



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 01:56 PM UTC

PDB ID : 8V7Z / pdb_00008v7z
EMDB ID : EMD-43011
Title : Phosphorylated, ATP-bound, E1371Q human cystic fibrosis transmembrane conductance regulator (E1371Q-CFTR)
Authors : Gao, X.; Hwang, T.
Deposited on : 2023-12-04
Resolution : 3.40 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

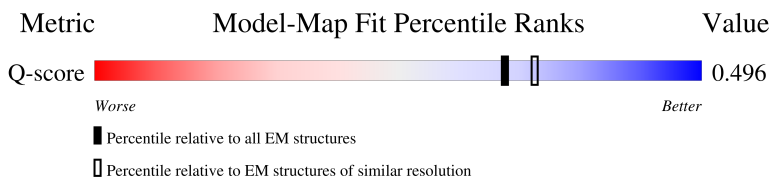
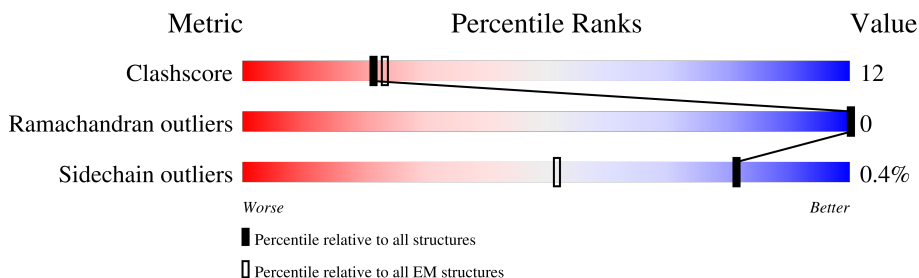
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	1421	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8977 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 Cystic fibrosis transmembrane conductance regulator.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1104	Total	C	N	O	S	0	0
			8846	5794	1462	1544	46		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	492	PRO	SER	conflict	UNP P13569
A	495	PRO	SER	conflict	UNP P13569
A	534	PRO	ALA	conflict	UNP P13569
A	539	THR	ILE	conflict	UNP P13569
A	555	LYS	ARG	conflict	UNP P13569
A	1371	GLN	GLU	engineered mutation	UNP P13569

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

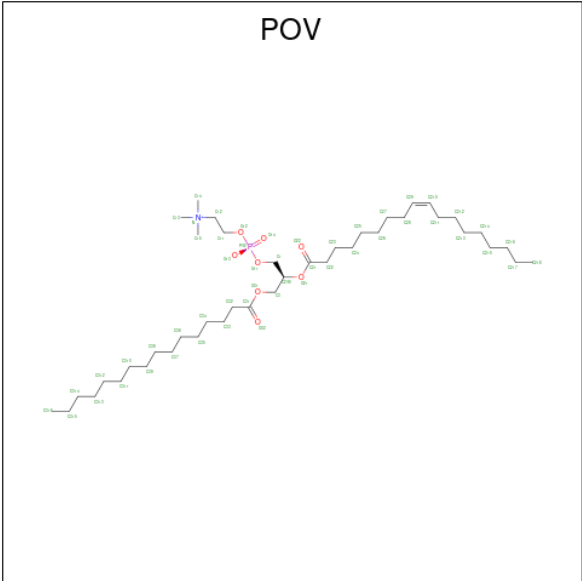
Mol	Chain	Residues	Atoms		AltConf
2	A	2	Total	Mg	0
			2	2	

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 4 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P).



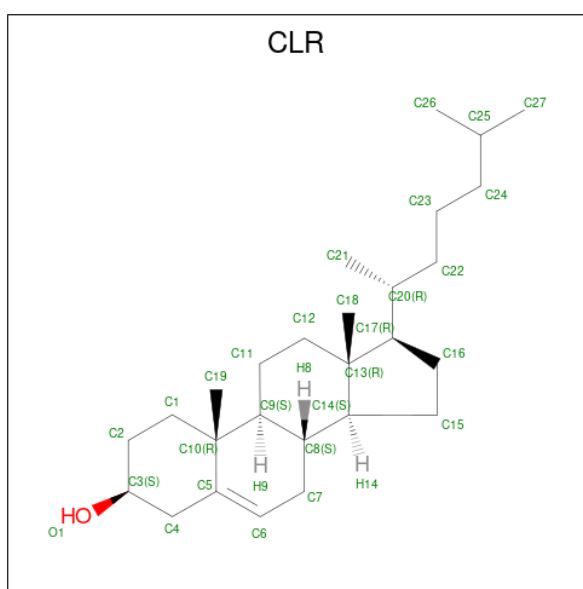
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	C	0
			9	9	

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Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	C	0
			9	9	
4	A	1	Total	C	0
			7	7	
4	A	1	Total	C	0
			9	9	
4	A	1	Total	C	0
			5	5	

- Molecule 5 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



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

R1245	R1368	T943	F1074	F166	R1245	R1368	T943
K1250	L1361	V944	E1075	M169	K1250	L1361	V944
T1252	S1251	S945	T1086	F1170	T1252	S1251	S945
L1253	K1365	K946	L1253	T1171	L1253	K1365	K946
L1254	L1366	M952	L1254	GLU	L1254	L1366	M952
F1257	L1367	L957	GLY	GLY	F1257	L1367	L957
L1258	L1368	Q958	LYS	LYS	L1258	L1368	Q958
R1259	L1369	A959	PRO	PRO	R1259	L1369	A959
L1260	D1370	P960	THR	THR	L1260	D1370	P960
L1261	Q1371	T963	LYS	LYS	L1261	Q1371	T963
M1262	P1372	L967	SER	SER	M1262	P1372	L967
T1263	D1377	K968	THR	THR	T1263	D1377	K968
I1267	P1378	A969	LYS	LYS	I1267	P1378	A969
G1287	Q1381	I972	ASN	ASN	G1287	Q1381	I972
I1295	I1382	S977	GLY	GLY	I1295	I1382	S977
F1300	I1383	L983	LEU	LEU	F1300	I1383	L983
K1301	R1384	P984	SER	SER	K1301	R1384	P984
K1302	T1386	D985	LYS	LYS	K1302	T1386	D985
P1306	L1387	P988	VAL	VAL	P1306	L1387	P988
E1308	L1388	Q996	MET	MET	E1308	L1388	Q996
S1311	Q1390	A1004	ILE	ILE	S1311	Q1390	A1004
D1312	A1391	I1005	ILE	ILE	D1312	A1391	I1005
I1315	F1392	I1015	GLU	GLU	I1315	F1392	I1015
V1318	C1395	F1016	ASN	ASN	V1318	C1395	F1016
A1319	E1401	T1019	SER	SER	A1319	E1401	T1019
D1320	H1402	V1022	HIS	HIS	D1320	H1402	V1022
E1321	R1403	A1025	VAL	VAL	E1321	R1403	A1025
V1322	M1407	F1026	LYS	LYS	V1322	M1407	F1026
R1325	V1415	L1029	ASP	ASP	R1325	V1415	L1029
L1335	L1430	F1033	THR	THR	L1335	L1430	F1033
D1336	L1431	L1034	GLY	GLY	D1336	L1431	L1034
F1337		Q1035	GLY	GLY	F1337		Q1035
V1345		L1040	GLY	GLY	V1345		L1040
L1346		L1043	ARG	ARG	L1346		L1043
S1347		P1050	V1129	V1129	S1347		P1050
H1348		T1053	G1130	G1130	H1348		T1053
G1349		R1066	I1131	I1131	G1349		R1066
H1350		R1070	M1137	M1137	H1350		R1070
K1351			N1138	N1138	K1351		
Q1352			I1139	I1139	Q1352		
L1353			M1140	M1140	L1353		
M1354			L1143	L1143	M1354		
C1355			V1147	V1147	C1355		
A1357			T1151	T1151	A1357		
			D1152	D1152			
			V1160	V1160			
			V1163	V1163			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	261806	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.33375	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.146	Depositor
Minimum map value	-0.106	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0103	Depositor
Map size ($\text{\AA}$)	275.08, 275.08, 275.08	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.058, 1.058, 1.058	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: CLR, POV, ATP, 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	0.12	0/9031	0.31	0/12208

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8846	0	9160	213	0
2	A	2	0	0	0	0
3	A	62	0	24	0	0
4	A	39	0	58	0	0
5	A	28	0	46	1	0
All	All	8977	0	9288	213	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 12.

All (213) 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:1241:GLY:HA3	1:A:1407:MET:HE1	1.65	0.76
1:A:1320:ASP:OD2	1:A:1325:ARG:NH1	2.21	0.72
1:A:1043:LEU:HB3	1:A:1088:ASN:HD21	1.53	0.71
1:A:307:SER:O	1:A:352:ARG:NH2	2.24	0.70
1:A:967:LEU:HD11	1:A:1169:MET:HE1	1.75	0.68
1:A:502:ILE:HG12	1:A:541:LEU:HD11	1.77	0.67
1:A:113:ASN:HD21	1:A:117:ARG:HB2	1.60	0.67
1:A:1300:PHE:HB2	1:A:1335:LEU:HA	1.78	0.66
1:A:1401:GLU:HG3	1:A:1403:ARG:H	1.59	0.66
1:A:113:ASN:O	1:A:113:ASN:ND2	2.30	0.65
1:A:198:ALA:O	1:A:361:TRP:NE1	2.29	0.65
1:A:153:ARG:HD2	1:A:188:LEU:HA	1.79	0.64
1:A:1356:LEU:HD11	1:A:1387:THR:HG21	1.79	0.64
1:A:180:LEU:O	1:A:184:LEU:HD12	1.98	0.63
1:A:1318:VAL:HG11	1:A:1361:LEU:HG	1.82	0.61
1:A:278:GLU:HG2	1:A:957:LEU:HB3	1.81	0.61
1:A:131:PHE:HB3	1:A:1109:ILE:HG23	1.82	0.61
1:A:333:LEU:HA	1:A:336:ILE:HG22	1.82	0.60
1:A:503:LYS:HE3	1:A:537:ASP:HB3	1.84	0.60
1:A:1217:ALA:HB1	1:A:1261:LEU:HD11	1.83	0.60
1:A:251:ARG:NH1	1:A:985:ASP:OD1	2.35	0.60
1:A:259:LEU:HD21	1:A:977:SER:HB2	1.84	0.60
1:A:28:TYR:O	1:A:1035:GLN:NE2	2.35	0.59
1:A:869:ILE:HG22	1:A:933:ARG:HH11	1.67	0.59
1:A:170:ARG:HH12	1:A:476:GLU:HB2	1.69	0.58
1:A:163:LYS:HG2	1:A:375:LEU:HA	1.84	0.58
1:A:20:THR:HG22	1:A:24:LEU:HD12	1.86	0.58
1:A:237:GLN:NE2	1:A:351:THR:O	2.37	0.57
1:A:575:PHE:HA	1:A:578:LEU:HD12	1.86	0.57
1:A:450:ARG:NH2	1:A:567:ASP:OD2	2.38	0.57
1:A:465:THR:O	1:A:469:MET:HG2	2.05	0.57
1:A:1022:VAL:HG11	1:A:1140:MET:HG3	1.85	0.57
1:A:1033:PHE:HE1	1:A:1095:THR:HG22	1.69	0.57
1:A:507:ILE:HG23	1:A:510:VAL:HG22	1.86	0.57
1:A:1337:PHE:HE2	1:A:1345:VAL:HG21	1.69	0.56
1:A:555:LYS:HG3	1:A:578:LEU:HD21	1.88	0.56
1:A:1242:LEU:HD22	1:A:1250:LYS:HB3	1.87	0.56
1:A:333:LEU:HD12	1:A:911:SER:HA	1.88	0.56
1:A:549:SER:OG	1:A:552:GLN:OE1	2.23	0.55
1:A:1377:ASP:OD1	1:A:1377:ASP:N	2.40	0.55
1:A:394:MET:HE2	1:A:397:VAL:HG11	1.89	0.55
1:A:1208:GLY:HA2	1:A:1366:ILE:HD11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:914:TYR:O	1:A:918:ILE:HG12	2.06	0.55
1:A:1232:PHE:HZ	1:A:1257:PHE:HZ	1.55	0.55
1:A:1267:ILE:O	1:A:1267:ILE:HG22	2.06	0.55
1:A:1102:ARG:HD3	1:A:1106:ILE:HG21	1.89	0.55
1:A:23:ILE:HD11	1:A:32:LEU:HD13	1.89	0.55
1:A:222:SER:HB3	1:A:324:PRO:HG2	1.90	0.54
1:A:1383:ILE:HG12	1:A:1386:ARG:NH2	2.22	0.54
1:A:1005:ILE:HD13	1:A:1139:ILE:HD13	1.89	0.54
1:A:245:MET:HG3	1:A:359:GLN:HE22	1.72	0.54
1:A:1312:ASP:HA	1:A:1315:ILE:HG12	1.90	0.54
1:A:920:VAL:HG23	1:A:1004:ALA:HB1	1.90	0.53
1:A:573:SER:O	1:A:573:SER:OG	2.25	0.53
1:A:1383:ILE:HG12	1:A:1386:ARG:HH22	1.74	0.53
1:A:116:GLU:HG3	1:A:116:GLU:O	2.09	0.53
1:A:100:LEU:HG	1:A:342:PHE:HZ	1.75	0.52
1:A:40:ILE:HD13	1:A:1087:ALA:HA	1.90	0.52
1:A:154:ILE:HD11	1:A:1086:THR:OG1	2.09	0.52
1:A:503:LYS:O	1:A:507:ILE:HD12	2.10	0.52
1:A:1040:LEU:HD13	1:A:1092:TYR:HA	1.90	0.52
1:A:1295:ILE:HD11	1:A:1351:LYS:HG2	1.90	0.51
1:A:85:GLY:HA3	1:A:199:HIS:CE1	2.46	0.51
1:A:496:TRP:O	1:A:560:ARG:NH2	2.30	0.51
1:A:1383:ILE:HA	1:A:1386:ARG:NH2	2.26	0.51
1:A:1043:LEU:HB3	1:A:1088:ASN:ND2	2.23	0.51
1:A:289:ARG:NH1	1:A:292:GLU:OE1	2.43	0.51
1:A:280:ALA:HB1	1:A:1306:PRO:HB2	1.92	0.51
1:A:1050:PRO:HA	1:A:1053:THR:HG22	1.92	0.51
1:A:318:VAL:HG21	1:A:340:ILE:HG12	1.92	0.51
1:A:607:MET:HA	1:A:610:LEU:HD12	1.91	0.50
1:A:474:GLU:OE1	1:A:1066:ARG:NH2	2.44	0.50
1:A:1259:ARG:HA	1:A:1263:THR:HG21	1.92	0.50
1:A:502:ILE:HG21	1:A:530:ILE:HD11	1.93	0.50
1:A:598:LYS:O	1:A:600:ARG:NH1	2.45	0.49
1:A:508:PHE:CD2	1:A:1070:ARG:HG3	2.46	0.49
1:A:242:ARG:HA	1:A:245:MET:HE3	1.93	0.49
1:A:1029:LEU:HB3	1:A:1103:ILE:HD11	1.95	0.49
1:A:1033:PHE:CE1	1:A:1095:THR:HG22	2.47	0.48
1:A:1108:VAL:HG12	1:A:1109:ILE:HD13	1.95	0.48
1:A:1388:LEU:HD23	1:A:1392:PHE:HD2	1.78	0.48
1:A:862:VAL:HG11	1:A:937:LEU:HA	1.95	0.48
1:A:1300:PHE:CD2	1:A:1354:MET:HE1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1321:GLU:O	1:A:1386:ARG:NH1	2.44	0.48
1:A:1112:ILE:HG22	1:A:1137:MET:SD	2.54	0.48
1:A:1117:ILE:HG13	1:A:1137:MET:HE2	1.95	0.48
1:A:558:LEU:HD22	1:A:574:PRO:HB2	1.96	0.47
1:A:1322:VAL:HG11	1:A:1357:ALA:HB2	1.94	0.47
1:A:571:LEU:HB3	1:A:574:PRO:HG3	1.96	0.47
1:A:1026:PHE:HD2	1:A:1147:VAL:HG21	1.79	0.47
1:A:960:PRO:HG2	1:A:963:THR:OG1	2.14	0.47
1:A:913:TYR:HB2	1:A:1131:ILE:HG21	1.96	0.47
1:A:1322:VAL:O	1:A:1383:ILE:HD13	2.15	0.47
1:A:332:ILE:HD11	1:A:335:LYS:NZ	2.29	0.47
1:A:1261:LEU:HD23	1:A:1261:LEU:H	1.79	0.47
1:A:1366:ILE:O	1:A:1366:ILE:HG22	2.14	0.47
1:A:19:TRP:H	1:A:19:TRP:CD1	2.30	0.47
1:A:941:LEU:HD13	1:A:988:PRO:HA	1.97	0.47
1:A:114:LYS:HD2	1:A:114:LYS:N	2.30	0.47
1:A:1377:ASP:O	1:A:1381:TYR:N	2.47	0.47
1:A:1287:GLY:O	1:A:1368:LEU:N	2.41	0.46
1:A:101:LEU:HD22	1:A:123:LEU:HD22	1.97	0.46
1:A:441:LEU:HD13	1:A:444:ILE:HD12	1.97	0.46
1:A:1243:LEU:HB2	1:A:1415:VAL:HG12	1.97	0.46
1:A:160:ILE:HD11	1:A:371:ILE:HG12	1.98	0.46
1:A:23:ILE:HG12	1:A:1091:LEU:HD11	1.98	0.46
1:A:110:ASP:OD1	1:A:110:ASP:N	2.36	0.46
1:A:1430:LEU:HB3	1:A:1431:LEU:HD22	1.98	0.46
1:A:108:SER:O	1:A:108:SER:OG	2.26	0.46
1:A:277:TRP:CH2	1:A:1358:ARG:HD2	2.51	0.46
1:A:293:LEU:CD2	1:A:946:LYS:HB2	2.45	0.46
1:A:466:SER:O	1:A:470:VAL:HG23	2.15	0.46
1:A:952:MET:HE1	1:A:1163:VAL:HG22	1.98	0.46
1:A:1347:SER:OG	1:A:1350:HIS:ND1	2.48	0.46
1:A:244:MET:HG3	1:A:303:ARG:HG2	1.98	0.45
1:A:132:ILE:O	1:A:136:LEU:HG	2.16	0.45
1:A:210:LEU:HA	5:A:1510:CLR:H213	1.97	0.45
1:A:297:ARG:HA	1:A:942:ILE:HD13	1.98	0.45
1:A:29:ARG:HG3	1:A:30:GLN:HG2	1.98	0.45
1:A:90:LEU:O	1:A:94:THR:HG23	2.16	0.45
1:A:929:MET:H	1:A:996:GLN:HE22	1.63	0.45
1:A:129:LEU:O	1:A:132:ILE:HG13	2.16	0.45
1:A:454:LEU:HD12	1:A:615:LYS:HB3	1.99	0.45
1:A:929:MET:CG	1:A:933:ARG:HE	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:ARG:HA	1:A:518:ARG:HD3	1.85	0.45
1:A:1356:LEU:HD22	1:A:1384:ILE:HD13	1.99	0.45
1:A:958:GLN:HB3	1:A:1171:THR:HG22	1.98	0.45
1:A:1243:LEU:HD21	1:A:1407:MET:HE2	1.99	0.45
1:A:390:THR:HG21	1:A:567:ASP:HB3	1.99	0.44
1:A:233:LEU:HD11	1:A:309:ALA:HB1	2.00	0.44
1:A:293:LEU:HA	1:A:296:THR:HB	2.00	0.44
1:A:280:ALA:HB2	1:A:1307:TYR:CE1	2.52	0.44
1:A:200:PHE:HA	1:A:203:ILE:HB	1.99	0.44
1:A:139:HIS:HE1	1:A:1105:MET:HE2	1.83	0.44
1:A:484:HIS:ND1	1:A:485:SER:O	2.46	0.44
1:A:908:THR:OG1	1:A:909:SER:N	2.51	0.44
1:A:1302:LYS:NZ	1:A:1308:GLU:OE2	2.43	0.44
1:A:89:TYR:CZ	1:A:206:LEU:HD23	2.52	0.44
1:A:266:ILE:HG21	1:A:972:ILE:HG21	2.00	0.44
1:A:526:LEU:HD21	1:A:556:ILE:HG12	1.99	0.44
1:A:1386:ARG:O	1:A:1390:GLN:HB2	2.18	0.44
1:A:200:PHE:HB2	1:A:357:ALA:HB2	1.99	0.43
1:A:347:ARG:O	1:A:351:THR:HB	2.18	0.43
1:A:969:ALA:O	1:A:972:ILE:HG22	2.18	0.43
1:A:1033:PHE:CD1	1:A:1099:PHE:HB2	2.53	0.43
1:A:131:PHE:CD1	1:A:1109:ILE:HD12	2.53	0.43
1:A:211:LEU:O	1:A:215:ILE:HG13	2.19	0.43
1:A:593:LYS:HA	1:A:593:LYS:HD3	1.71	0.43
1:A:1239:ARG:NH2	1:A:1392:PHE:O	2.45	0.43
1:A:139:HIS:CD2	1:A:1097:ARG:HH11	2.37	0.43
1:A:445:ASN:OD1	1:A:445:ASN:N	2.52	0.43
1:A:499:PRO:HD3	1:A:543:GLU:HA	2.00	0.43
1:A:130:LEU:O	1:A:133:VAL:HG12	2.18	0.43
1:A:277:TRP:HH2	1:A:1358:ARG:HH11	1.66	0.43
1:A:856:HIS:HB2	1:A:944:VAL:HG22	2.00	0.43
1:A:468:LEU:HD22	1:A:570:LEU:HD23	2.00	0.43
1:A:20:THR:HG21	1:A:1095:THR:HA	2.01	0.43
1:A:513:ASP:HB3	1:A:516:ARG:HB3	1.99	0.43
1:A:1099:PHE:HE2	1:A:1151:ILE:HG21	1.84	0.43
1:A:37:ILE:HD11	1:A:1043:LEU:HD13	2.00	0.43
1:A:1022:VAL:HG11	1:A:1112:ILE:HD11	2.01	0.43
1:A:396:ASN:H	1:A:445:ASN:HB3	1.84	0.42
1:A:859:LEU:HD22	1:A:944:VAL:HG21	1.99	0.42
1:A:85:GLY:HA3	1:A:199:HIS:NE2	2.34	0.42
1:A:160:ILE:HD13	1:A:183:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1226:ILE:HB	1:A:1252:THR:HG21	2.01	0.42
1:A:178:GLY:HA2	1:A:181:VAL:HG12	2.01	0.42
1:A:983:LEU:HD11	1:A:1160:VAL:HG23	2.02	0.42
1:A:1311:SER:O	1:A:1315:ILE:HG23	2.19	0.42
1:A:1043:LEU:C	1:A:1088:ASN:HD21	2.28	0.42
1:A:57:TRP:O	1:A:61:LEU:HG	2.20	0.42
1:A:266:ILE:HG21	1:A:972:ILE:HG12	2.02	0.42
1:A:299:ALA:O	1:A:303:ARG:HG3	2.19	0.42
1:A:397:VAL:HA	1:A:479:GLU:O	2.20	0.42
1:A:446:PHE:HE2	1:A:467:LEU:HD11	1.85	0.42
1:A:161:TYR:OH	1:A:1074:PHE:HB3	2.20	0.42
1:A:1102:ARG:HA	1:A:1106:ILE:HB	2.01	0.42
1:A:1140:MET:SD	1:A:1143:LEU:HD13	2.60	0.42
1:A:1388:LEU:HD23	1:A:1392:PHE:CD2	2.55	0.41
1:A:33:GLU:H	1:A:33:GLU:HG2	1.65	0.41
1:A:536:LYS:HD3	1:A:536:LYS:HA	1.89	0.41
1:A:102:LEU:O	1:A:106:ILE:HG23	2.20	0.41
1:A:135:THR:HG22	1:A:136:LEU:HD23	2.02	0.41
1:A:139:HIS:NE2	1:A:1100:GLN:O	2.54	0.41
1:A:935:LEU:HD23	1:A:935:LEU:HA	1.87	0.41
1:A:323:LEU:O	1:A:327:LEU:HB2	2.20	0.41
1:A:92:GLU:HB3	1:A:207:GLN:NE2	2.35	0.41
1:A:1215:LEU:HD22	1:A:1230:ILE:HD11	2.02	0.41
1:A:73:LEU:HD22	1:A:152:MET:HG2	2.01	0.41
1:A:172:LEU:HD23	1:A:172:LEU:HA	1.90	0.41
1:A:459:SER:HA	1:A:1377:ASP:OD2	2.21	0.41
1:A:1112:ILE:O	1:A:1116:PHE:HB2	2.20	0.41
1:A:14:LYS:HA	1:A:14:LYS:HD3	1.87	0.41
1:A:1015:ILE:O	1:A:1019:THR:HG23	2.20	0.41
1:A:1034:LEU:HD23	1:A:1034:LEU:HA	1.82	0.41
1:A:1230:ILE:O	1:A:1230:ILE:HG13	2.20	0.41
1:A:161:TYR:HE2	1:A:1075:GLU:HA	1.86	0.41
1:A:505:ASN:O	1:A:560:ARG:HD3	2.21	0.41
1:A:571:LEU:HD12	1:A:602:LEU:HB3	2.03	0.41
1:A:1369:LEU:HD23	1:A:1372:PRO:HG2	2.03	0.41
1:A:448:ILE:HD11	1:A:454:LEU:HD13	2.02	0.41
1:A:579:ASP:OD2	1:A:1245:ARG:HD3	2.20	0.41
1:A:1348:HIS:O	1:A:1352:GLN:HG2	2.21	0.41
1:A:945:SER:HB2	1:A:983:LEU:HB3	2.02	0.40
1:A:1254:LEU:HD23	1:A:1370:ASP:HB2	2.02	0.40
1:A:1365:LYS:HG3	1:A:1395:CYS:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ALA:HB2	1:A:1307:TYR:CZ	2.57	0.40
1:A:230:LEU:HD23	1:A:230:LEU:HA	1.83	0.40
1:A:389:THR:O	1:A:450:ARG:HB2	2.21	0.40
1:A:972:ILE:HD11	1:A:1166:PHE:CZ	2.57	0.40
1:A:244:MET:HB2	1:A:302:VAL:HG11	2.03	0.40
1:A:1378:PRO:HA	1:A:1381:TYR:HB3	2.04	0.40
1:A:102:LEU:HD12	1:A:102:LEU:HA	1.90	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	1059/1421 (74%)	1010 (95%)	49 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	900/1259 (72%)	896 (100%)	4 (0%)	84	83

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	286	GLU
1	A	323	LEU
1	A	856	HIS
1	A	1096	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	ASN
1	A	139	HIS
1	A	179	GLN
1	A	186	ASN
1	A	187	ASN
1	A	359	GLN
1	A	847	ASN
1	A	856	HIS
1	A	996	GLN
1	A	1088	ASN
1	A	1238	GLN
1	A	1262	ASN
1	A	1268	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	$\# Z > 2$
4	POV	A	1506	-	8,8,51	0.24	0	7,7,59	0.23	0
3	ATP	A	1504	2	32,33,33	0.29	0	48,52,52	0.29	0
3	ATP	A	1503	2	32,33,33	0.30	0	48,52,52	0.28	0
5	CLR	A	1510	-	31,31,31	0.37	0	48,48,48	0.75	2 (4%)
4	POV	A	1505	-	8,8,51	0.23	0	7,7,59	0.25	0
4	POV	A	1509	-	4,4,51	0.28	0	3,3,59	0.23	0
4	POV	A	1507	-	6,6,51	0.25	0	5,5,59	0.22	0
4	POV	A	1508	-	8,8,51	0.24	0	7,7,59	0.21	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
4	POV	A	1506	-	-	0/6/6/55	-
3	ATP	A	1504	2	-	5/22/38/38	0/3/3/3
3	ATP	A	1503	2	-	1/22/38/38	0/3/3/3
5	CLR	A	1510	-	-	7/10/68/68	0/4/4/4
4	POV	A	1505	-	-	0/6/6/55	-
4	POV	A	1509	-	-	0/2/2/55	-
4	POV	A	1507	-	-	0/4/4/55	-
4	POV	A	1508	-	-	2/6/6/55	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1510	CLR	C10-C9-C8	-2.23	109.46	112.71
5	A	1510	CLR	C14-C8-C9	2.06	111.78	109.09

There are no chirality outliers.

All (15) torsion outliers are listed below:

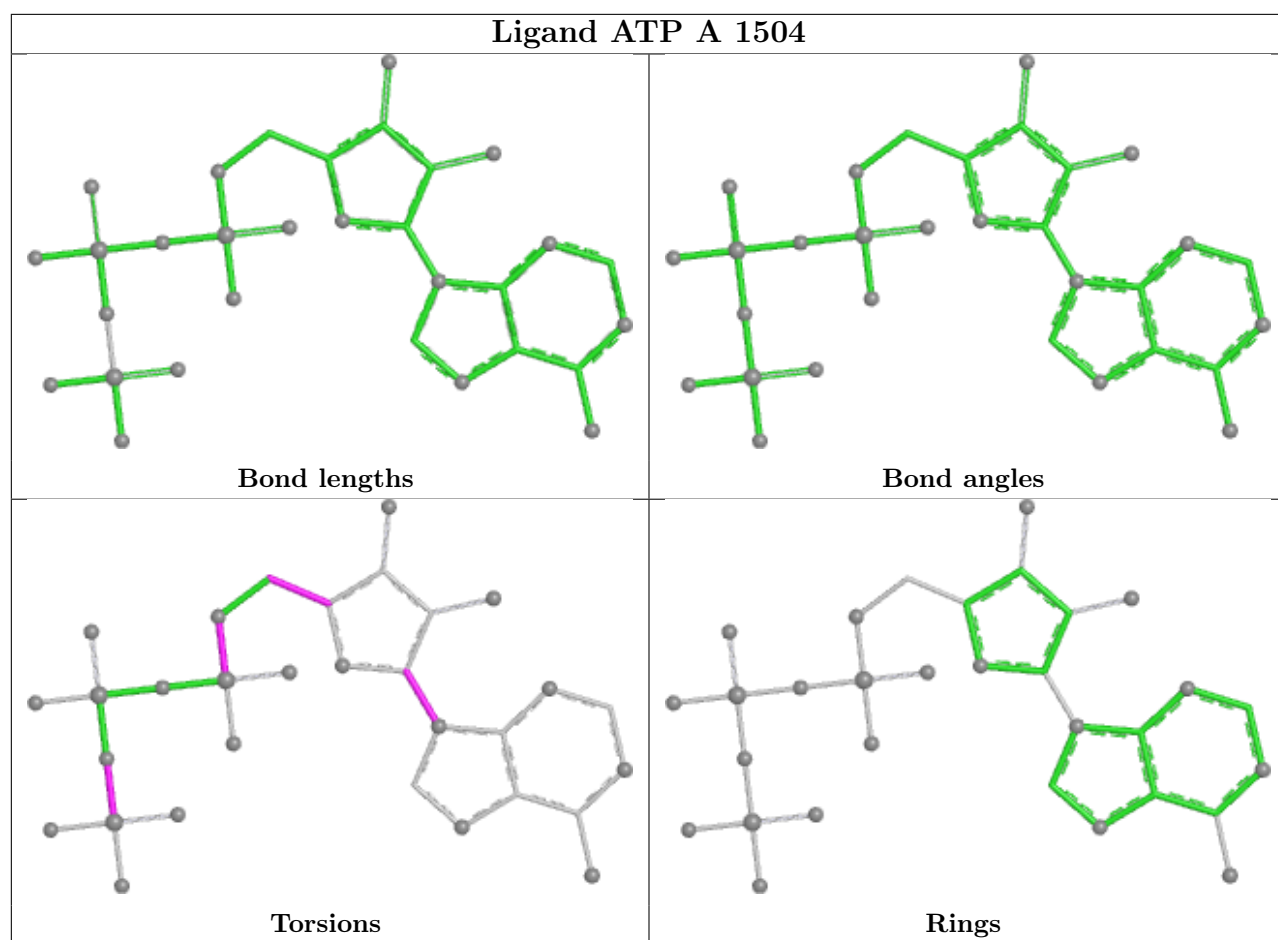
Mol	Chain	Res	Type	Atoms
3	A	1504	ATP	C5'-O5'-PA-O2A
5	A	1510	CLR	C17-C20-C22-C23
5	A	1510	CLR	C21-C20-C22-C23
3	A	1504	ATP	O4'-C4'-C5'-O5'
3	A	1504	ATP	C3'-C4'-C5'-O5'
4	A	1508	POV	C36-C37-C38-C39
5	A	1510	CLR	C13-C17-C20-C22
5	A	1510	CLR	C13-C17-C20-C21
3	A	1503	ATP	PA-O3A-PB-O2B
3	A	1504	ATP	C2'-C1'-N9-C8
5	A	1510	CLR	C16-C17-C20-C22
4	A	1508	POV	C34-C35-C36-C37
3	A	1504	ATP	PB-O3B-PG-O2G
5	A	1510	CLR	C20-C22-C23-C24
5	A	1510	CLR	C16-C17-C20-C21

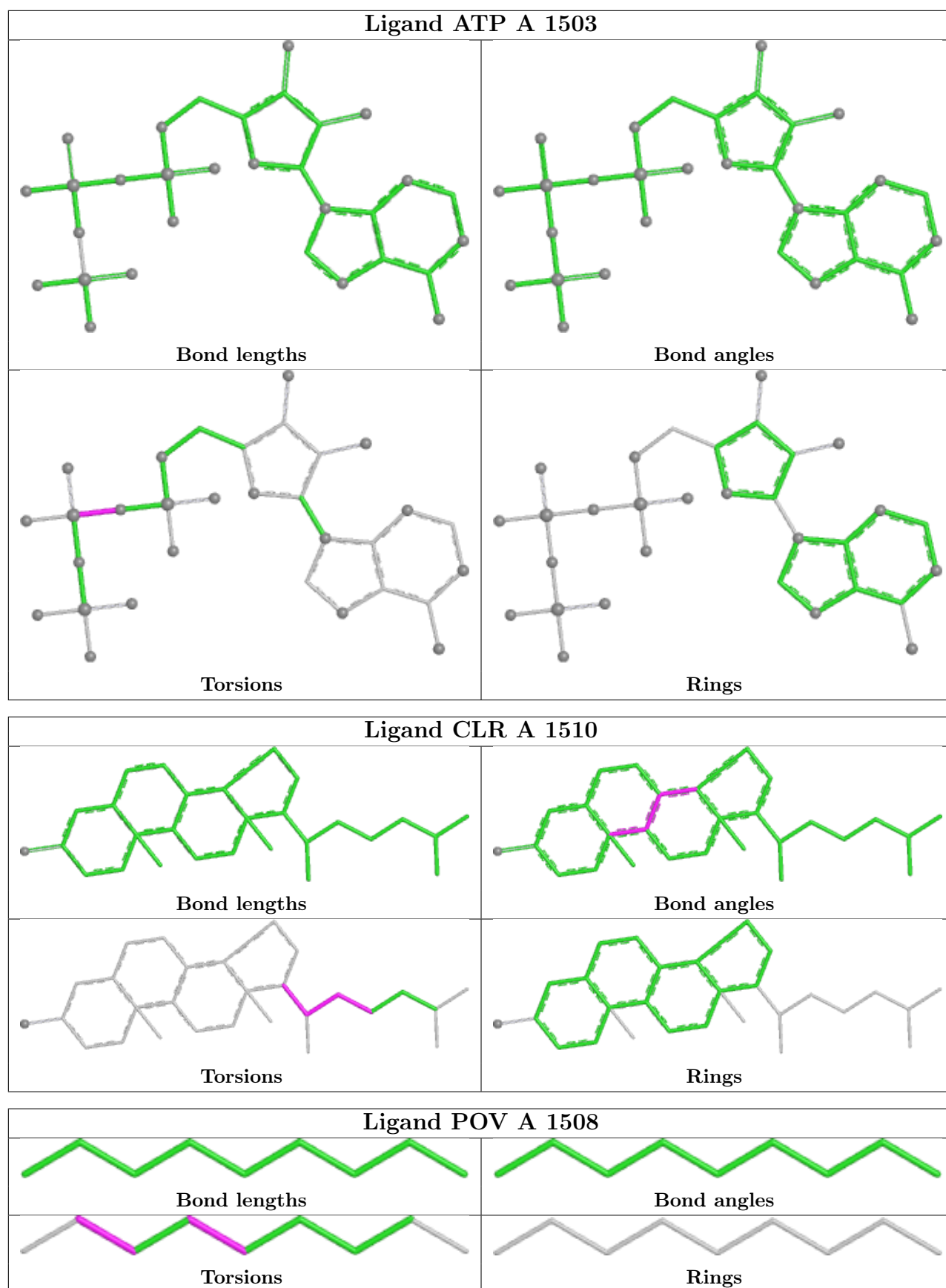
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1510	CLR	1	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43011. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

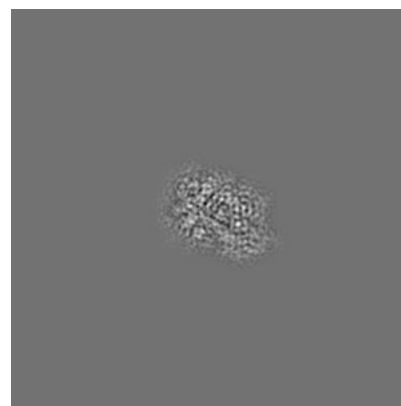
6.1.1 Primary map



X

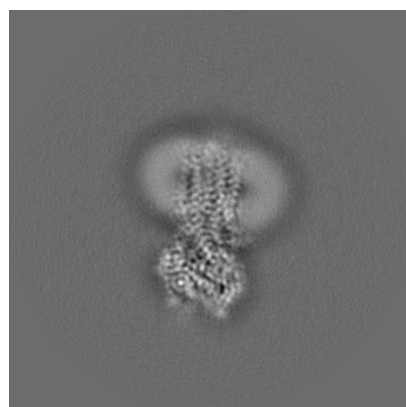


Y

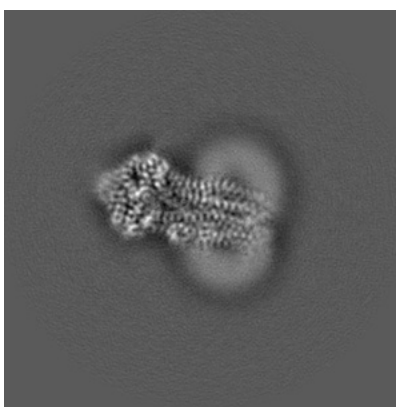


Z

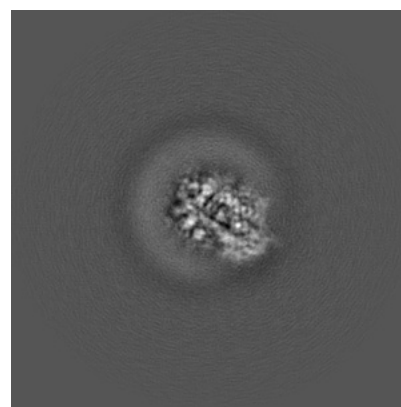
6.1.2 Raw map



X



Y

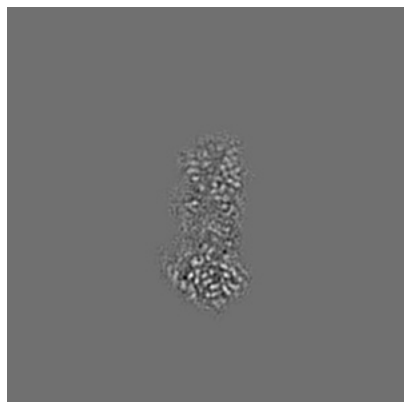


Z

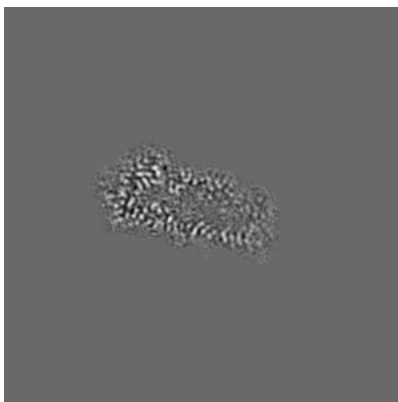
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

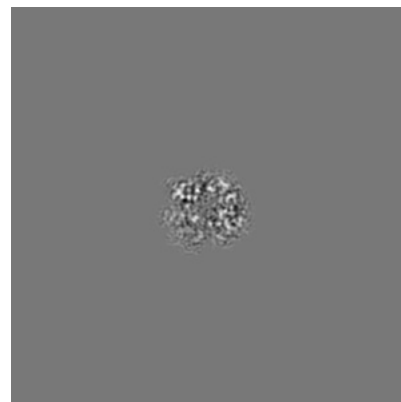
6.2.1 Primary map



X Index: 130

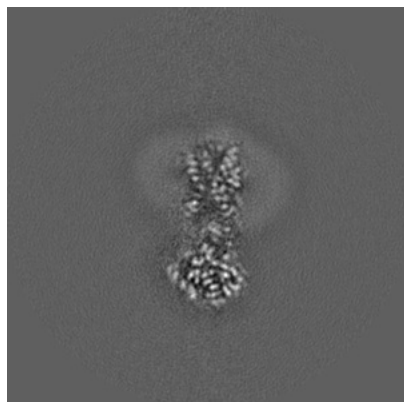


Y Index: 130

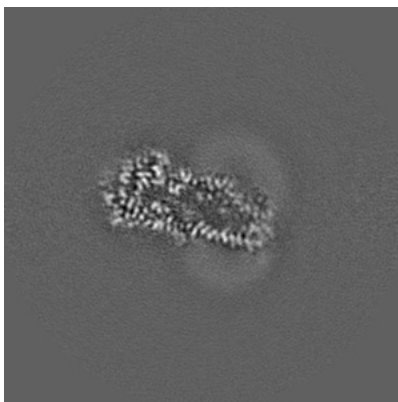


Z Index: 130

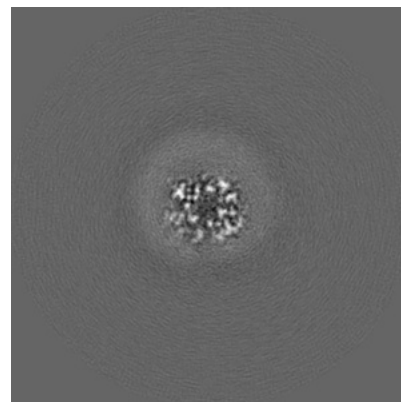
6.2.2 Raw map



X Index: 130



Y Index: 130

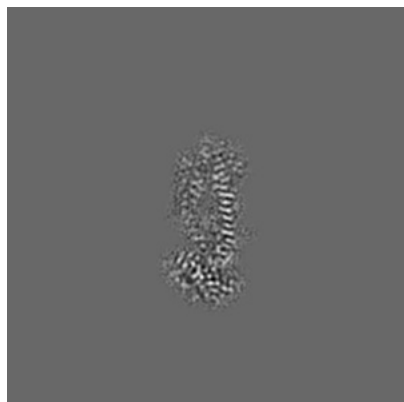


Z Index: 130

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

6.3 Largest variance slices [i](#)

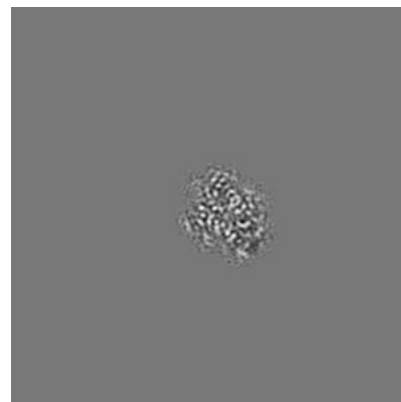
6.3.1 Primary map



X Index: 125

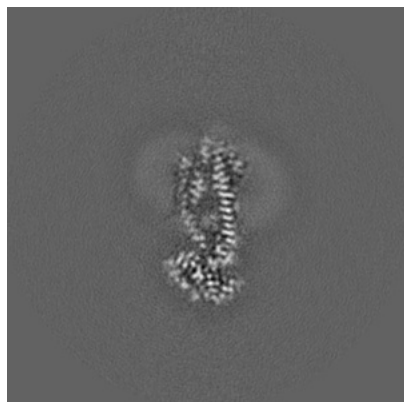


Y Index: 134

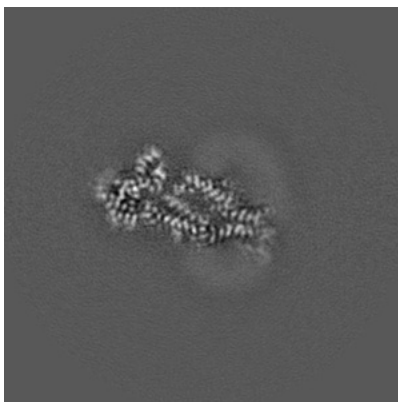


Z Index: 88

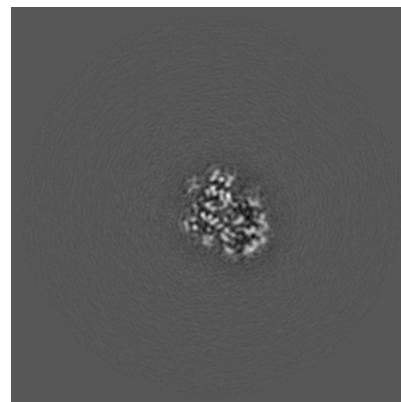
6.3.2 Raw map



X Index: 125



Y Index: 135

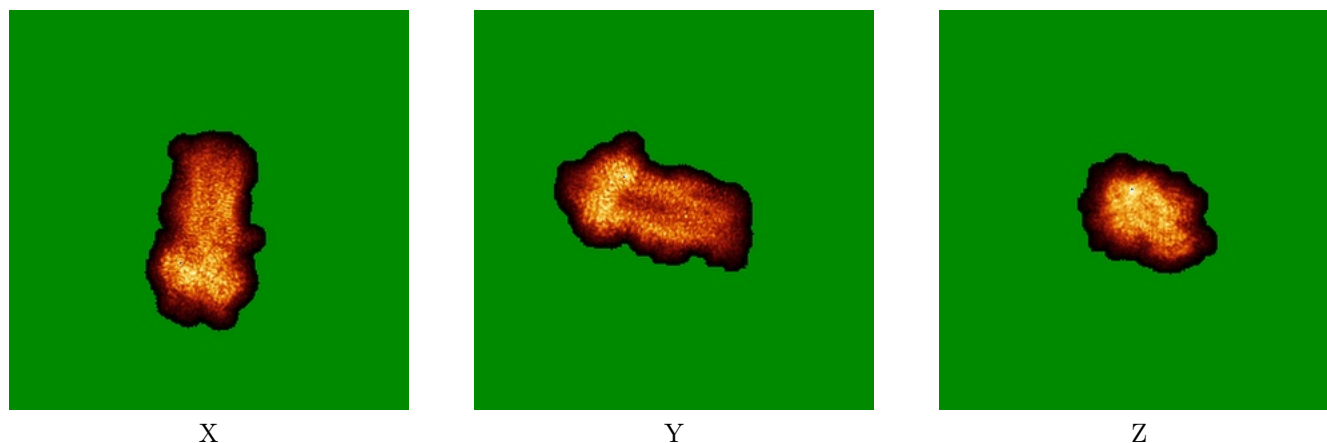


Z Index: 86

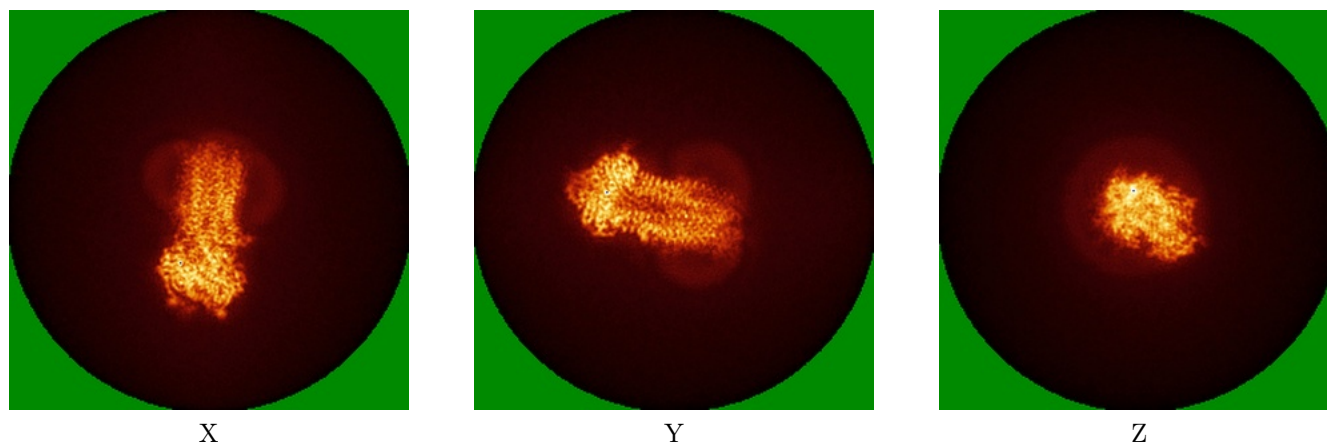
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

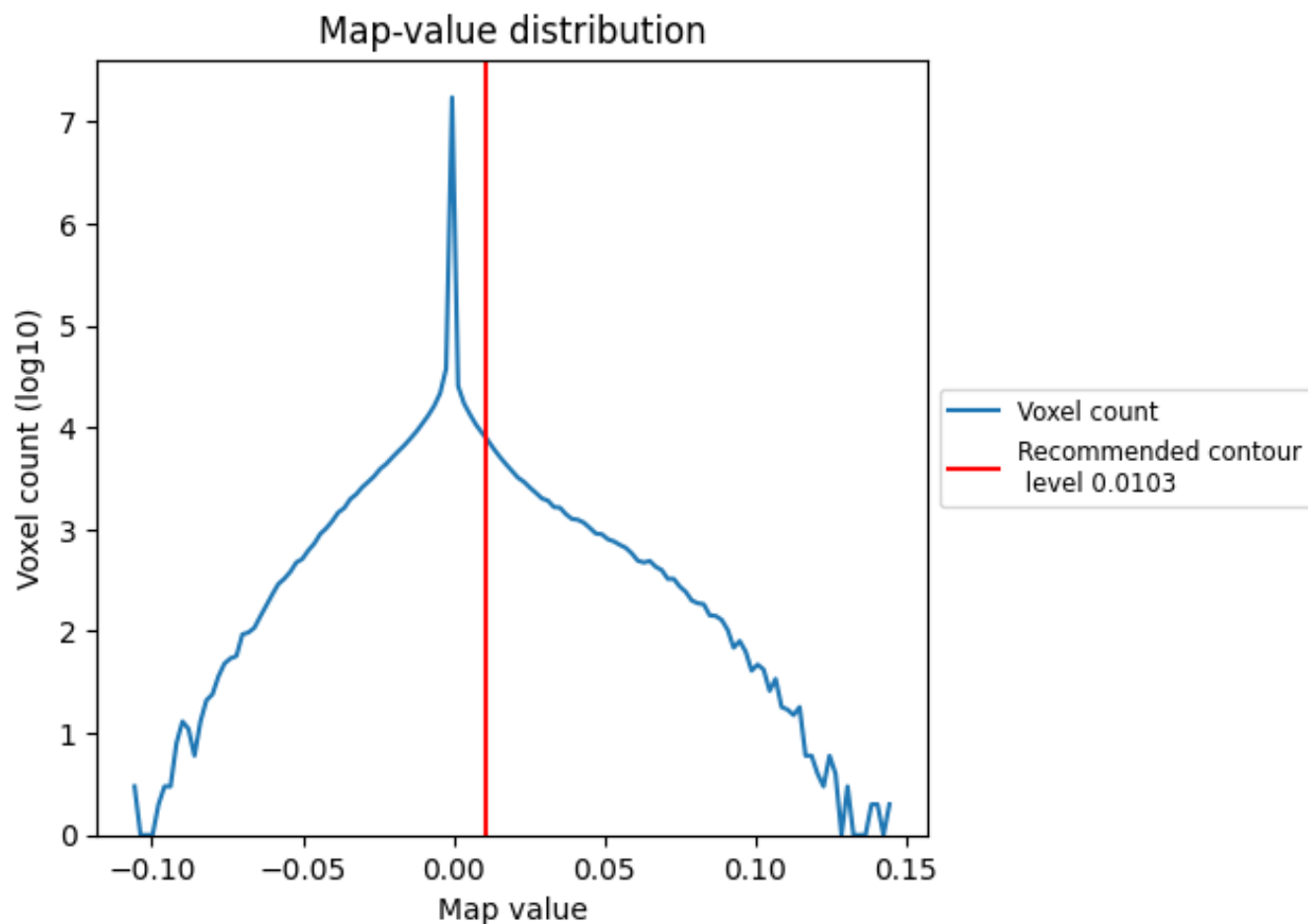
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

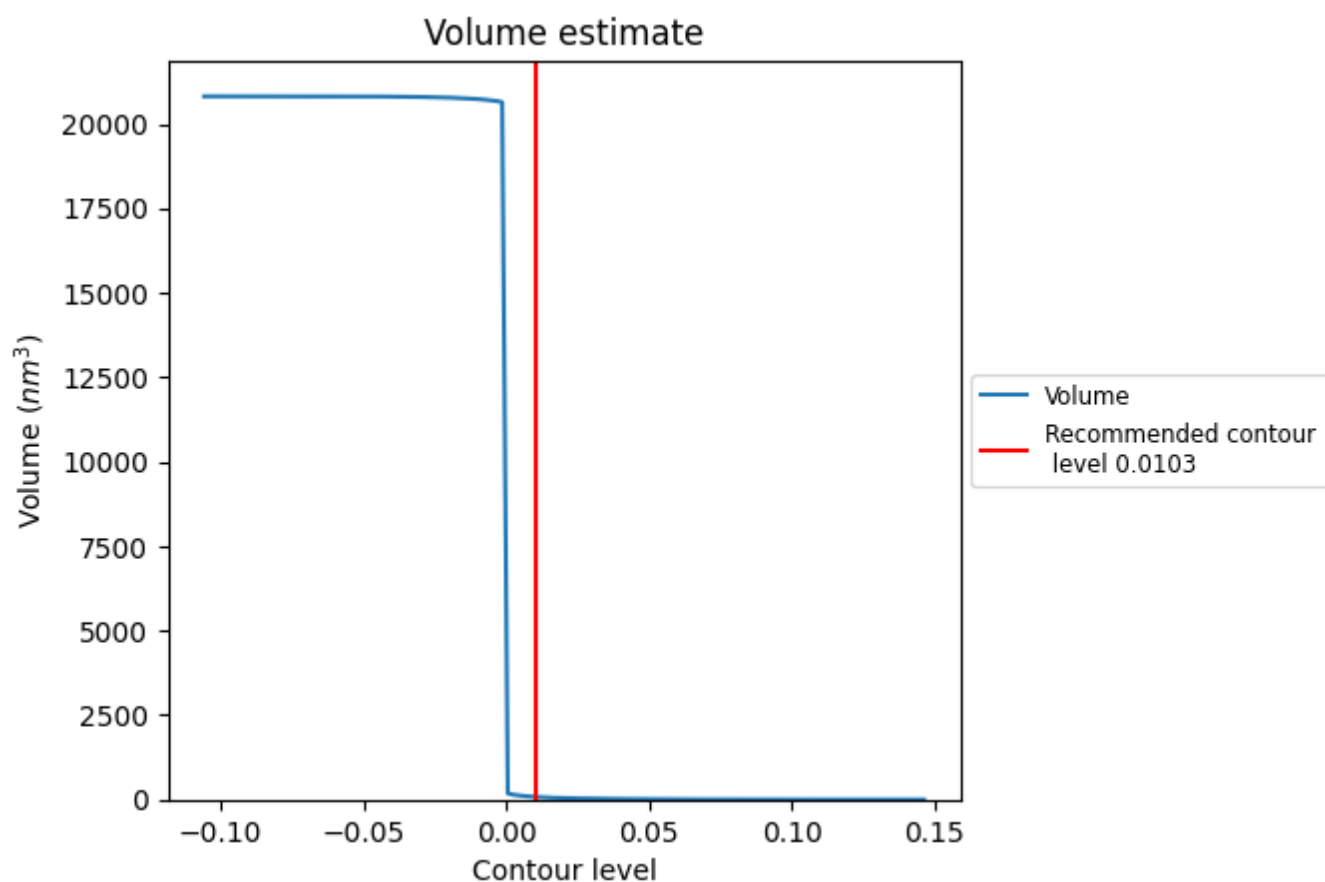
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

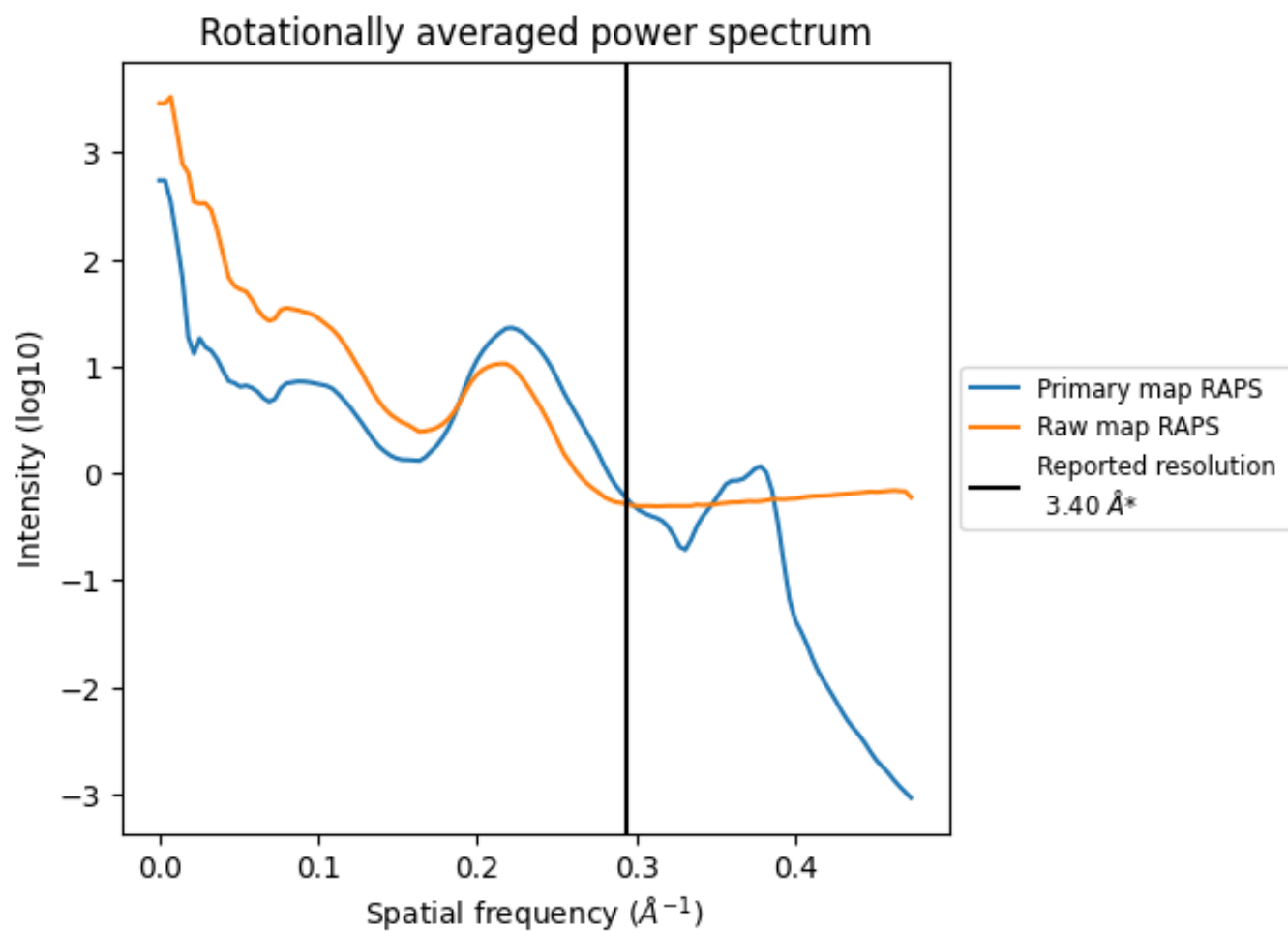
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 78 nm^3 ; this corresponds to an approximate mass of 71 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 ⓘ

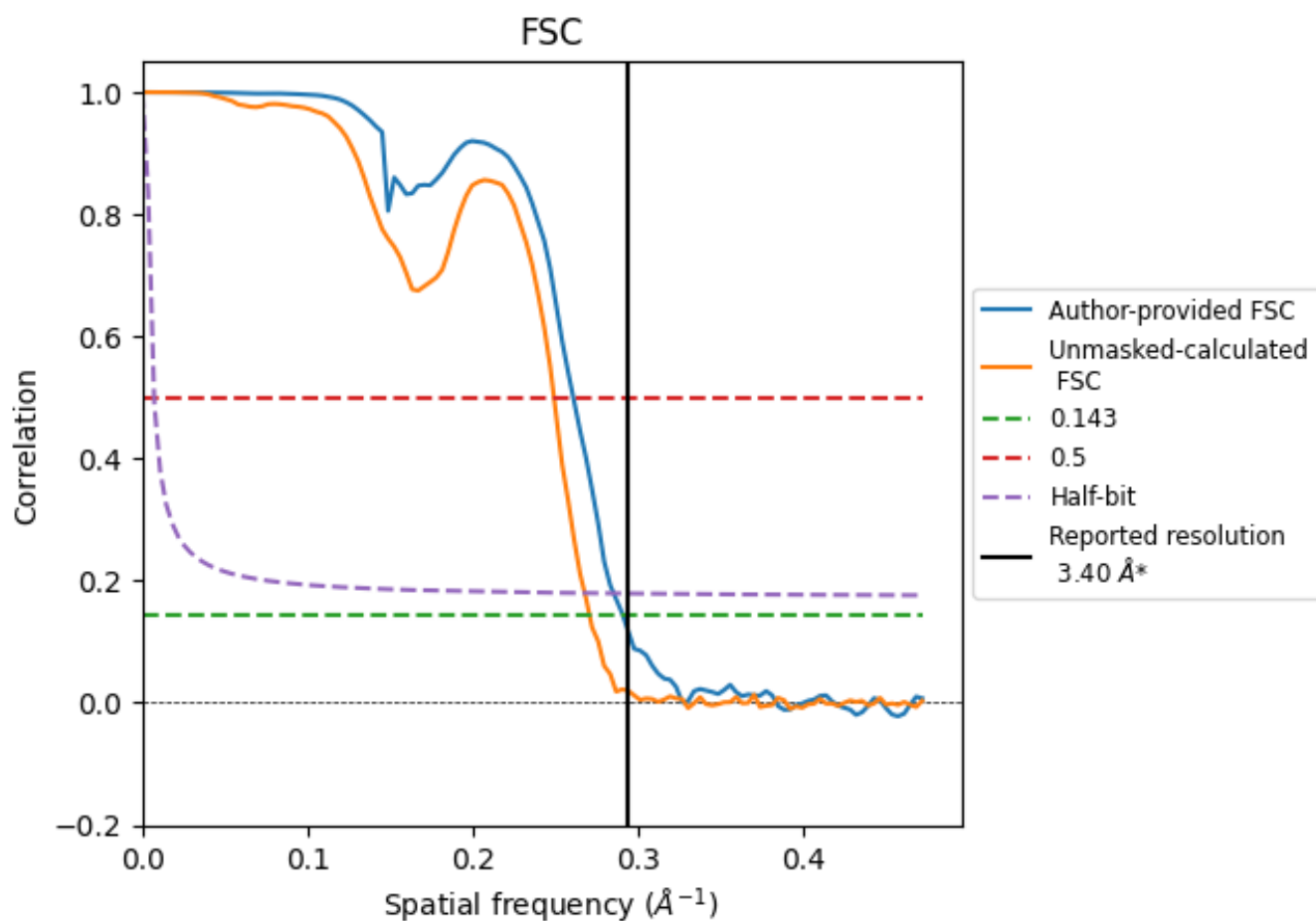


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.294 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.43	3.83	3.50
Unmasked-calculated*	3.69	4.01	3.73

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

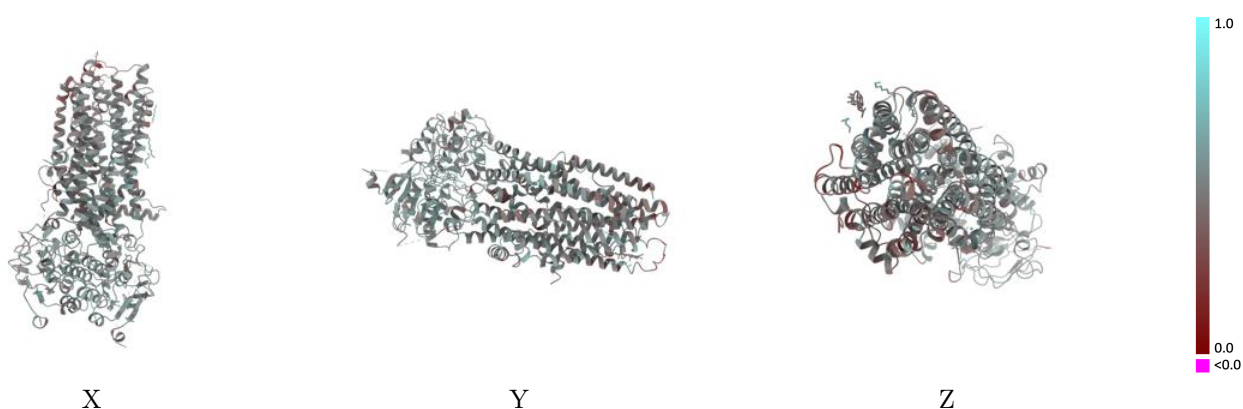
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-43011 and PDB model 8V7Z. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

This section was not generated.

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

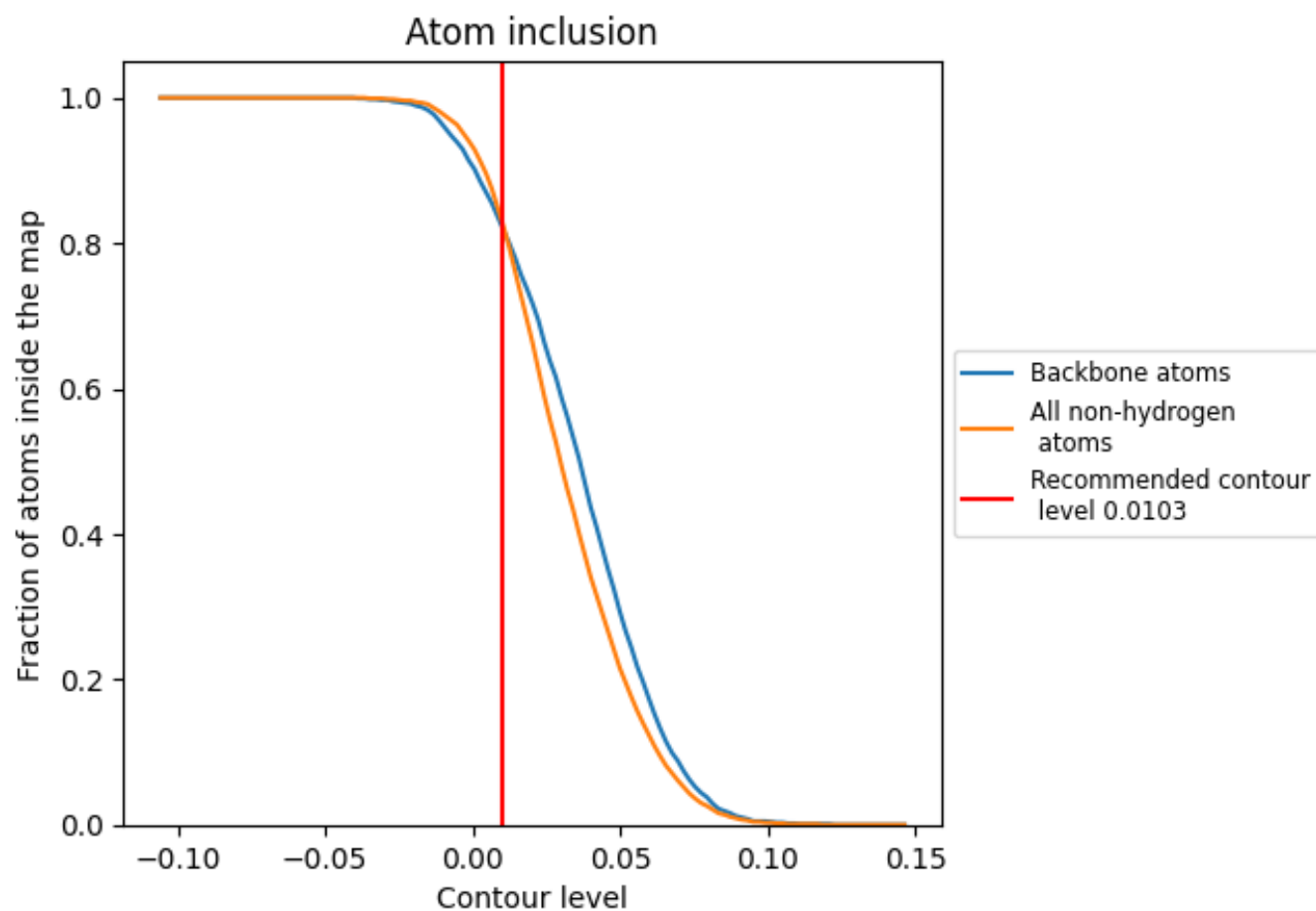


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 83% 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 (0.0103) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8260	0.4960
A	0.8260	0.4960

