



wwPDB EM Validation Summary Report

Dec 7, 2024 – 06:45 am GMT

PDB ID : 8QKV
EMDB ID : EMD-18472
Title : SWR1-nucleosome complex in configuration 2
Authors : Jalal, A.S.B.; Wigley, D.B.
Deposited on : 2023-09-18
Resolution : 4.70 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.dev113
Mogul : 1.8.4, CSD as541be (2020)
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

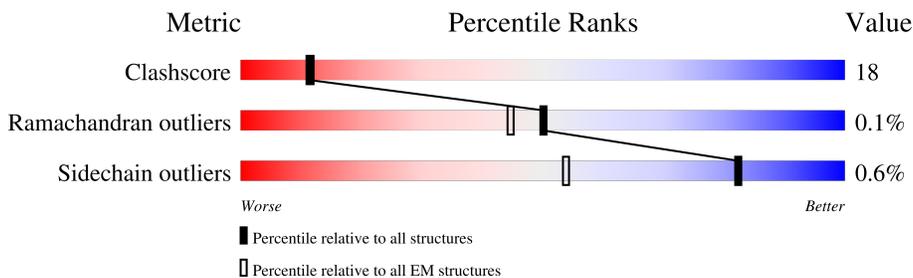
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.70 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 ≥ 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	136	
1	B	136	
2	C	103	
2	D	103	
3	E	158	
3	F	158	
4	G	131	
4	H	131	

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Mol	Chain	Length	Quality of chain
5	I	194	41% 59%
6	J	194	30% 70%
7	Z	180	5% 73% 24%
8	M	1514	28% 17% 55%
9	R	438	60% 34% 6%
10	S	280	42% 24% 34%
11	T	463	60% 35% 5%
11	V	463	52% 41% 6%
11	X	463	57% 39% 5%
12	U	471	53% 38% 9%
12	W	471	50% 42% 8%
12	Y	471	62% 32% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	BEF	M	1602	-	-	X	-

2 Entry composition i

There are 16 unique types of molecules in this entry. The entry contains 45846 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 Histone H3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	B	97	796	506	152	138	0	0
1	A	97	796	506	152	138	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	123	GLU	ASP	conflict	UNP P61830
A	123	GLU	ASP	conflict	UNP P61830

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	C	82	651	410	126	115	0	0
2	D	80	638	401	124	113	0	0

- Molecule 3 is a protein called Histone H2A.2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	F	101	767	482	149	136	0	0
3	E	103	795	499	156	140	0	0

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	127	GLU	-	expression tag	UNP P04912
F	128	VAL	-	expression tag	UNP P04912
F	129	CYS	-	expression tag	UNP P04912

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Chain	Residue	Modelled	Actual	Comment	Reference
F	130	GLN	-	expression tag	UNP P04912
F	131	ASP	-	expression tag	UNP P04912
F	132	CYS	-	expression tag	UNP P04912
F	133	GLN	-	expression tag	UNP P04912
F	134	SER	-	expression tag	UNP P04912
F	135	PHE	-	expression tag	UNP P04912
F	136	SER	-	expression tag	UNP P04912
F	137	ARG	-	expression tag	UNP P04912
F	138	THR	-	expression tag	UNP P04912
F	139	VAL	-	expression tag	UNP P04912
F	140	ARG	-	expression tag	UNP P04912
F	141	THR	-	expression tag	UNP P04912
F	142	GLU	-	expression tag	UNP P04912
F	143	LEU	-	expression tag	UNP P04912
F	144	LYS	-	expression tag	UNP P04912
F	145	ARG	-	expression tag	UNP P04912
F	146	ASN	-	expression tag	UNP P04912
F	147	LYS	-	expression tag	UNP P04912
F	148	ALA	-	expression tag	UNP P04912
F	149	ASN	-	expression tag	UNP P04912
F	150	GLN	-	expression tag	UNP P04912
F	151	THR	-	expression tag	UNP P04912
F	152	PHE	-	expression tag	UNP P04912
F	153	LEU	-	expression tag	UNP P04912
F	154	SER	-	expression tag	UNP P04912
F	155	PHE	-	expression tag	UNP P04912
F	156	GLY	-	expression tag	UNP P04912
F	157	VAL	-	expression tag	UNP P04912
E	127	GLU	-	expression tag	UNP P04912
E	128	VAL	-	expression tag	UNP P04912
E	129	CYS	-	expression tag	UNP P04912
E	130	GLN	-	expression tag	UNP P04912
E	131	ASP	-	expression tag	UNP P04912
E	132	CYS	-	expression tag	UNP P04912
E	133	GLN	-	expression tag	UNP P04912
E	134	SER	-	expression tag	UNP P04912
E	135	PHE	-	expression tag	UNP P04912
E	136	SER	-	expression tag	UNP P04912
E	137	ARG	-	expression tag	UNP P04912
E	138	THR	-	expression tag	UNP P04912
E	139	VAL	-	expression tag	UNP P04912
E	140	ARG	-	expression tag	UNP P04912

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Chain	Residue	Modelled	Actual	Comment	Reference
E	141	THR	-	expression tag	UNP P04912
E	142	GLU	-	expression tag	UNP P04912
E	143	LEU	-	expression tag	UNP P04912
E	144	LYS	-	expression tag	UNP P04912
E	145	ARG	-	expression tag	UNP P04912
E	146	ASN	-	expression tag	UNP P04912
E	147	LYS	-	expression tag	UNP P04912
E	148	ALA	-	expression tag	UNP P04912
E	149	ASN	-	expression tag	UNP P04912
E	150	GLN	-	expression tag	UNP P04912
E	151	THR	-	expression tag	UNP P04912
E	152	PHE	-	expression tag	UNP P04912
E	153	LEU	-	expression tag	UNP P04912
E	154	SER	-	expression tag	UNP P04912
E	155	PHE	-	expression tag	UNP P04912
E	156	GLY	-	expression tag	UNP P04912
E	157	VAL	-	expression tag	UNP P04912

- Molecule 4 is a protein called Histone H2B.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	G	96	746	468	131	146	1	0	0
4	H	91	712	449	125	137	1	0	0

- Molecule 5 is a DNA chain called DNA (194-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	I	194	3960	1879	716	1171	194	0	0

- Molecule 6 is a DNA chain called DNA (194-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	J	194	3994	1888	755	1157	194	0	0

- Molecule 7 is a protein called Vacuolar protein sorting-associated protein 72.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	Z	180	1367	854	248	262	3	0	0

- Molecule 8 is a protein called Helicase SWR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	M	688	5398	3438	960	974	26	0	0

- Molecule 9 is a protein called Actin-like protein ARP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	R	411	3335	2156	544	619	16	0	0

- Molecule 10 is a protein called Vacuolar protein sorting-associated protein 71.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	S	185	1499	947	265	277	10	0	0

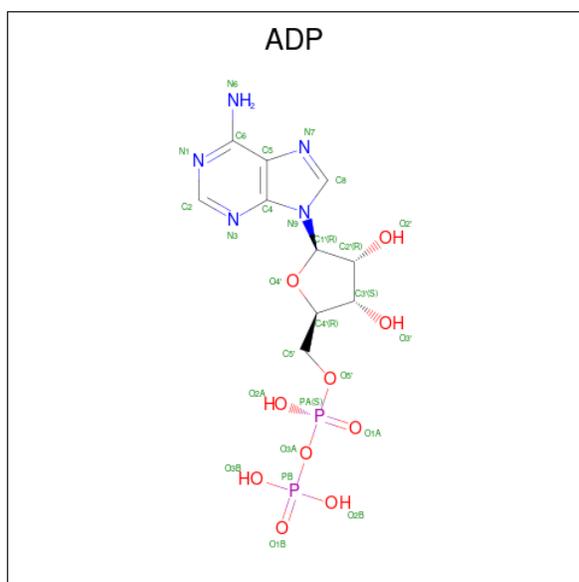
- Molecule 11 is a protein called RuvB-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	T	443	3391	2140	584	657	10	0	0
11	V	434	3336	2107	574	645	10	0	0
11	X	442	3397	2144	584	659	10	0	0

- Molecule 12 is a protein called RuvB-like protein 2.

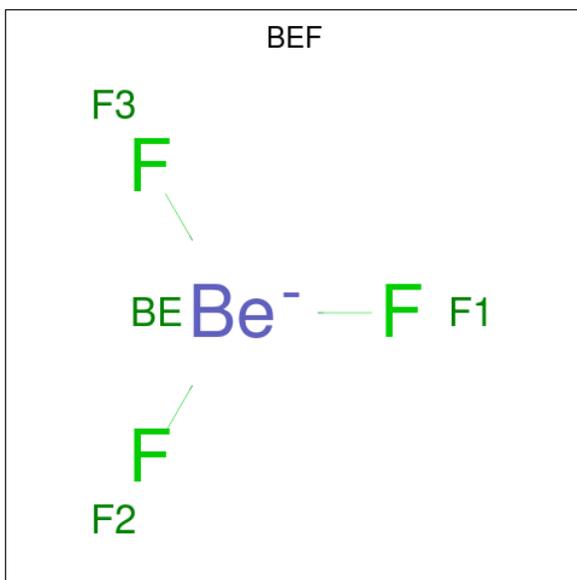
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	U	430	3299	2063	570	655	11	0	0
12	W	433	3325	2085	572	657	11	0	0
12	Y	447	3410	2133	590	675	12	0	0

- Molecule 13 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
13	M	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	R	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	T	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	U	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	V	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	W	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	X	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	Y	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 14 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	Be	F	
14	M	1	4	1	3	0
14	R	1	4	1	3	0

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
15	M	1	1	1	0
15	R	1	1	1	0
15	T	1	1	1	0
15	U	1	1	1	0
15	V	1	1	1	0
15	W	1	1	1	0
15	X	1	1	1	0
15	Y	1	1	1	0

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

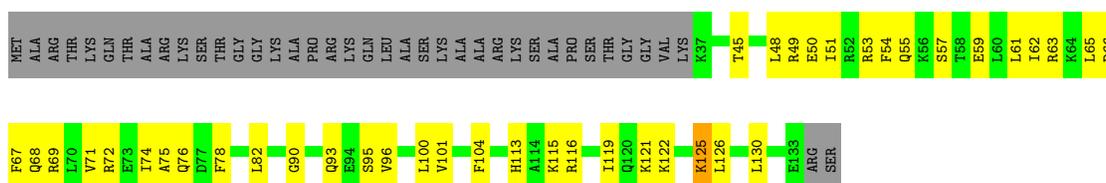
Mol	Chain	Residues	Atoms		AltConf
16	S	2	Total 2	Zn 2	0

3 Residue-property plots [i](#)

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

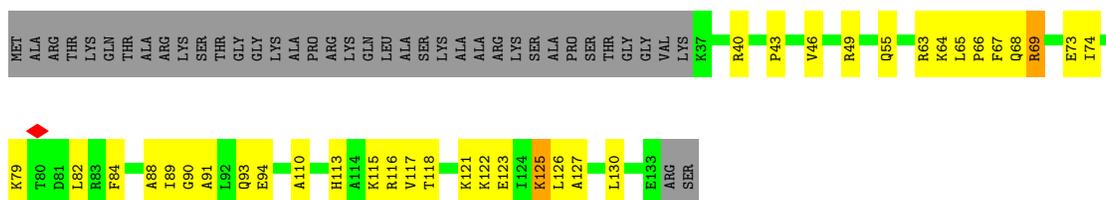
- Molecule 1: Histone H3

Chain B: 



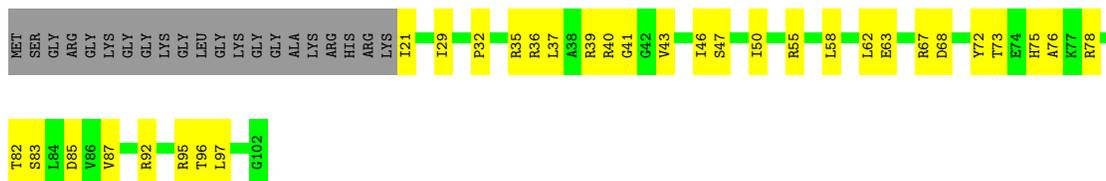
- Molecule 1: Histone H3

Chain A: 



- Molecule 2: Histone H4

Chain C: 



- Molecule 2: Histone H4

Chain D: 





• Molecule 3: Histone H2A.2

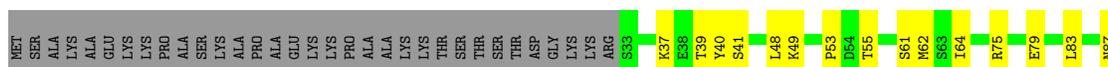


• Molecule 3: Histone H2A.2



VAL

• Molecule 4: Histone H2B.1



• Molecule 4: Histone H2B.1



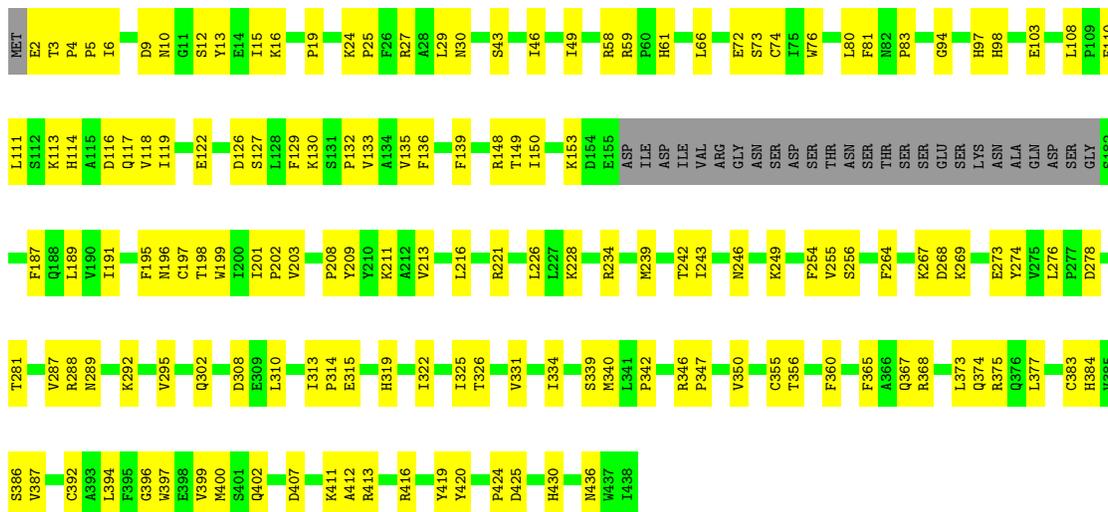
• Molecule 5: DNA (194-MER)



ALA	THR	R1313	C1217	L1198	A1015	K939	T862	S756	ASN	GLY	SER	ASP	TRP	HIS	ARG	ARG
MET	ASP	I1314	V1220	R1129	S1016	Q940	G853	V756	ARG	LEU	SER	VAL	ASN	MET	LEU	LEU
ARG	TYR	I1315	W1221	R1130	S1017	M841	T854	L757	ASP	SER	THR	LEU	MET	SER	LEU	ALA
GLU	PHE	I1316	N1222	R1133	K1019	P942	L860	L758	ASP	LEU	ALA	GLU	ALA	LYS	LYS	LYS
VAL	SER	I1318	N1223	R1134	D1020	P943	L861	M769	ILE	LEU	TYR	GLU	GLU	PHE	LEU	GLY
GLY	LYS	I1319	L1231	I1141	D1021	K944	E862	M768	LYS	PHE	ASP	GLY	ALA	LYS	ILE	ILE
ILE	LEU	S1323	L1232	D1142	R1023	Y945	L863	E761	ASP	GLY	SER	ASP	ASP	ARG	ARG	ASN
ASP	SER	I1328	A1234	L1143	R1024	E946	L864	F764	VAL	GLY	ASN	ASP	TYR	SER	ASN	GLY
ASN	VAL	I1329	F1235	L1144	T1024	H947	L865	F765	GLU	GLY	GLY	ASP	ARG	SER	GLY	THR
ASP	ARG	M1329	F1236	L1145	L1025	I948	L866	P769	GLU	GLU	LEU	MET	LEU	THR	ALA	ALA
ASP	ASP	L1330	P1237	T1146	L1026	I949	L867	P769	ASP	GLU	GLU	ASP	GLU	LYS	LYS	LYS
PHE	LEU	D1330	D1237	L1147	Q1034	I948	L868	P769	ASP	GLU	GLU	ASP	ARG	ALA	ALA	ALA
LEU	LEU	A1333	K1238	D1148	Q1035	I949	L869	P769	ASP	SER	ASP	ASP	GLY	ARG	ARG	THR
GLY	GLY	D1334	L1239	R1149	R1037	I949	L870	V773	THR	GLY	PHE	LEU	ASP	ILE	ILE	ASP
SER	SER	I1337	Y1243	R1150	F1042	K954	T874	G779	LYS	ASP	THR	SER	GLU	ALA	ALA	LYS
GLU	GLU	F1338	G1246	V1150	F1043	K955	V875	G779	LYS	ASP	THR	THR	GLU	ARG	ARG	LYS
LEU	LEU	F1339	G1247	K1151	F1044	R956	V875	Q782	VAL	LEU	PRO	GLU	GLU	THR	THR	GLY
PRO	PRO	Y1339	K1247	K1152	L1045	Q957	A885	Q782	GLN	ASP	LEU	SER	GLU	ALA	ALA	THR
GLY	GLY	F1340	L1248	D1163	L1046	F959	A885	K792	GLU	LEU	GLU	ASP	GLN	LYS	LYS	ASP
ALA	ASN	D1340	Q1249	D1164	L1047	R960	A885	K792	GLU	ASP	LEU	SER	GLN	ALA	ALA	THR
ALA	ASN	S1341	Q1250	K1165	L1048	Y961	A885	P793	GLN	ASP	LEU	ASP	GLN	LYS	LYS	SER
ALA	ALA	D1342	L1251	S1155	M1050	Y961	A885	D794	GLN	ASP	LEU	ASP	LYS	VAL	VAL	LEU
ASN	SER	D1343	L1252	D1159	D1051	Y961	A885	A795	LEU	SER	GLN	ASP	ARG	ARG	ARG	GLN
GLY	GLY	K1349	L1254	D1160	K1052	F964	A885	A795	LEU	SER	GLN	ASP	ARG	ARG	ARG	GLN
GLY	GLY	Q1350	L1255	L1162	K1053	M965	A885	V798	LEU	SER	GLN	ASP	ARG	ARG	ARG	GLN
LYS	LYS	D1353	L1256	L1163	D1054	S966	A885	C799	LEU	SER	GLN	ASP	ARG	ARG	ARG	GLN
ASN	PRO	R1353	R1264	K1164	A1059	R967	A885	T800	LEU	ASN	THR	VAL	GLN	GLN	GLN	LYS
LEU	LEU	R1354	I1267	P1165	K1064	Q969	A885	V801	LEU	SER	ASP	ALA	GLN	GLN	GLN	LYS
ALA	ALA	H1355	I1268	L1166	L1065	T970	A885	S802	LEU	SER	VAL	VAL	ALA	HIS	HIS	LYS
LEU	ASP	R1357	T1272	R1169	L1066	K971	A885	R803	LEU	SER	VAL	VAL	ALA	GLY	GLY	LYS
ASP	ASP	Q1360	L1273	R1170	T1067	A972	A885	Q808	LEU	SER	VAL	VAL	ALA	GLY	GLY	LYS
ASP	ASP	T1361	V1274	R1171	V1068	A972	A885	Q809	LEU	SER	VAL	VAL	ALA	GLY	GLY	LYS
TYR	VAL	R1362	L1275	I1177	K1069	A972	A885	Q810	LEU	SER	VAL	VAL	ALA	GLY	GLY	LYS
GLY	ALA	D1363	D1276	L1183	M1070	N978	A885	Y820	LEU	SER	VAL	VAL	ALA	GLY	GLY	LYS
THR	LYS	D1364	V1277	T1184	F1071	S981	A885	V821	LEU	SER	VAL	VAL	ALA	GLY	GLY	LYS
ALA	ASP	I1366	L1282	P1185	E1073	I982	A885	L823	LEU	SER	VAL	VAL	ALA	GLY	GLY	LYS
PRO	PRO	Y1367	G1286	A1187	M1076	V983	A885	D824	LEU	SER	VAL	VAL	ALA	GLY	GLY	LYS
VAL	ARG	R1368	Y1287	V1188	R1079	N984	A885	E825	LEU	SER	VAL	VAL	ALA	GLY	GLY	LYS
ASP	GLN	M1378	L1288	A1189	E1080	C985	A885	A826	LEU	SER	VAL	VAL	ALA	GLY	GLY	LYS
GLY	LEU	M1379	Y1289	V1188	L1085	M987	A885	H827	LEU	SER	VAL	VAL	ALA	GLY	GLY	LYS
TYR	GLU	K1381	M1290	R1183	L1086	Q988	A885	N828	LEU	SER	VAL	VAL	ALA	GLY	GLY	LYS
MET	ARG	K1382	R1291	K1194	L1087	L989	A885	L829	LEU	SER	VAL	VAL	ALA	GLY	GLY	LYS
ILE	LEU	A1383	L1292	L1199	M1101	L990	A885	K630	LEU	SER	VAL	VAL	ALA	GLY	GLY	LYS
ARG	LEU	K1384	D1293	M1200	M1102	R990	A885	D721	LEU	SER	VAL	VAL	ALA	GLY	GLY	LYS
PHE	ALA	K1385	T1296	D1201	F1104	K991	A885	K727	LEU	SER	VAL	VAL	ALA	GLY	GLY	LYS
ILE	ALA	R1387	K1297	L1201	F1105	L998	A885	K727	LEU	SER	VAL	VAL	ALA	GLY	GLY	LYS
ALA	ALA	Q1388	L1298	G1206	F1106	F999	A885	L738	LEU	SER	VAL	VAL	ALA	GLY	GLY	LYS
ASP	ASP	L1389	E1207	E1207	M1108	L925	A885	L738	LEU	SER	VAL	VAL	ALA	GLY	GLY	LYS
TYR	GLU	D1390	M1208	M1208	M1109	L926	A885	K742	LEU	SER	VAL	VAL	ALA	GLY	GLY	LYS
TYR	ASP	R1391	T1209	T1209	R1114	R926	A885	E743	LEU	SER	VAL	VAL	ALA	GLY	GLY	LYS
TYR	ASP	I1394	R1301	M1209	G1114	R926	A885	M744	LEU	SER	VAL	VAL	ALA	GLY	GLY	LYS
VAL	VAL	Q1395	Q1302	L1210	L1114	P1003	A885	M744	LEU	SER	VAL	VAL	ALA	GLY	GLY	LYS
LYS	LYS	E1396	L1303	R1210	M1118	L1004	A885	M744	LEU	SER	VAL	VAL	ALA	GLY	GLY	LYS
ALA	ALA	GLY	L1304	K1212	M1118	L1005	A885	L749	LEU	SER	VAL	VAL	ALA	GLY	GLY	LYS
ASP	ASP	PHE	R1307	V1213	M1124	L1005	A885	I750	LEU	SER	VAL	VAL	ALA	GLY	GLY	LYS
THR	LEU	THR	T1310	M1216	K1127	L1009	A885	P753	LEU	SER	VAL	VAL	ALA	GLY	GLY	LYS
						L1010	A885	T754	LEU	SER	VAL	VAL	ALA	GLY	GLY	LYS

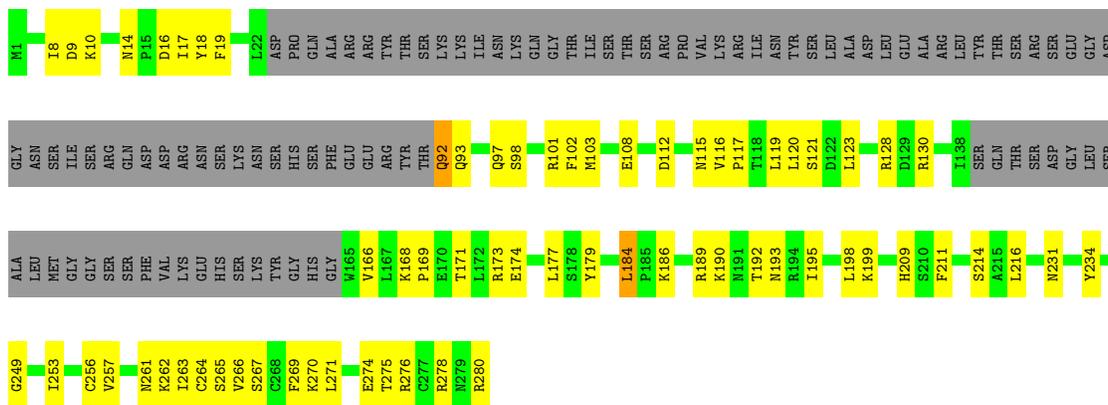
● Molecule 9: Actin-like protein ARP6





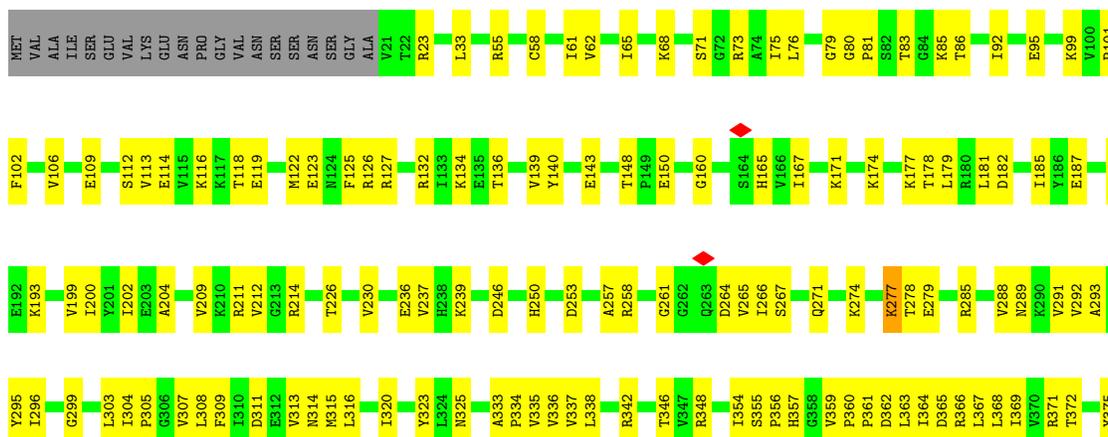
• Molecule 10: Vacuolar protein sorting-associated protein 71

Chain S: 42% 24% 34%



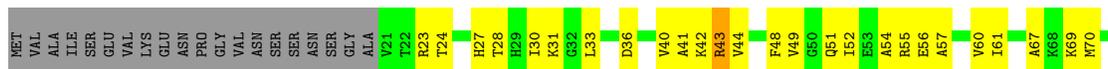
• Molecule 11: RuvB-like protein 1

Chain T: 60% 35%





• Molecule 11: RuvB-like protein 1



• Molecule 11: RuvB-like protein 1



• Molecule 12: RuvB-like protein 2

L111	L112	K113	T114	E115	Q119	R122	K123	S124	I125	G126	I127	K130	L135	I136	V141	K157	L158	T159	L160	K161	T162	M165	E166	T167	I168	L171	G172	M175	I176	V184	L185	A186	G187	D188	V189	I190	S191	I192	D193	K194	A195	S196	K201	R204	R208	Y212	D213	A214	M215	G216	A217	D218	T219	R220	F221	V222	Q223	L229	V236	H237	S240	L241	H242	E243	I244	D245	V246	I247	R250	G253	F254	L255	A256	L257	G263	R266	S267	E268	V269	R270	I273	K281	I288	L283	F294	V298	H299	M300	L301	D302	I303	E304	C305	F306	R311	D315	E316	P319	I320	V321	M322	M323	A324	T325	M326	R327	K331	T332	T335	K338	S339	P340	H341	P344	L345	D346	L347	L348	D349	R350	S351	I352	Y359	I364	I367	R371	E378	D382	L387	V392	L396	R397	M401	L402	I403	Q408	I409	A410	M411	K414	M415	M416	T417	D432	R435	S436	V437	V440	Q446	Y447	I448	N453	V454	K460	SER	ALA	ASP	PRO	ASP	ALA	MET	ASP	THR	THR	GLU
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33595	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.042	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00157	Depositor
Map size (\AA)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1, 1.1, 1.1	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: MG, BEF, ADP, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/807	0.53	0/1081
1	B	0.24	0/807	0.55	0/1081
2	C	0.23	0/658	0.59	0/880
2	D	0.24	0/645	0.58	0/862
3	E	0.25	0/806	0.56	0/1091
3	F	0.25	0/777	0.52	0/1053
4	G	0.25	0/756	0.48	0/1017
4	H	0.26	0/722	0.51	0/972
5	I	0.54	0/4436	0.93	0/6841
6	J	0.54	0/4486	0.90	0/6925
7	Z	0.25	0/1385	0.51	0/1863
8	M	0.25	0/5495	0.52	1/7442 (0.0%)
9	R	0.25	0/3429	0.48	0/4650
10	S	0.24	0/1523	0.52	0/2052
11	T	0.25	0/3433	0.53	0/4646
11	V	0.24	0/3375	0.52	0/4565
11	X	0.24	0/3439	0.52	0/4652
12	U	0.25	0/3333	0.52	0/4492
12	W	0.25	0/3361	0.51	0/4530
12	Y	0.24	0/3447	0.50	0/4649
All	All	0.32	0/47120	0.62	1/65344 (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
3	E	0	1
7	Z	0	1
10	S	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
11	T	0	1
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	953	LEU	CA-CB-CG	5.49	127.93	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	26	PHE	Peptide
10	S	211	PHE	Peptide
11	T	160	GLY	Peptide
7	Z	298	THR	Peptide

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	796	0	841	34	0
1	B	796	0	841	43	0
2	C	651	0	690	35	0
2	D	638	0	677	28	0
3	E	795	0	834	39	0
3	F	767	0	792	26	0
4	G	746	0	771	25	0
4	H	712	0	736	30	0
5	I	3960	0	2179	106	0
6	J	3994	0	2172	129	0
7	Z	1367	0	1291	40	0
8	M	5398	0	5352	215	0
9	R	3335	0	3256	109	0
10	S	1499	0	1544	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	T	3391	0	3513	139	0
11	V	3336	0	3474	167	0
11	X	3397	0	3533	157	0
12	U	3299	0	3387	137	0
12	W	3325	0	3410	155	0
12	Y	3410	0	3465	129	0
13	M	27	0	12	5	0
13	R	27	0	12	1	0
13	T	27	0	12	1	0
13	U	27	0	12	5	0
13	V	27	0	12	8	0
13	W	27	0	12	4	0
13	X	27	0	12	7	0
13	Y	27	0	12	5	0
14	M	4	0	0	2	0
14	R	4	0	0	1	0
15	M	1	0	0	0	0
15	R	1	0	0	0	0
15	T	1	0	0	0	0
15	U	1	0	0	0	0
15	V	1	0	0	0	0
15	W	1	0	0	0	0
15	X	1	0	0	0	0
15	Y	1	0	0	0	0
16	S	2	0	0	0	0
All	All	45846	0	42854	1560	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 18.

The worst 5 of 1560 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)
10:S:92:GLN:N	10:S:92:GLN:HE21	1.36	1.20
10:S:92:GLN:N	10:S:92:GLN:NE2	2.16	0.92
5:I:-51:DC:O2	6:J:51:DG:N2	2.03	0.92
5:I:-51:DC:N3	6:J:51:DG:N1	2.23	0.85
8:M:758:LEU:HB3	8:M:1302:GLN:HG2	1.56	0.85

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	95/136 (70%)	93 (98%)	2 (2%)	0	100	100
1	B	95/136 (70%)	92 (97%)	3 (3%)	0	100	100
2	C	80/103 (78%)	75 (94%)	5 (6%)	0	100	100
2	D	78/103 (76%)	76 (97%)	2 (3%)	0	100	100
3	E	101/158 (64%)	96 (95%)	5 (5%)	0	100	100
3	F	99/158 (63%)	96 (97%)	3 (3%)	0	100	100
4	G	94/131 (72%)	92 (98%)	2 (2%)	0	100	100
4	H	89/131 (68%)	84 (94%)	5 (6%)	0	100	100
7	Z	176/180 (98%)	157 (89%)	17 (10%)	2 (1%)	12	46
8	M	684/1514 (45%)	629 (92%)	54 (8%)	1 (0%)	48	83
9	R	407/438 (93%)	386 (95%)	21 (5%)	0	100	100
10	S	179/280 (64%)	163 (91%)	15 (8%)	1 (1%)	22	60
11	T	441/463 (95%)	412 (93%)	29 (7%)	0	100	100
11	V	430/463 (93%)	415 (96%)	15 (4%)	0	100	100
11	X	440/463 (95%)	425 (97%)	15 (3%)	0	100	100
12	U	426/471 (90%)	413 (97%)	13 (3%)	0	100	100
12	W	429/471 (91%)	420 (98%)	9 (2%)	0	100	100
12	Y	445/471 (94%)	430 (97%)	14 (3%)	1 (0%)	44	78
All	All	4788/6270 (76%)	4554 (95%)	229 (5%)	5 (0%)	50	83

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	Z	299	PRO
10	S	184	LEU
7	Z	326	LYS
12	Y	416	ASN

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Mol	Chain	Res	Type
8	M	972	ALA

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	84/113 (74%)	82 (98%)	2 (2%)	44	63
1	B	84/113 (74%)	83 (99%)	1 (1%)	67	79
2	C	68/81 (84%)	67 (98%)	1 (2%)	60	75
2	D	67/81 (83%)	65 (97%)	2 (3%)	36	56
3	E	82/124 (66%)	82 (100%)	0	100	100
3	F	77/124 (62%)	77 (100%)	0	100	100
4	G	83/109 (76%)	83 (100%)	0	100	100
4	H	78/109 (72%)	77 (99%)	1 (1%)	65	77
7	Z	134/171 (78%)	132 (98%)	2 (2%)	60	75
8	M	574/1376 (42%)	567 (99%)	7 (1%)	67	79
9	R	372/396 (94%)	372 (100%)	0	100	100
10	S	178/261 (68%)	177 (99%)	1 (1%)	84	88
11	T	371/391 (95%)	369 (100%)	2 (0%)	86	90
11	V	368/391 (94%)	365 (99%)	3 (1%)	79	85
11	X	374/391 (96%)	373 (100%)	1 (0%)	91	92
12	U	367/403 (91%)	366 (100%)	1 (0%)	91	92
12	W	369/403 (92%)	369 (100%)	0	100	100
12	Y	372/403 (92%)	372 (100%)	0	100	100
All	All	4102/5440 (75%)	4078 (99%)	24 (1%)	82	88

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	M	1146	LYS

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Mol	Chain	Res	Type
11	T	277	LYS
10	S	92	GLN
11	T	392	ARG
7	Z	216	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
12	W	310	ASN
12	Y	119	GLN
11	X	325	ASN
9	R	246	ASN
12	W	90	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 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 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
13	ADP	W	501	15	24,29,29	0.94	1 (4%)	29,45,45	1.47	5 (17%)
14	BEF	R	502	13	0,3,3	-	-	-	-	-
14	BEF	M	1602	-	0,3,3	-	-	-	-	-
13	ADP	V	501	15	24,29,29	0.93	1 (4%)	29,45,45	1.50	4 (13%)
13	ADP	T	501	15	24,29,29	0.97	1 (4%)	29,45,45	1.48	4 (13%)
13	ADP	Y	501	15	24,29,29	0.98	1 (4%)	29,45,45	1.44	4 (13%)
13	ADP	U	501	15	24,29,29	0.97	1 (4%)	29,45,45	1.50	4 (13%)
13	ADP	M	1601	15	24,29,29	0.96	1 (4%)	29,45,45	1.41	4 (13%)
13	ADP	R	501	15,14	24,29,29	0.96	1 (4%)	29,45,45	1.46	4 (13%)
13	ADP	X	501	15	24,29,29	0.98	1 (4%)	29,45,45	1.38	4 (13%)

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
13	ADP	W	501	15	-	6/12/32/32	0/3/3/3
13	ADP	V	501	15	-	5/12/32/32	0/3/3/3
13	ADP	T	501	15	-	0/12/32/32	0/3/3/3
13	ADP	Y	501	15	-	2/12/32/32	0/3/3/3
13	ADP	U	501	15	-	1/12/32/32	0/3/3/3
13	ADP	M	1601	15	-	5/12/32/32	0/3/3/3
13	ADP	R	501	15,14	-	4/12/32/32	0/3/3/3
13	ADP	X	501	15	-	1/12/32/32	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	W	501	ADP	C5-C4	2.58	1.47	1.40
13	X	501	ADP	C5-C4	2.58	1.47	1.40
13	U	501	ADP	C5-C4	2.51	1.47	1.40
13	T	501	ADP	C5-C4	2.51	1.47	1.40
13	V	501	ADP	C5-C4	2.50	1.47	1.40

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	U	501	ADP	PA-O3A-PB	-3.92	119.38	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	V	501	ADP	PA-O3A-PB	-3.85	119.60	132.83
13	W	501	ADP	C3'-C2'-C1'	3.70	106.55	100.98
13	T	501	ADP	PA-O3A-PB	-3.67	120.23	132.83
13	Y	501	ADP	PA-O3A-PB	-3.61	120.45	132.83

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

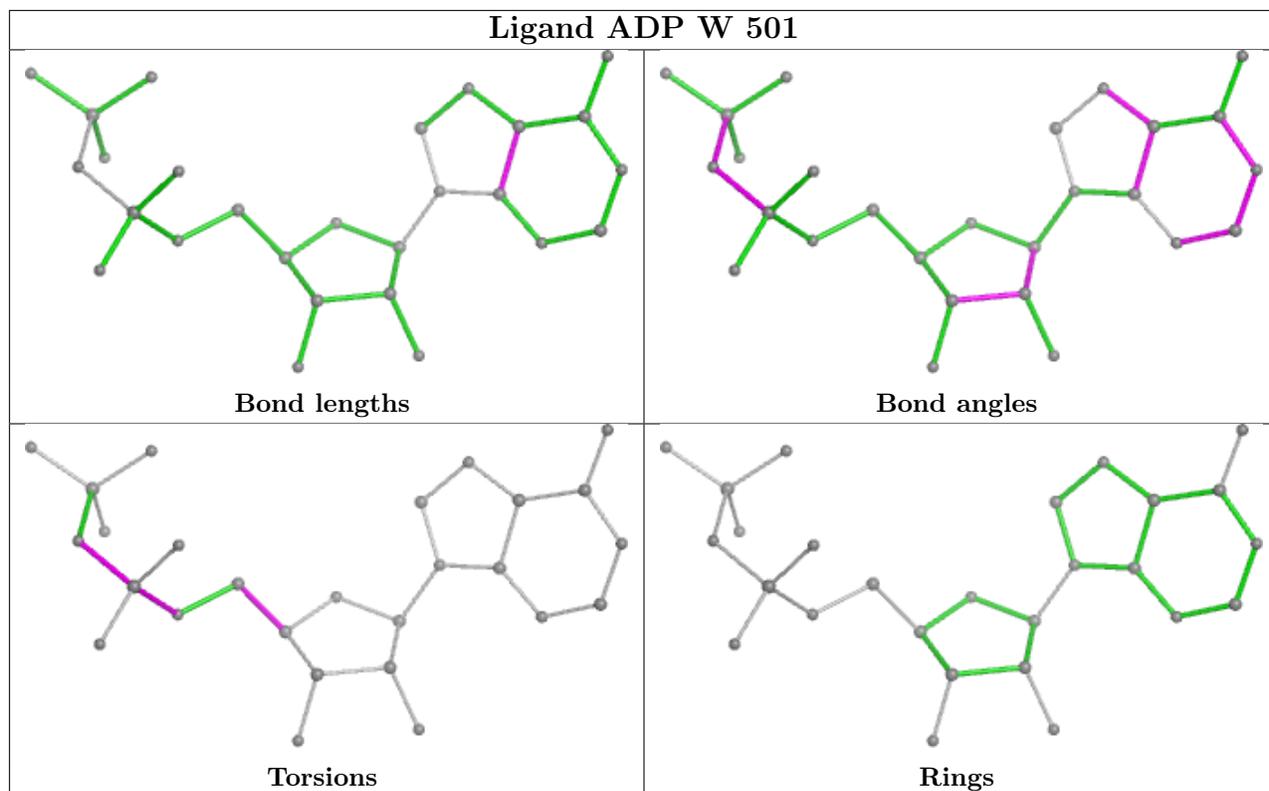
Mol	Chain	Res	Type	Atoms
13	M	1601	ADP	PB-O3A-PA-O5'
13	M	1601	ADP	C5'-O5'-PA-O2A
13	R	501	ADP	C5'-O5'-PA-O3A
13	R	501	ADP	C3'-C4'-C5'-O5'
13	V	501	ADP	C5'-O5'-PA-O3A

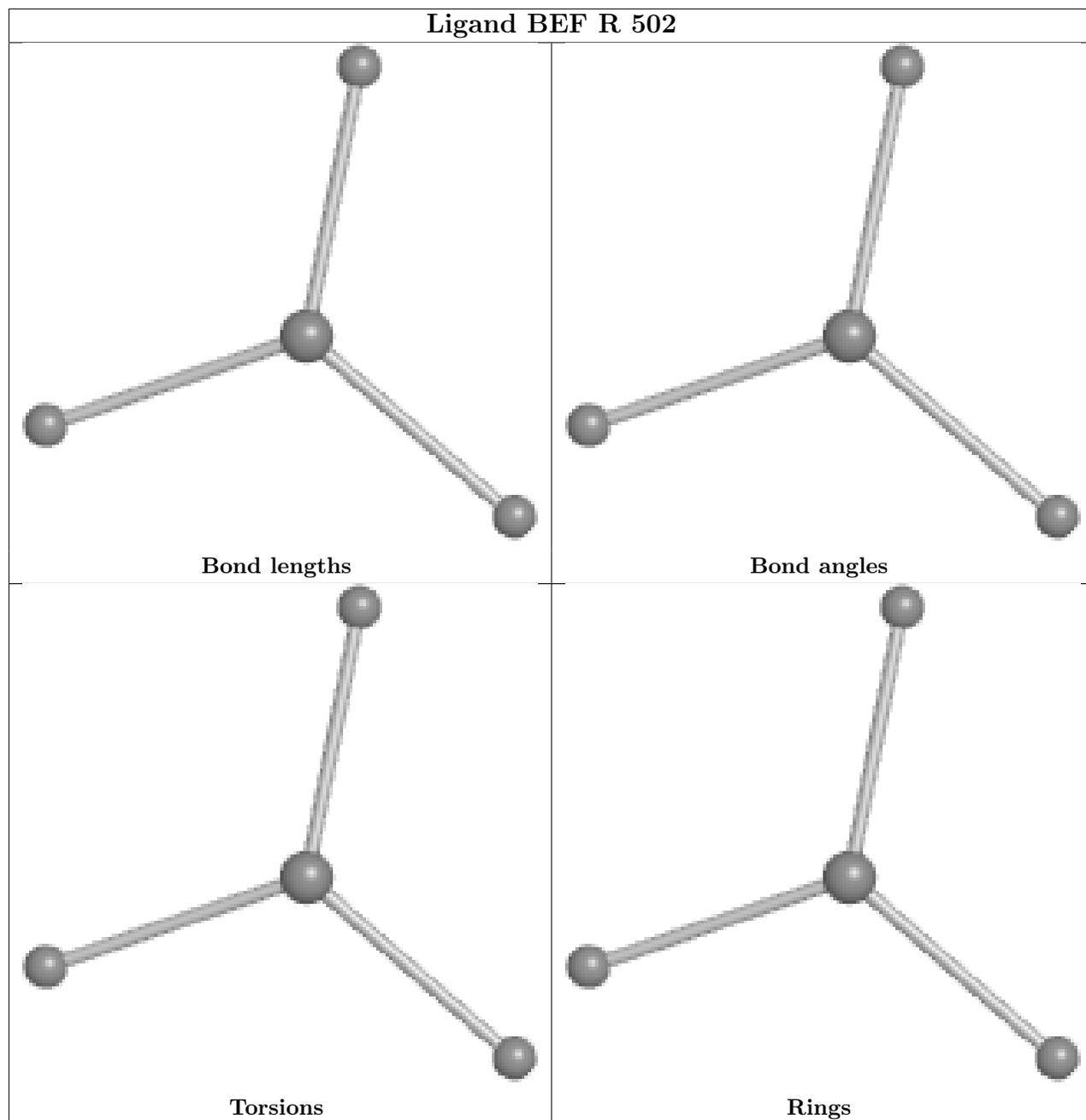
There are no ring outliers.

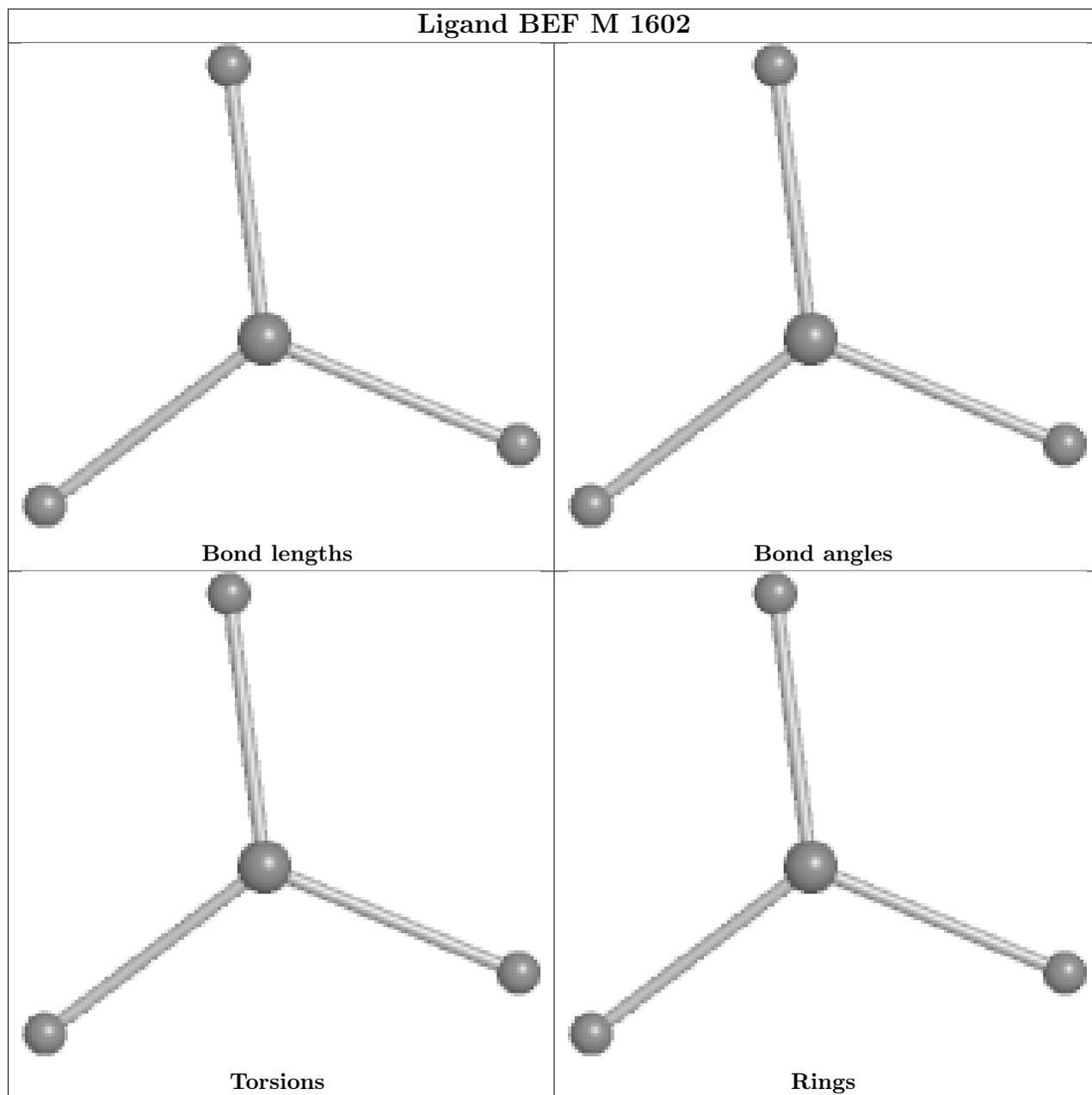
10 monomers are involved in 37 short contacts:

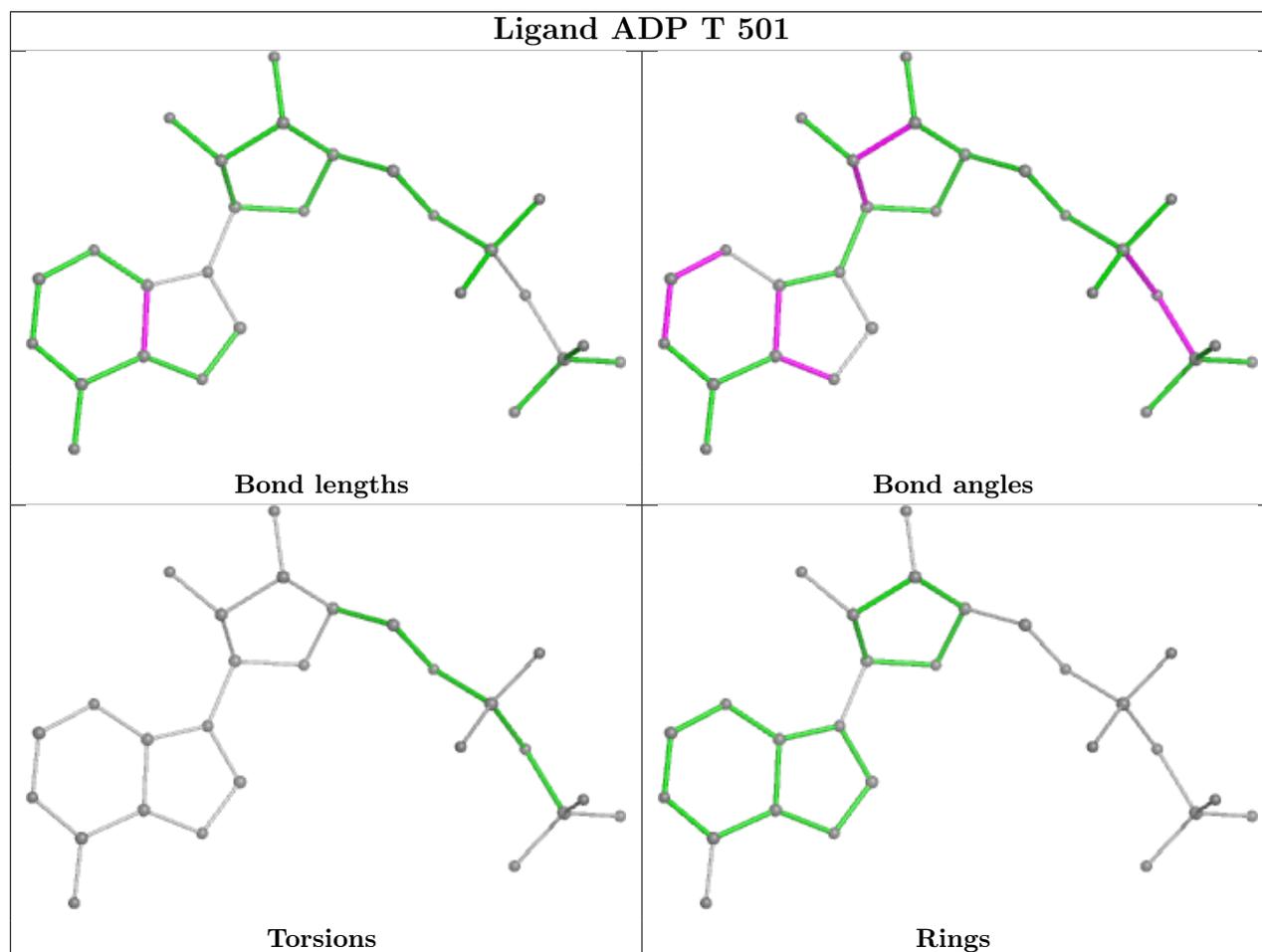
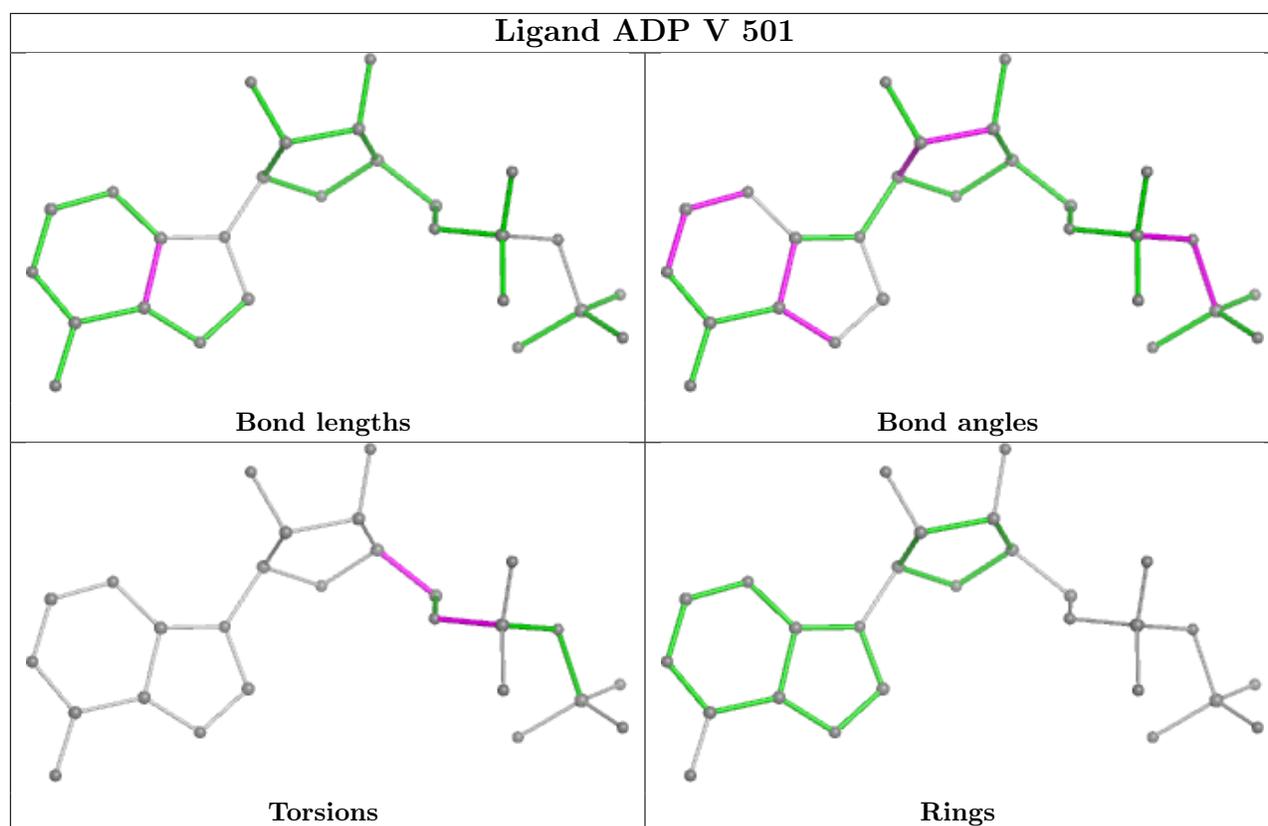
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	W	501	ADP	4	0
14	R	502	BEF	1	0
14	M	1602	BEF	2	0
13	V	501	ADP	8	0
13	T	501	ADP	1	0
13	Y	501	ADP	5	0
13	U	501	ADP	5	0
13	M	1601	ADP	5	0
13	R	501	ADP	1	0
13	X	501	ADP	7	0

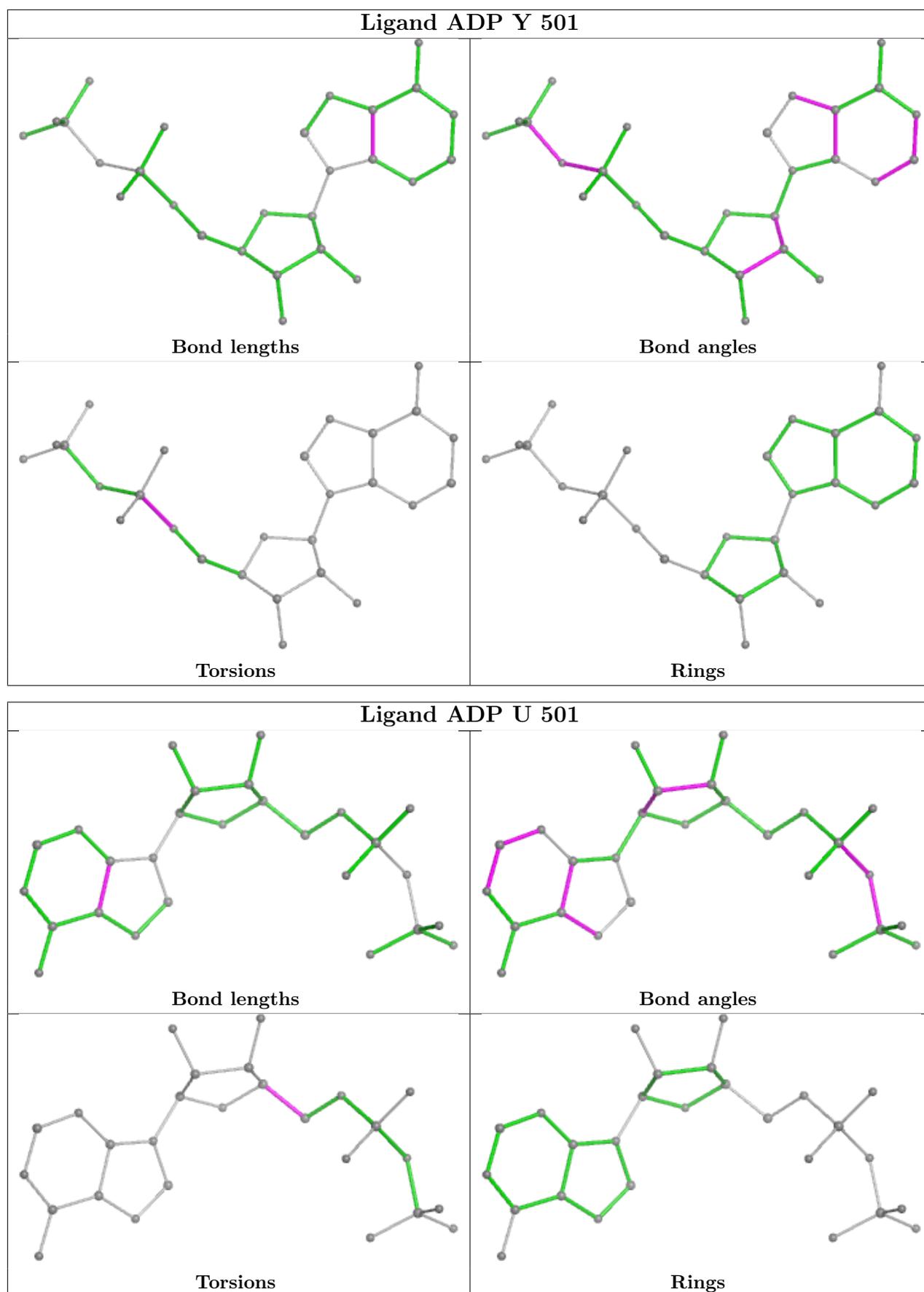
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

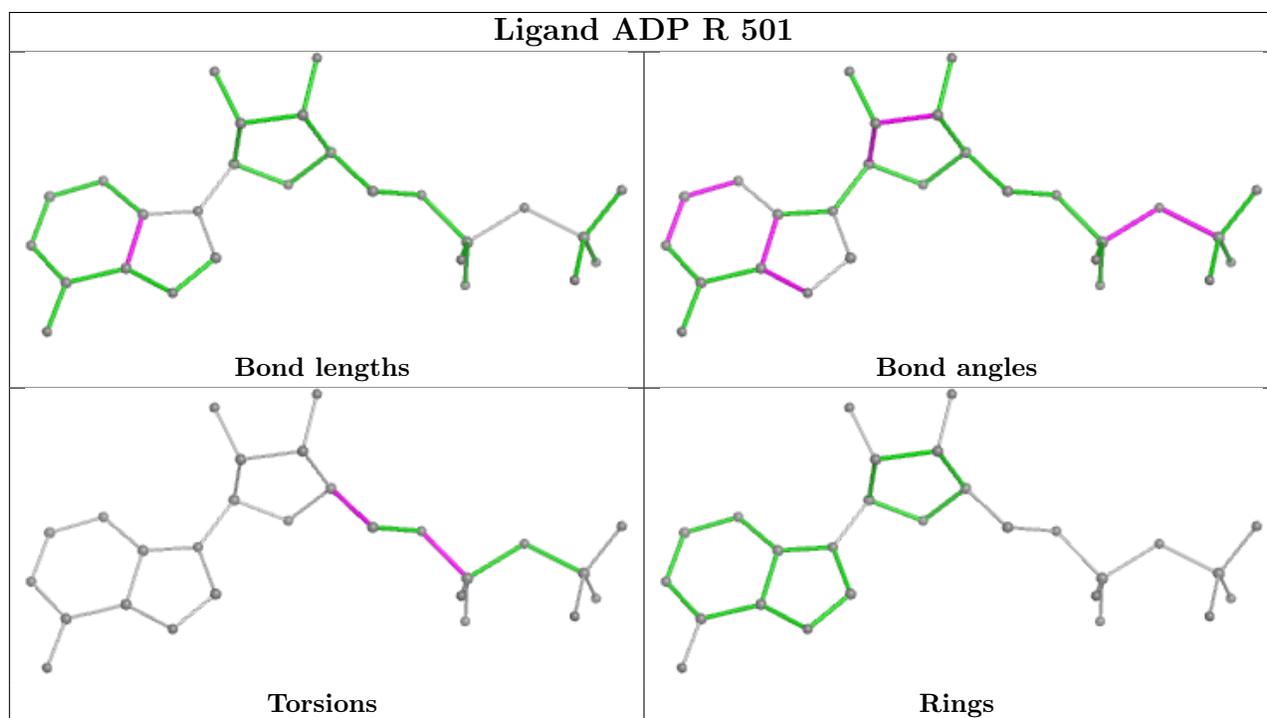
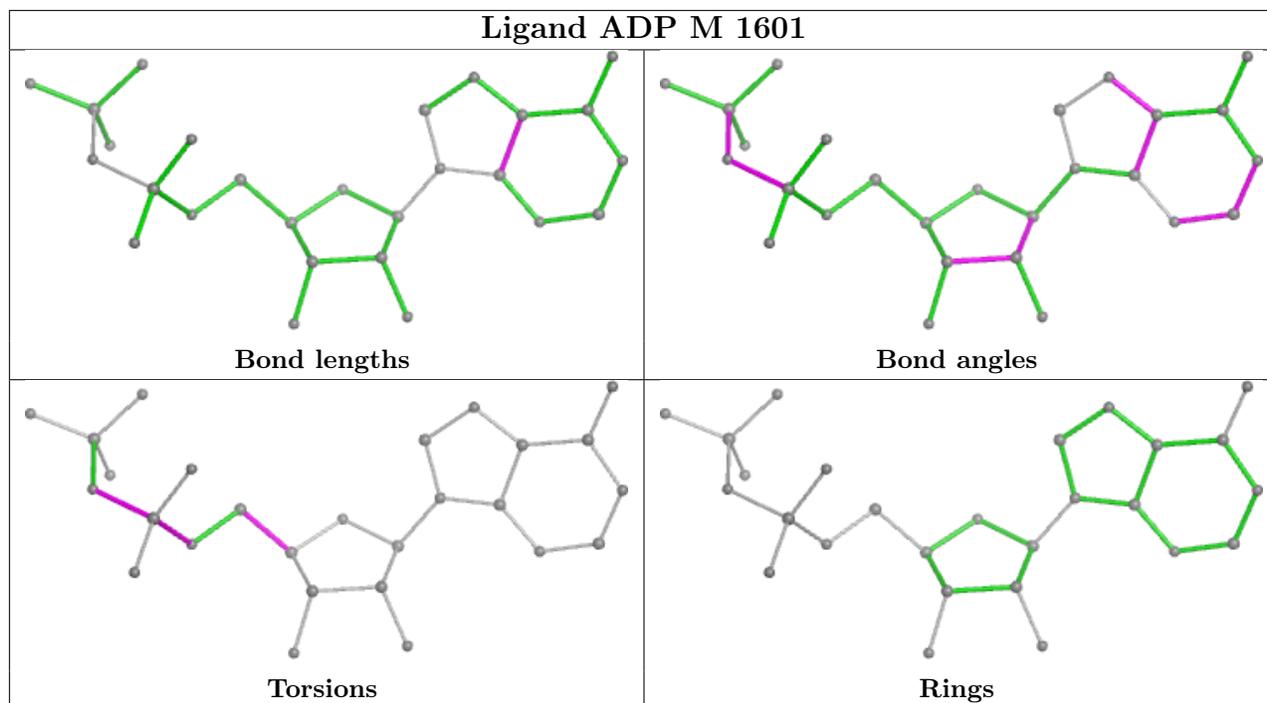


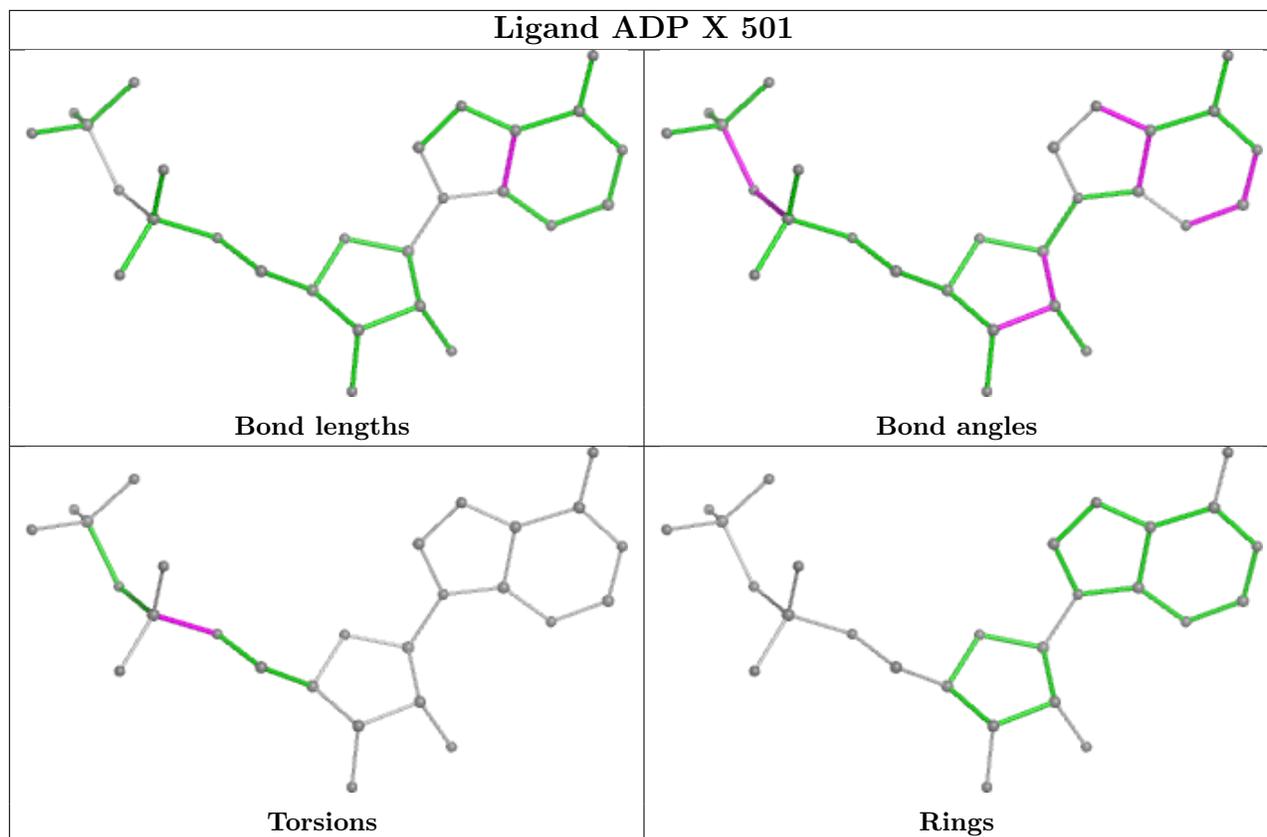












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
7	Z	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Z	329:LYS	C	581:THR	N	57.91

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18472. These allow visual inspection of the internal detail of the map and identification of artifacts.

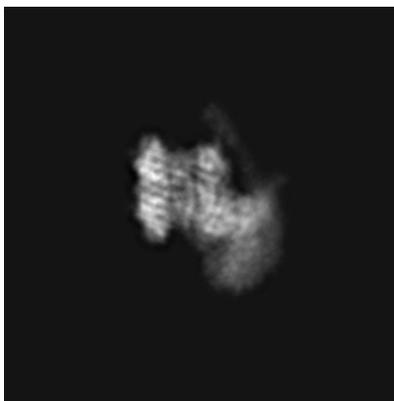
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

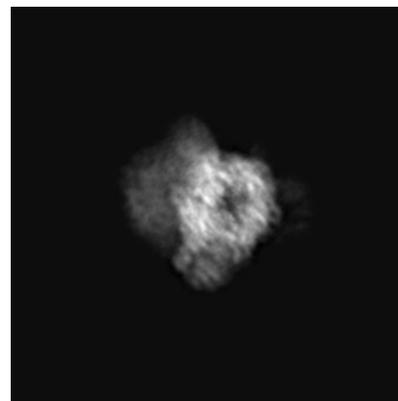
6.1.1 Primary map



X

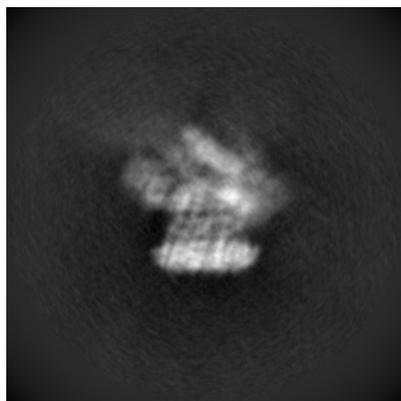


Y

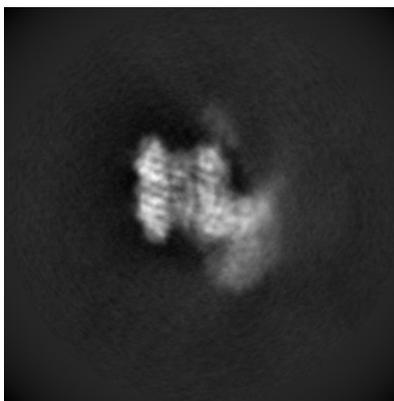


Z

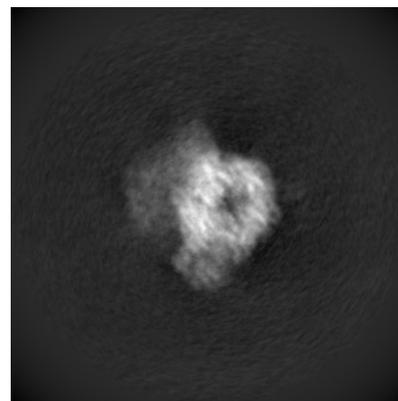
6.1.2 Raw map



X



Y

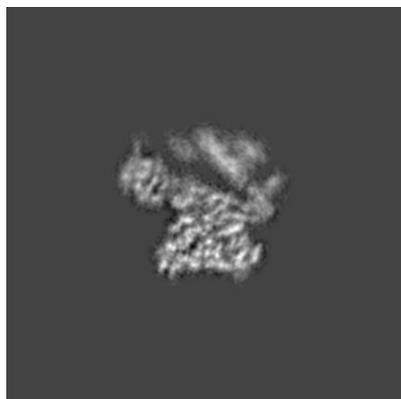


Z

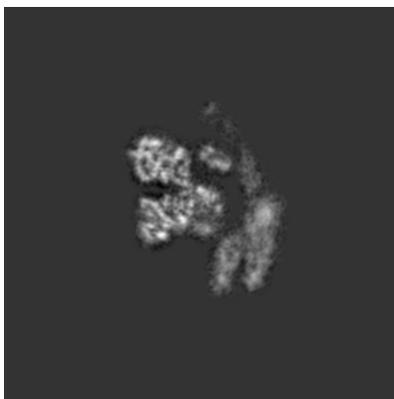
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

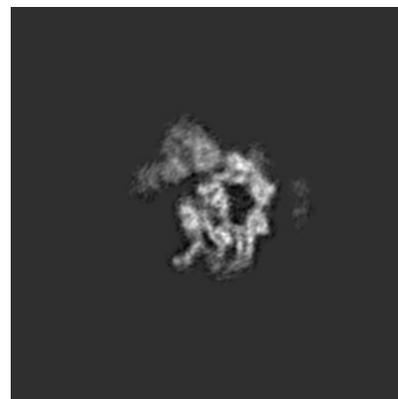
6.2.1 Primary map



X Index: 192

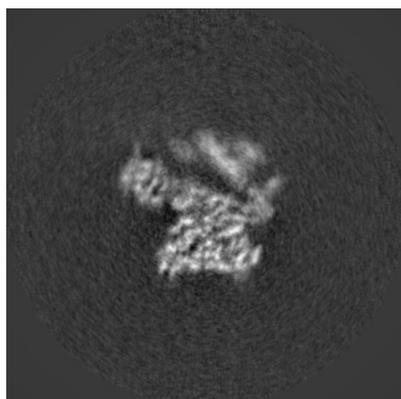


Y Index: 192

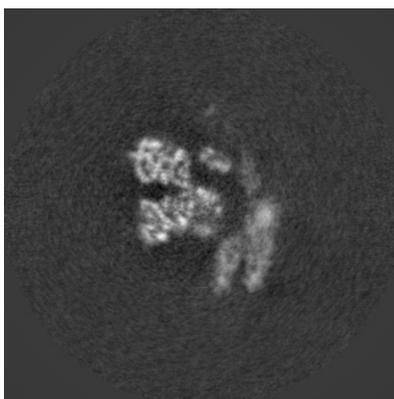


Z Index: 192

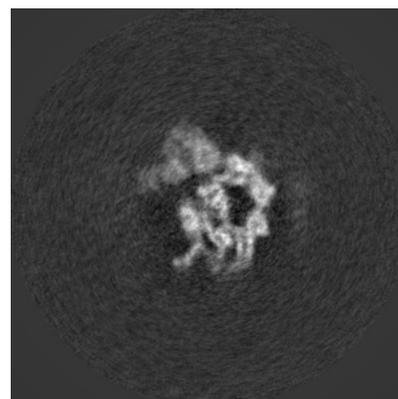
6.2.2 Raw map



X Index: 192



Y Index: 192



Z Index: 192

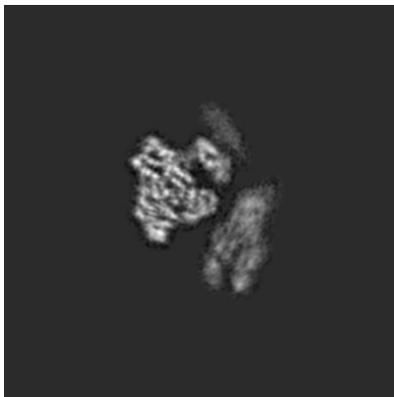
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

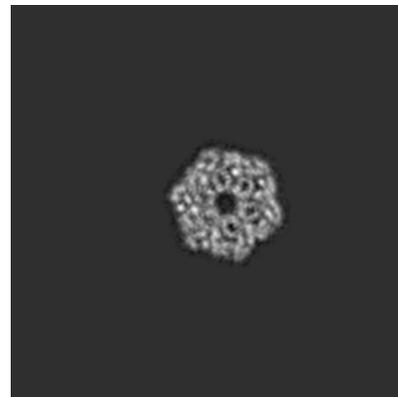
6.3.1 Primary map



X Index: 187

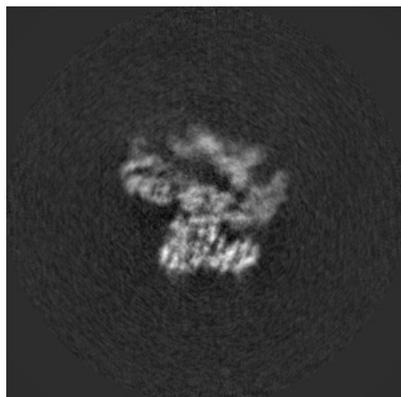


Y Index: 207

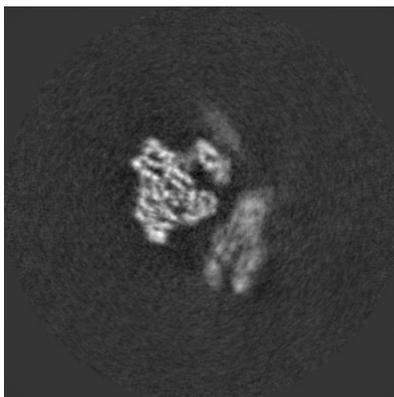


Z Index: 144

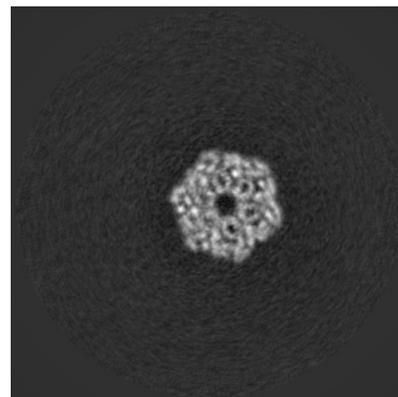
6.3.2 Raw map



X Index: 187



Y Index: 207

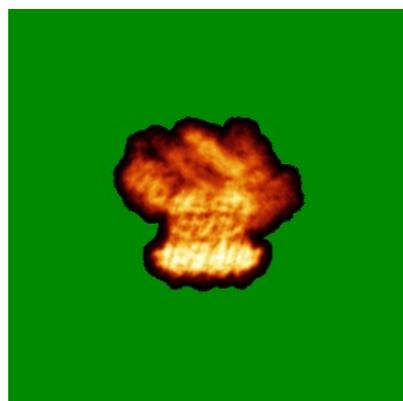


Z Index: 144

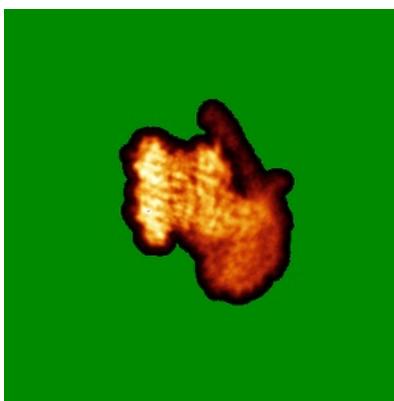
The images above show the largest variance slices of the map in three orthogonal directions.

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

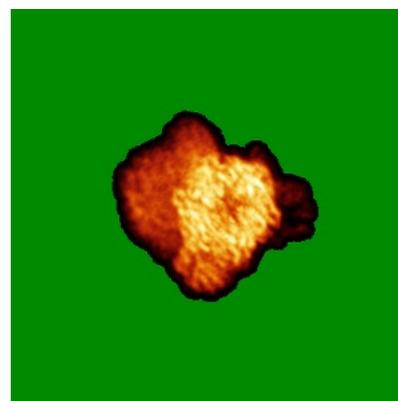
6.4.1 Primary map



X

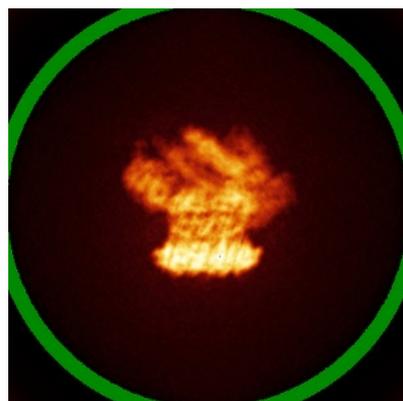


Y

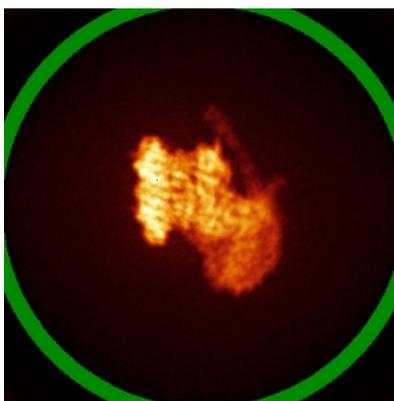


Z

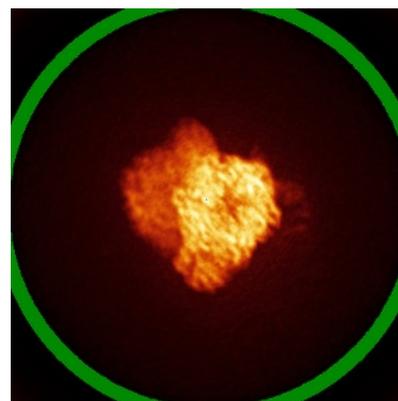
6.4.2 Raw map



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.

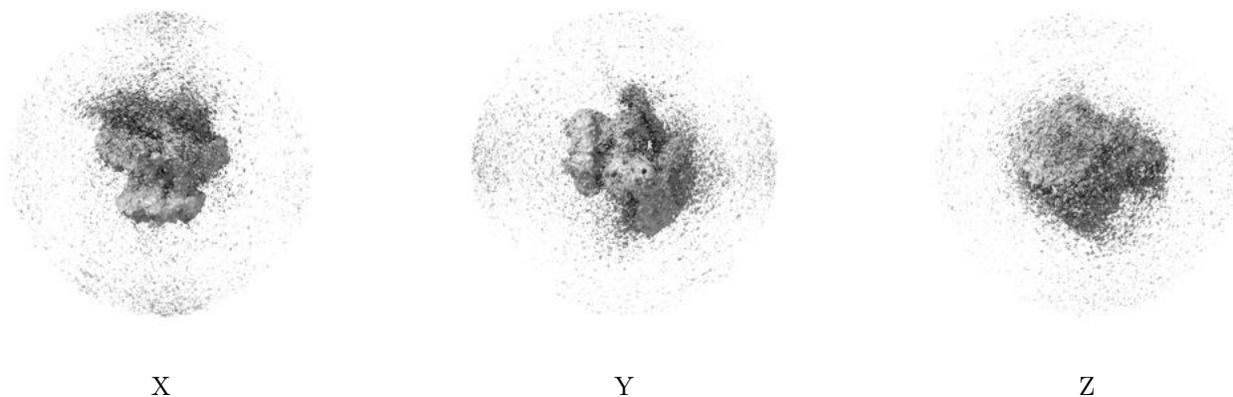
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00157. 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.

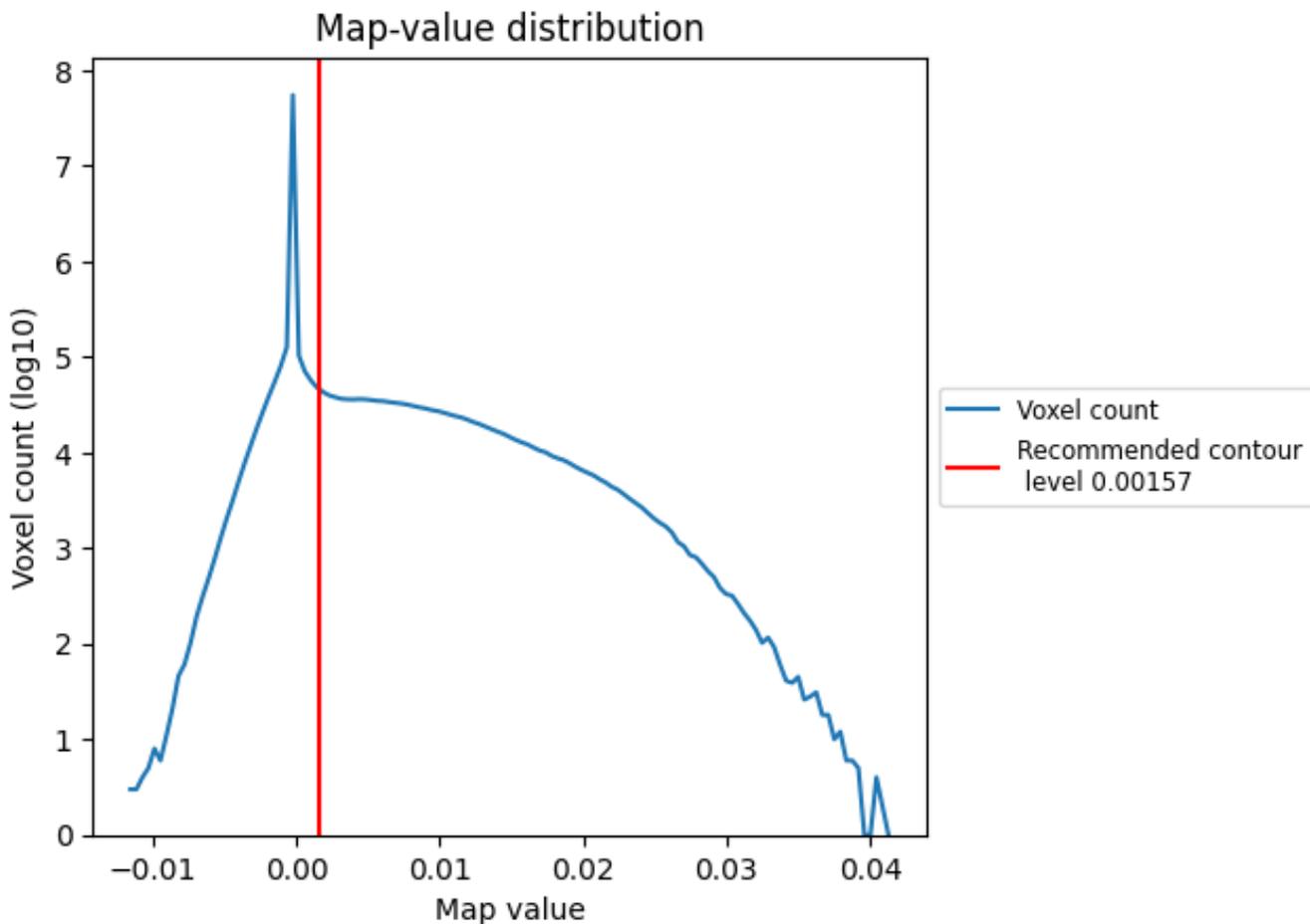
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

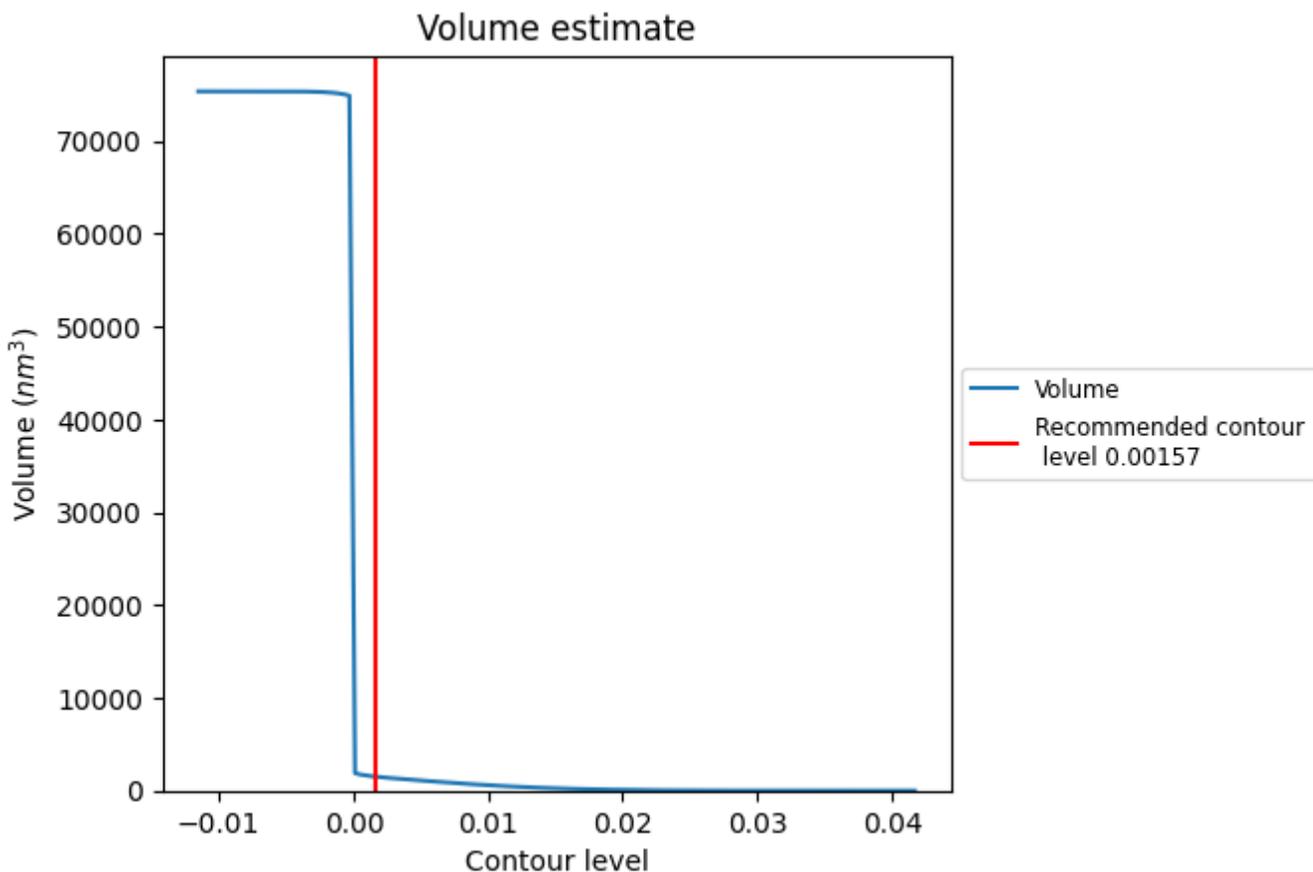
This section contains the results of statistical analysis of the map.

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.

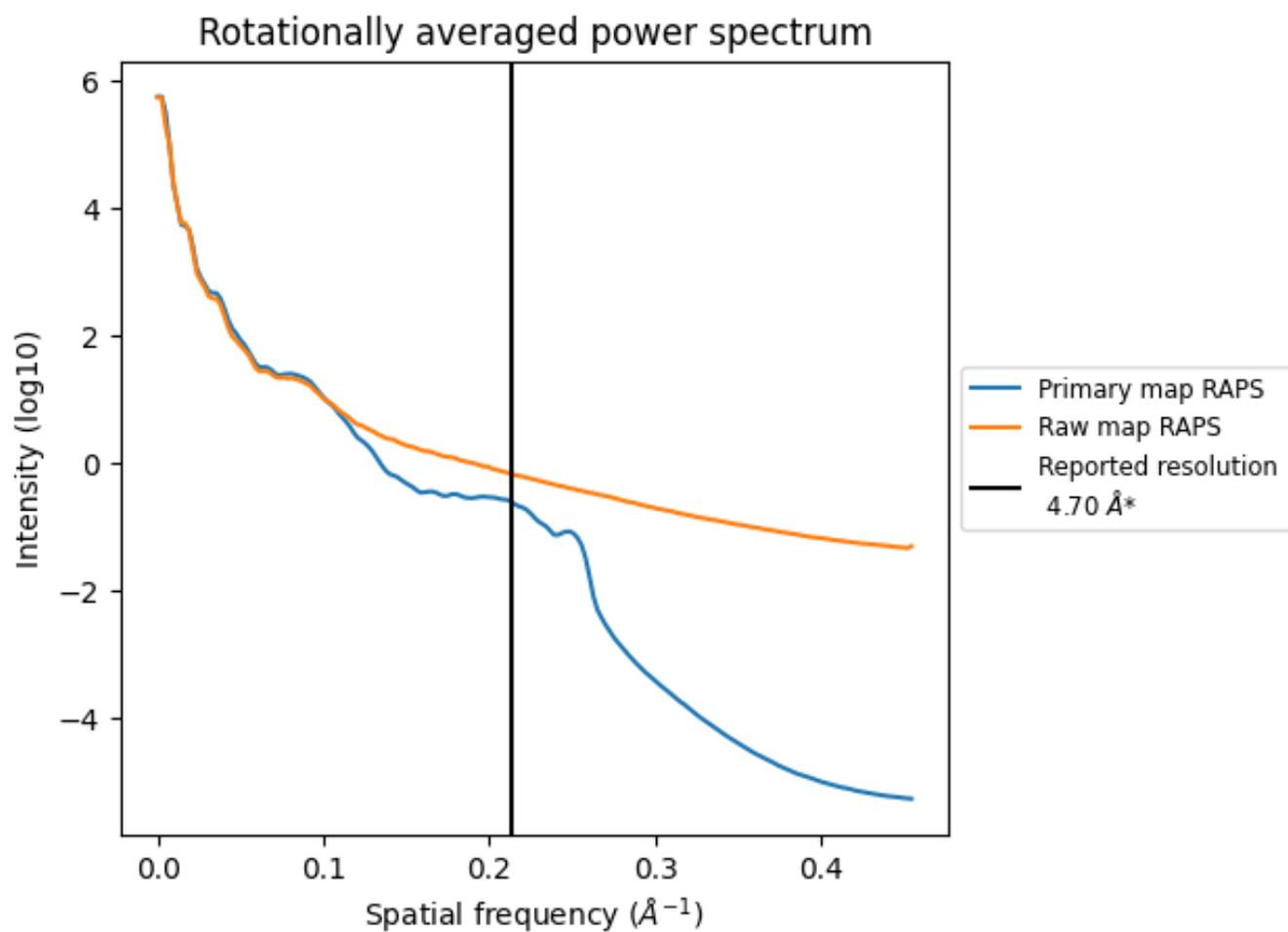
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1517 nm³; this corresponds to an approximate mass of 1370 kDa.

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

7.3 Rotationally averaged power spectrum i

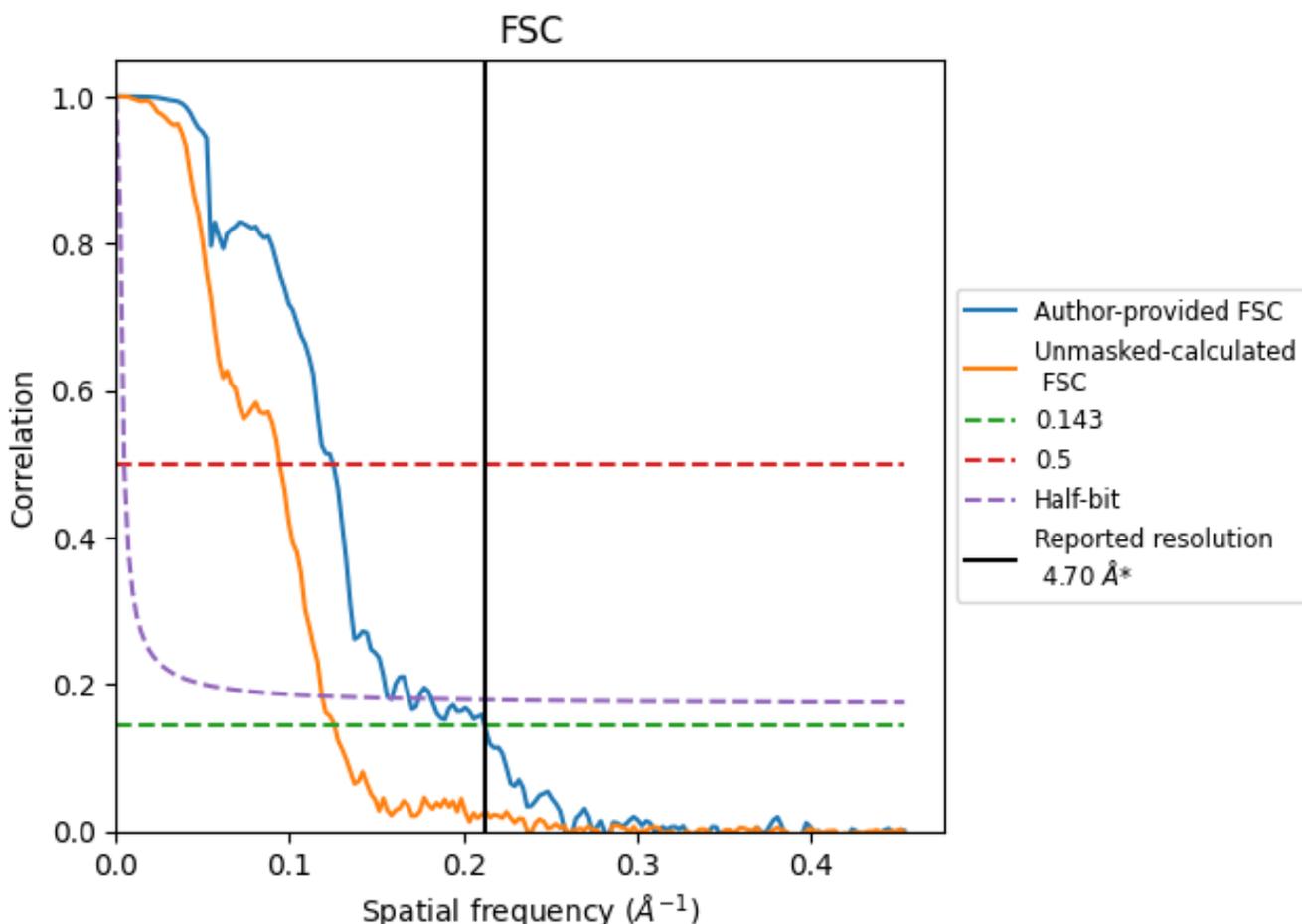


*Reported resolution corresponds to spatial frequency of 0.213 Å⁻¹

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 0.213 Å⁻¹

8.2 Resolution estimates [i](#)

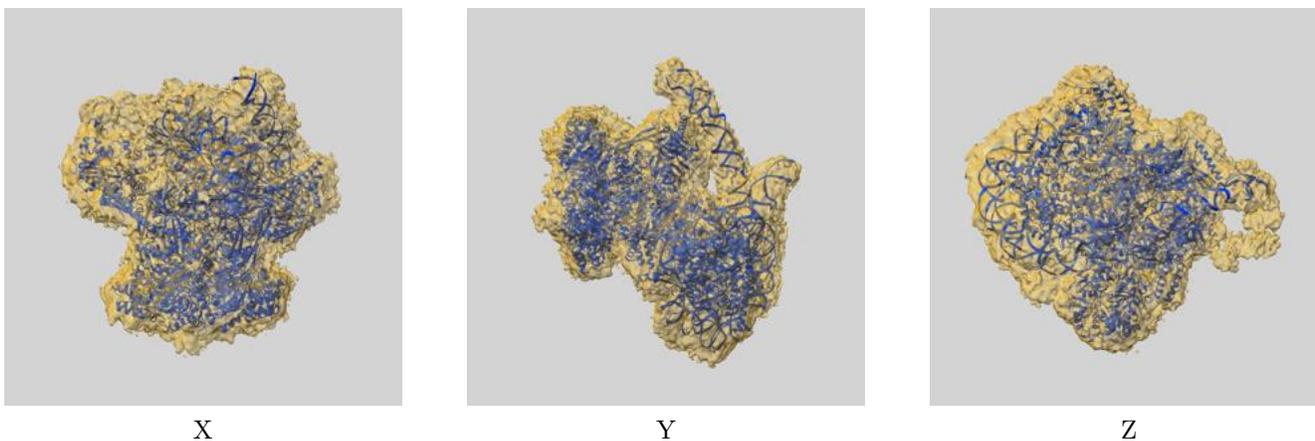
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	4.71	8.01	6.35
Unmasked-calculated*	7.95	10.60	8.42

*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 7.95 differs from the reported value 4.7 by more than 10 %

9 Map-model fit [i](#)

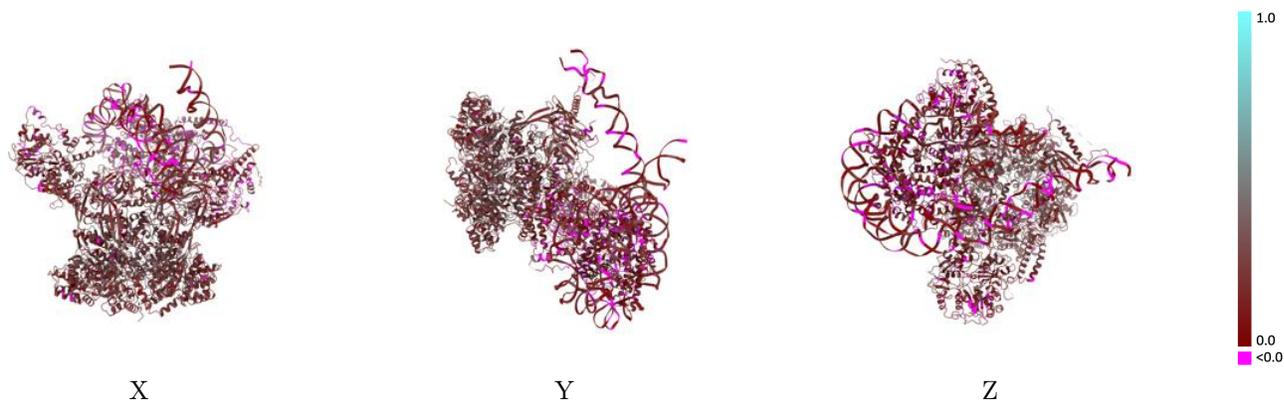
This section contains information regarding the fit between EMDB map EMD-18472 and PDB model 8QKV. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



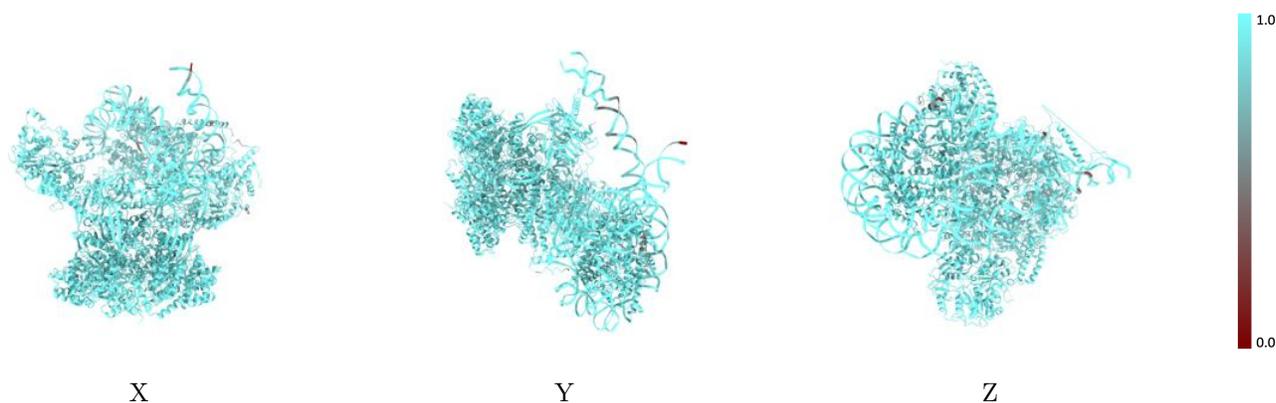
The images above show the 3D surface view of the map at the recommended contour level 0.00157 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



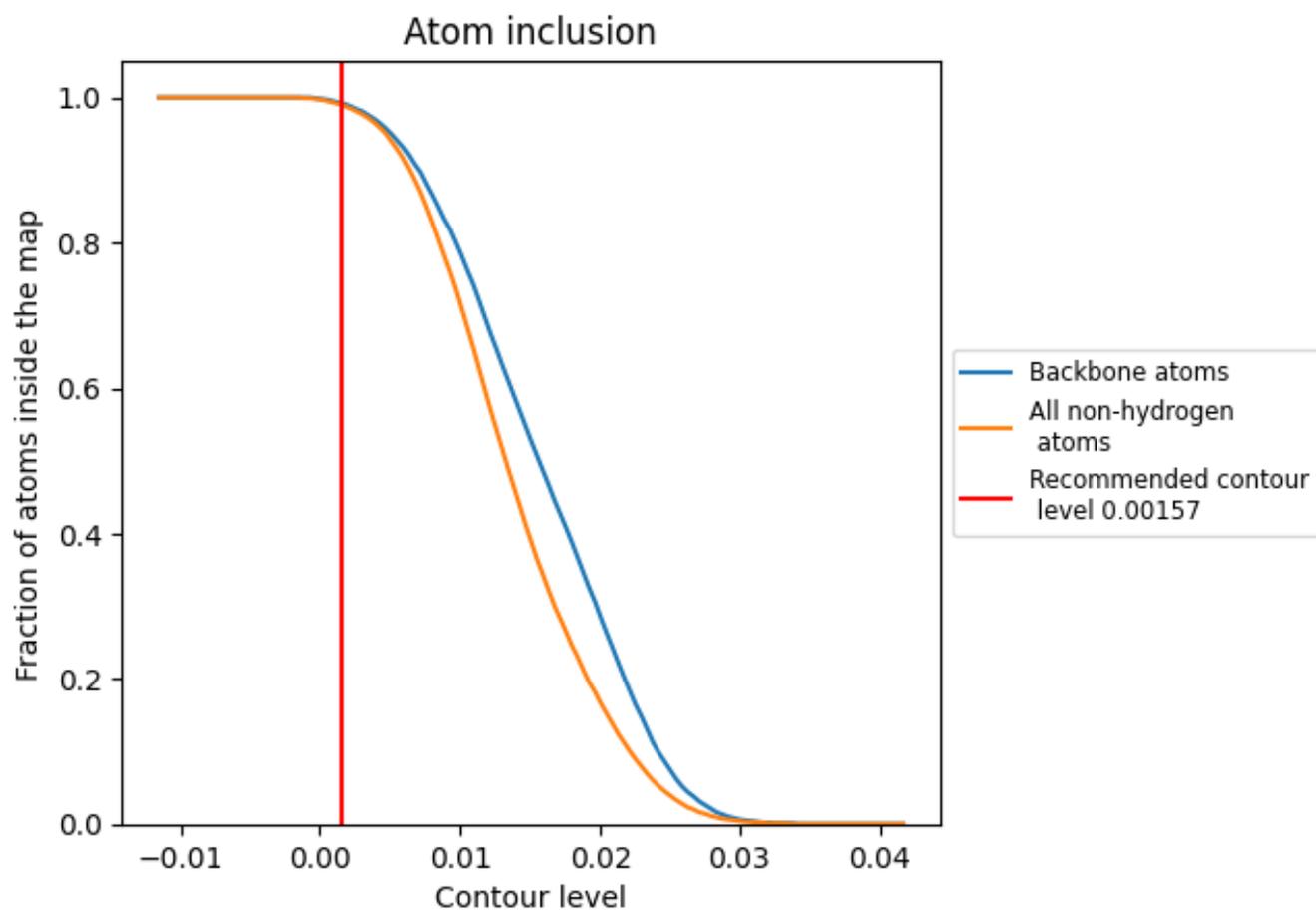
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00157).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.00157) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9900	 0.1850
A	 0.9870	 0.0990
B	 0.9970	 0.1270
C	 0.9980	 0.1380
D	 0.9790	 0.0630
E	 1.0000	 0.1340
F	 0.9890	 0.0960
G	 0.9900	 0.1180
H	 0.9970	 0.1260
I	 0.9720	 0.0980
J	 0.9720	 0.1160
M	 0.9910	 0.1810
R	 0.9960	 0.1810
S	 0.9940	 0.1710
T	 0.9930	 0.2280
U	 1.0000	 0.2460
V	 0.9990	 0.2470
W	 0.9990	 0.2450
X	 0.9990	 0.2430
Y	 0.9990	 0.2490
Z	 0.9340	 0.1360

