



## wwPDB EM Validation Summary Report ⓘ

Feb 8, 2025 – 07:59 PM EST

PDB ID : 9CGP  
EMDB ID : EMD-45584  
Title : RyR1 disease mutant Y523S with FKBP12.6, nanodisc and inhibitor dantrolene in the absence of calcium with refined P1 domain  
Authors : Iyer, K.A.; Samso, M.  
Deposited on : 2024-06-30  
Resolution : 3.34 Å(reported)  
Based on initial model : 7T64

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

---

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

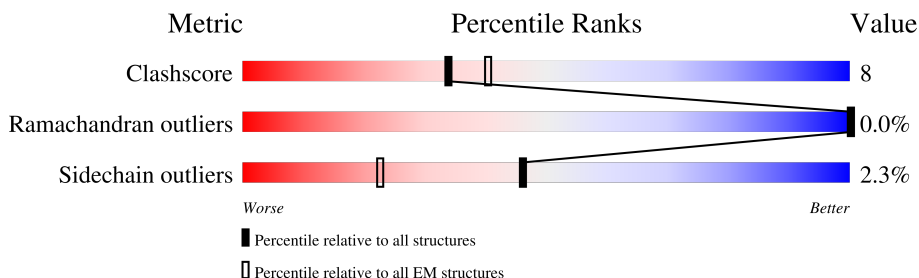
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

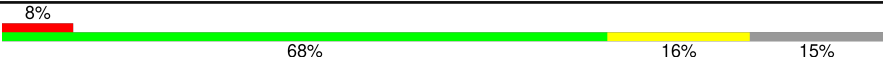




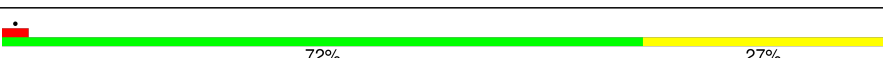


The reported resolution of this entry is 3.34 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	5037	
1	B	5037	
1	C	5037	
1	D	5037	
2	E	107	
2	F	107	
2	G	107	
2	H	107	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 132860 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 Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4258	Total 32374	C 20609	N 5541	O 6025	S 199	0	0
1	B	4258	Total 32374	C 20609	N 5541	O 6025	S 199	0	0
1	C	4258	Total 32374	C 20609	N 5541	O 6025	S 199	0	0
1	D	4258	Total 32374	C 20609	N 5541	O 6025	S 199	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	523	SER	TYR	engineered mutation	UNP P11716
B	523	SER	TYR	engineered mutation	UNP P11716
C	523	SER	TYR	engineered mutation	UNP P11716
D	523	SER	TYR	engineered mutation	UNP P11716

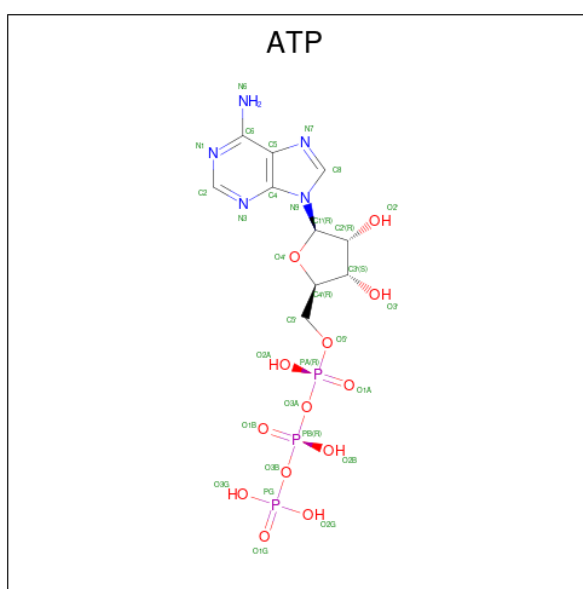
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total 786	C 498	N 137	O 148	S 3	0	0
2	F	107	Total 786	C 498	N 137	O 148	S 3	0	0
2	G	107	Total 786	C 498	N 137	O 148	S 3	0	0
2	H	107	Total 786	C 498	N 137	O 148	S 3	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

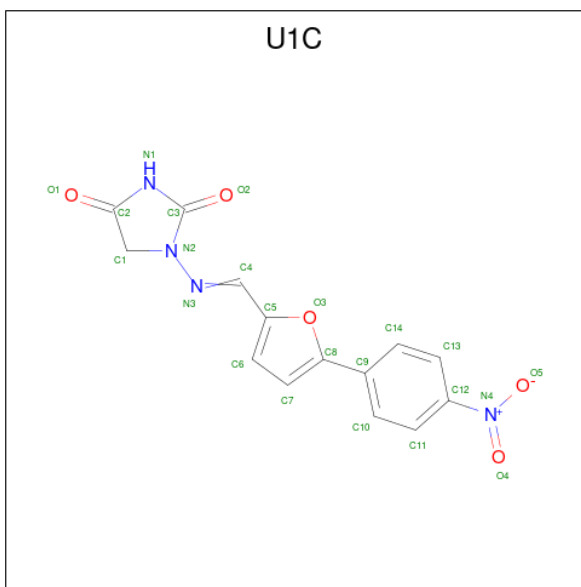
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is Dantrolene (three-letter code: U1C) (formula:  $C_{14}H_{10}N_4O_5$ ) (labeled as "Ligand of Interest" by depositor).

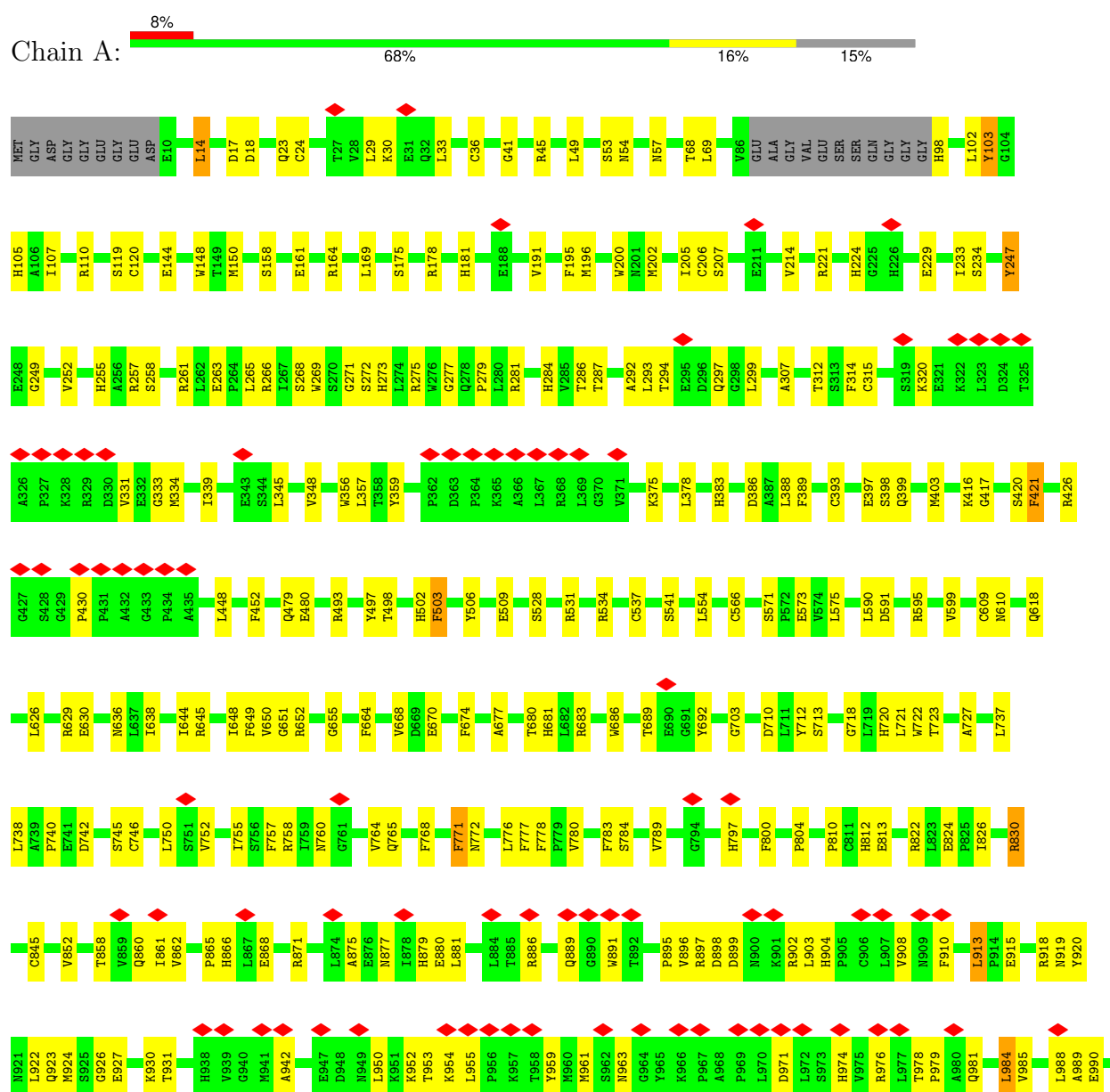


Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			23	14	4	5	
5	B	1	Total	C	N	O	0
			23	14	4	5	
5	C	1	Total	C	N	O	0
			23	14	4	5	
5	D	1	Total	C	N	O	0
			23	14	4	5	

### 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: Ryanodine receptor 1

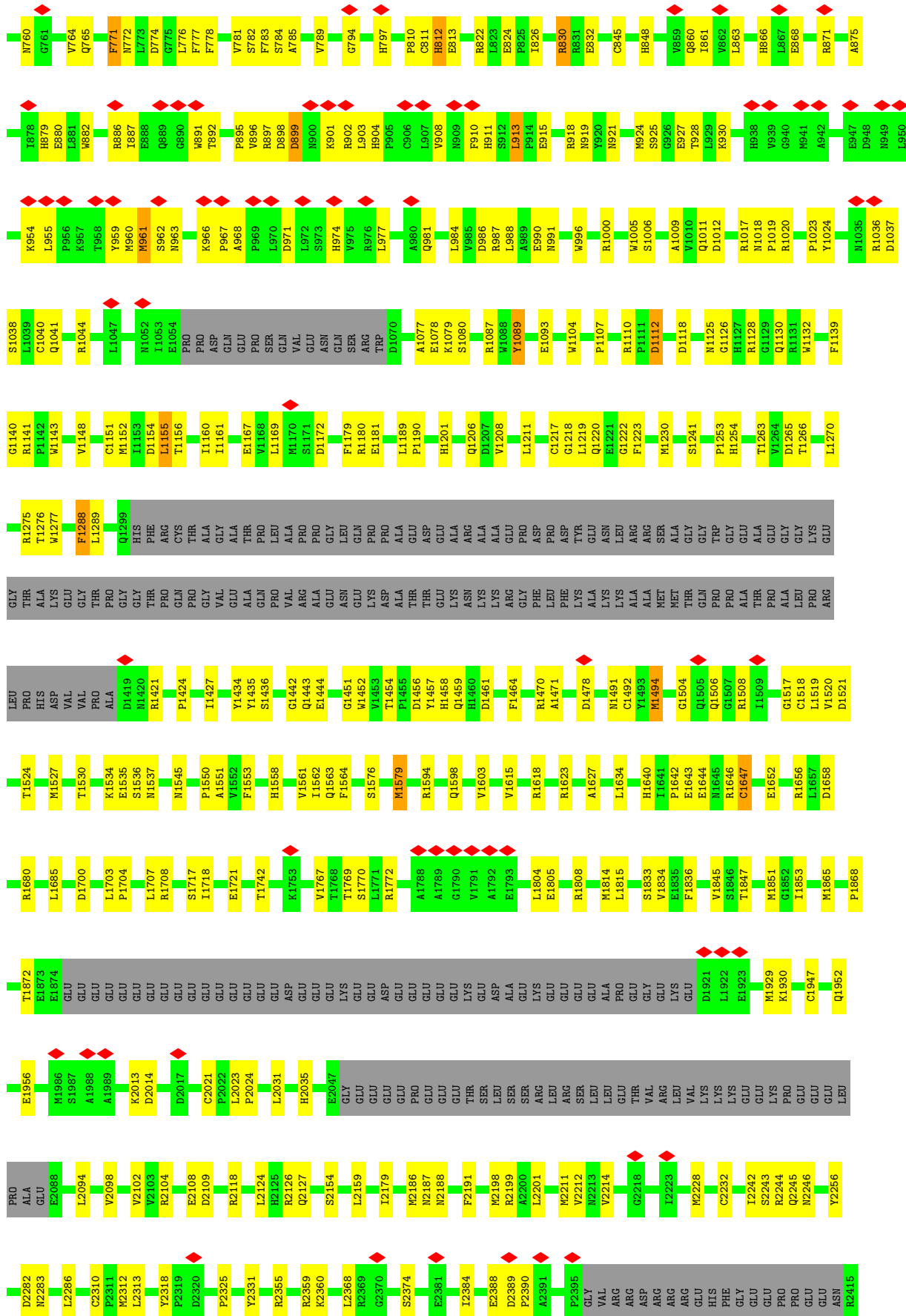


H993	E1093	E1221	TYR	LYS	N1482	V1615	M1814	GLU	SER	R2199	T2384	I2476	H2584
R1000	E1093	G1222	GLU	ALA	S1486	R1618	L1815	GLU	LEU	A2200	E2388	P2477	T2585
W1005	W1104	F1223	ASN	LYS	S1833	R1623	S1833	ALA	GLU	L2201	D2389	T2478	T2585
S1006	P1107	M1230	LEU	LYS	N1491	R1623	E1835	PRO	THR	M2211	D2390	L2478	R2591
A1009	R1110	S1241	ARG	ALA	M1494	A1627	F1836	GLY	VAL	V2212	A2391	L2478	S2594
V1010	P1111	P1253	ALA	THR	G1504	L1634	V1845	LYS	LEU	G2218	P2395	A2487	R2597
Q1011	D1112	H1254	GLY	GLN	Q1505	H1640	T1847	LYS	GLY	I2223	VAL	Q2487	C2606
D1012	D1118	T1263	TRP	PRO	R1508	P1642	L1848	LYS	LYS	M2228	ARG	S2491	L2607
I1013	D1118	T1266	GLY	PRO	I1509	E1643	V1850	GLU	GLU	L2233	ARG	S2491	I2614
V1022	N1125	T1266	ALA	THR	G1517	E1643	M1851	LYS	GLU	M2238	ASP	A2492	R2615
P1023	G1126	L1270	GLU	PRO	C1518	E1644	M1865	PRO	PRO	L2236	ARG	S2492	P2618
Y1024	W1132	L1270	GLY	LEU	L1519	E1646	P1868	ARG	GLU	L2266	ARG	F2494	S2617
L1027	F1139	R1275	LYS	PRO	D1521	C1647	P1868	GLU	GLU	I2242	ARG	D2497	N2618
D1028	G1140	T1276	GLY	ARG	T1524	E1652	T1872	LEU	LEU	S2243	HIS	A2500	L2622
K1032	W1143	W1277	THR	LEU	M1527	R1656	E1873	GLU	PRO	R2244	PHE	A2500	L2626
N1035	V1148	V1284	LYS	HIS	M1527	D1658	E1874	ALA	ALA	Q2245	GLY	L2506	L2626
R1036	C1151	F1288	GLY	VAL	T1530	M1678	E1874	GLU	GLU	N2246	GLU	L2507	L2627
L1039	M1152	L1289	THR	PRO	T1530	N1678	E1874	GLU	ALA	M2250	PRO	L2508	F2628
R1044	I1153	Q1299	GLY	ALA	E1535	D1700	E1874	GLU	GLU	Y2256	GLU	L2509	L2633
L1047	D1154	PHE	THR	ASP	S1536	L1703	E1874	GLU	GLU	L2257	GLU	L2509	R2650
G1048	T1156	ARG	PRO	VAL	N1537	P1704	E1874	GLU	GLU	L2258	ASN	L2510	C2651
N1052	I1160	CYS	GLN	VAL	N1545	L1707	E1874	GLU	GLU	V2275	GLU	D2516	R2652
E1054	I1161	THR	GLY	VAL	L1548	R1708	E1874	GLU	GLU	D2282	GLU	L2519	Y2654
PRO	L1169	ALA	ALA	PRO	F1549	R1708	E1874	GLU	GLU	N2283	GLU	H2520	R2657
ASP	M1170	ALA	GLN	GLY	P1550	S1717	E1874	GLU	GLU	L2286	PRO	V2524	T2659
ASN	S1171	LEU	GLN	ASP	A1551	E1721	E1874	GLU	GLU	C2310	PRO	L2527	N2663
GLN	D1172	PRO	VAL	VAL	V1554	T1742	E1874	GLU	GLU	M2311	GLU	M2530	L2672
GLU	F1179	ALA	ALA	ALA	L1555	K1753	E1874	GLU	GLU	L2312	GLU	R2531	R2677
PRO	R1180	PRO	GLY	GLY	H1558	V1767	E1874	GLU	GLU	L2313	GLU	L2536	C2681
SER	E1181	LEU	ASN	ASN	V1561	T1769	E1874	GLU	GLU	Y2318	GLU	L2536	K2677
GLN	L1189	GLN	GLN	GLN	I1562	A1788	E1874	GLU	GLU	P2319	GLU	L2536	L2681
VAL	P1190	ALA	GLY	ALA	Q1563	A1789	E1874	GLU	GLU	D2320	GLU	A2547	R2690
THR	H1201	ASP	THR	THR	F1564	T1772	E1874	GLU	GLU	P2325	GLU	L2550	TYR
ASP	Q1206	GLU	THR	THR	T1572	S1576	E1874	GLU	GLU	Y2331	GLU	L2556	ASP
TRP	D1207	ASP	THR	THR	S1579	M1579	E1874	GLU	GLU	R2355	GLU	L2556	GLN
A1077	S1209	ARG	LYS	LYS	P1593	P1593	E1874	GLU	GLU	R2359	GLU	L2556	LEU
E1078	L1210	ALA	LYS	LYS	R1470	A1792	E1874	GLU	GLU	L2368	GLU	L2556	TYR
K1079	L1211	ALA	ARG	ARG	A1471	E1793	E1874	GLU	GLU	R2369	GLU	L2556	ARG
S1080	C1217	PRO	GLY	GLY	G1477	E1805	E1874	GLU	GLU	G2370	GLU	L2556	ARG
R1087	L1219	PRO	PHE	PHE	D1478	R1808	E1874	GLU	GLU	S2374	GLU	L2556	ALA
W1088	Q1220	ASP	LEU	LEU				GLU	GLU		GLU	L2556	ALA
Y1089								ARG	ARG		GLU	L2556	ALA

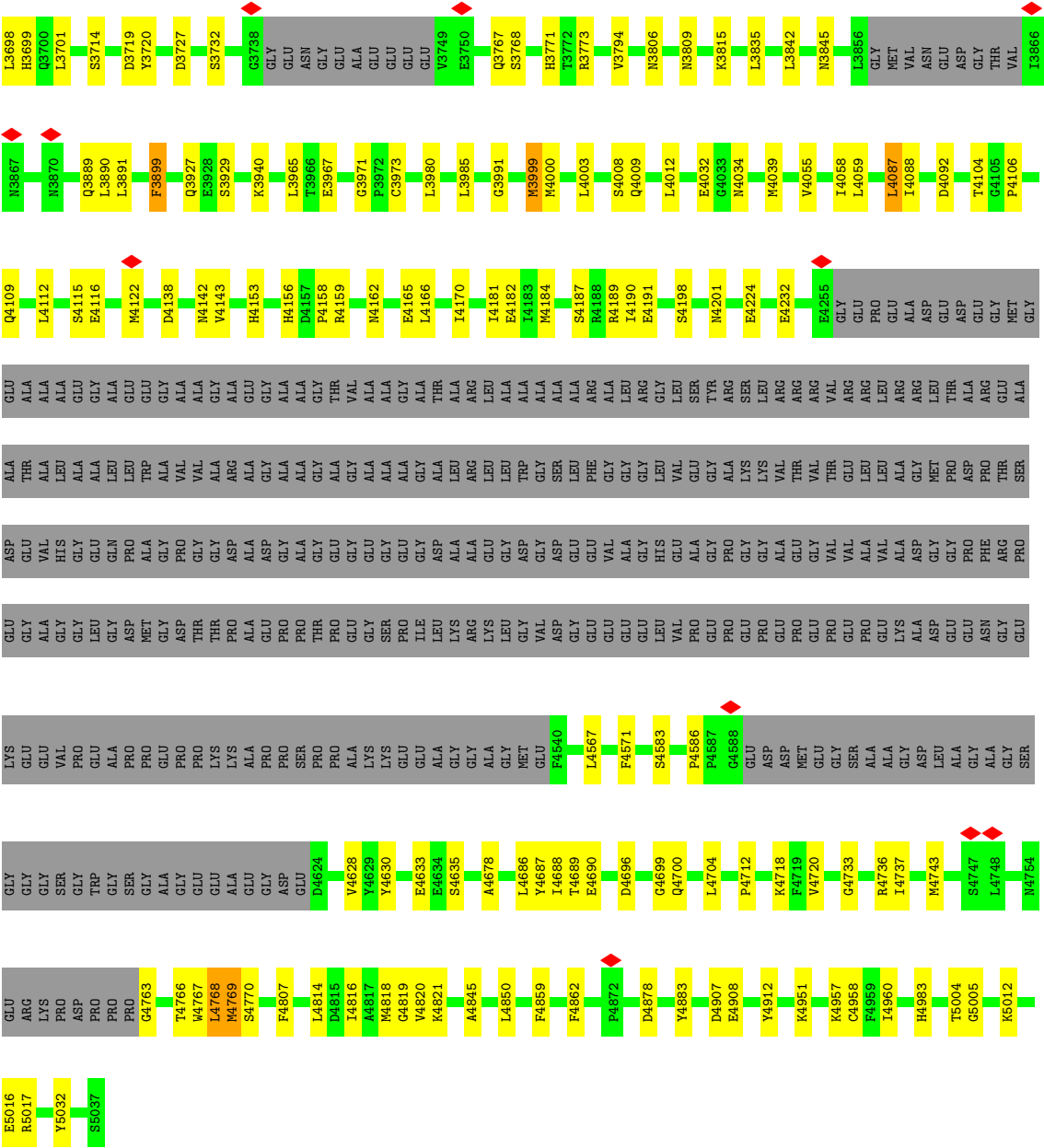




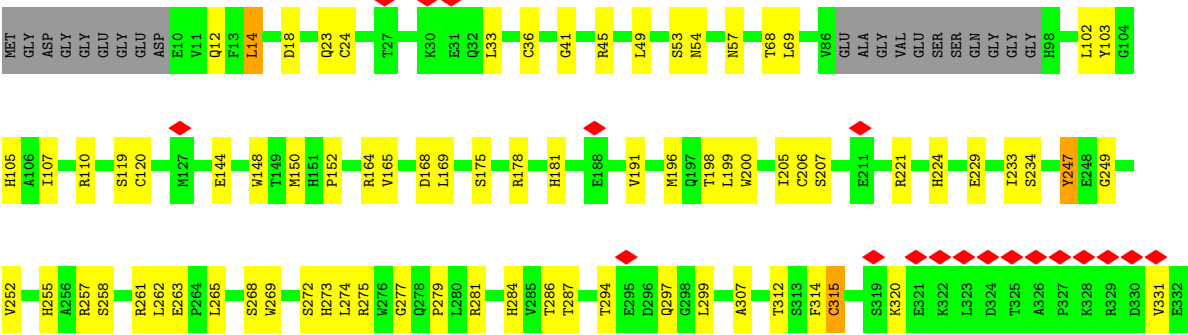


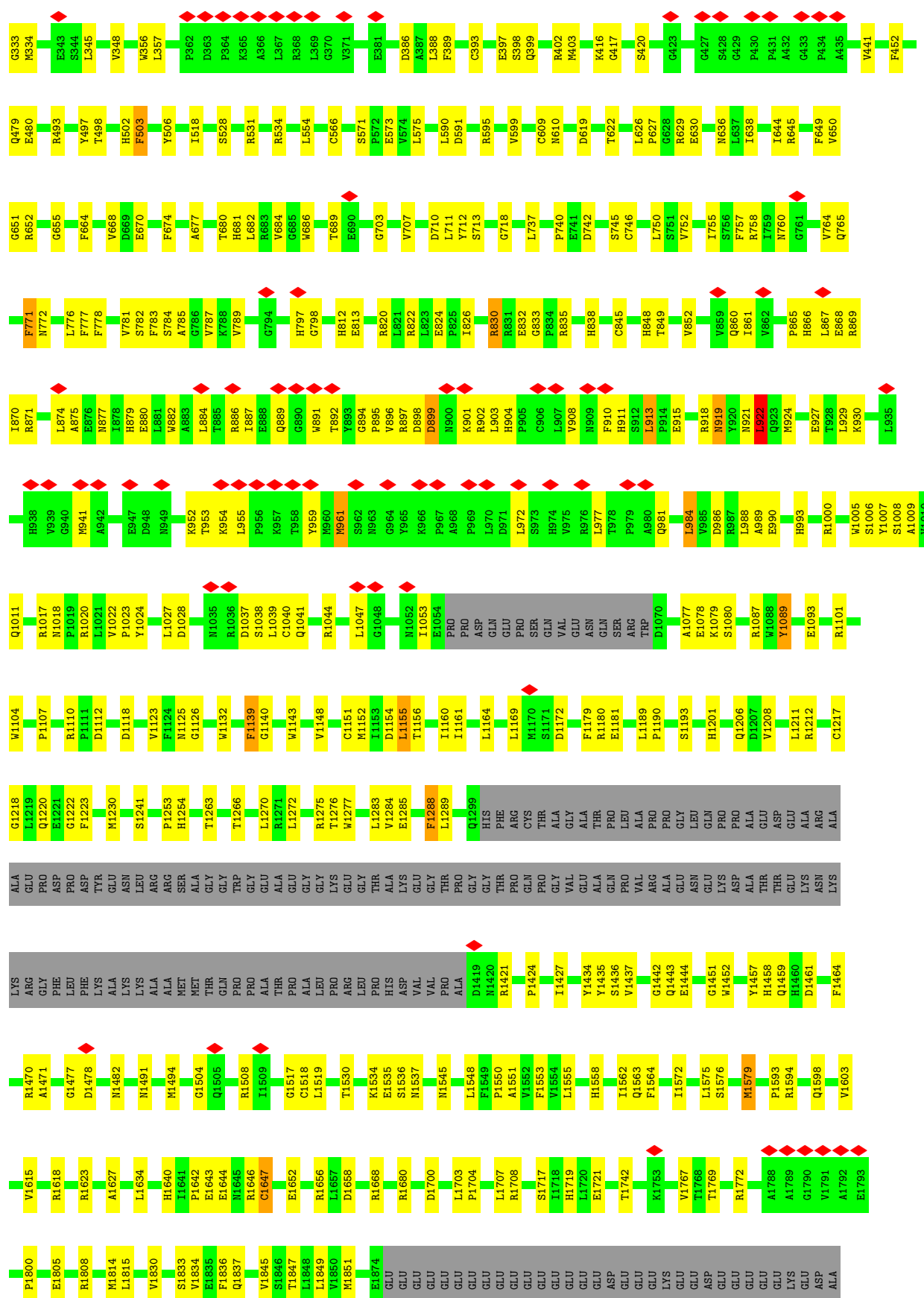






● Molecule 1: Ryanodine receptor 1











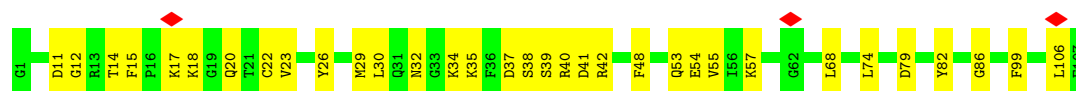




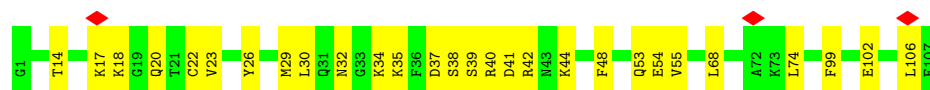




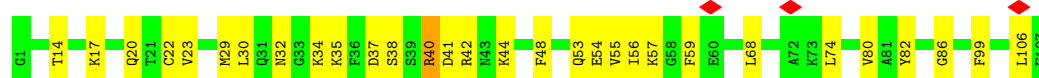
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



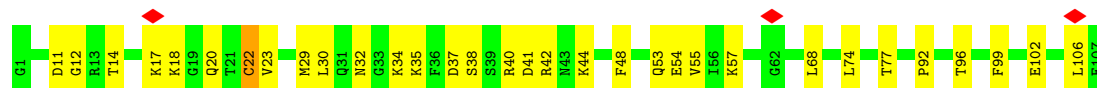
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	249034	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.277	Depositor
Minimum map value	0.000	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.072	Depositor
Recommended contour level	0.32	Depositor
Map size ( $\text{\AA}$ )	501.12003, 501.12003, 501.12003	wwPDB
Map dimensions	464, 464, 464	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.08, 1.08, 1.08	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ATP, U1C

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.25	0/33082	0.48	3/45015 (0.0%)
1	B	0.24	0/33082	0.47	2/45015 (0.0%)
1	C	0.24	0/33082	0.48	4/45015 (0.0%)
1	D	0.25	0/33082	0.48	5/45015 (0.0%)
2	E	0.26	0/802	0.52	0/1086
2	F	0.27	0/802	0.54	0/1086
2	G	0.27	0/802	0.55	0/1086
2	H	0.26	0/802	0.52	0/1086
All	All	0.25	0/135536	0.48	14/184404 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3003	LEU	CA-CB-CG	7.13	131.69	115.30
1	C	3003	LEU	CA-CB-CG	7.11	131.64	115.30
1	D	3003	LEU	CA-CB-CG	7.03	131.48	115.30
1	A	3003	LEU	CA-CB-CG	7.00	131.39	115.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	922	LEU	CA-CB-CG	6.73	130.77	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	626	LEU	Peptide
1	B	626	LEU	Peptide
1	C	626	LEU	Peptide
1	D	626	LEU	Peptide

## 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	32374	0	30869	505	0
1	B	32374	0	30869	488	0
1	C	32374	0	30869	498	0
1	D	32374	0	30869	514	0
2	E	786	0	766	22	0
2	F	786	0	766	20	0
2	G	786	0	766	21	0
2	H	786	0	766	26	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	31	0	12	0	0
4	B	31	0	12	0	0
4	C	31	0	12	0	0
4	D	31	0	12	0	0
5	A	23	0	0	0	0
5	B	23	0	0	0	0
5	C	23	0	0	0	0
5	D	23	0	0	0	0
All	All	132860	0	126588	2070	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 8.

The worst 5 of 2070 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:830:ARG:HD3	1:D:1612:PHE:CE2	1.70	1.26
1:D:1454:THR:CG2	1:D:1456:ASP:OD1	2.09	0.99
1:D:830:ARG:CD	1:D:1612:PHE:CE2	2.45	0.99
1:D:1454:THR:HG23	1:D:1456:ASP:OD1	1.63	0.97
1:B:4763:GLY:N	1:B:4766:THR:HG1	1.62	0.95

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	4214/5037 (84%)	3883 (92%)	329 (8%)	2 (0%)	100	100
1	B	4214/5037 (84%)	3873 (92%)	340 (8%)	1 (0%)	100	100
1	C	4214/5037 (84%)	3878 (92%)	334 (8%)	2 (0%)	100	100
1	D	4214/5037 (84%)	3886 (92%)	327 (8%)	1 (0%)	100	100
2	E	105/107 (98%)	90 (86%)	15 (14%)	0	100	100
2	F	105/107 (98%)	89 (85%)	16 (15%)	0	100	100
2	G	105/107 (98%)	89 (85%)	16 (15%)	0	100	100
2	H	105/107 (98%)	90 (86%)	15 (14%)	0	100	100
All	All	17276/20576 (84%)	15878 (92%)	1392 (8%)	6 (0%)	100	100

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	862	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	899	ASP
1	A	1023	PRO
1	C	1023	PRO
1	D	1023	PRO

### 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	3334/4276 (78%)	3266 (98%)	68 (2%)	50	72
1	B	3334/4276 (78%)	3244 (97%)	90 (3%)	40	65
1	C	3334/4276 (78%)	3260 (98%)	74 (2%)	47	70
1	D	3334/4276 (78%)	3259 (98%)	75 (2%)	47	70
2	E	80/88 (91%)	78 (98%)	2 (2%)	42	67
2	F	80/88 (91%)	79 (99%)	1 (1%)	65	79
2	G	80/88 (91%)	79 (99%)	1 (1%)	65	79
2	H	80/88 (91%)	79 (99%)	1 (1%)	65	79
All	All	13656/17456 (78%)	13344 (98%)	312 (2%)	46	69

5 of 312 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	4807	PHE
1	D	3003	LEU
1	D	315	CYS
1	D	1143	TRP
1	D	4156	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	2005	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	D	2176	ASN
1	D	3837	GLN
1	B	2112	GLN
1	B	2005	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 12 ligands modelled in this entry, 4 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	ATP	B	5102	-	28,33,33	0.66	0	34,52,52	0.58	1 (2%)
5	U1C	D	5103	-	23,25,25	6.20	12 (52%)	26,35,35	3.19	9 (34%)
5	U1C	B	5103	-	23,25,25	6.19	12 (52%)	26,35,35	3.20	9 (34%)
5	U1C	A	5103	-	23,25,25	6.21	12 (52%)	26,35,35	3.20	9 (34%)
4	ATP	C	5102	-	28,33,33	0.63	0	34,52,52	0.59	1 (2%)
5	U1C	C	5103	-	23,25,25	6.21	12 (52%)	26,35,35	3.18	9 (34%)
4	ATP	A	5102	-	28,33,33	0.65	0	34,52,52	0.58	1 (2%)
4	ATP	D	5102	-	28,33,33	0.65	0	34,52,52	0.58	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
4	ATP	B	5102	-	-	9/18/38/38	0/3/3/3
5	U1C	D	5103	-	-	1/7/25/25	0/3/3/3
5	U1C	B	5103	-	-	1/7/25/25	0/3/3/3
5	U1C	A	5103	-	-	1/7/25/25	0/3/3/3
4	ATP	C	5102	-	-	9/18/38/38	0/3/3/3
5	U1C	C	5103	-	-	1/7/25/25	0/3/3/3
4	ATP	A	5102	-	-	9/18/38/38	0/3/3/3
4	ATP	D	5102	-	-	9/18/38/38	0/3/3/3

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	5103	U1C	C1-N2	-18.77	1.32	1.45
5	A	5103	U1C	C1-N2	-18.76	1.32	1.45
5	D	5103	U1C	C1-N2	-18.64	1.32	1.45
5	B	5103	U1C	C1-N2	-18.59	1.32	1.45
5	B	5103	U1C	C1-C2	-10.54	1.39	1.51

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	5103	U1C	C2-C1-N2	8.41	106.93	101.45
5	B	5103	U1C	C2-C1-N2	8.40	106.92	101.45
5	A	5103	U1C	C2-C1-N2	8.38	106.91	101.45
5	D	5103	U1C	C2-C1-N2	8.37	106.90	101.45
5	B	5103	U1C	C1-N2-C3	-7.36	108.27	112.31

There are no chirality outliers.

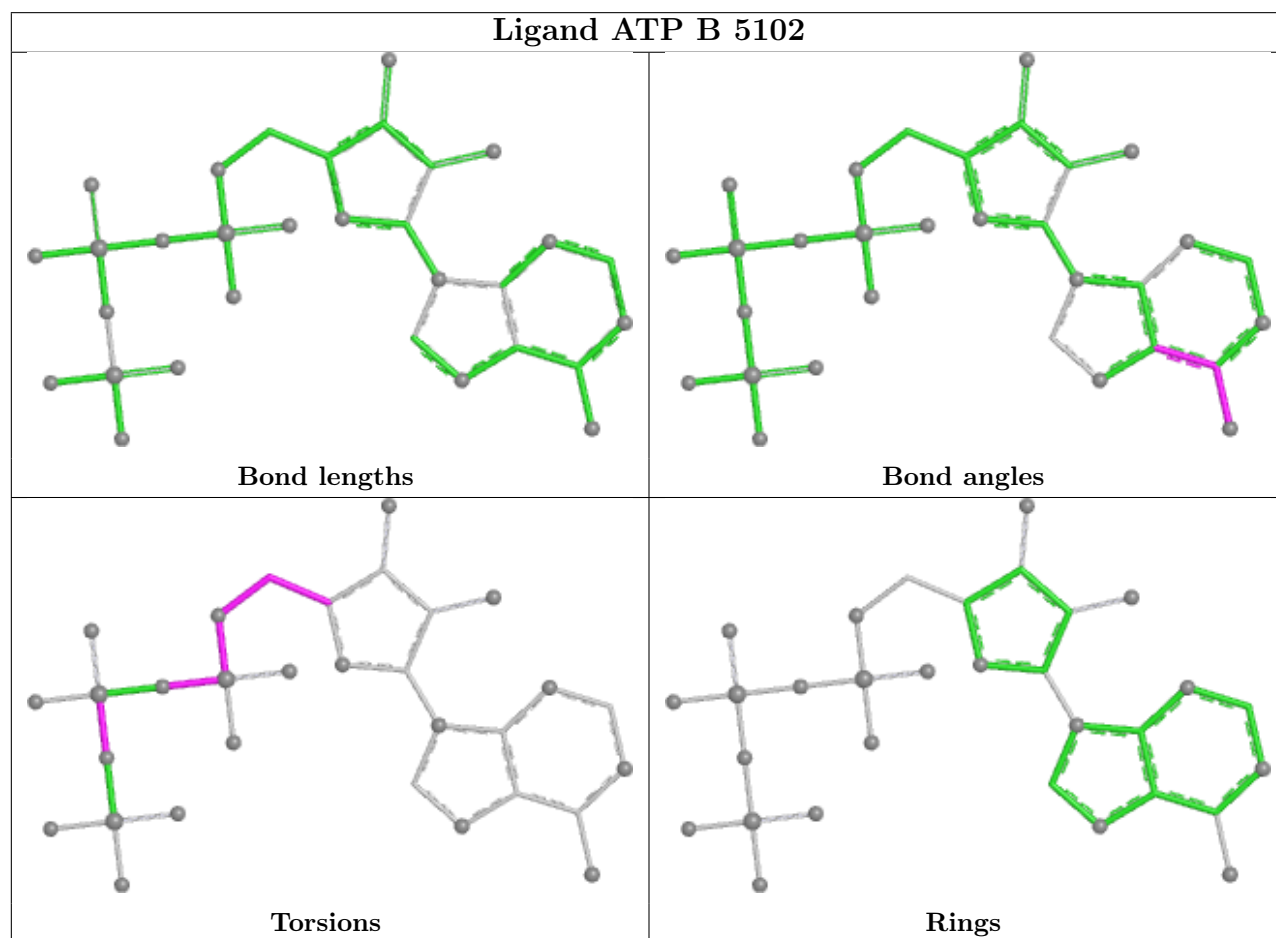
5 of 40 torsion outliers are listed below:

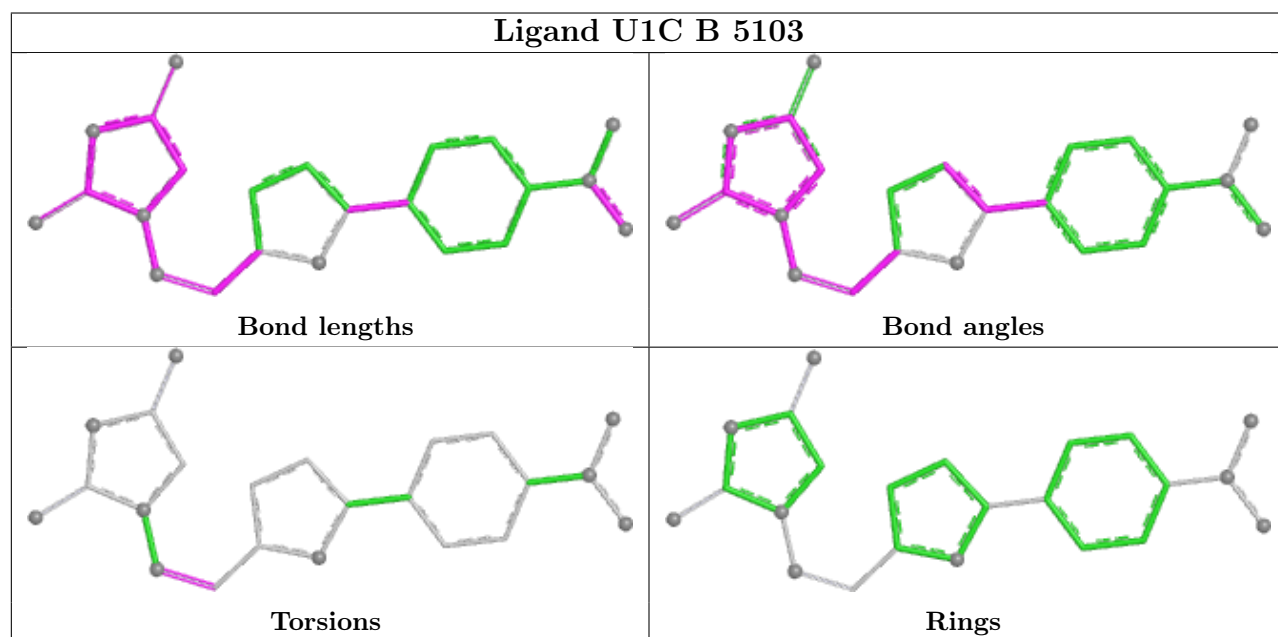
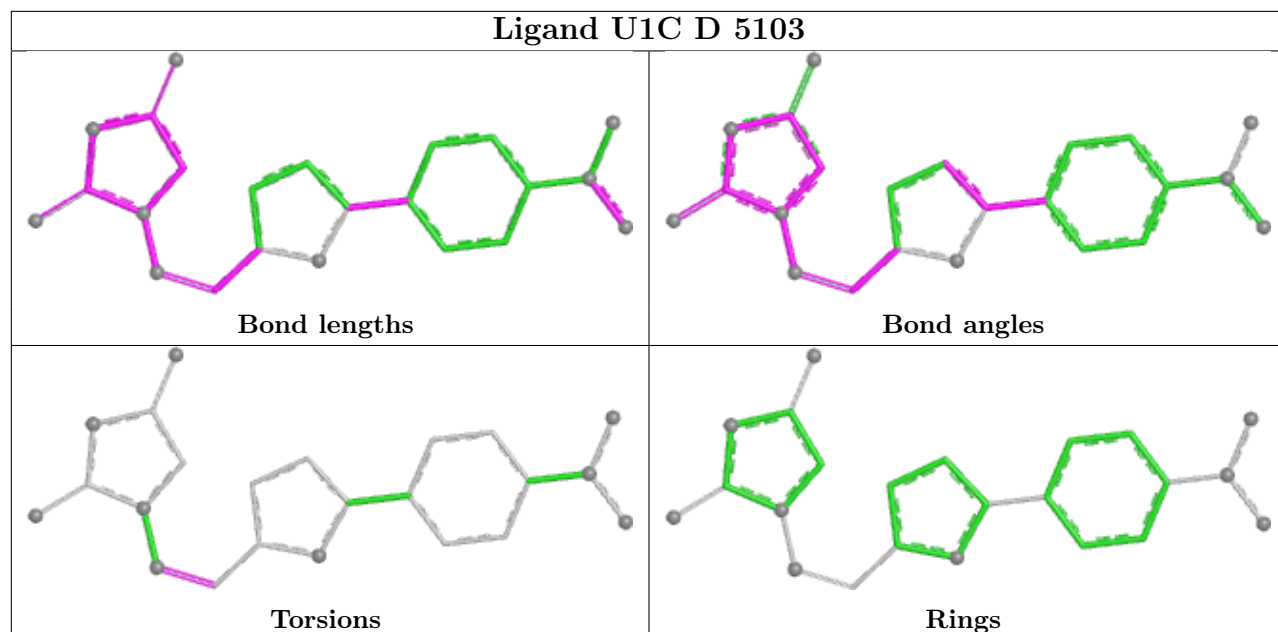
Mol	Chain	Res	Type	Atoms
4	A	5102	ATP	C5'-O5'-PA-O1A
4	A	5102	ATP	C5'-O5'-PA-O2A
4	A	5102	ATP	C5'-O5'-PA-O3A
4	A	5102	ATP	O4'-C4'-C5'-O5'
4	B	5102	ATP	C5'-O5'-PA-O1A

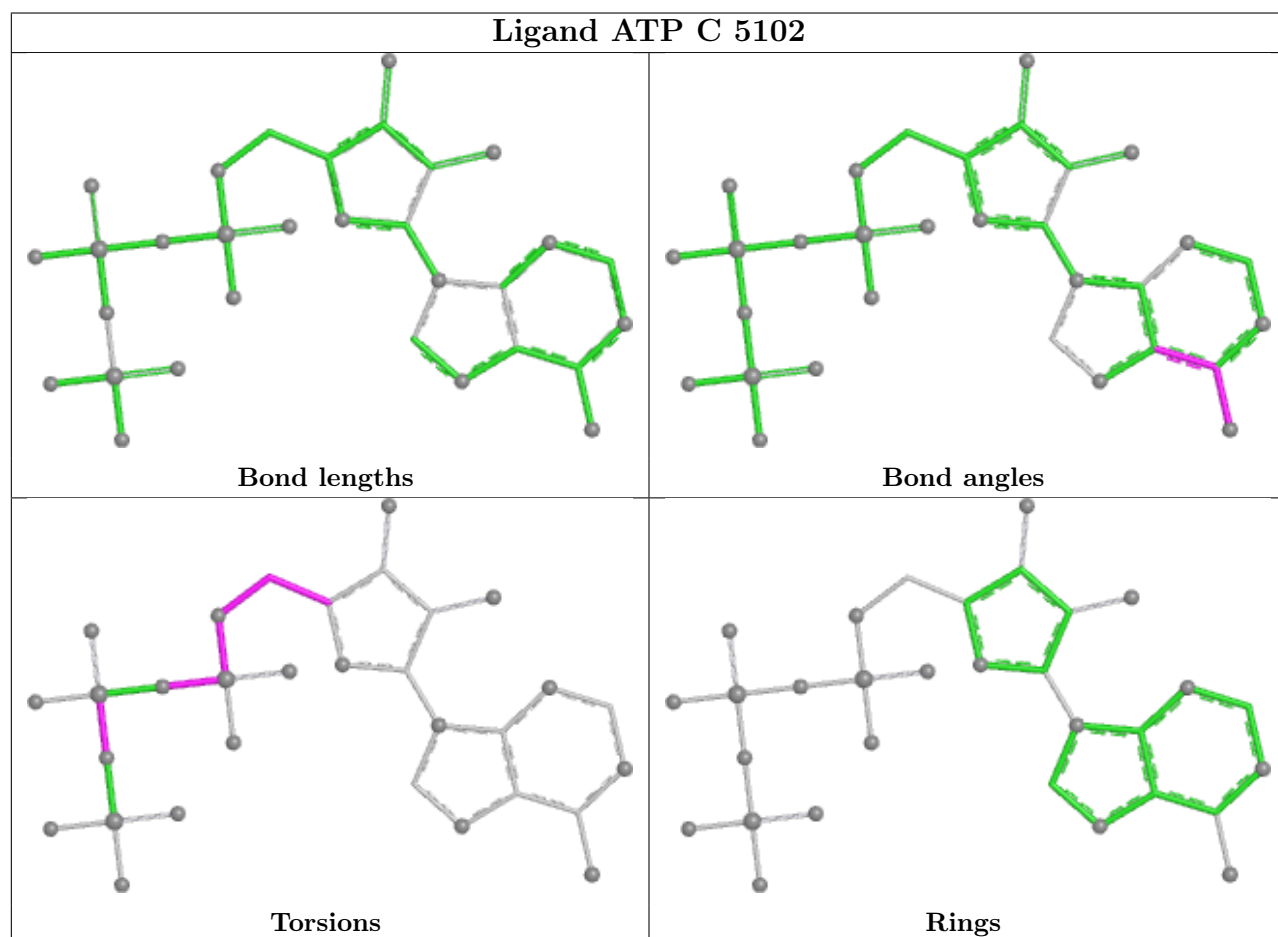
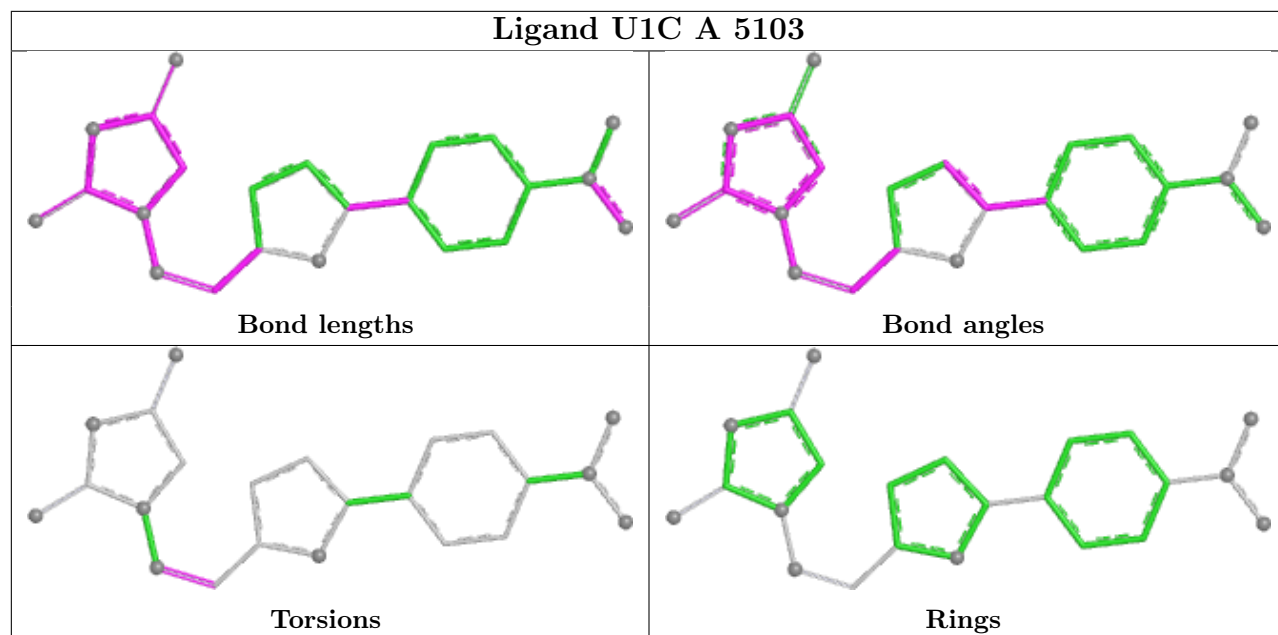
There are no ring outliers.

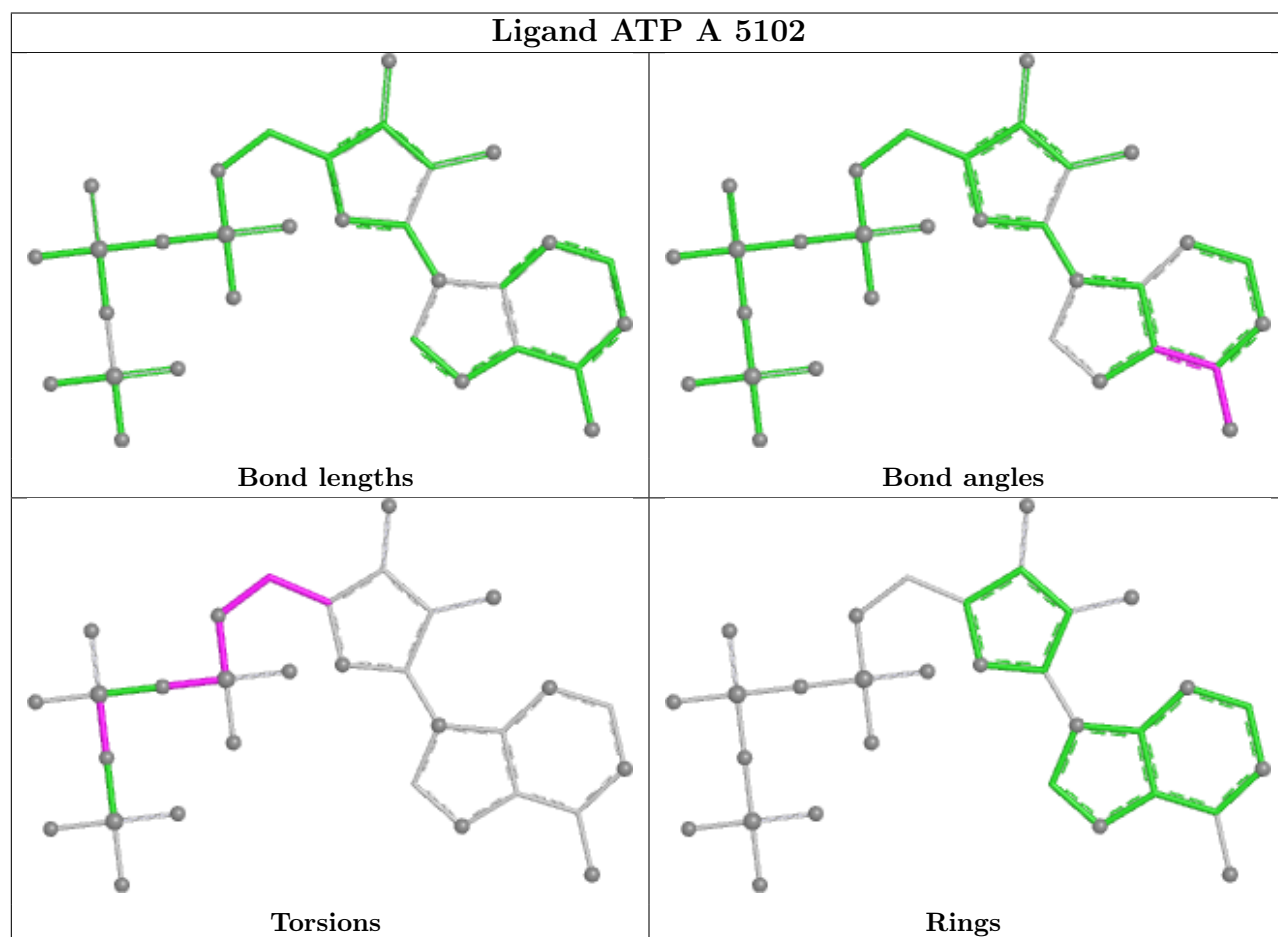
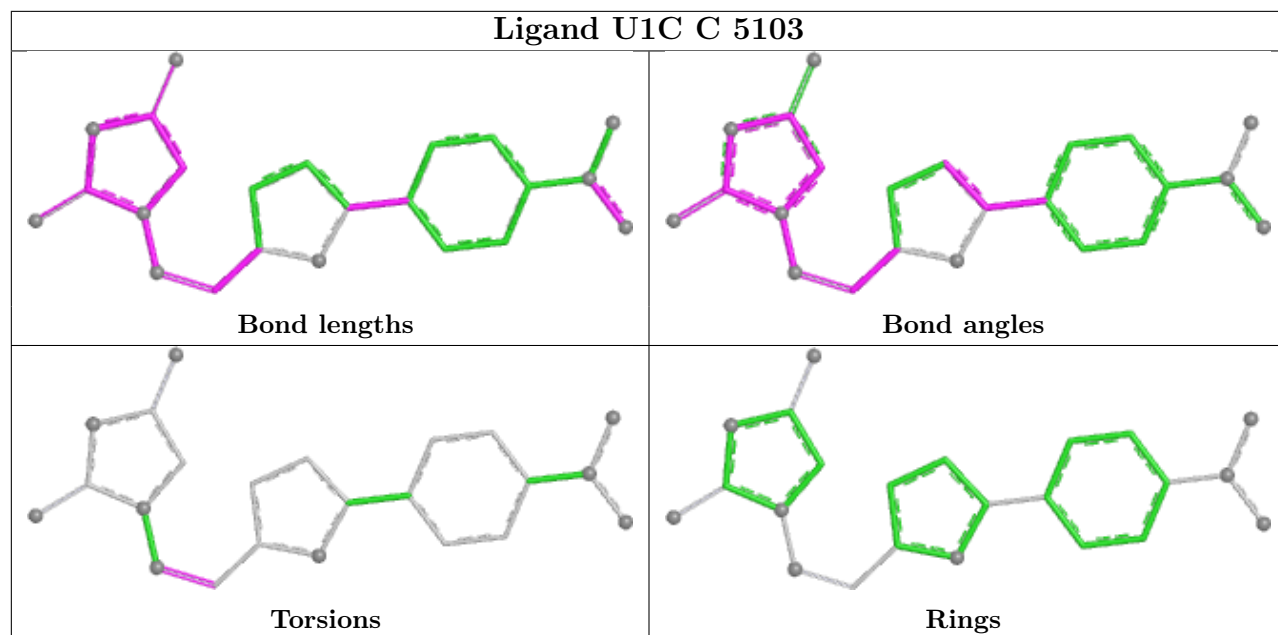
No monomer is involved in short contacts.

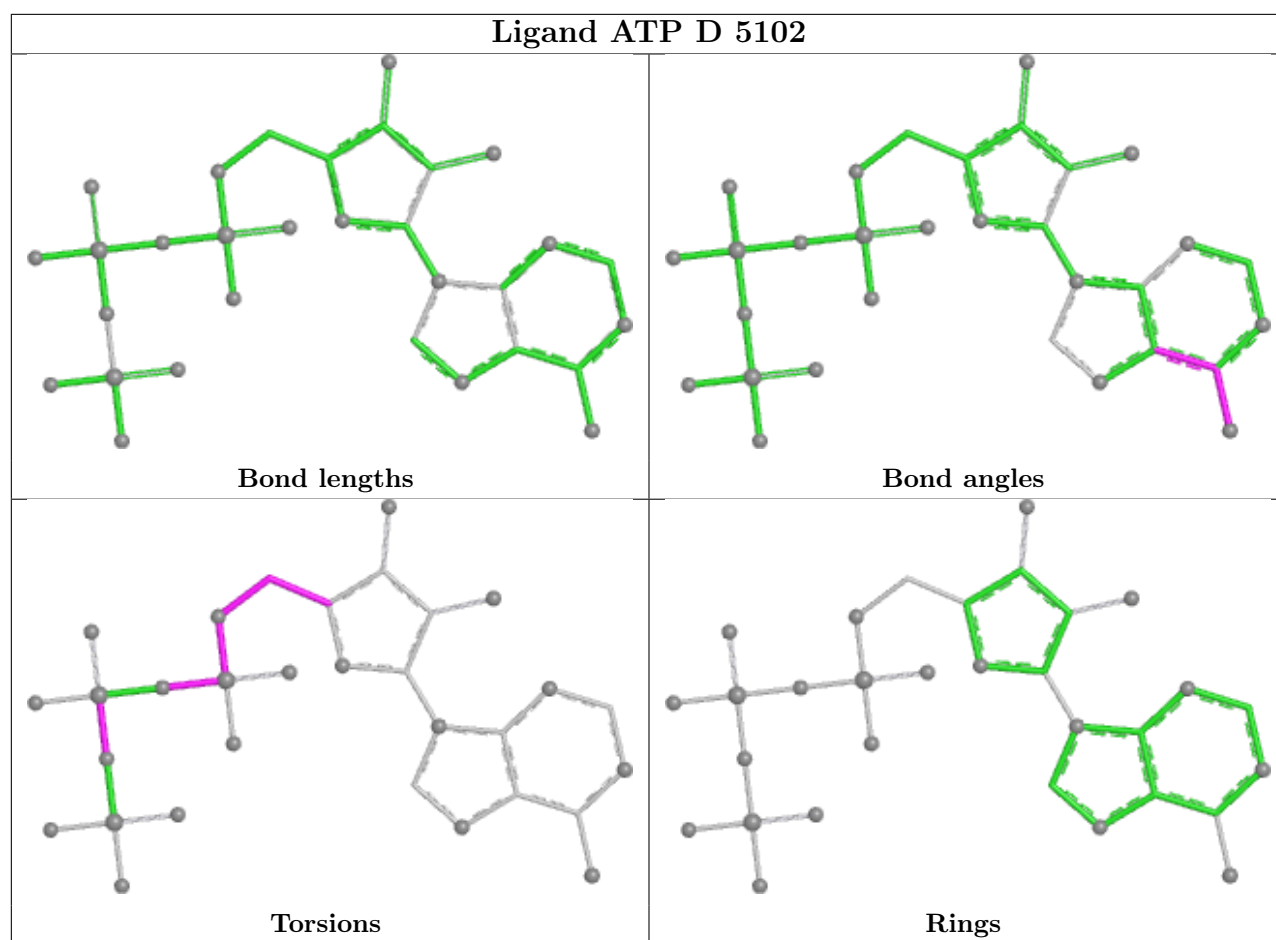
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

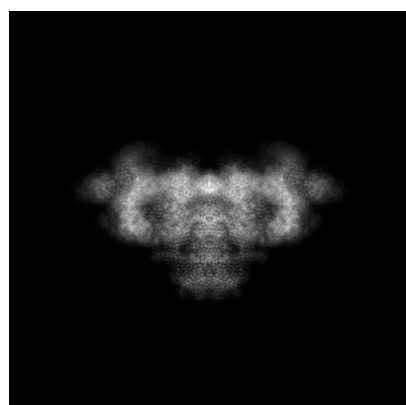
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45584. These allow visual inspection of the internal detail of the map and identification of artifacts.

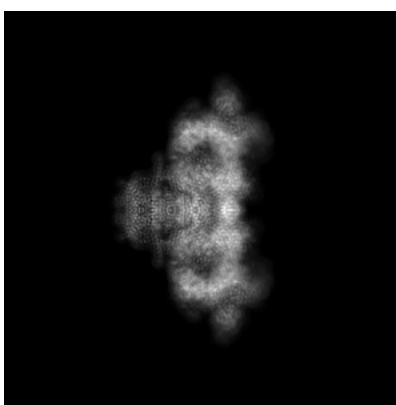
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

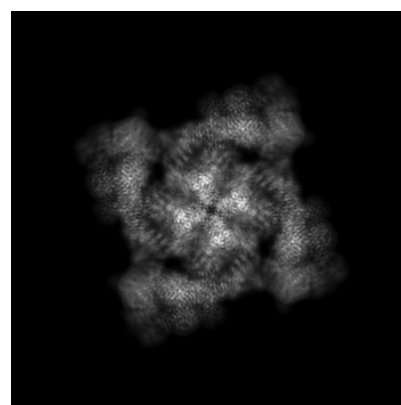
#### 6.1.1 Primary map



X



Y

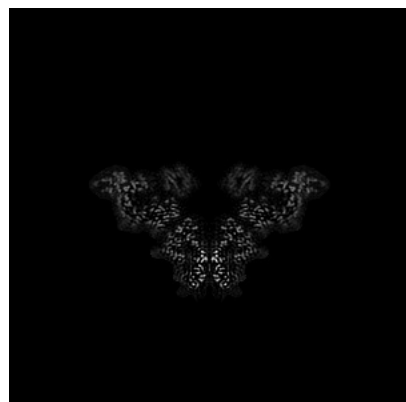


Z

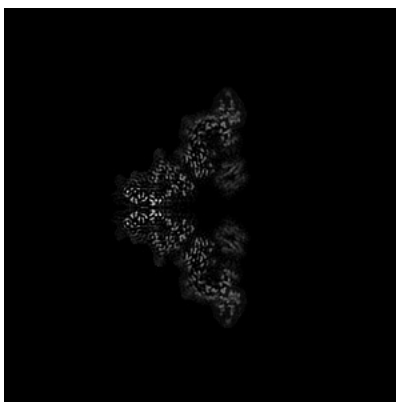
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

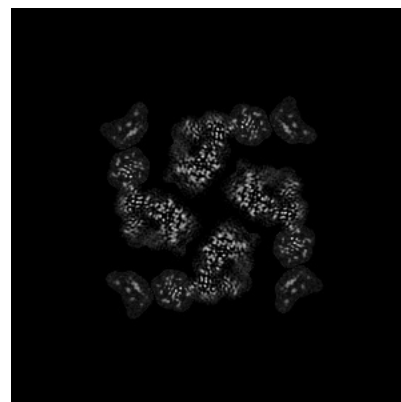
#### 6.2.1 Primary map



X Index: 232



Y Index: 232



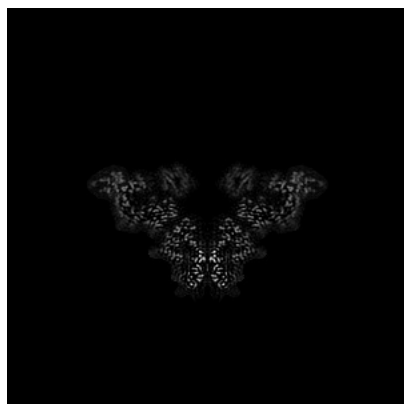
Z Index: 232



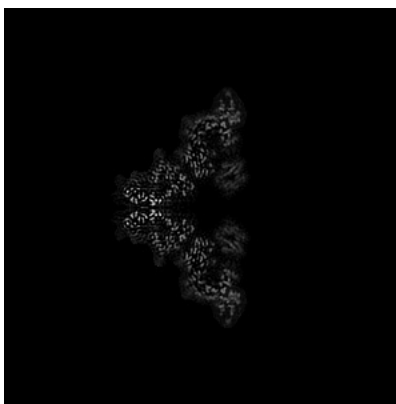
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

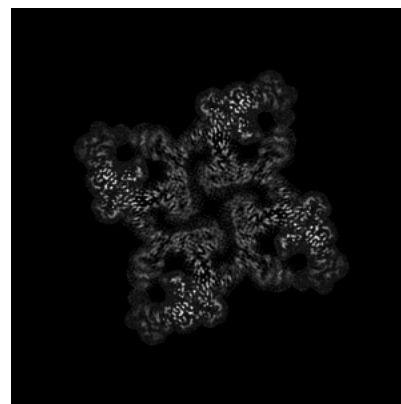
### 6.3.1 Primary map



X Index: 232



Y Index: 232

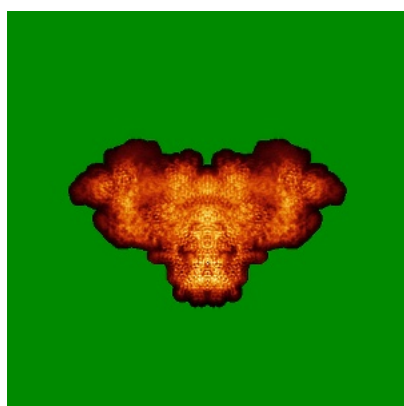


Z Index: 261

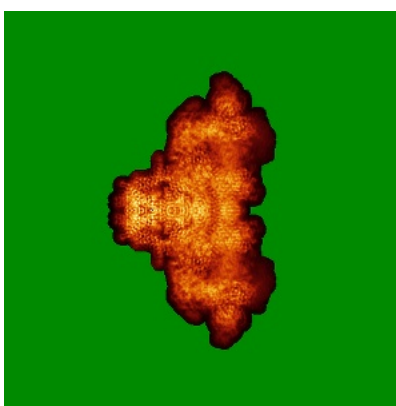
The images above show the largest variance slices of the map in three orthogonal directions.

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

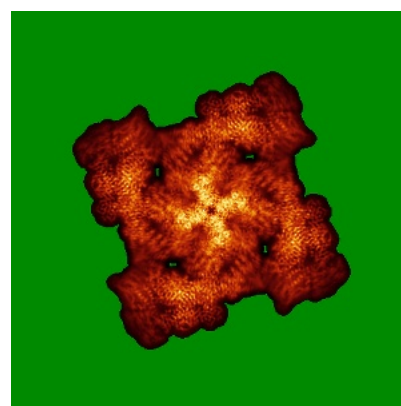
### 6.4.1 Primary map



X



Y

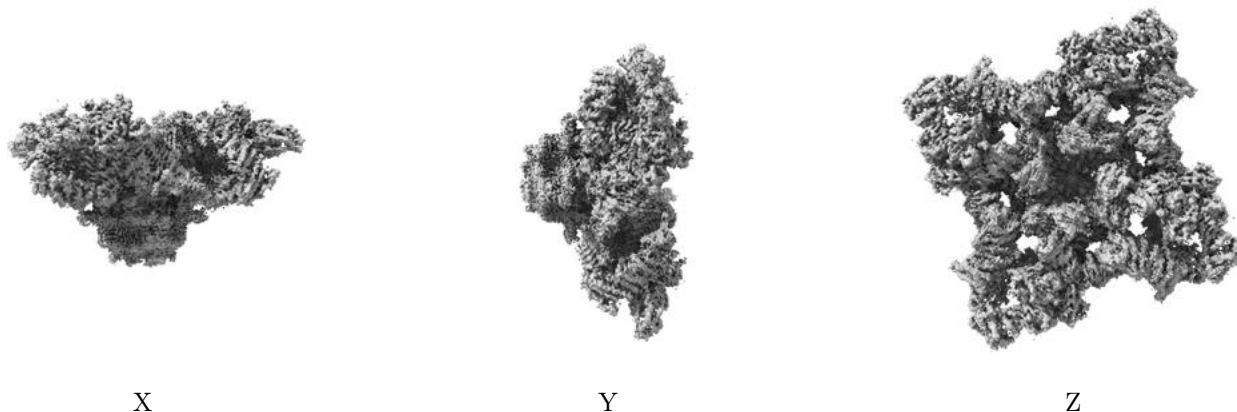


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.32. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

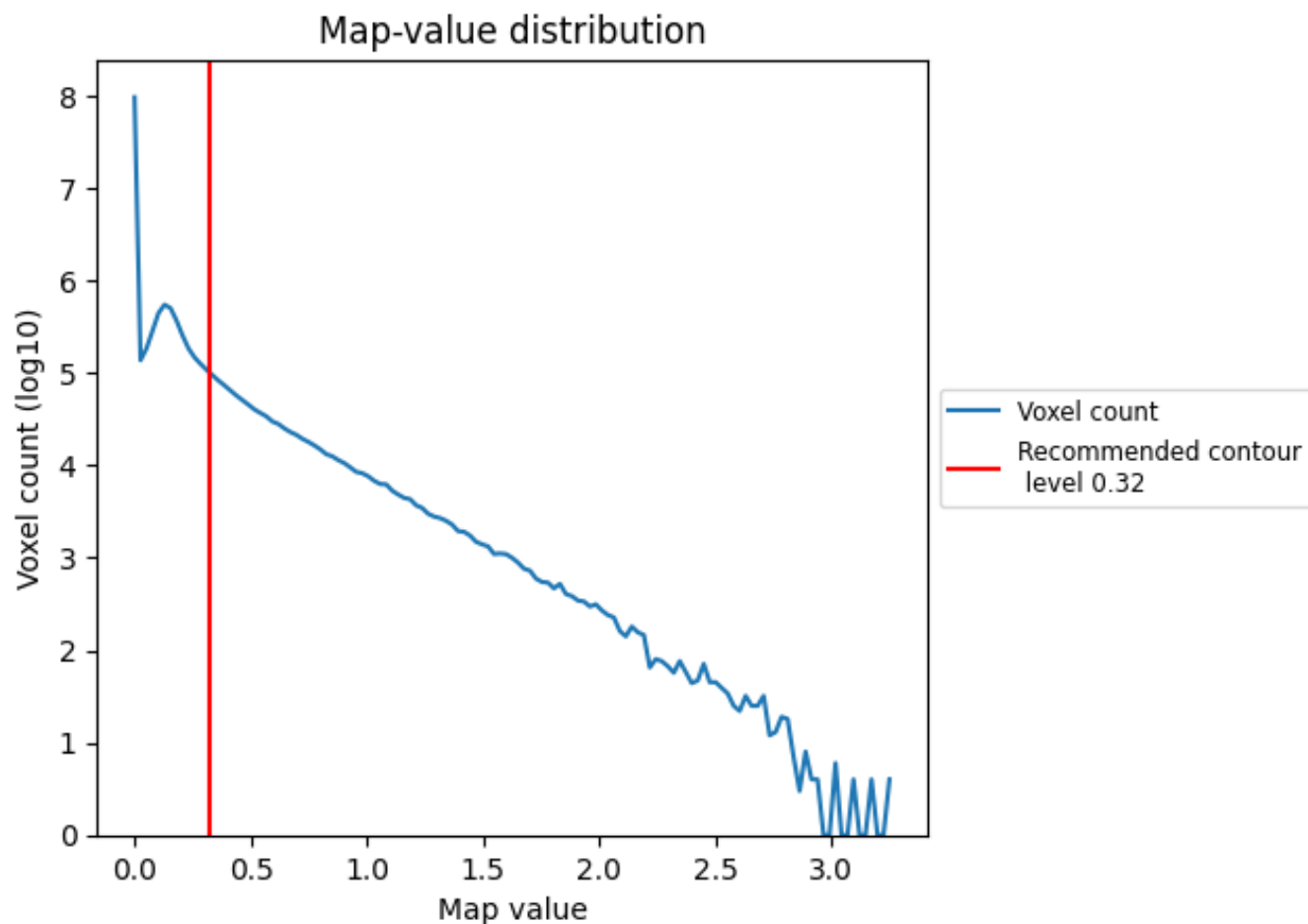
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

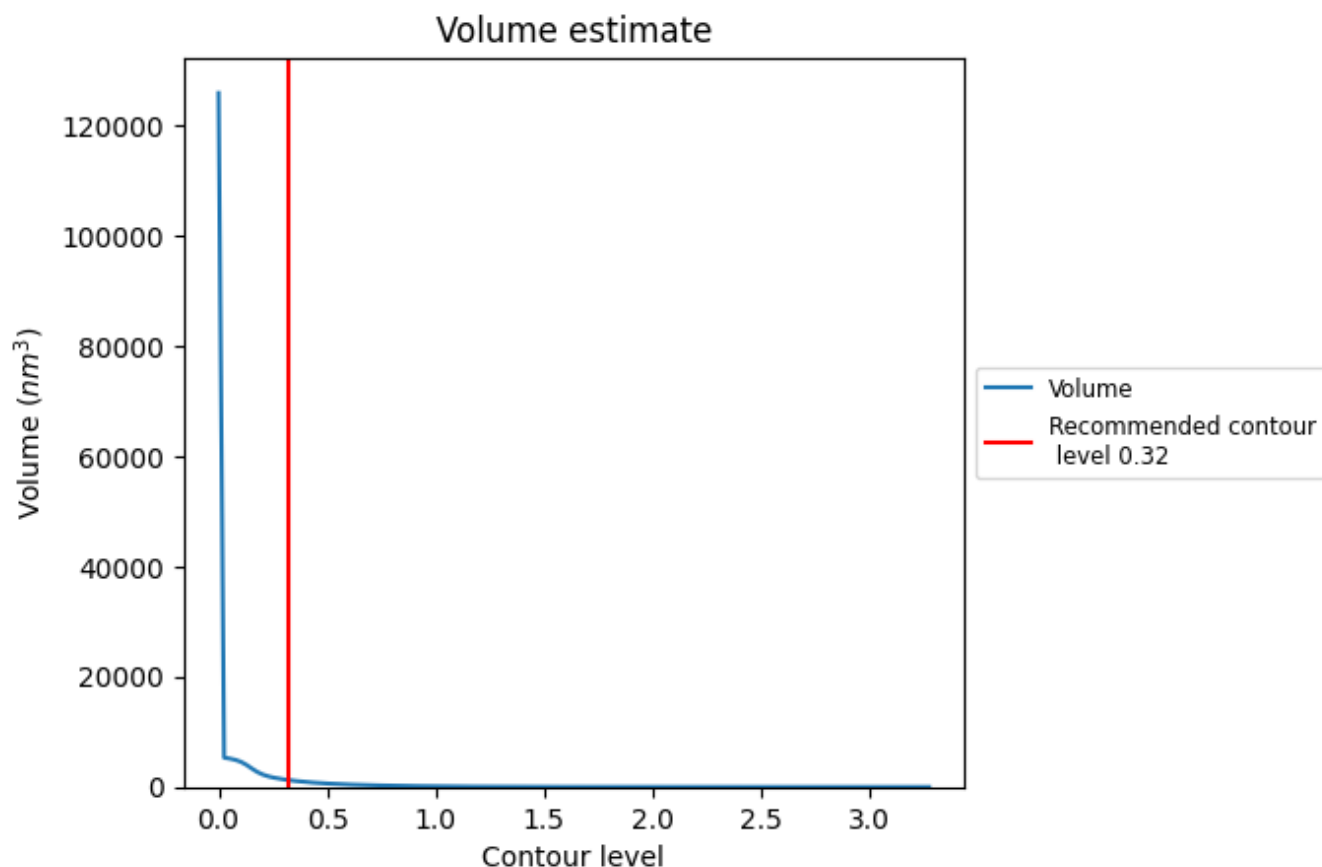
This section contains the results of statistical analysis of the map.

### 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.

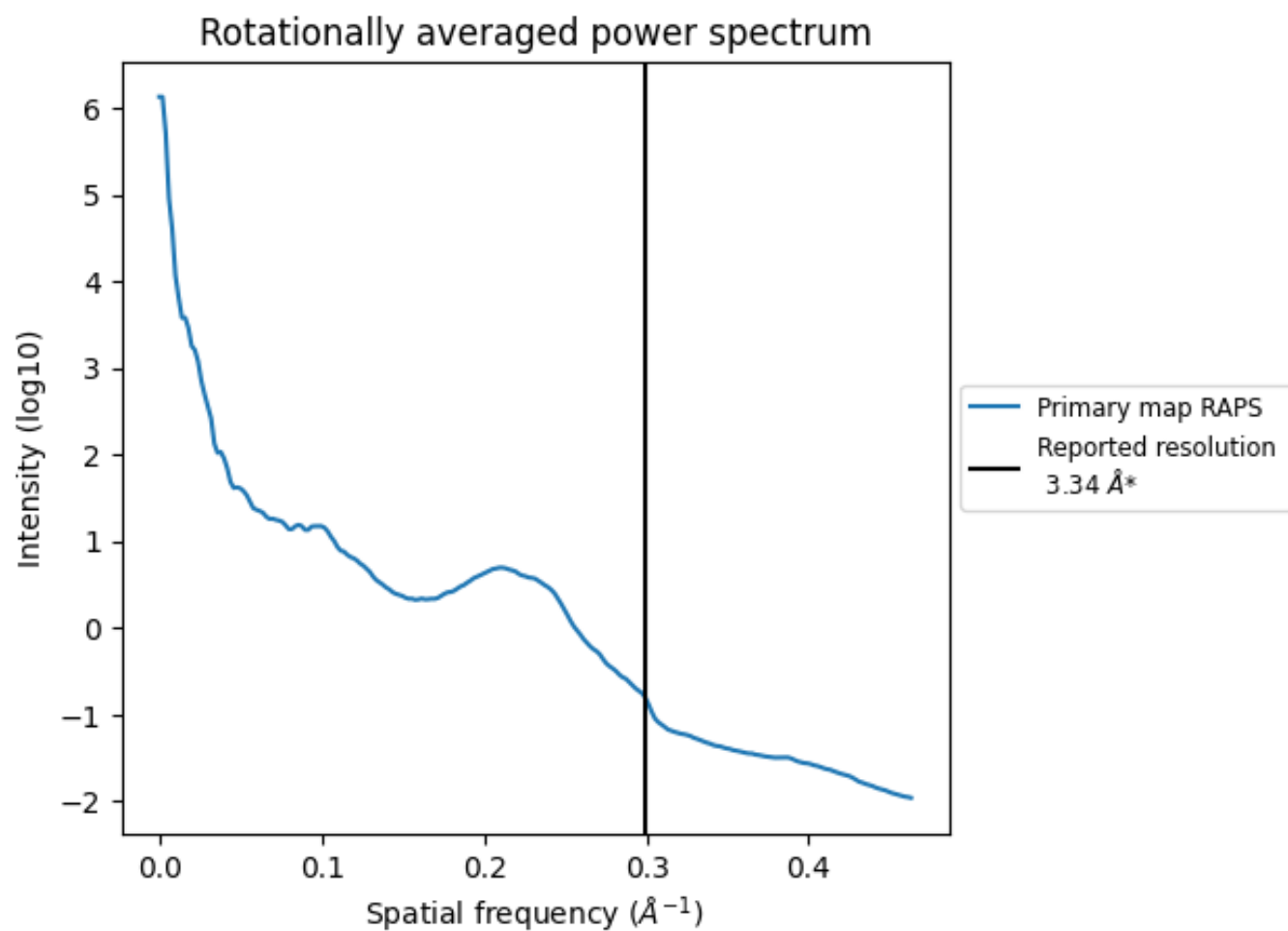
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1262  $\text{nm}^3$ ; this corresponds to an approximate mass of 1140 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 0.299 Å<sup>-1</sup>

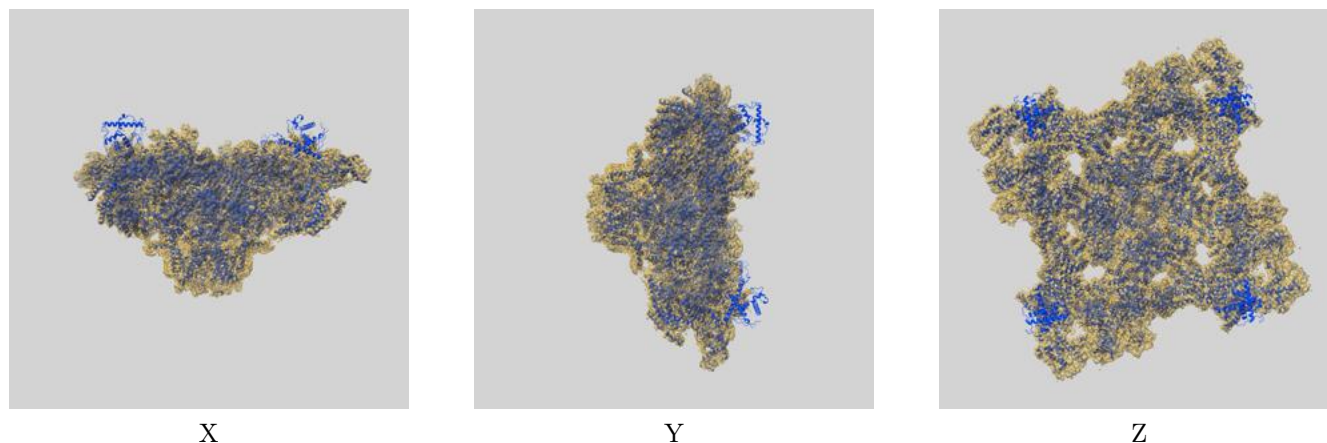
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

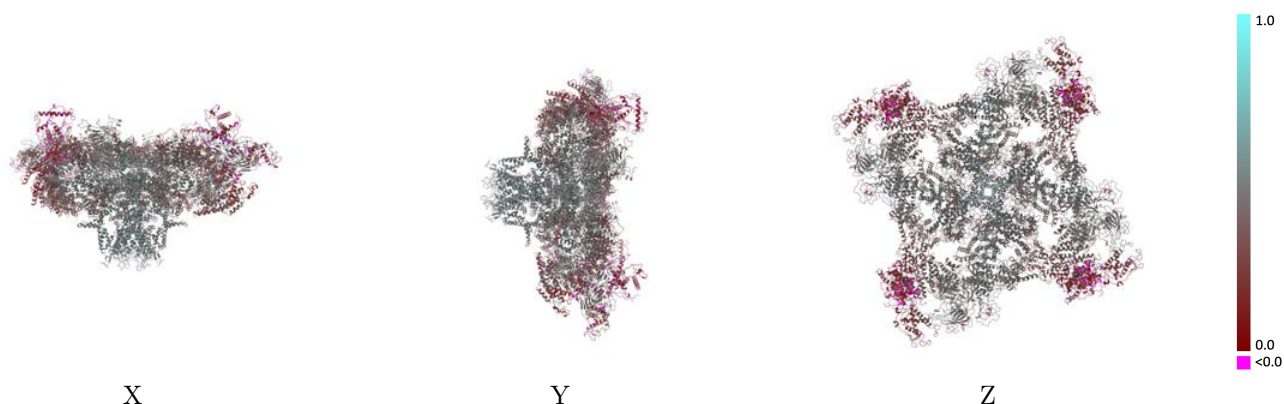
This section contains information regarding the fit between EMDB map EMD-45584 and PDB model 9CGP. Per-residue inclusion information can be found in section [3](#) on page [6](#).

### 9.1 Map-model overlay [i](#)



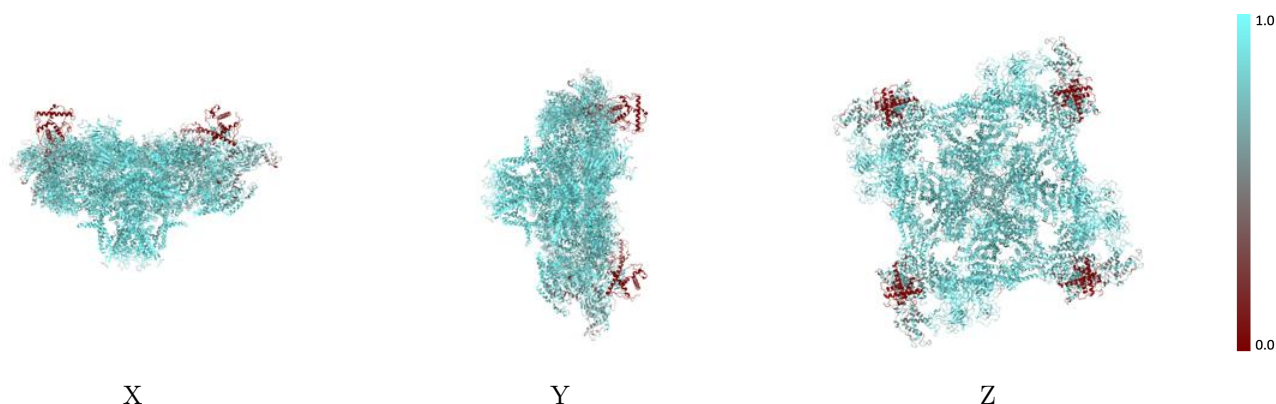
The images above show the 3D surface view of the map at the recommended contour level 0.32 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



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

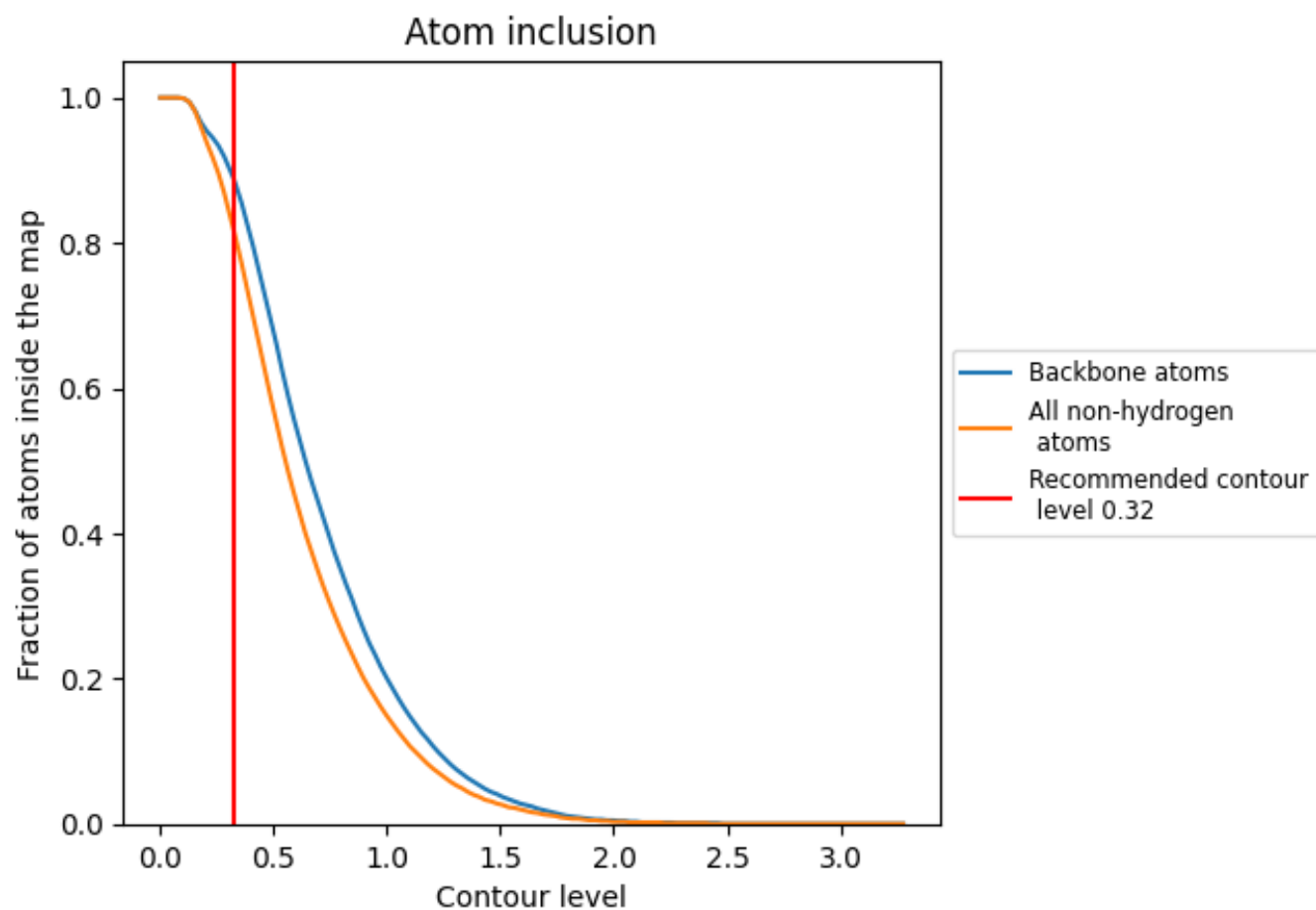
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.32).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 82% 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 (0.32) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8220	<div><div></div></div> 0.4080
A	<div><div></div></div> 0.8210	<div><div></div></div> 0.4070
B	<div><div></div></div> 0.8220	<div><div></div></div> 0.4080
C	<div><div></div></div> 0.8210	<div><div></div></div> 0.4070
D	<div><div></div></div> 0.8230	<div><div></div></div> 0.4080
E	<div><div></div></div> 0.8530	<div><div></div></div> 0.4190
F	<div><div></div></div> 0.8480	<div><div></div></div> 0.4210
G	<div><div></div></div> 0.8490	<div><div></div></div> 0.4200
H	<div><div></div></div> 0.8490	<div><div></div></div> 0.4230

1.0

0.0

<0.0