



wwPDB EM Validation Summary Report ⓘ

Mar 7, 2026 – 02:31 AM UTC

PDB ID : 8TLA / pdb_00008tla
EMDB ID : EMD-41366
Title : Human Type 3 IP3 Receptor - Higher-Order Inhibited State - Symmetry Mate
1
Authors : Paknejad, N.; Sapuru, V.; Hite, R.K.
Deposited on : 2023-07-26
Resolution : 3.20 Å(reported)

This is a wwPDB EM Validation Summary 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

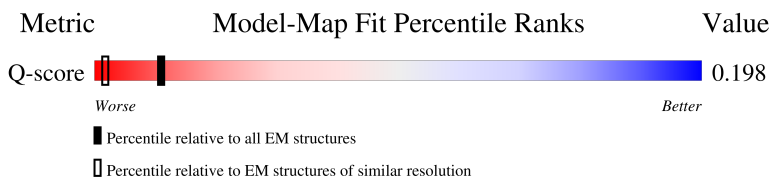
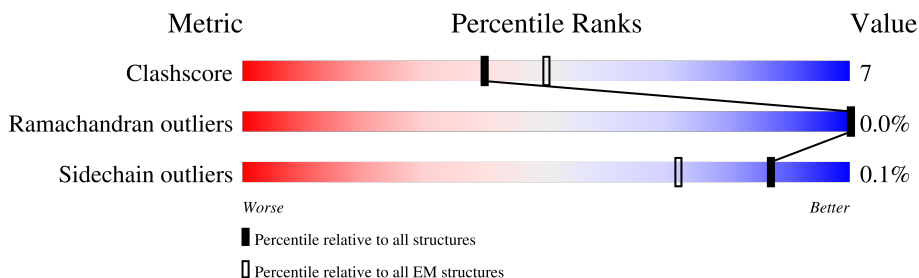
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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	2671	30% 61% 13% 26%
1	B	2671	34% 61% 13% 26%
1	C	2671	17% 65% 10% 25%
1	D	2671	14% 65% 11% 24%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 130502 atoms, of which 65433 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.

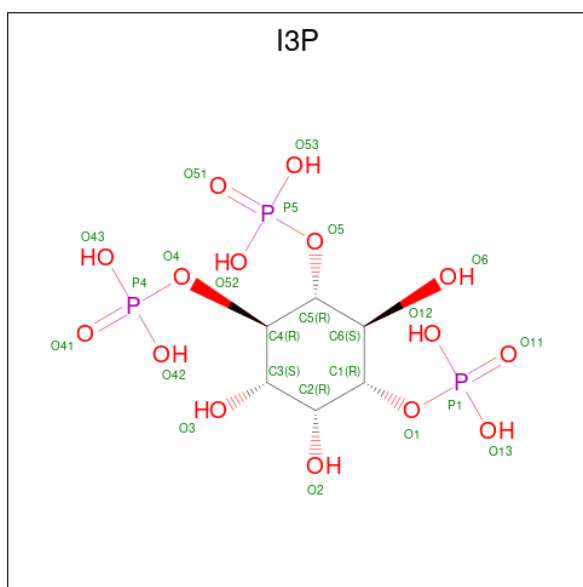
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1989	Total	C	H	N	O	S	0	0
			32350	10293	16244	2749	2960	104		
1	B	1987	Total	C	H	N	O	S	0	0
			32312	10283	16225	2743	2957	104		
1	C	2004	Total	C	H	N	O	S	0	0
			32571	10370	16344	2767	2986	104		
1	D	2034	Total	C	H	N	O	S	0	0
			32957	10480	16536	2807	3029	105		

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Zn	0
			1	1	
2	B	1	Total	Zn	0
			1	1	
2	C	1	Total	Zn	0
			1	1	
2	D	1	Total	Zn	0
			1	1	

- Molecule 3 is D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (CCD ID: I3P) (formula: C₆H₁₅O₁₅P₃) (labeled as "Ligand of Interest" by depositor).

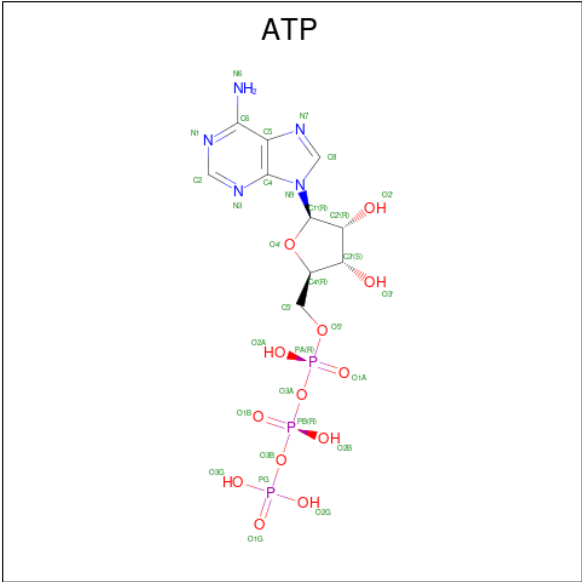


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	B	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	C	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	D	1	Total	C	H	O	P	0
			33	6	9	15	3	

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Ca	0
			1	1	
4	B	1	Total	Ca	0
			1	1	
4	C	1	Total	Ca	0
			1	1	
4	D	1	Total	Ca	0
			1	1	

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

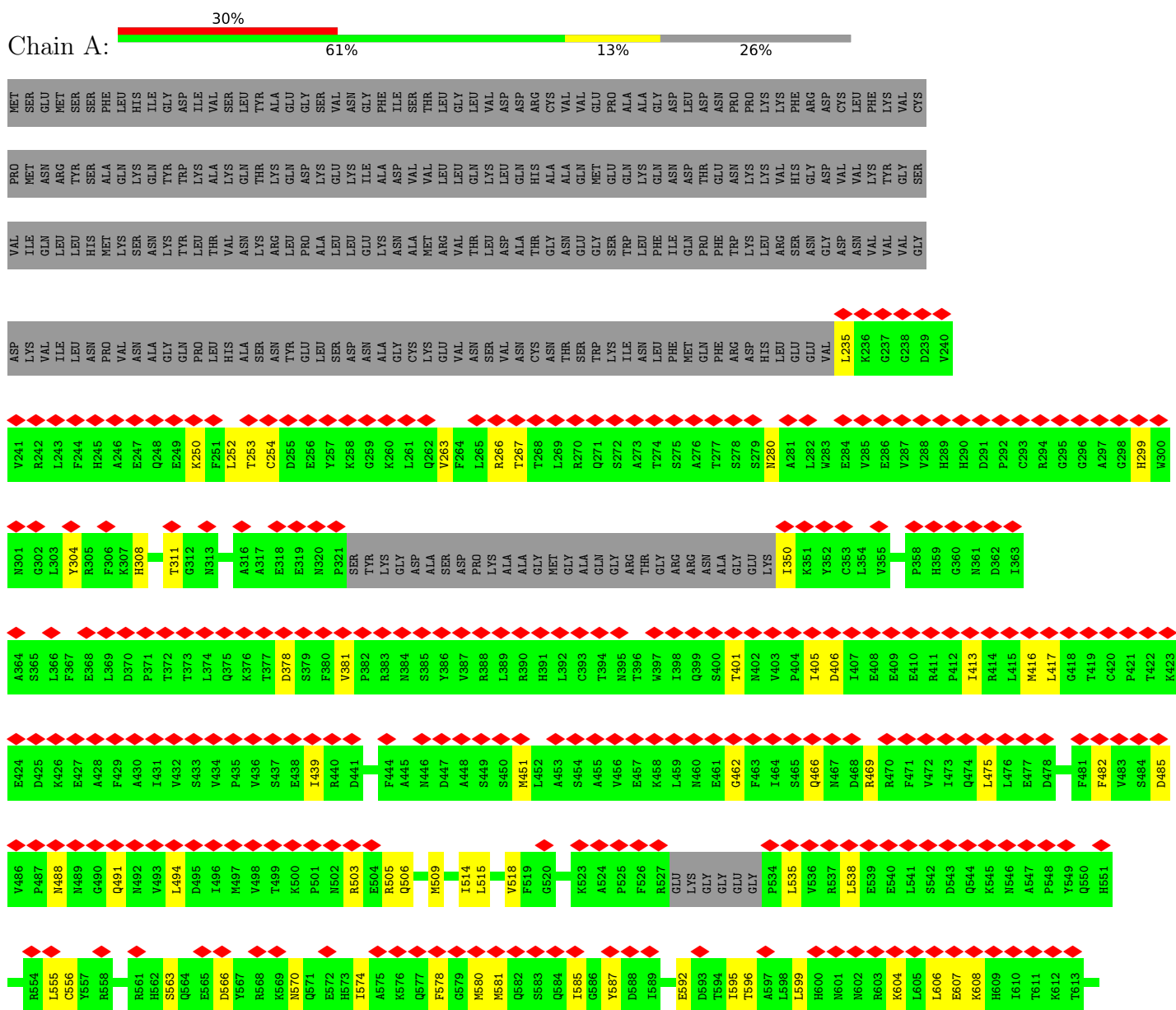


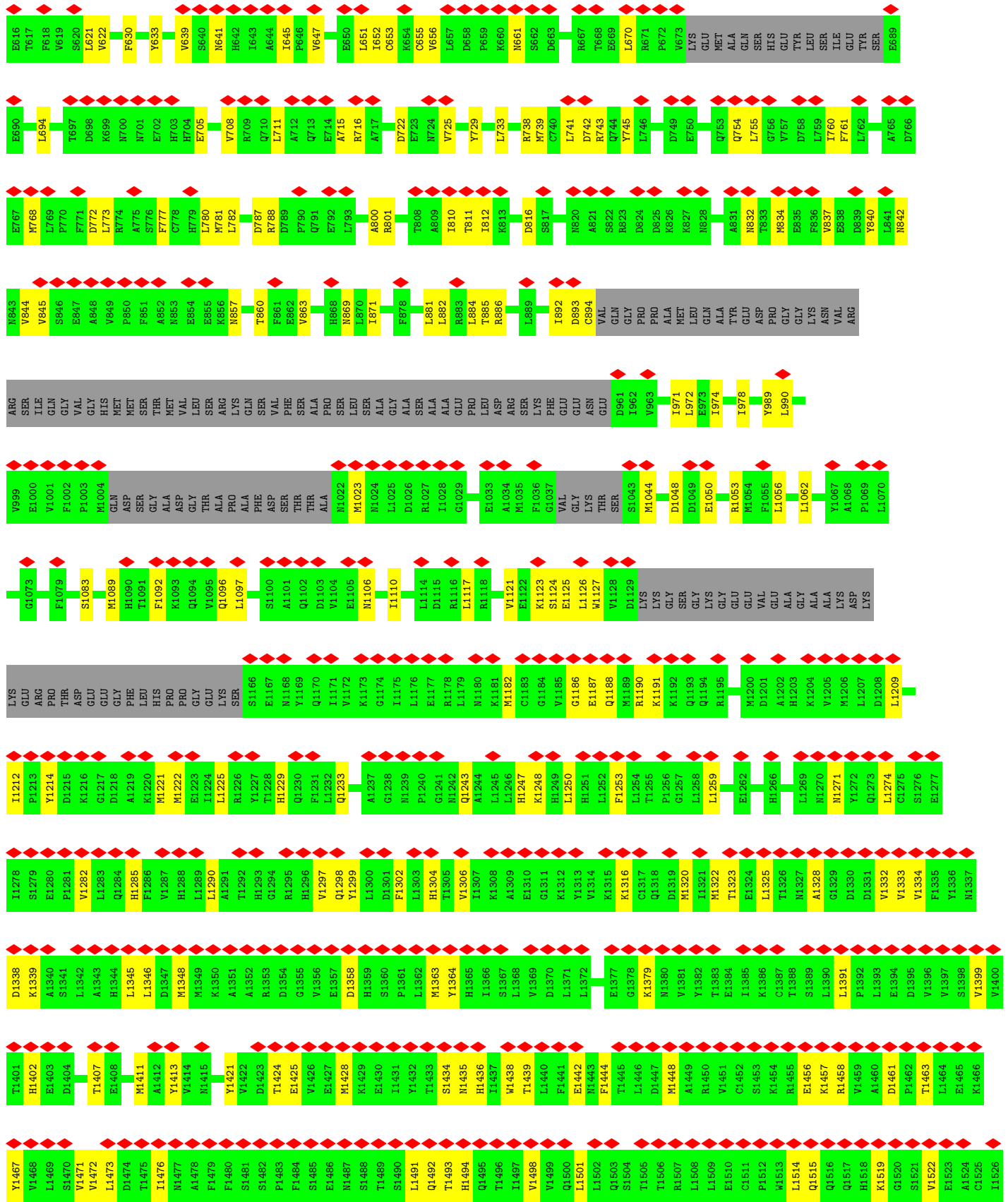
Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
5	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
5	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
5	D	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3





V241	N301	D362	T422	F482	S542	N602	T668	L735	B801	H868	ARG	GLY
R242	G302	I363	K423	V483	D543	R603	E669	L736	T804	N869	LYS	THR
L243	L303	A364	E424	S484	Q544	K604	L670	F736	E805	L870	GLN	ALA
F244	Y304	S365	D425	D485	K545	L605	R671	M739	T808	I871	VAL	ALA
H245	H305	L366	D426	V486	K546	L606	P672	D742	A809	H872	PHE	ASP
A246	F306	F367	E427	P487	N546	E607	P673	R743	I810	G873	SER	THR
E247	K307	E368	A428	N488	P548	K608	L746	Y745	T811	F874	ALA	THR
Q248	H308	L369	F429	G490	Q550	H609	A747	L748	D814	S877	LEU	ALA
Q249	L309	P371	A430	Q491	H551	I610	GLN	A749	E814	F878	SER	ALA
K250	A310	P372	V432	N492	N552	K612	HIS	E749	S817	L881	GLY	N1022
F251	G312	T372	S433	V493	F553	T613	GLU	E750	N818	L884	ALA	M1023
L252	N313	T373	L494	L494	R554	E614	GLU	E751	L819	T885	SER	M1024
T253	Y314	L374	D495	L496	L555	V615	LEU	W751	N820	L888	ALA	L1025
C254	L315	Q375	P435	I496	C556	E616	ILE	S752	A821	L889	ALA	D1026
D255	A316	K376	V436	M497	Y557	T617	GLU	Q753	S822	L890	GLU	R1027
E256	A317	T377	E437	V498	R558	F618	TYR	Q754	R823	Q890	ASP	E1030
Y257	E318	D378	E438	T499	V559	V619	SER	L755	D824	I891	LYS	Q1031
K258	E319	S379	I439	K500	R561	S620	E689	W757	D825	I892	LYS	A1032
G259	N320	F380	R440	P501	H562	L621	E690	D758	K326	D893	PHE	M1035
K260	P321	V381	D441	N502	S563	K624	E691	L759	R327	C894	GLU	F1036
L261	SER	P382	L442	R503	Q564	N625	V692	W760	N828	L894	GLU	G1037
Q262	TYR	R383	D443	R504	E565	R626	L694	F761	K329	L895	ASN	VAL
V263	GLY	N384	F444	E504	D566	E627	T695	L762	N832	L896	GLY	VAL
F264	ASP	S385	A445	R505	Y567	F630	V696	C763	N834	D898	PRO	L961
L265	ALA	Y386	N446	K506	R568	L634	T697	W764	T833	D899	ALA	I962
R266	SER	V387	D447	K507	K569	S635	D698	A765	N834	L899	LEU	V963
T267	PRO	R388	A448	L508	N570	D636	K699	D766	E835	D900	GLN	E566
T268	LYS	L389	S449	M509	Q571	L637	W700	E767	F836	L901	ALA	L969
L269	ALA	R390	S450	E511	E572	L637	N701	W768	W837	L902	TYR	K370
R270	ALA	H391	M451	Q512	H573	C638	E702	L769	E838	L903	ASP	I971
Q271	GLY	L392	L452	N513	I574	V639	H703	P770	D839	L904	GLY	L372
S272	GLY	C393	A453	L515	I574	S640	H704	F771	N840	L905	PRO	E973
A273	ALA	T394	S454	K516	A575	N641	E705	D772	L841	L906	GLY	I974
L274	GLN	N395	A455	Q517	K576	H642	K706	L773	N842	L907	LYS	I978
S275	ARG	T396	V456	V518	Q577	L643	S707	R774	N843	L908	ASN	D984
A276	THR	W397	E457	F519	F578	T643	V708	A775	W844	L909	VAL	L991
T277	GLY	I398	K458	G520	G579	A644	R709	C778	V845	L910	ARG	E1000
S278	ARG	Q399	L459	I521	M580	T645	E710	H779	S846	L911	SER	V1001
N279	ASN	S400	N460	L522	M581	P646	L711	L780	E847	L912	ILE	P1002
N280	ALA	T401	E461	K523	Q582	V647	A712	M781	A848	L913	GLY	M1004
A281	GLU	N402	G462	A524	S583	L651	Q713	L782	P850	L914	VAL	E1008
L282	LYS	V403	F463	P525	T585	I652	E714	H785	F851	L915	GLY	V1001
W283	LYS	P404	I464	F526	G586	I652	A715	W786	A852	L916	HIS	P1002
E284	GLY	I405	S465	R527	G587	K654	R716	Q791	N853	L917	MET	L1070
V285	GLY	D406	Q466	GLU	D588	V655	A717	E792	N854	L918	SER	V1071
E286	GLY	I407	N467	LYS	T589	V656	G718	E793	E854	L919	THR	L1077
V287	GLY	E408	D468	GLY	L590	L657	N719	L793	E855	L920	THR	L1078
V288	GLY	E409	R469	GLU	L591	D658	A720	W794	K856	L921	VAL	F1079
H289	GLY	E410	F471	GLY	E592	P659	H721	T795	N857	L922	LEU	Q1086
H290	GLY	R411	V472	P534	D593	K660	D722	Y797	F861	L923	SER	H1090
D291	GLY	P412	I413	L535	T594	N661	E723	K798	E862	L924	ASP	T1091
P292	GLY	I413	R414	V536	T595	S662	N724	F799	W863	L925	GLY	
C293	GLY	R414	L415	R537	T596	D663	I664	L665	W864	L926	ALA	
R294	GLY	L415	L475	L538	A597	I664	L665	I666	S865	L927	ALA	
G295	GLY	M416	L476	E539	L598	L665	I666	R667	L866	L928	ALA	
C296	GLY	L417	E477	E540	H600	R667	N601		A867	L929	ALA	
A297	GLY	G418	D478	L541						L930	ALA	
C298	GLY	T419	L479							L931	ALA	
H299	GLY	C420	V480							L932	ALA	
V300	GLY	P421	F481							L933	ALA	







L1988	L1994	A2002	L2003	M2004	R2007	H2008	D2009	R2015	L2016	L2017	L2018	R2021	P2022	Q2023	E2024	D2027	Y2033	L2034	Q2035	E2048	N2052	L2060	N2064	K2065	Q2066	V2074	L922	G1923	L1924	E1931	D1932	N1933	V1934	G1950	P1951	Q1956	H1962	E1963	S1964	I1978	M1986	D1987											
SER	LEU	GLY	PRO	SER	LEU	ARG	ARG	GLY	HIS	VAL	SER	GLU	ARG	VAL	GLN	SER	GLU	ASN	ASP	LEU	GLY	SER	GLN	PRO	PRO	HIS	GLU	ASP	ARG	GLU	PRO	VAL	ASP	PRO	THR	THR	LYS	GLY	ARG	VAL	ALA	ALA	PHE	SER	ILE	PRO	GLY	SER	ASN	ASN	LYS	GLN	
V1737	L1740	I1741	T1744	E1747	E1752	S1753	I1754	A1757	H1773	F1785	E1799	A1805	V1806	N1807	MET	ASN	ASP	LEU	GLY	SER	GLN	PRO	PRO	HIS	GLU	ASP	ARG	GLU	PRO	ARG	ASP	LEU	GLY	ASP	PRO	THR	THR	LYS	GLY	ARG	VAL	ALA	ALA	PHE	SER	ILE	PRO	GLY	SER	ASN	ASN	LYS	GLN
K1589	I1592	E1593	K1594	L1595	Q1596	L1602	L1606	L1609	V1610	L1626	Y1635	S1640	T1651	L1654	V1665	L1666	Q1670	L1695	R1698	LYS	THR	SER	ARG	GLU	PRO	ARG	ASP	GLY	ASP	ASP	LEU	PRO	ASP	ASP	LEU	PRO	ASP	PRO	ILE	GLY	THR	GLY	LEU	ASP	PRO	ASP	ASP	ASP	ASP	ASP	ASP	ASP	
H1518	V1522	I1526	A1530	M1531	V1532	A1533	K1534	A1537	I1538	L1539	L1540	P1541	M1542	D1543	L1544	D1545	A1546	H1547	I1548	S1549	S1550	M1551	L1552	S1553	S1554	G1555	A1556	S1557	C1558	A1559	A1560	A1561	A1562	Q1563	R1564	N1565	A1566	S1567	S1568	Y1569	K1570	A1571	S1572	T1573	R1574	A1575	F1576	P1577	V1578	T1580	P1581	T1582	A1583
Y1432	T1433	S1434	M1435	H1436	T1439	E1442	M1448	S1453	K1454	R1455	E1456	K1457	R1458	V1459	A1460	D1461	L1464	E1465	K1466	Y1467	V1468	L1469	S1470	Y1471	V1472	L1473	D1474	T1475	I1476	F1480	F1484	S1485	E1486	M1487	S1488	T1489	Q1492	T1493	H1494	Q1495	T1496	I1497	T1505	L1508	L1509	W1513	L1514	Q1515					
D1347	M1348	M1349	K1350	A1351	A1352	R1353	D1354	G1355	V1356	E1357	D1358	H1359	L1362	L1371	C1375	A1376	E1377	N1380	V1381	Y1382	I1385	K1386	C1387	T1388	S1389	L1393	E1394	D1395	V1396	V1397	T1401	H1402	E1403	D1404	T1407	E1408	V1409	K1410	Y1413	M1418	Y1421	V1426	E1427	M1428	K1429	E1430	I1431						
L1246	H1251	L1252	F1253	L1254	L1255	P1256	G1257	L1258	T1263	I1267	C1275	I1278	Q1284	V1287	H1288	L1289	L1290	A1291	T1292	H1296	V1297	Q1298	Y1299	L1300	I1307	E1310	K1315	M1322	T1326	N1327	A1328	G1329	D1330	V1334	N1337	D1338	K1339	A1340	S1341	L1342	A1343	H1344	L1345	L1346									
GLY	GLU	VAL	GLU	ALA	GLY	ALA	LYS	LYS	GLU	ARG	PRO	THR	ASP	GLU	GLU	GLY	PHE	LEU	HIS	PRO	PRO	GLY	GLU	LYS	SER	E1166	E1167	I1175	L1176	M1182	Q1188	M1206	L1209	L1210	O1211	I1212	D1215	K1216	G1217	D1218	A1219	K1220	M1221	M1222	T1228	C1236							
F1016	D1017	S1018	A1021	N1022	M1023	N1024	L1025	I1028	E1033	A1034	M1035	F1036	G1037	VAL	GLY	LYS	THR	SER	S1043	M1044	L1045	E1046	V1047	D1066	Y1067	A1068	P1069	L1070	V1071	L1077	R1085	Q1086	E1087	A1088	L1097	L1117	R1118	K1123	S1124	E1125	W1127	V1128	D1129	LYS	LYS	GLY	GLY	LYS					
LEU	SER	ARG	LYS	GLN	SER	VAL	PHE	ALA	PRO	SER	LEU	SER	ALA	ALA	GLU	PRO	LEU	LEU	ASP	ARG	SER	LYS	PHE	GLU	ASN	GLU	PRO	ALA	GLN	TRP	ASP	PRO	GLY	LYS	ASN	VAL	ARG	ARG	SER	ILE	GLN	GLY	VAL	GLY	HIS	MET	MET	SER	LYS	THR	MET	VAL	
S822	R823	K826	N832	T833	M834	E835	F851	E854	L866	A867	H868	I871	L881	L884	C894	VAL	GLN	GLY	PRO	PRO	ALA	MET	LEU	GLN	ALA	TRP	GLU	ASP	PRO	GLY	LYS	ASN	VAL	ARG	ARG	SER	ILE	GLN	GLY	VAL	GLY	HIS	MET	MET	SER	LYS	THR	MET	VAL				



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	85139	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	66	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	4300	Depositor
Magnification	29000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.885	Depositor
Minimum map value	-0.441	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	422.912, 422.912, 422.912	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.826, 0.826, 0.826	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: ZN, I3P, CA, ATP

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	0.11	0/16403	0.28	0/22156
1	B	0.11	0/16384	0.28	0/22131
1	C	0.11	0/16528	0.27	0/22327
1	D	0.11	0/16726	0.27	0/22603
All	All	0.11	0/66041	0.27	0/89217

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	16106	16244	16243	258	0
1	B	16087	16225	16224	258	0
1	C	16227	16344	16353	196	0
1	D	16421	16536	16535	217	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	24	9	9	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	9	9	1	0
3	C	24	9	9	1	0
3	D	24	9	9	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	31	12	12	0	0
5	B	31	12	12	0	0
5	C	31	12	12	0	0
5	D	31	12	12	0	0
All	All	65069	65433	65439	923	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 923 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:D:1962:HIS:HD1	1:D:1964:SER:HG	1.08	0.99
1:A:1962:HIS:HD1	1:A:1964:SER:HG	1.06	0.96
1:C:885:THR:HG22	1:C:978:ILE:HD13	1.48	0.93
1:A:729:TYR:CE1	1:A:733:LEU:HD21	2.04	0.92
1:C:2203:LEU:O	1:C:2207:ILE:HD12	1.73	0.89

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	1961/2671 (73%)	1930 (98%)	30 (2%)	1 (0%)	48 79

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1959/2671 (73%)	1933 (99%)	26 (1%)	0	100	100
1	C	1978/2671 (74%)	1951 (99%)	27 (1%)	0	100	100
1	D	2010/2671 (75%)	1979 (98%)	30 (2%)	1 (0%)	100	100
All	All	7908/10684 (74%)	7793 (98%)	113 (1%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1514	LEU
1	A	1697	ASN

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	1807/2385 (76%)	1805 (100%)	2 (0%)	88	91
1	B	1805/2385 (76%)	1804 (100%)	1 (0%)	88	91
1	C	1820/2385 (76%)	1819 (100%)	1 (0%)	88	91
1	D	1838/2385 (77%)	1836 (100%)	2 (0%)	88	91
All	All	7270/9540 (76%)	7264 (100%)	6 (0%)	87	91

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	703	HIS
1	D	1022	ASN
1	D	2297	VAL
1	A	2331	VAL
1	A	1731	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2579	ASN
1	D	1380	ASN
1	D	384	ASN
1	D	1096	GLN
1	D	1622	HIS

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 16 ligands modelled in this entry, 8 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	$\# Z > 2$
5	ATP	D	3004	-	32,33,33	0.26	0	48,52,52	0.67	0
3	I3P	D	3002	-	24,24,24	2.19	3 (12%)	39,39,39	0.85	0
5	ATP	C	3004	-	32,33,33	0.26	0	48,52,52	0.67	0
3	I3P	A	3002	-	24,24,24	2.19	3 (12%)	39,39,39	0.86	0
5	ATP	B	3004	-	32,33,33	0.26	0	48,52,52	0.67	0
3	I3P	C	3002	-	24,24,24	2.19	3 (12%)	39,39,39	0.86	0
5	ATP	A	3004	-	32,33,33	0.26	0	48,52,52	0.67	0
3	I3P	B	3002	-	24,24,24	2.19	3 (12%)	39,39,39	0.86	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
5	ATP	D	3004	-	-	5/22/38/38	0/3/3/3
3	I3P	D	3002	-	-	3/15/39/39	0/1/1/1
5	ATP	C	3004	-	-	10/22/38/38	0/3/3/3
3	I3P	A	3002	-	-	1/15/39/39	0/1/1/1
5	ATP	B	3004	-	-	6/22/38/38	0/3/3/3
3	I3P	C	3002	-	-	2/15/39/39	0/1/1/1
5	ATP	A	3004	-	-	7/22/38/38	0/3/3/3
3	I3P	B	3002	-	-	2/15/39/39	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3002	I3P	P4-O4	6.06	1.70	1.59
3	B	3002	I3P	P4-O4	6.06	1.70	1.59
3	A	3002	I3P	P4-O4	6.05	1.70	1.59
3	D	3002	I3P	P4-O4	6.05	1.70	1.59
3	D	3002	I3P	P5-O5	5.97	1.70	1.59

There are no bond angle outliers.

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	3004	ATP	C5'-O5'-PA-O2A
5	A	3004	ATP	C5'-O5'-PA-O3A
5	B	3004	ATP	C5'-O5'-PA-O2A
5	C	3004	ATP	PB-O3B-PG-O2G
5	C	3004	ATP	C5'-O5'-PA-O1A

There are no ring outliers.

4 monomers are involved in 4 short contacts:

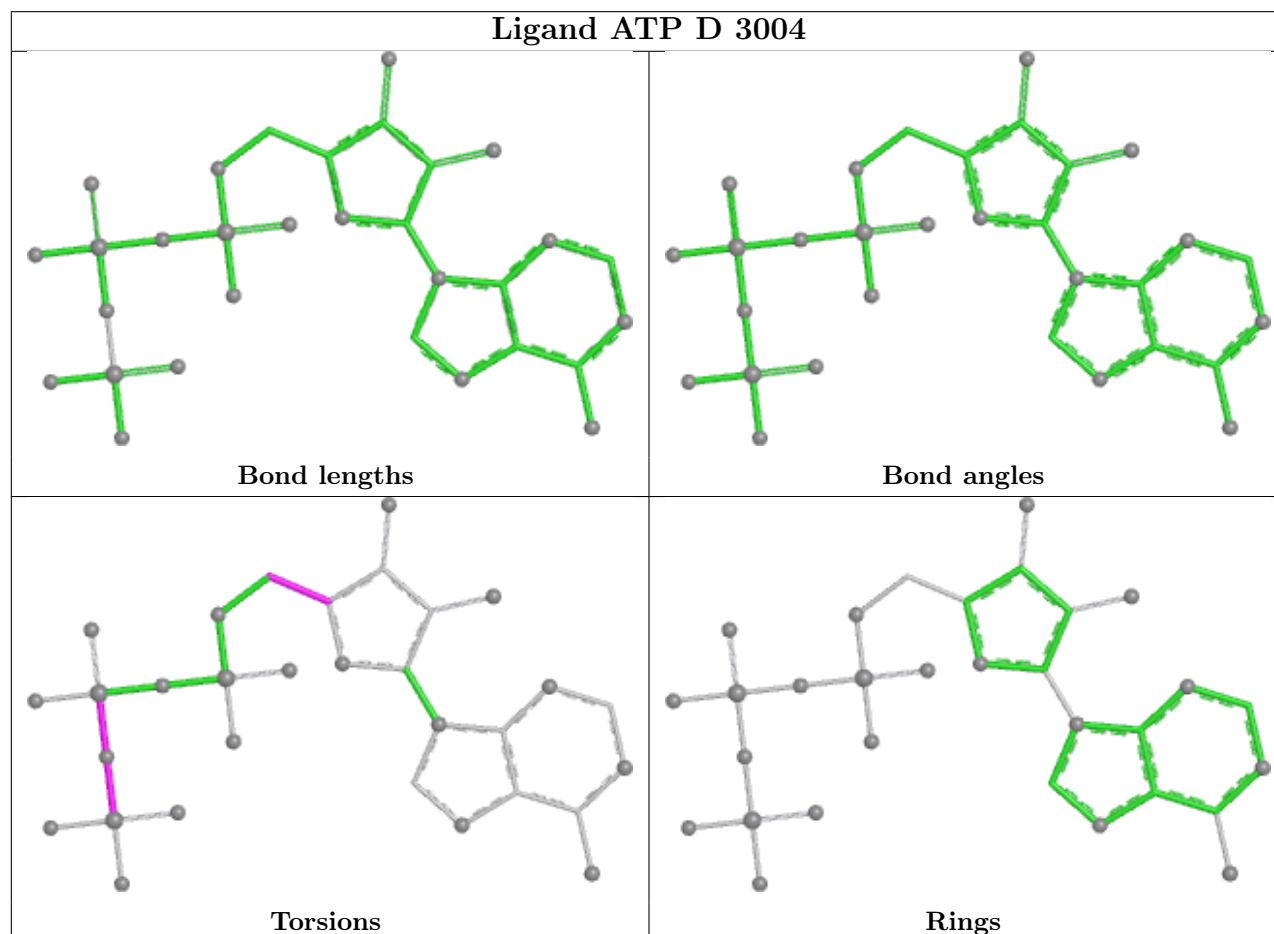
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	3002	I3P	1	0
3	A	3002	I3P	1	0
3	C	3002	I3P	1	0

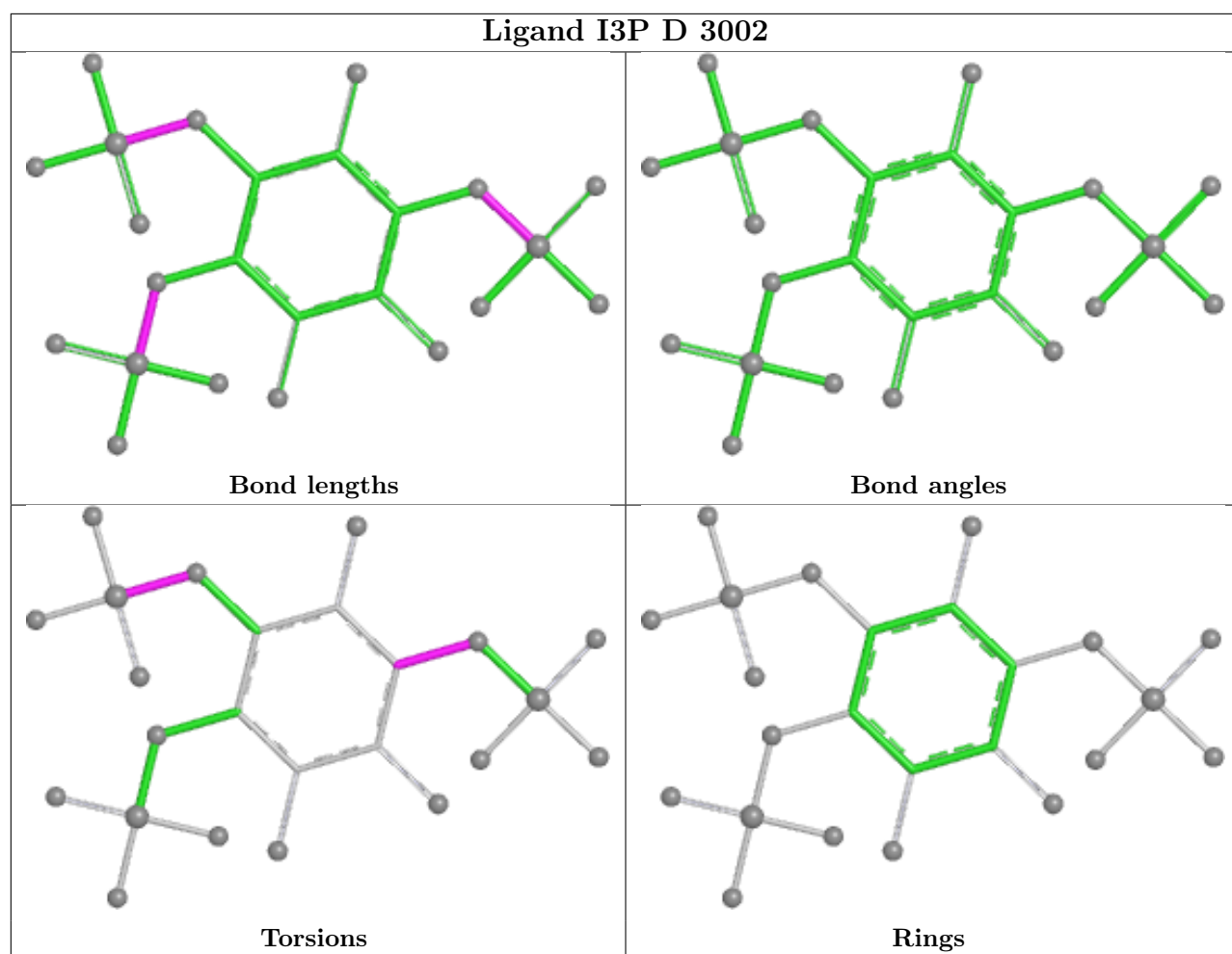
Continued on next page...

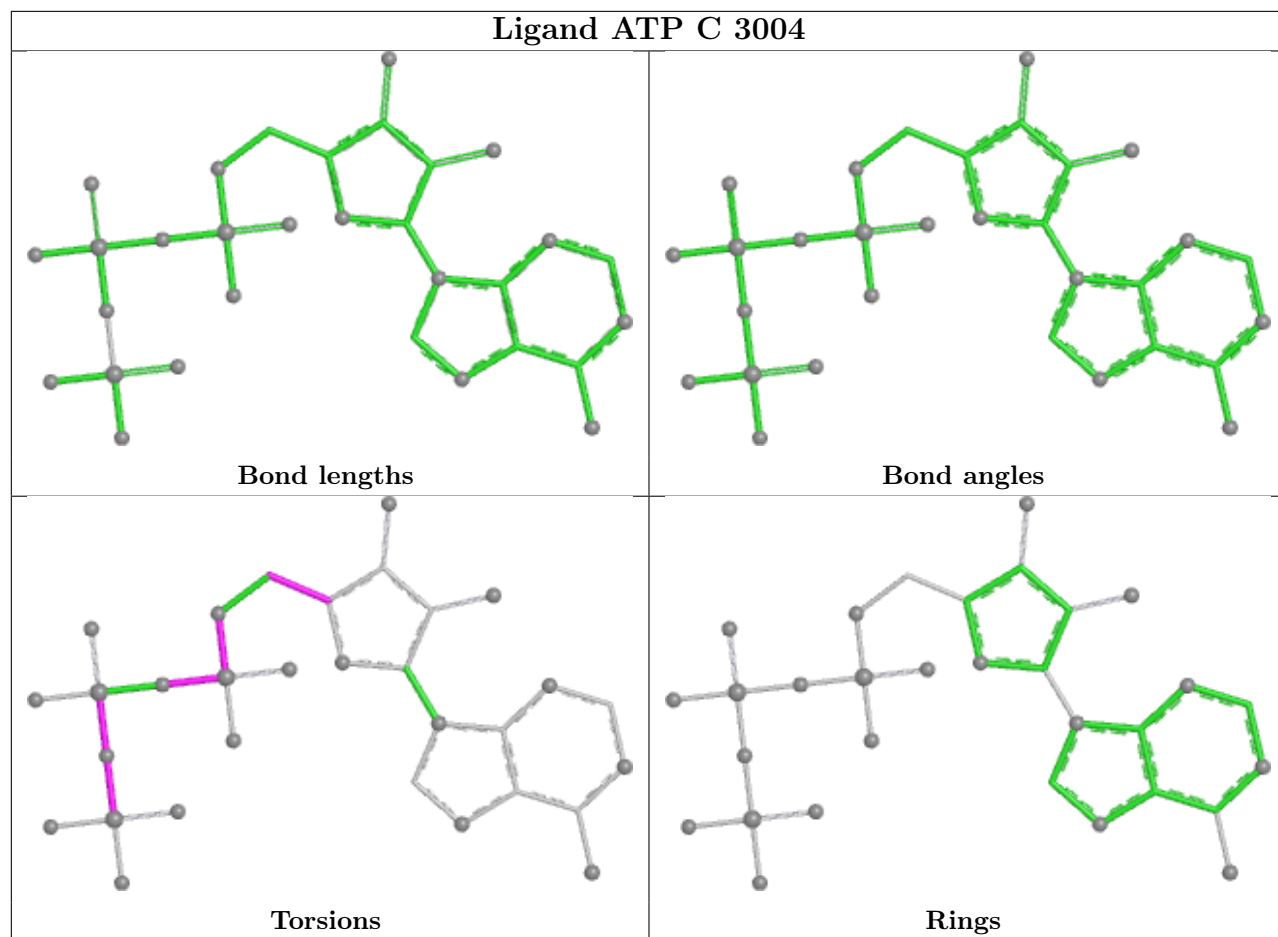
Continued from previous page...

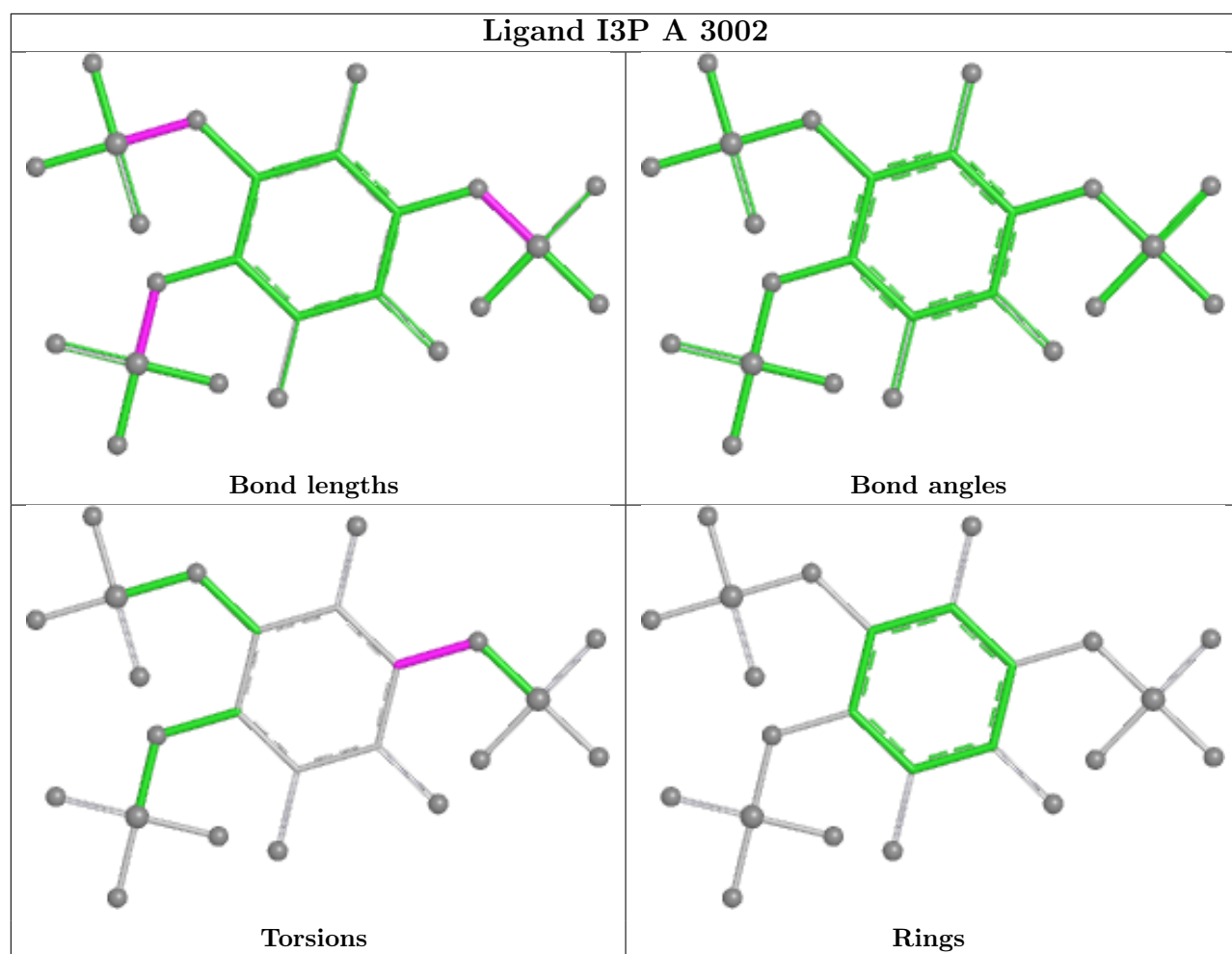
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	3002	I3P	1	0

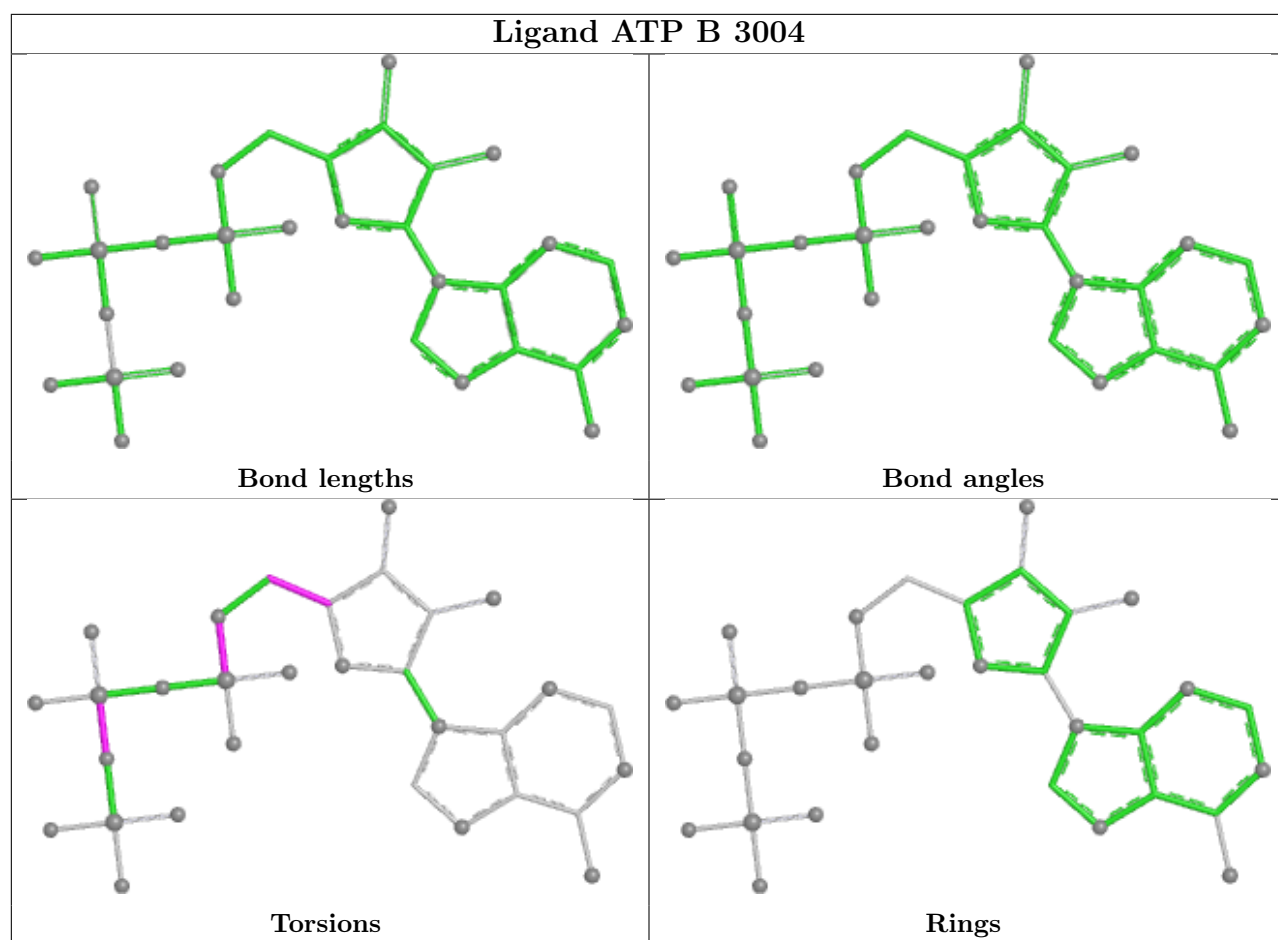
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

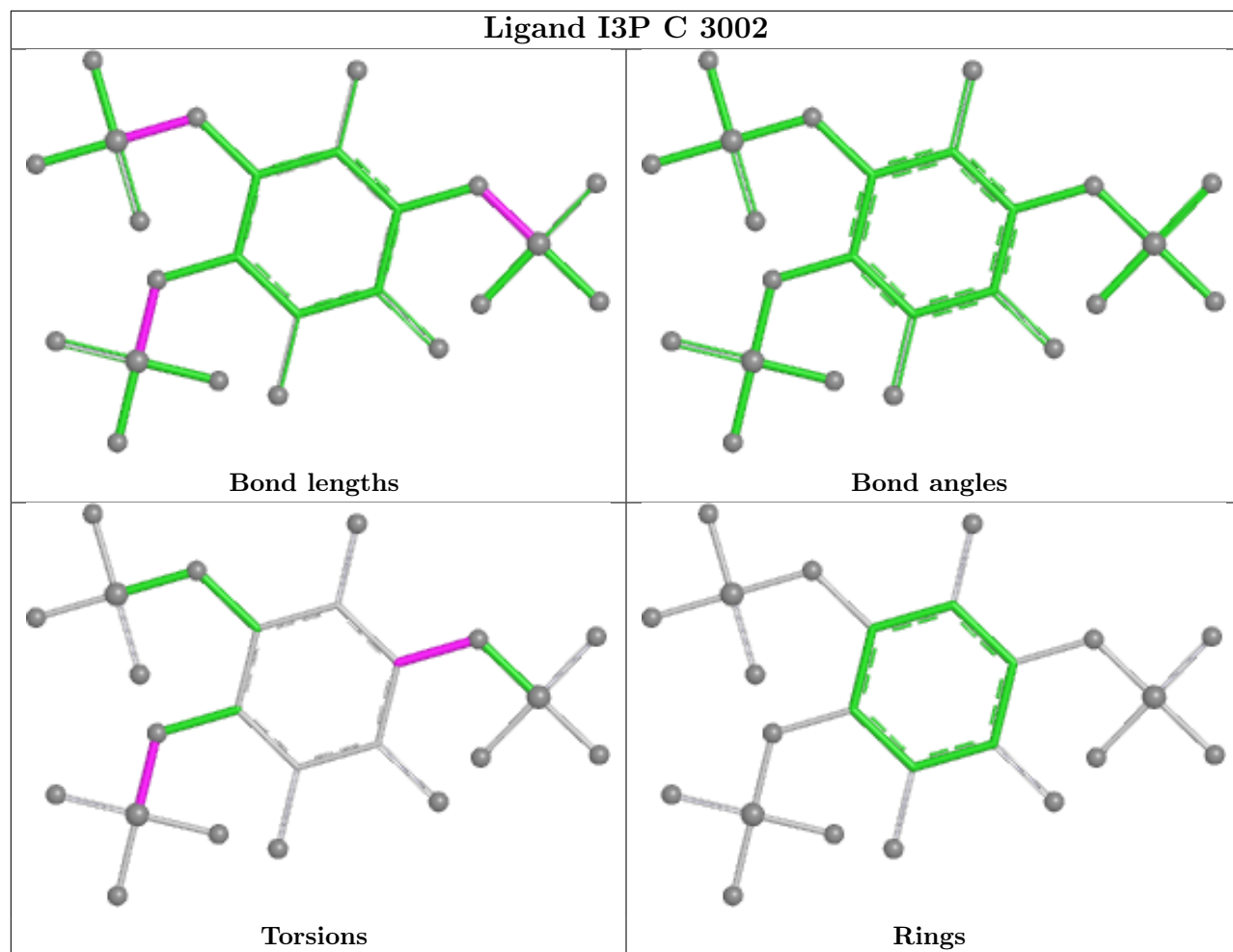


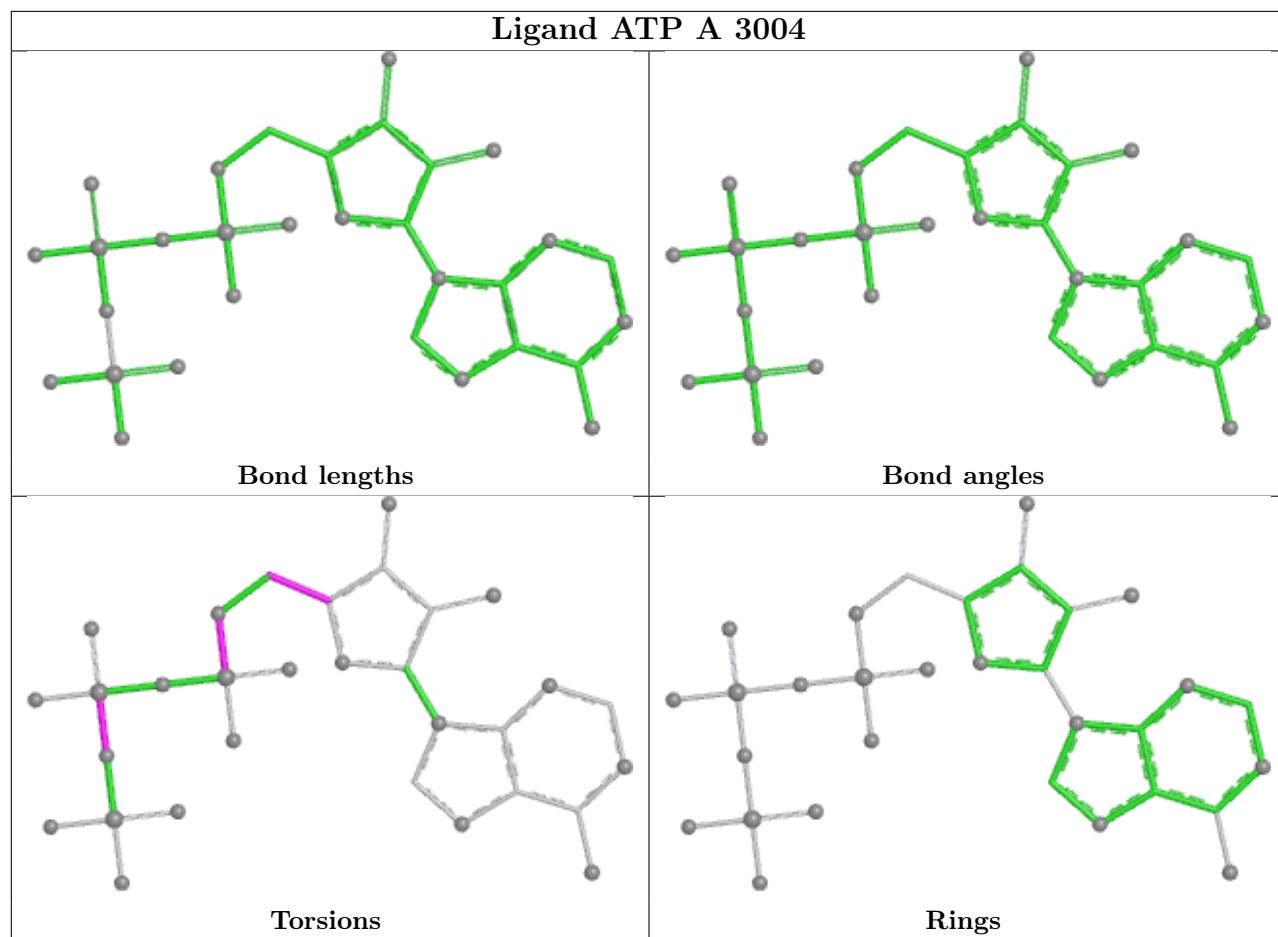


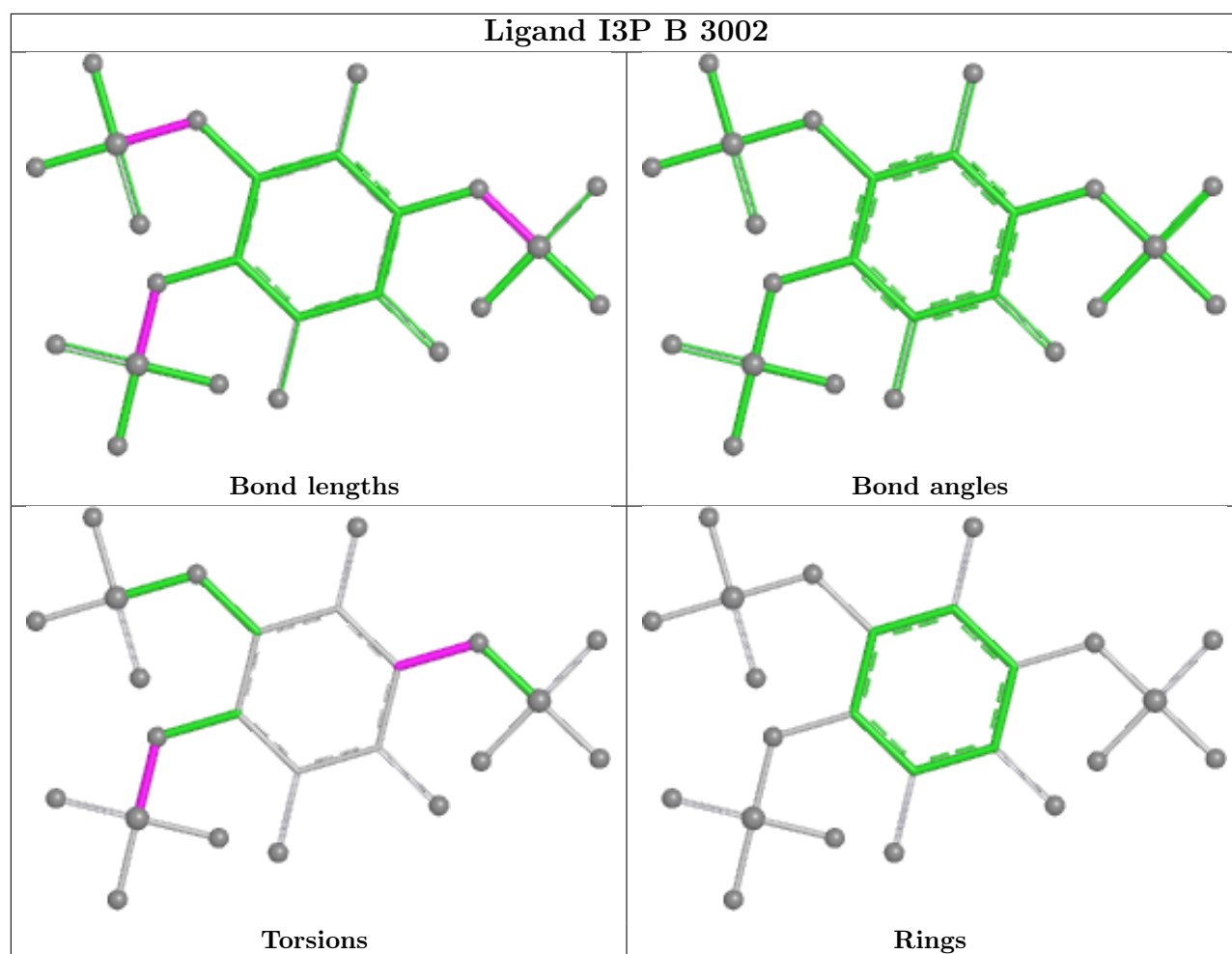












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

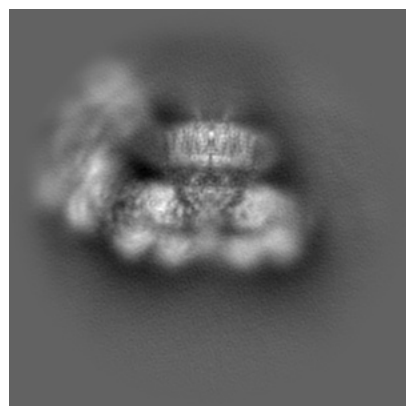
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41366. These allow visual inspection of the internal detail of the map and identification of artifacts.

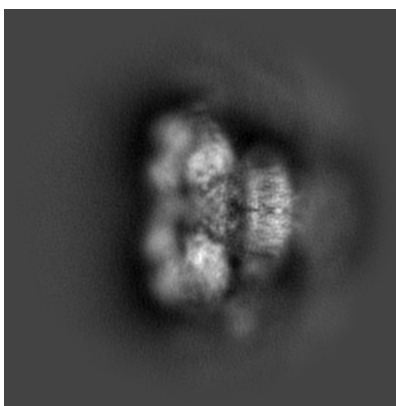
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

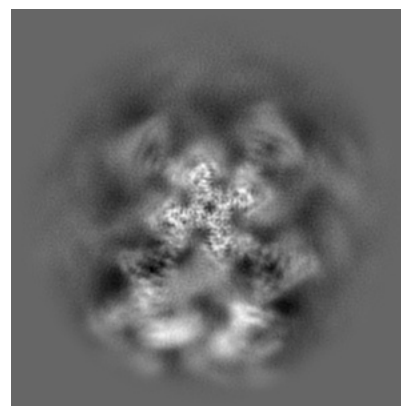
6.1.1 Primary map



X

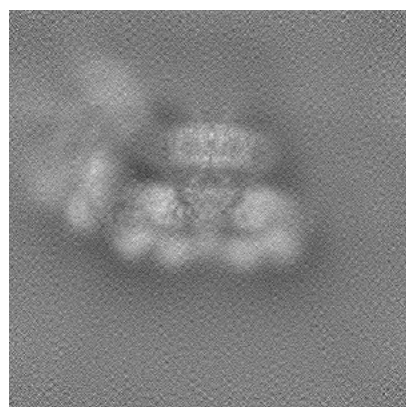


Y

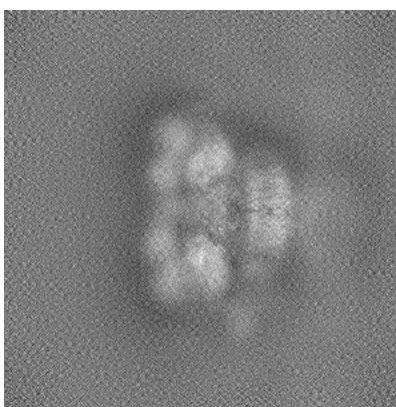


Z

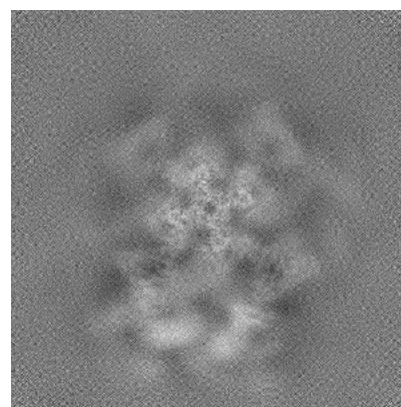
6.1.2 Raw map



X



Y

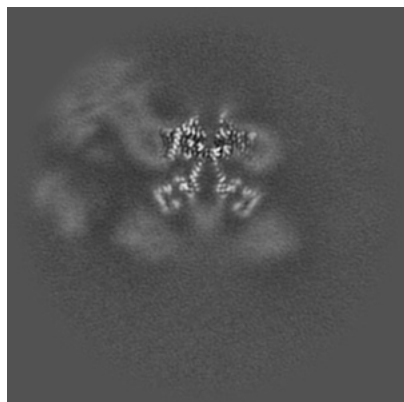


Z

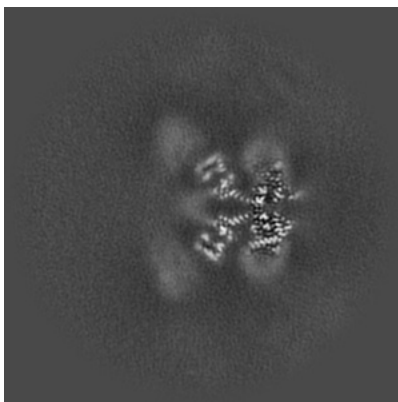
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

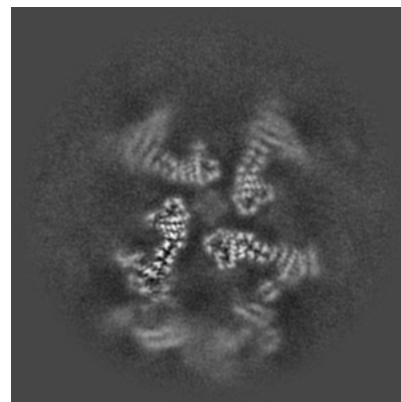
6.2.1 Primary map



X Index: 256

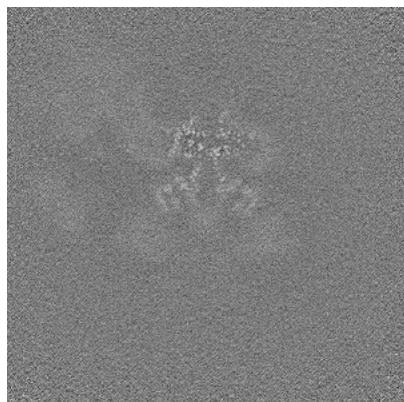


Y Index: 256



Z Index: 256

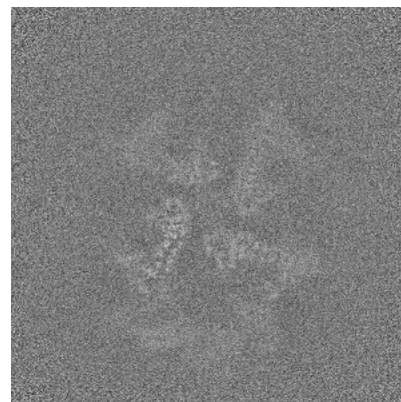
6.2.2 Raw map



X Index: 256



Y Index: 256

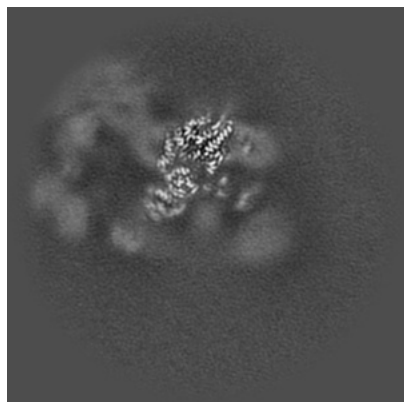


Z Index: 256

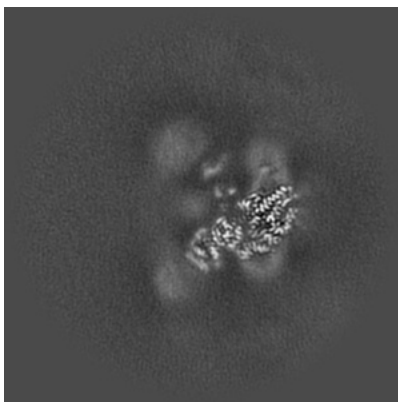
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

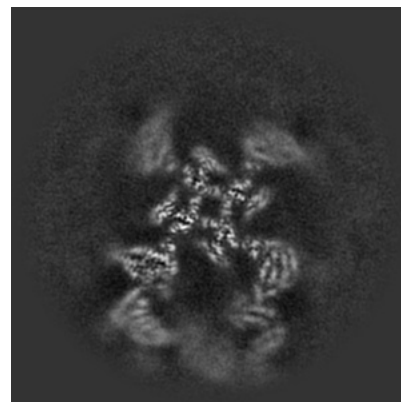
6.3.1 Primary map



X Index: 266

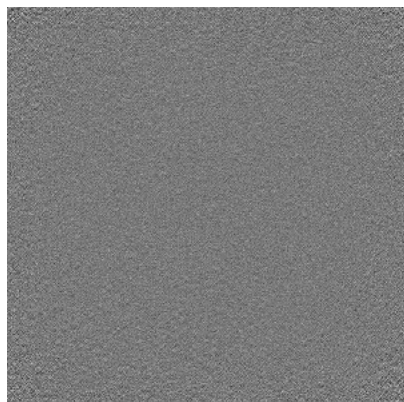


Y Index: 246

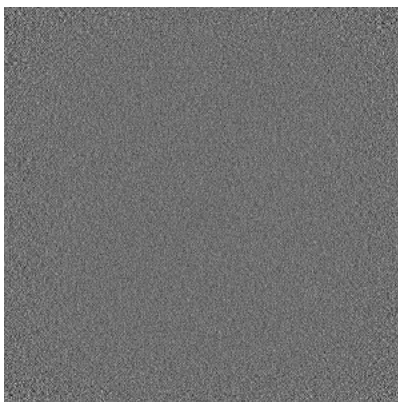


Z Index: 271

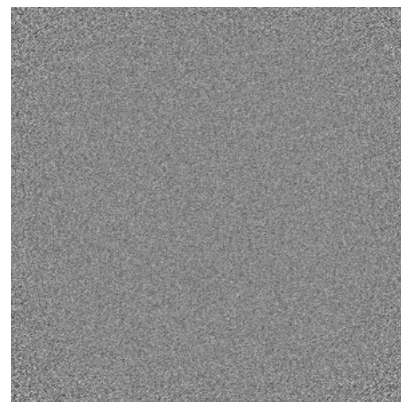
6.3.2 Raw map



X Index: 0



Y Index: 0

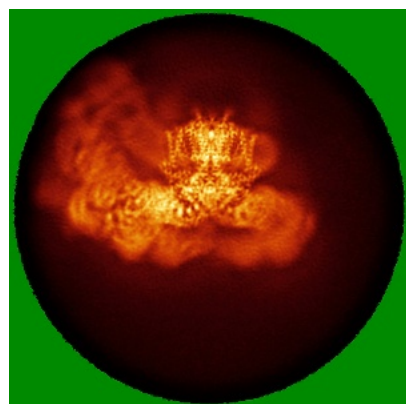


Z Index: 0

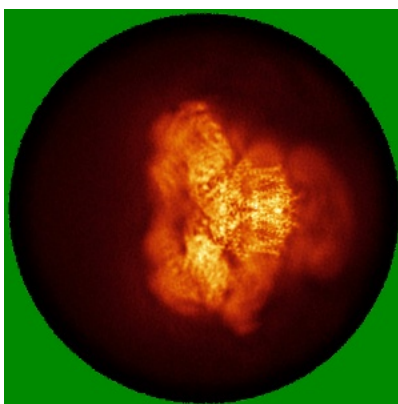
The images above show the largest variance slices of the map in three orthogonal directions.

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

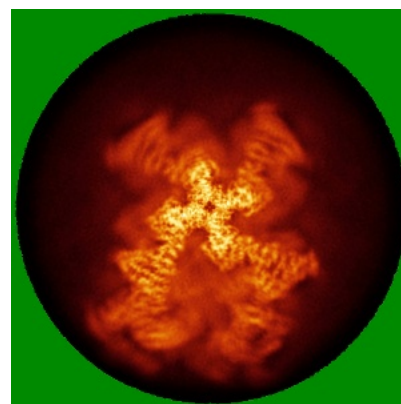
6.4.1 Primary map



X

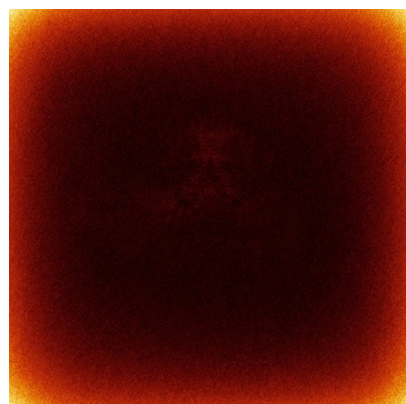


Y

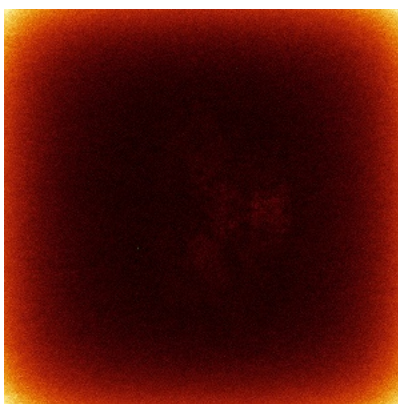


Z

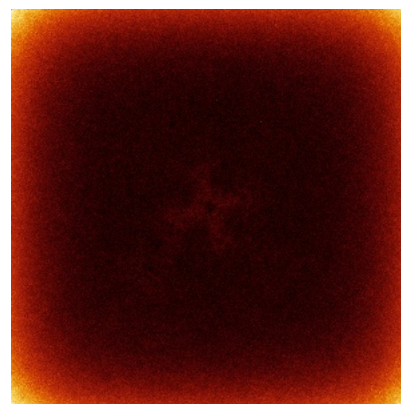
6.4.2 Raw map



X



Y

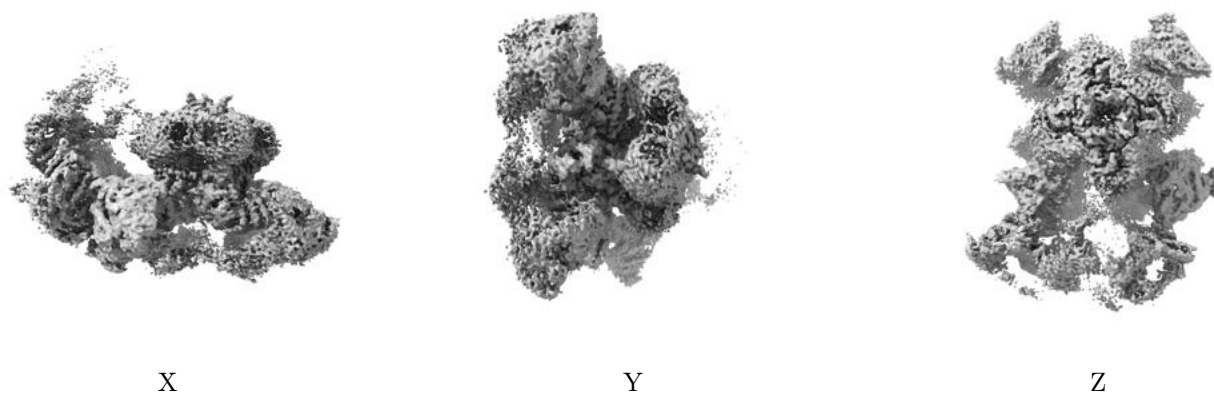


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

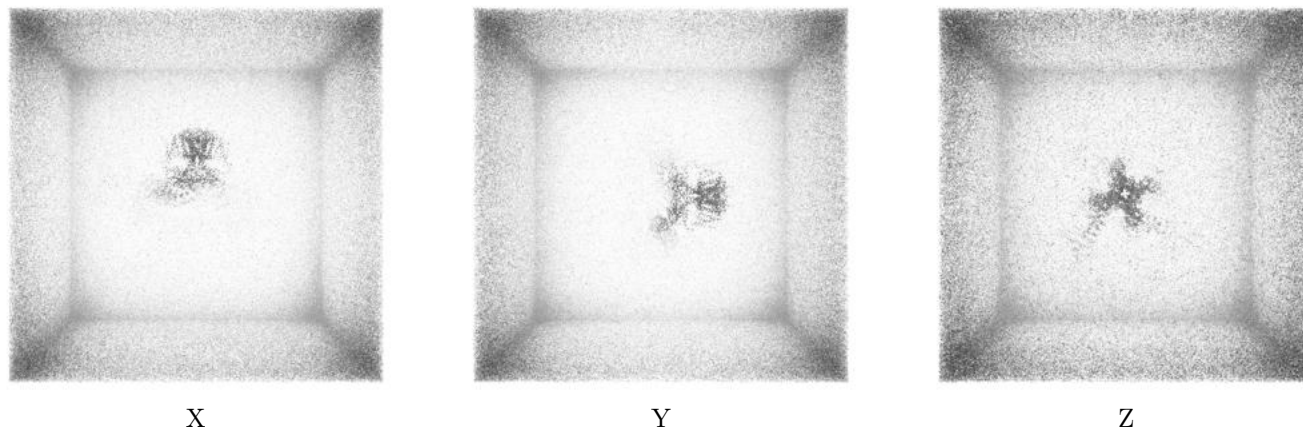
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

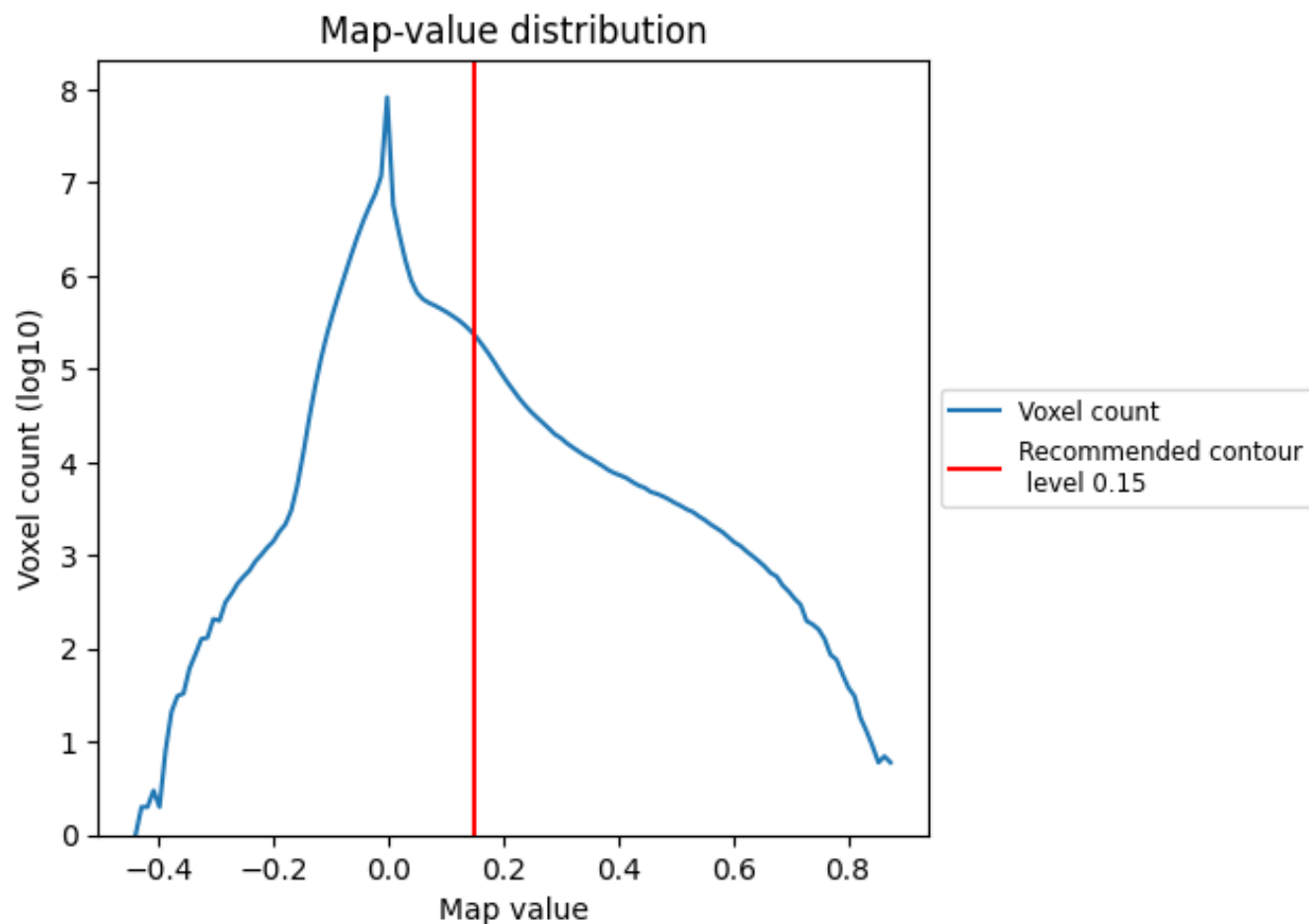
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

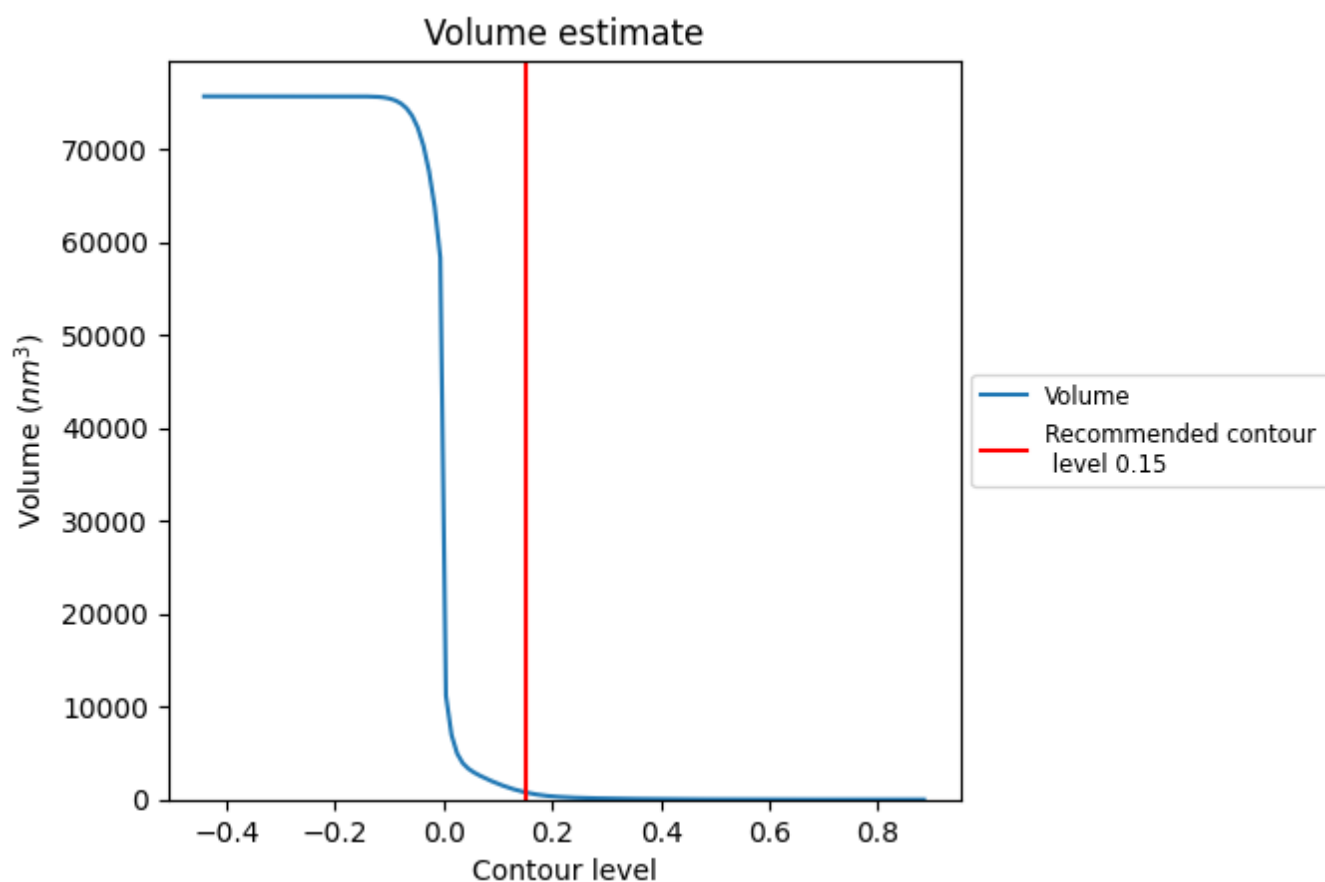
This section contains the results of statistical analysis of the map.

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.

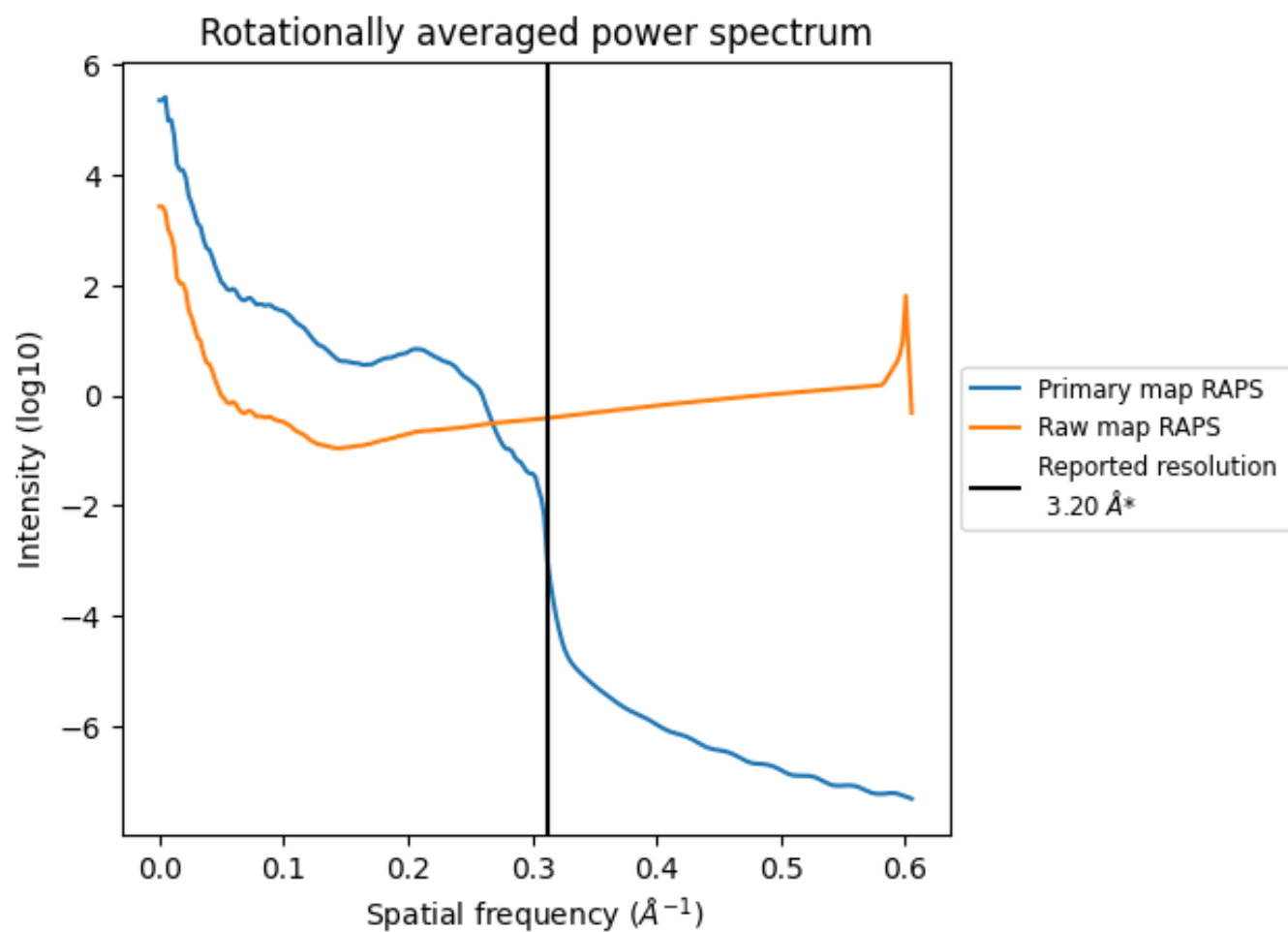
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 788 nm³; this corresponds to an approximate mass of 712 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 ⓘ

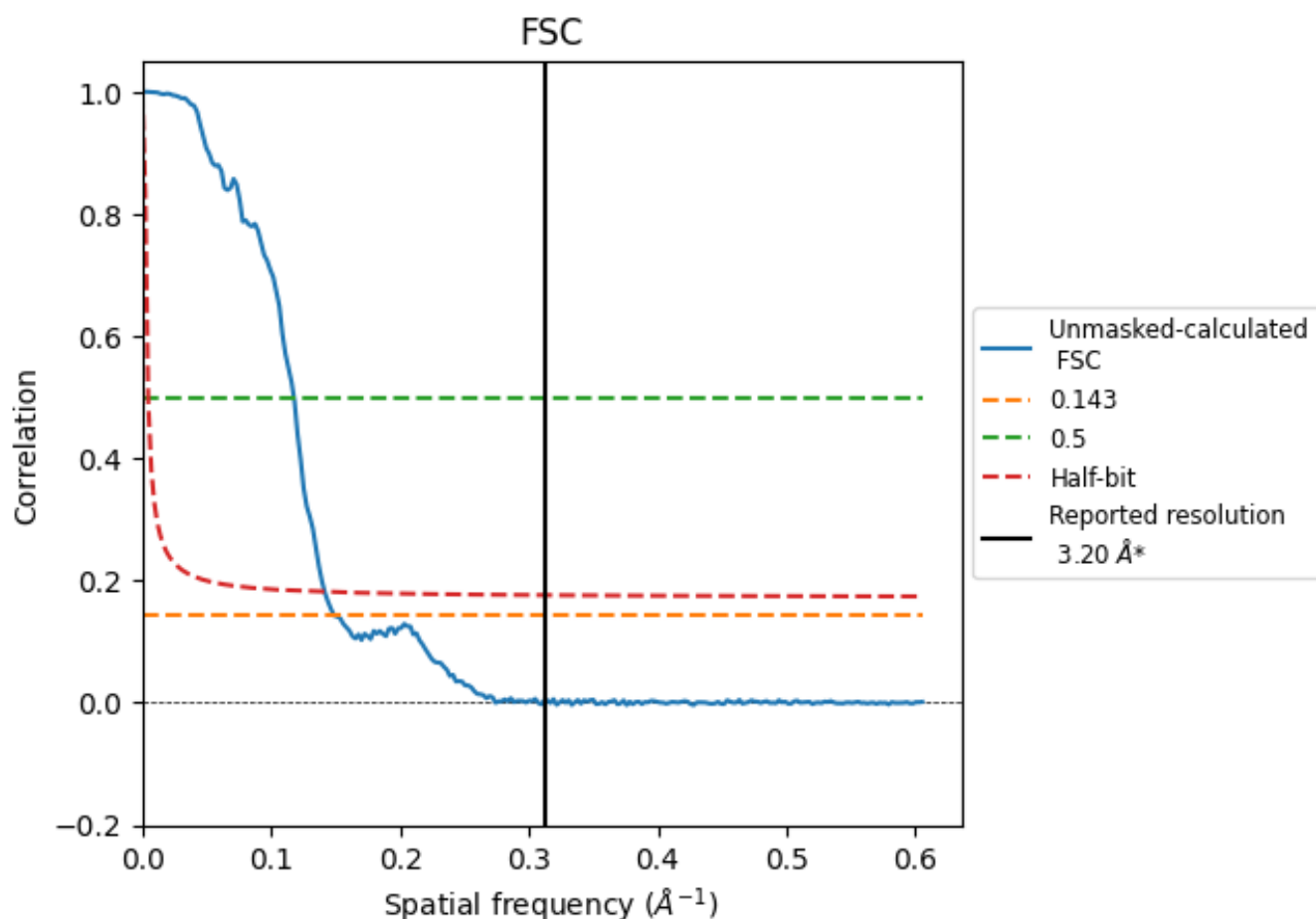


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

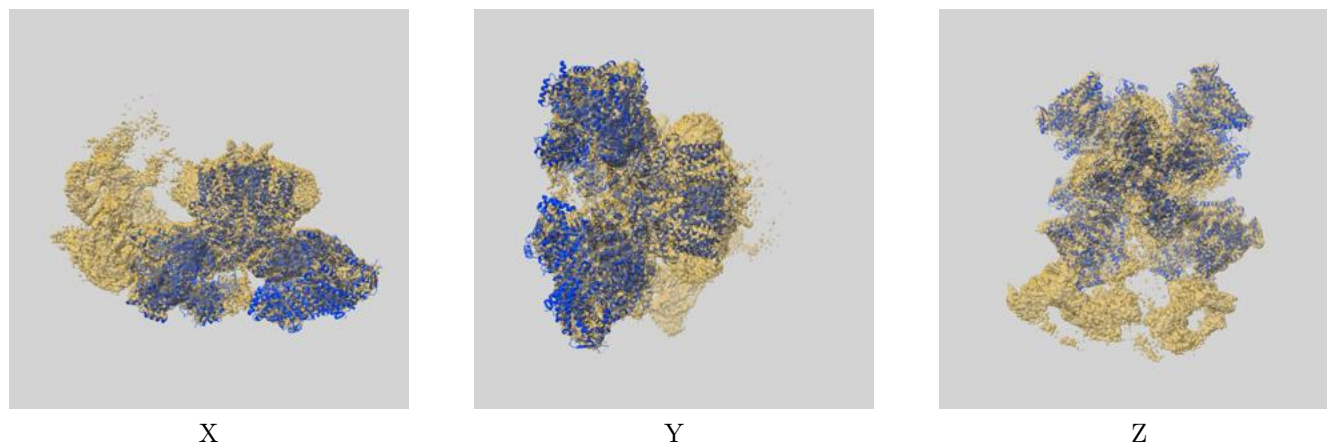
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.72	8.50	7.06

*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 6.72 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

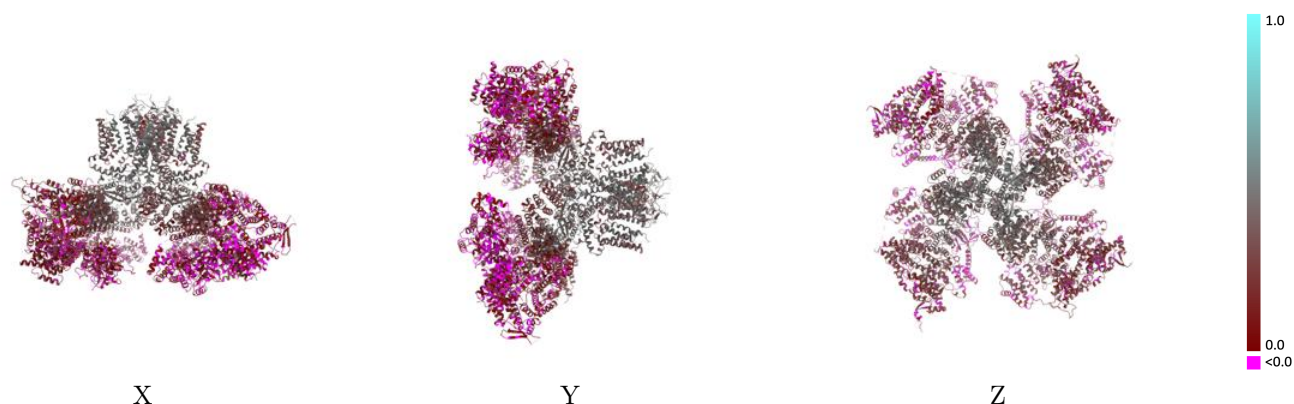
This section contains information regarding the fit between EMDB map EMD-41366 and PDB model 8TLA. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



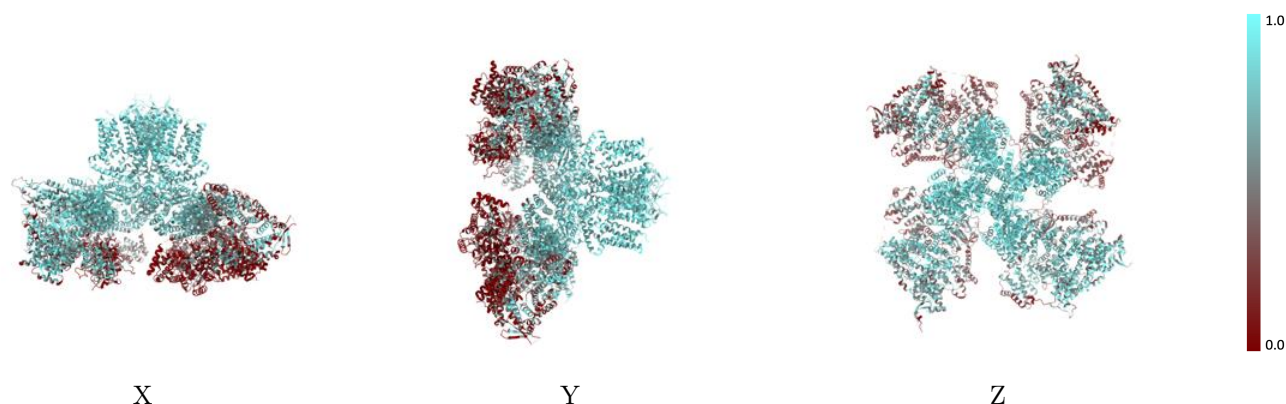
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



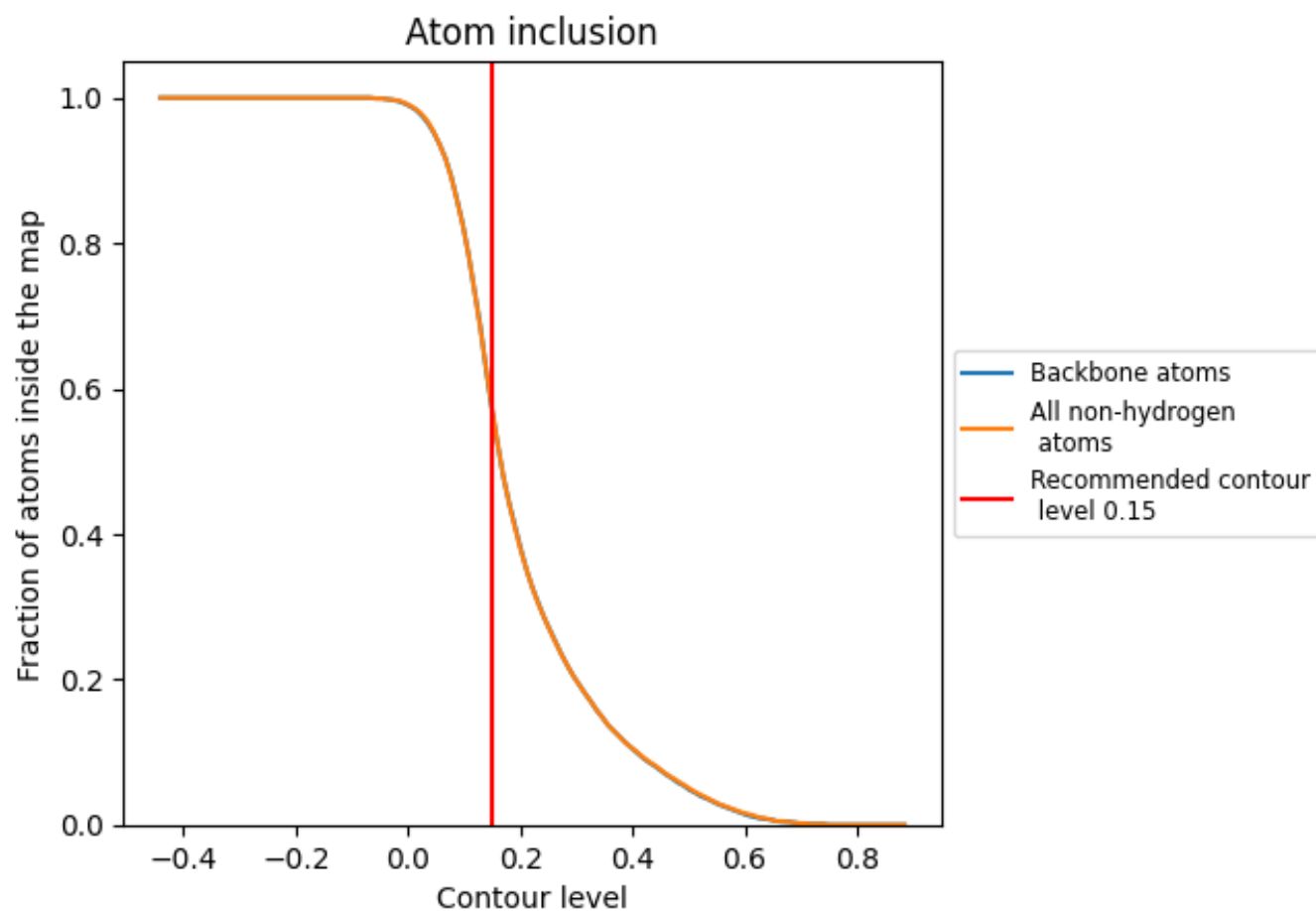
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 57% of all backbone atoms, 57% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5720	0.1980
A	0.5100	0.1710
B	0.4700	0.1640
C	0.6520	0.2320
D	0.6740	0.2250

