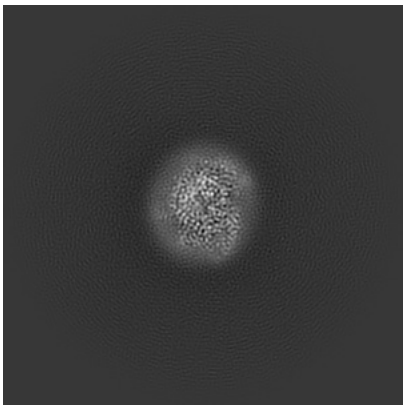
6.1.1 Primary map



X

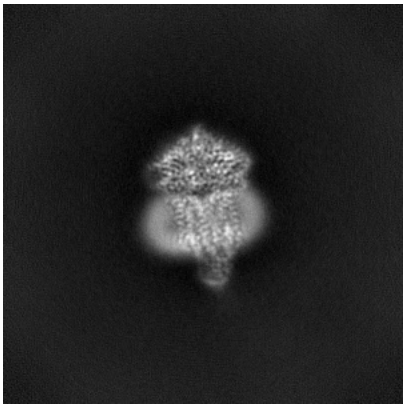


Y

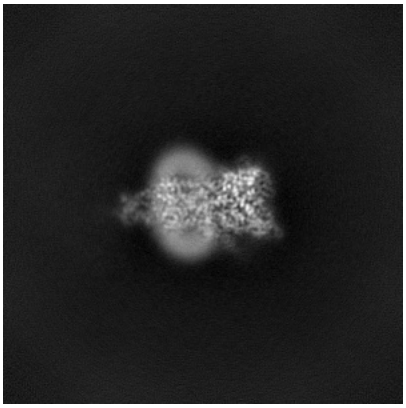


Z

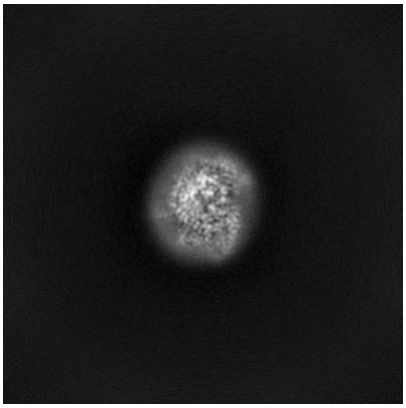
6.1.2 Raw map



X



Y

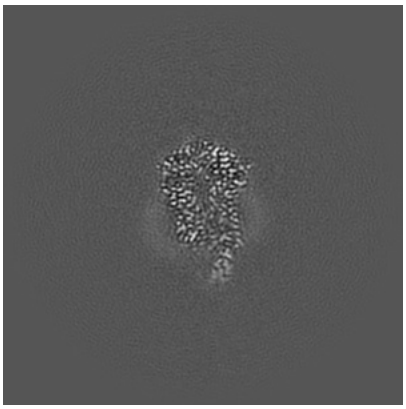


Z

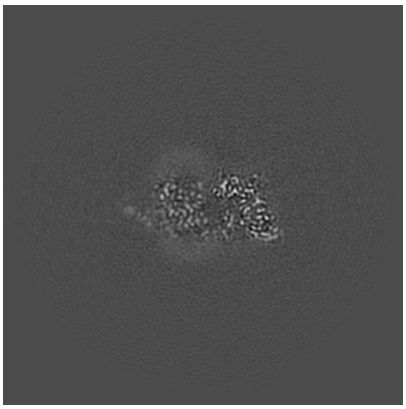
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

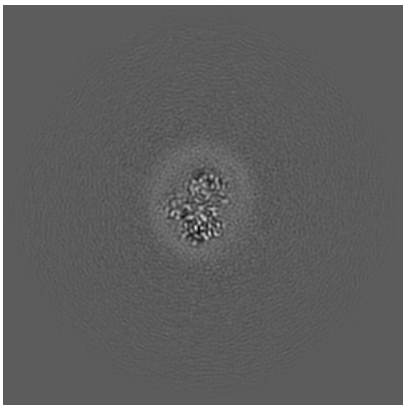
6.2.1 Primary map



X Index: 192

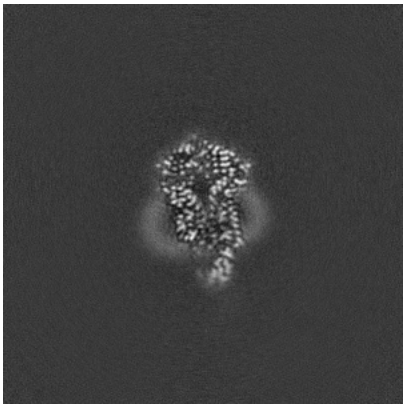


Y Index: 192

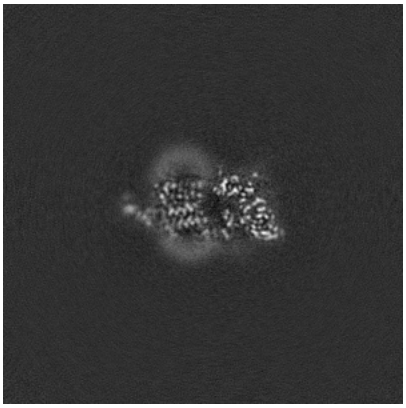


Z Index: 192

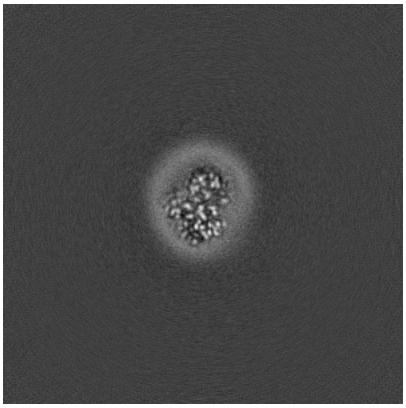
6.2.2 Raw map



X Index: 192



Y Index: 192

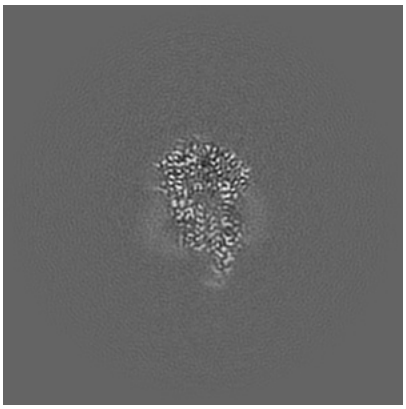


Z Index: 192

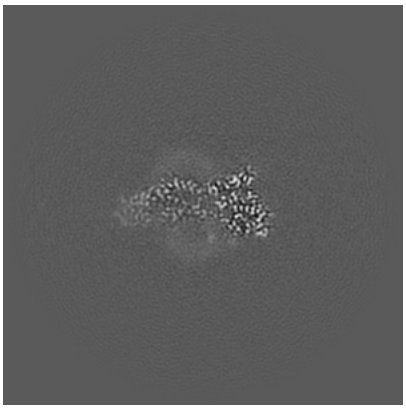
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

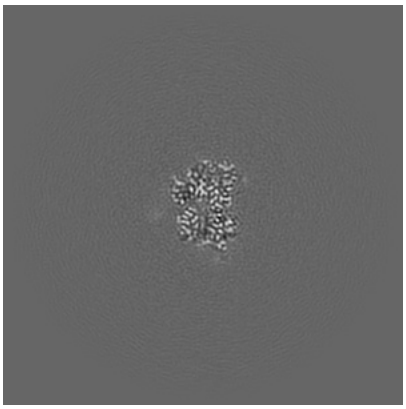
6.3.1 Primary map



X Index: 198

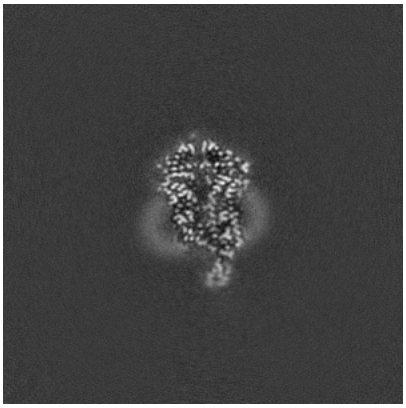


Y Index: 207

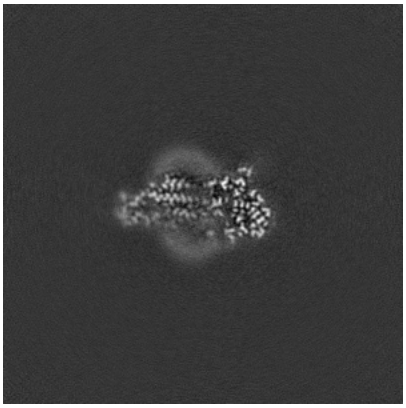


Z Index: 223

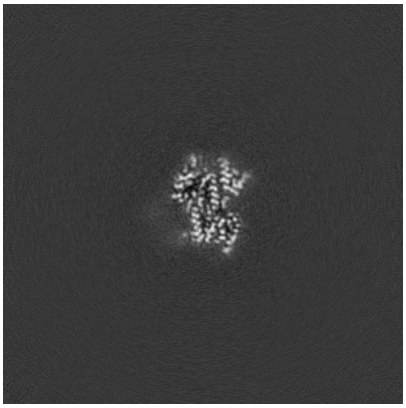
6.3.2 Raw map



X Index: 194



Y Index: 203

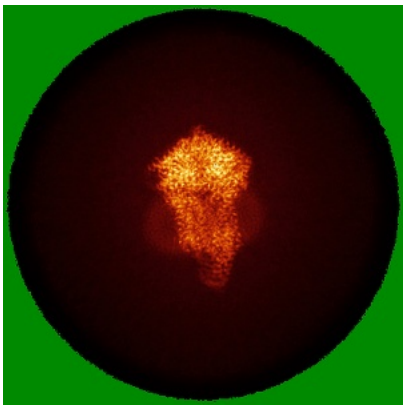


Z Index: 236

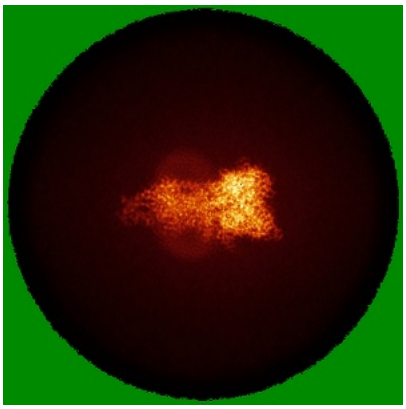
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

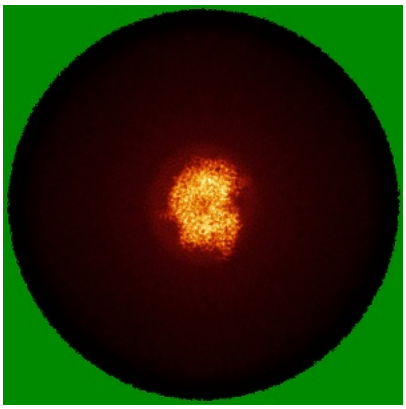
6.4.1 Primary map



X

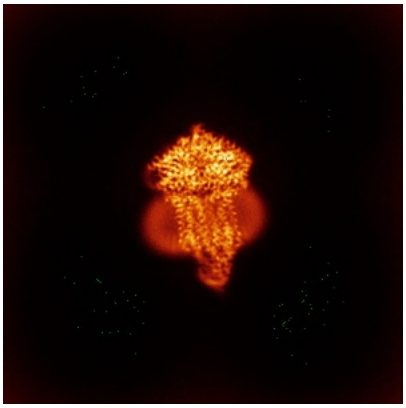


Y

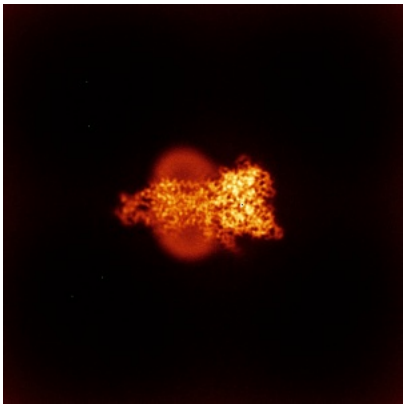


Z

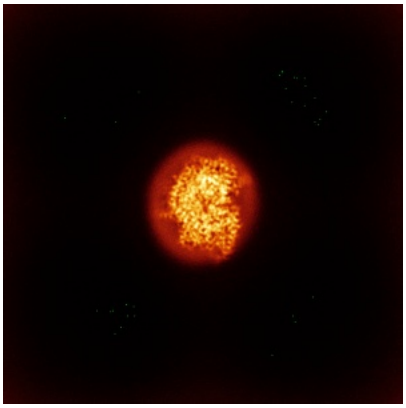
6.4.2 Raw map



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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. 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



X Y Z

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.

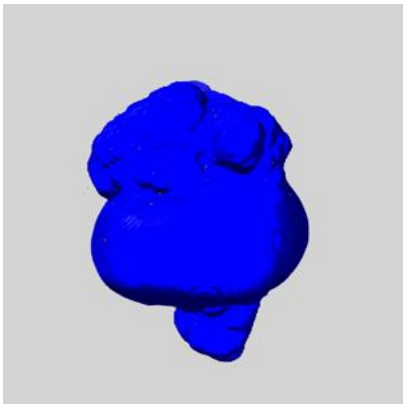
6.6 Mask visualisation

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

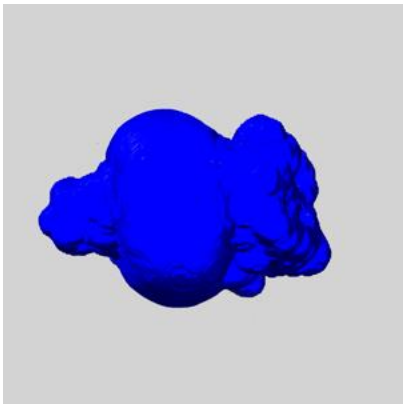
A mask typically either:

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

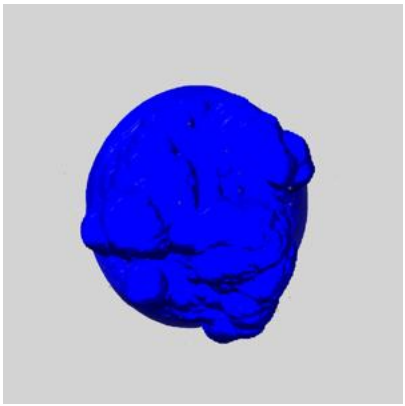
6.6.1 emd_54488_msk_1.map



X



Y

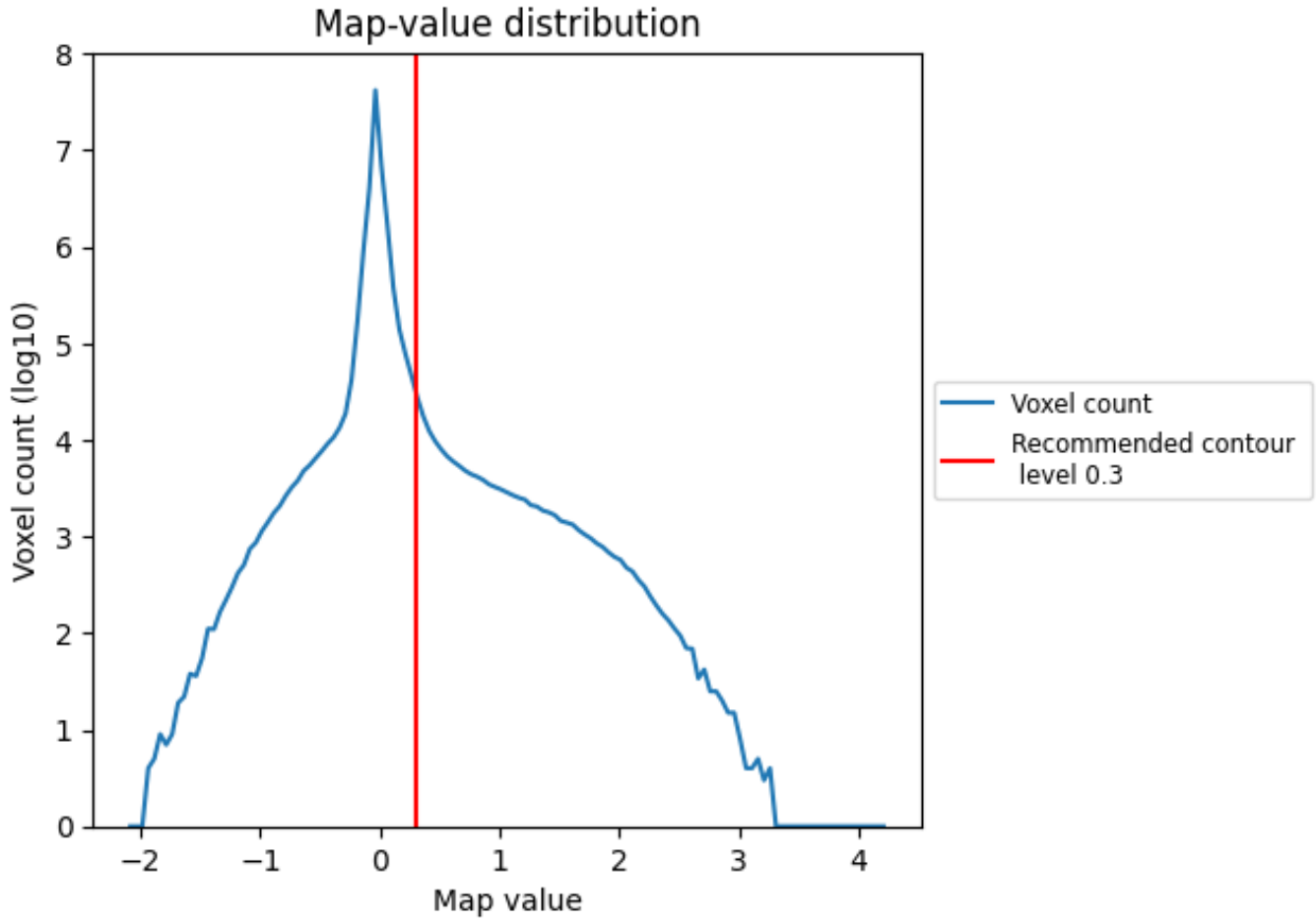


Z

7 Map analysis

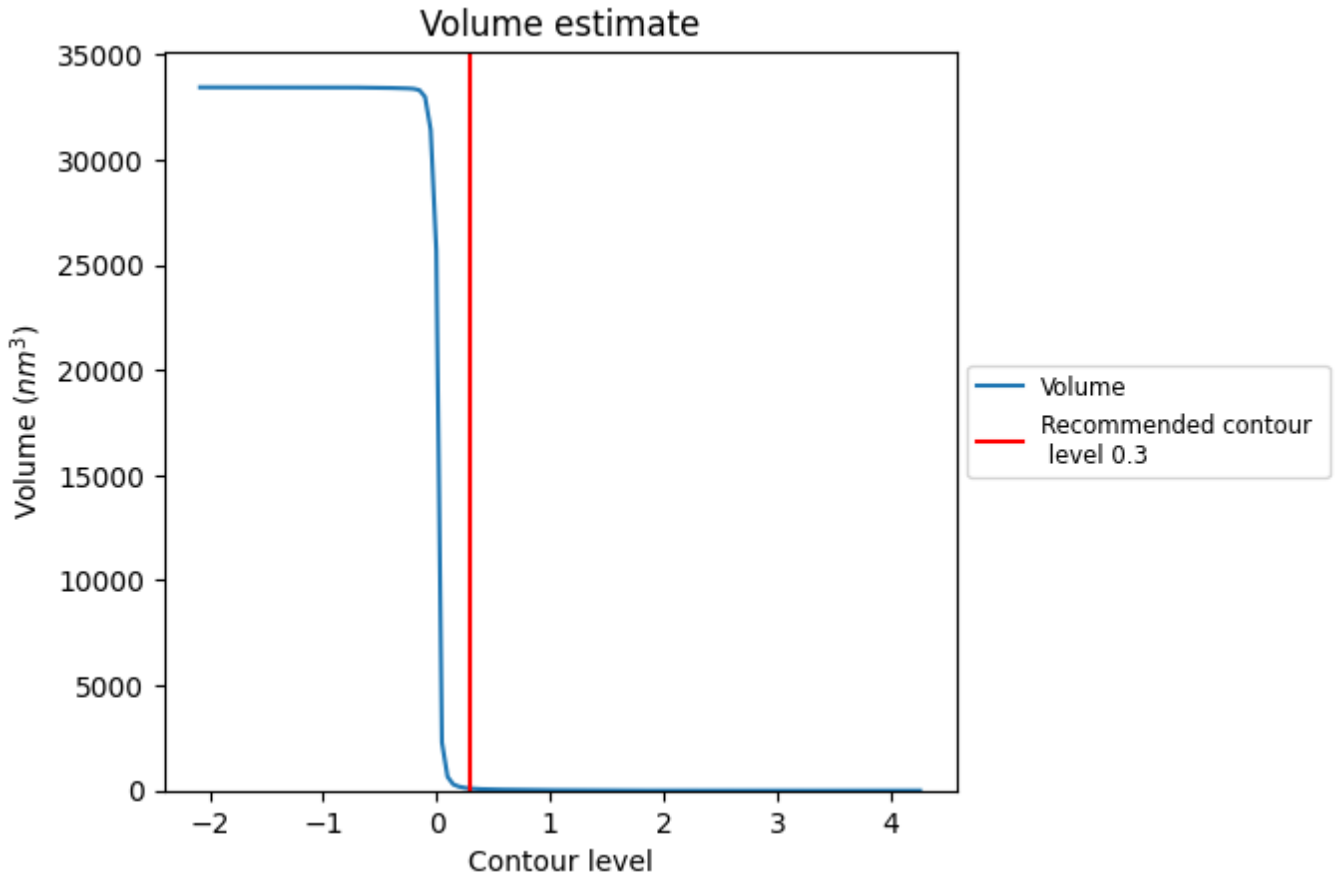
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

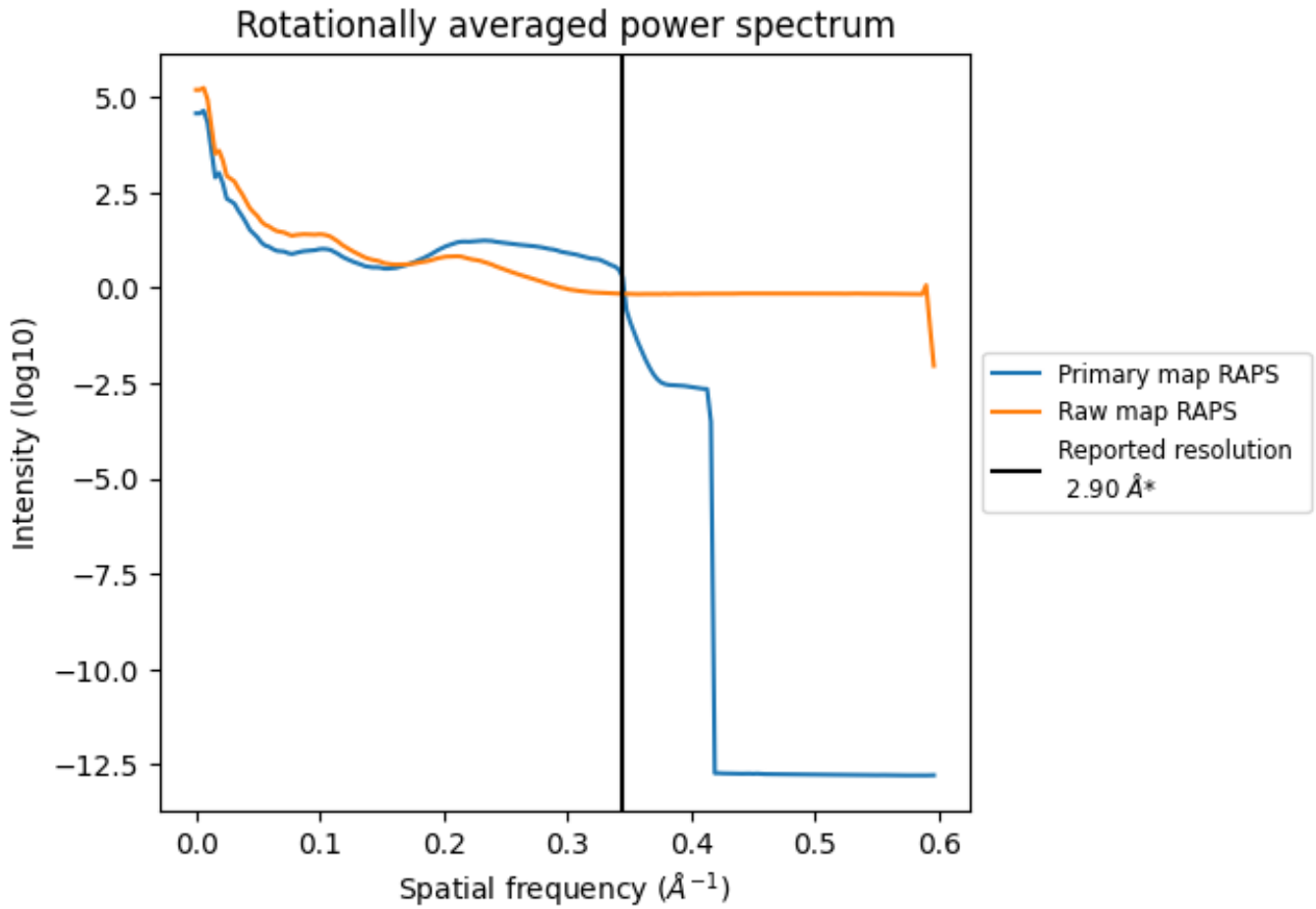
7.2 Volume estimate



The volume at the recommended contour level is 98 nm^3; this corresponds to an approximate mass of 88 kDa.

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

7.3 Rotationally averaged power spectrum (i)

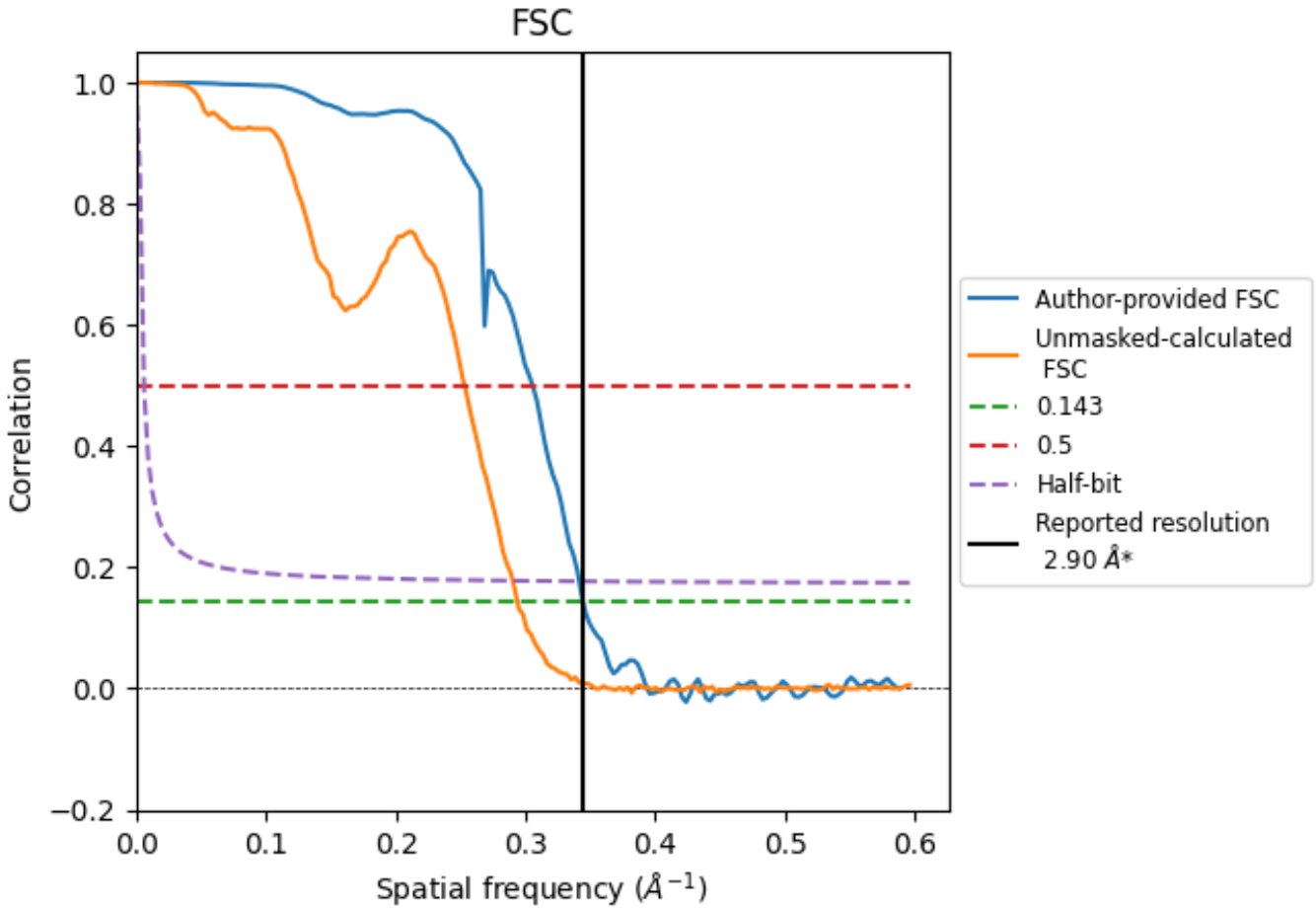


*Reported resolution corresponds to spatial frequency of 0.345 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8.2 Resolution estimates (i)

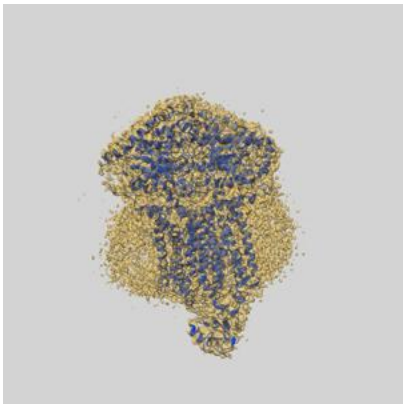
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.27	2.93
Unmasked-calculated*	3.40	3.95	3.45

*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 3.40 differs from the reported value 2.9 by more than 10 %

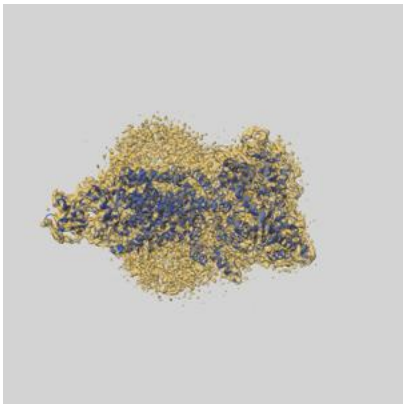
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-54488 and PDB model 9S2C. Per-residue inclusion information can be found in section 3 on page 7.

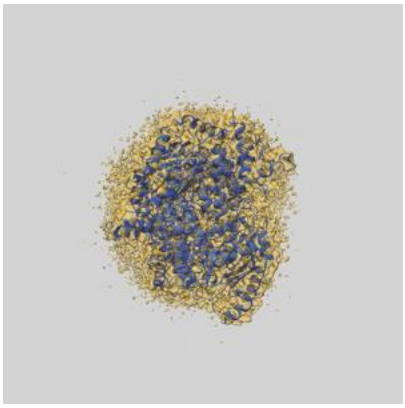
9.1 Map-model overlay



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 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.

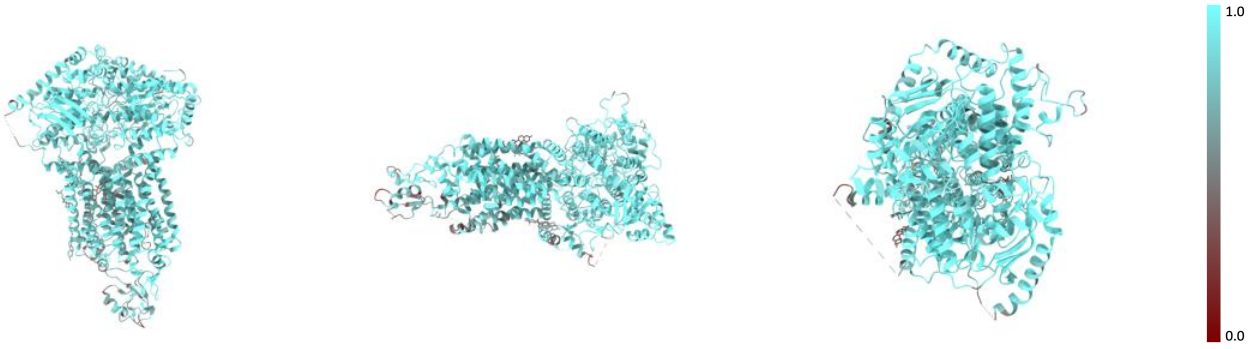
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

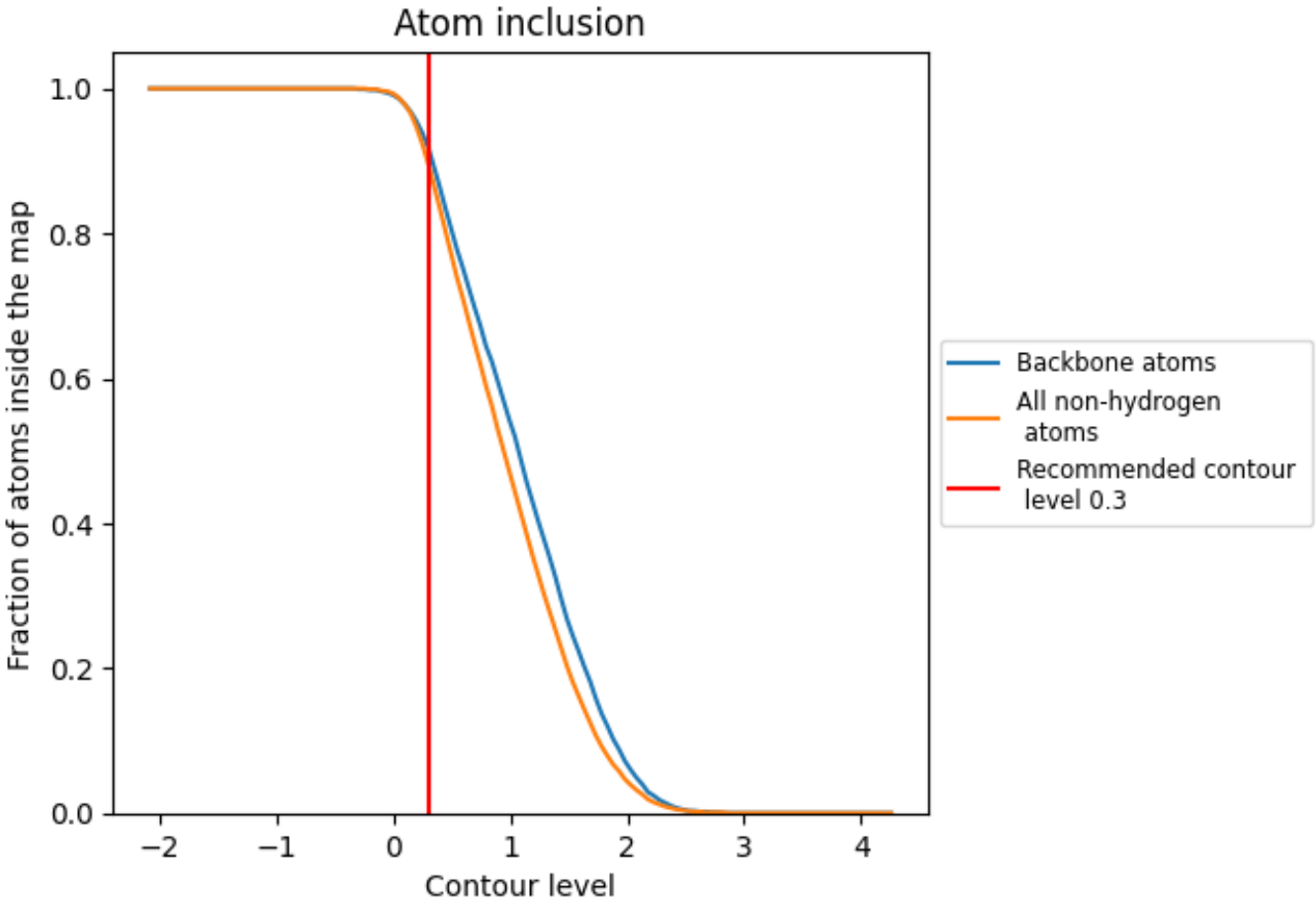
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.3).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.8940	0.5650
A	0.8940	0.5650