



Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 08:16 AM EST

PDB ID : 6BCU
EMDB ID : EMD-7086
Title : Cryo-EM structure of the activated RHEB-mTORC1 refined to 3.4 angstrom
Authors : Pavletich, N.P.; Yang, H.
Deposited on : 2017-10-20
Resolution : 3.43 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

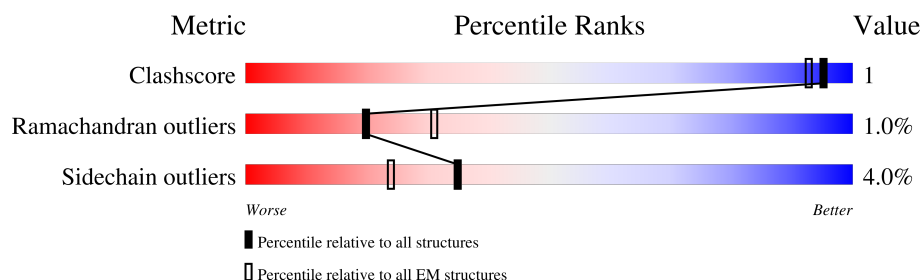
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.43 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	2549	<div> <div>21%</div> <div>80%</div> <div>6%</div> <div>14%</div> </div>
1	B	2549	<div> <div>21%</div> <div>79%</div> <div>7%</div> <div>14%</div> </div>
2	D	326	<div> <div>71%</div> <div>91%</div> <div>6%</div> <div>•</div> </div>
2	E	326	<div> <div>73%</div> <div>90%</div> <div>7%</div> <div>•</div> </div>
3	W	1343	<div> <div>43%</div> <div>72%</div> <div>6%</div> <div>22%</div> </div>
3	Y	1343	<div> <div>43%</div> <div>72%</div> <div>6%</div> <div>22%</div> </div>
4	X	122	<div> <div>6%</div> <div>•</div> <div>93%</div> </div>
4	Z	122	<div> <div>6%</div> <div>•</div> <div>93%</div> </div>

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Mol	Chain	Length	Quality of chain
5	R	188	<div><div>66%</div><div><div></div><div></div><div></div></div><div>84%</div><div>12%</div></div>
5	S	188	<div><div>66%</div><div><div></div><div></div><div></div></div><div>84%</div><div>12%</div></div>

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 119740 atoms, of which 60078 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 Serine/threonine-protein kinase mTOR,Serine/threonine-protein kinase mTOR.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2204	Total	C	H	N	O	S	0	0
			35397	11194	17859	3074	3157	113		
1	B	2204	Total	C	H	N	O	S	0	0
			35397	11194	17859	3074	3157	113		

- Molecule 2 is a protein called Target of rapamycin complex subunit LST8.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	317	Total	C	H	N	O	S	0	0
			4809	1526	2353	436	476	18		
2	E	317	Total	C	H	N	O	S	0	0
			4809	1526	2353	436	476	18		

- Molecule 3 is a protein called Regulatory-associated protein of mTOR,Regulatory-associated protein of mTOR.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	W	1052	Total	C	H	N	O	S	0	0
			16791	5361	8406	1450	1518	56		
3	Y	1052	Total	C	H	N	O	S	0	0
			16791	5361	8406	1450	1518	56		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	-7	MET	-	initiating methionine	UNP Q8N122
W	-6	ASP	-	expression tag	UNP Q8N122
W	-5	TYR	-	expression tag	UNP Q8N122
W	-4	LYS	-	expression tag	UNP Q8N122
W	-3	ASP	-	expression tag	UNP Q8N122
W	-2	ASP	-	expression tag	UNP Q8N122
W	-1	ASP	-	expression tag	UNP Q8N122

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Chain	Residue	Modelled	Actual	Comment	Reference
W	0	ASP	-	expression tag	UNP Q8N122
W	1	LYS	-	expression tag	UNP Q8N122
Y	-7	MET	-	initiating methionine	UNP Q8N122
Y	-6	ASP	-	expression tag	UNP Q8N122
Y	-5	TYR	-	expression tag	UNP Q8N122
Y	-4	LYS	-	expression tag	UNP Q8N122
Y	-3	ASP	-	expression tag	UNP Q8N122
Y	-2	ASP	-	expression tag	UNP Q8N122
Y	-1	ASP	-	expression tag	UNP Q8N122
Y	0	ASP	-	expression tag	UNP Q8N122
Y	1	LYS	-	expression tag	UNP Q8N122

- Molecule 4 is a protein called Eukaryotic translation initiation factor 4E-binding protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	X	8	Total	C	H	N	O	S	0	0
			126	42	58	9	16	1		
4	Z	8	Total	C	H	N	O	S	0	0
			126	42	58	9	16	1		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	-3	GLY	-	expression tag	UNP Q13541
X	-2	SER	-	expression tag	UNP Q13541
X	-1	GLY	-	expression tag	UNP Q13541
X	0	ARG	-	expression tag	UNP Q13541
Z	-3	GLY	-	expression tag	UNP Q13541
Z	-2	SER	-	expression tag	UNP Q13541
Z	-1	GLY	-	expression tag	UNP Q13541
Z	0	ARG	-	expression tag	UNP Q13541

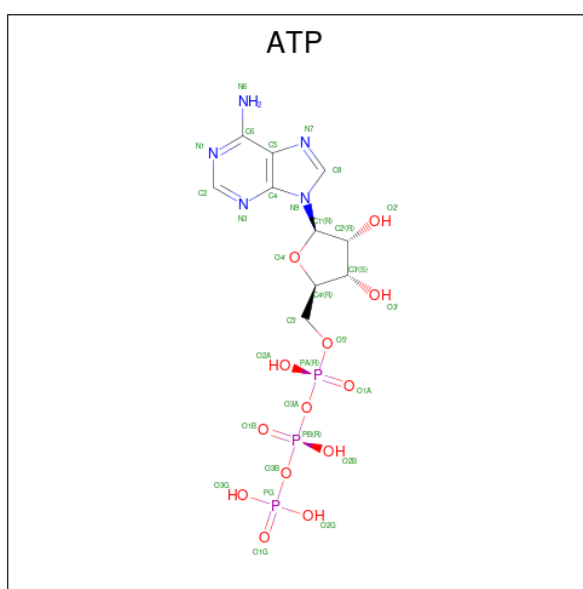
- Molecule 5 is a protein called GTP-binding protein Rheb.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	S	166	Total	C	H	N	O	S	0	0
			2657	846	1339	215	254	3		
5	R	166	Total	C	H	N	O	S	0	0
			2657	846	1339	215	254	3		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	-3	GLY	-	expression tag	UNP Q15382
S	-2	SER	-	expression tag	UNP Q15382
S	-1	GLY	-	expression tag	UNP Q15382
S	0	ARG	-	expression tag	UNP Q15382
R	-3	GLY	-	expression tag	UNP Q15382
R	-2	SER	-	expression tag	UNP Q15382
R	-1	GLY	-	expression tag	UNP Q15382
R	0	ARG	-	expression tag	UNP Q15382

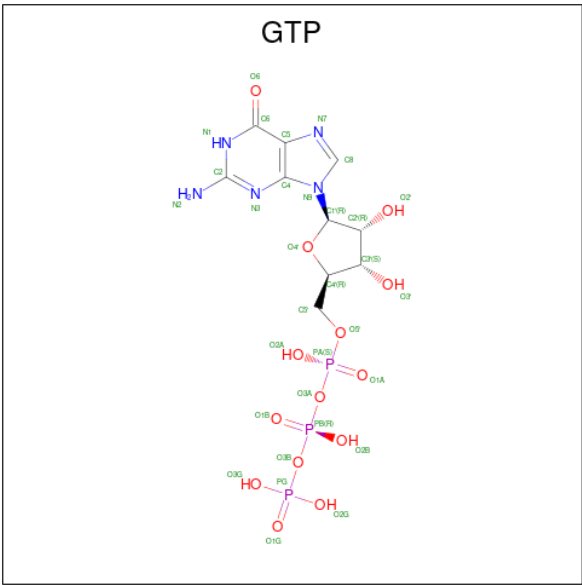
- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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Mol	Chain	Residues	Atoms		AltConf
7	R	1	Total	Mg	0
			1	1	

- Molecule 8 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

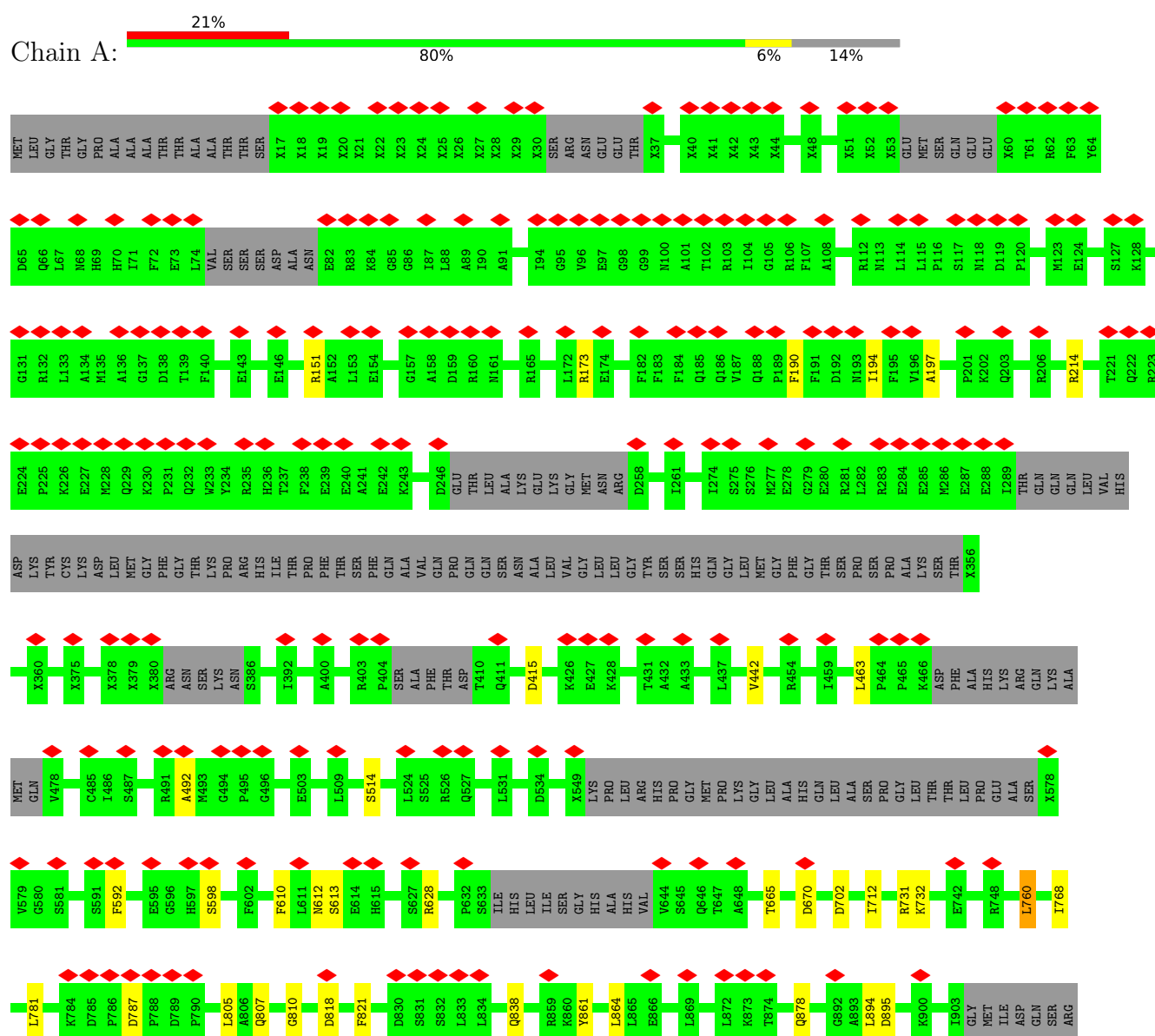


Mol	Chain	Residues	Atoms						AltConf
8	S	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	
8	R	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	

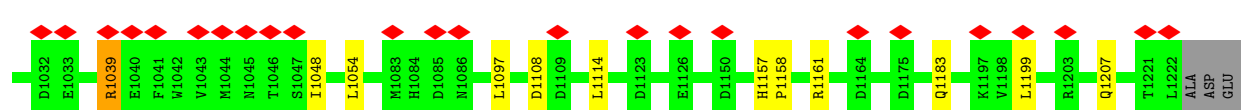
3 Residue-property plots

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.

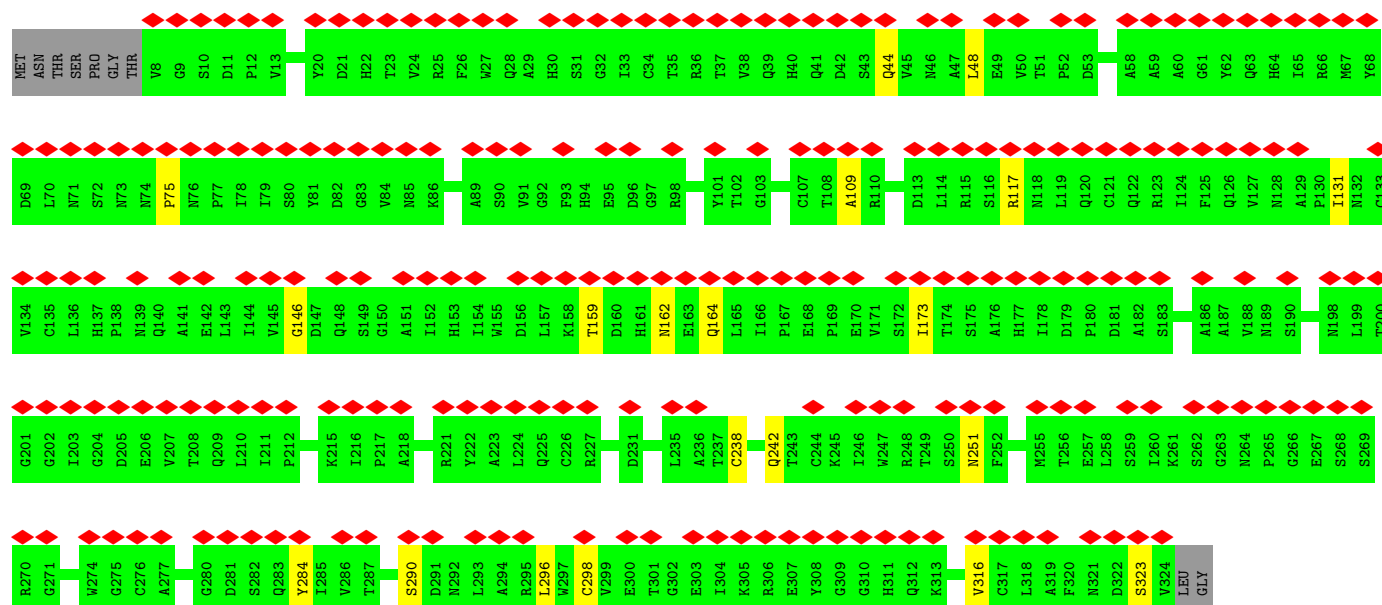
- Molecule 1: Serine/threonine-protein kinase mTOR,Serine/threonine-protein kinase mTOR



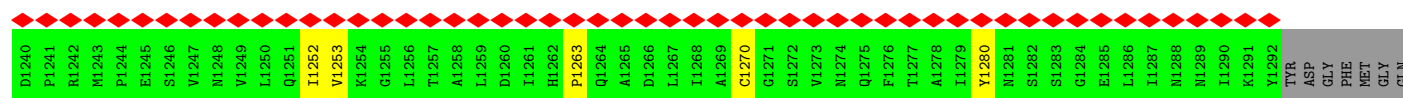




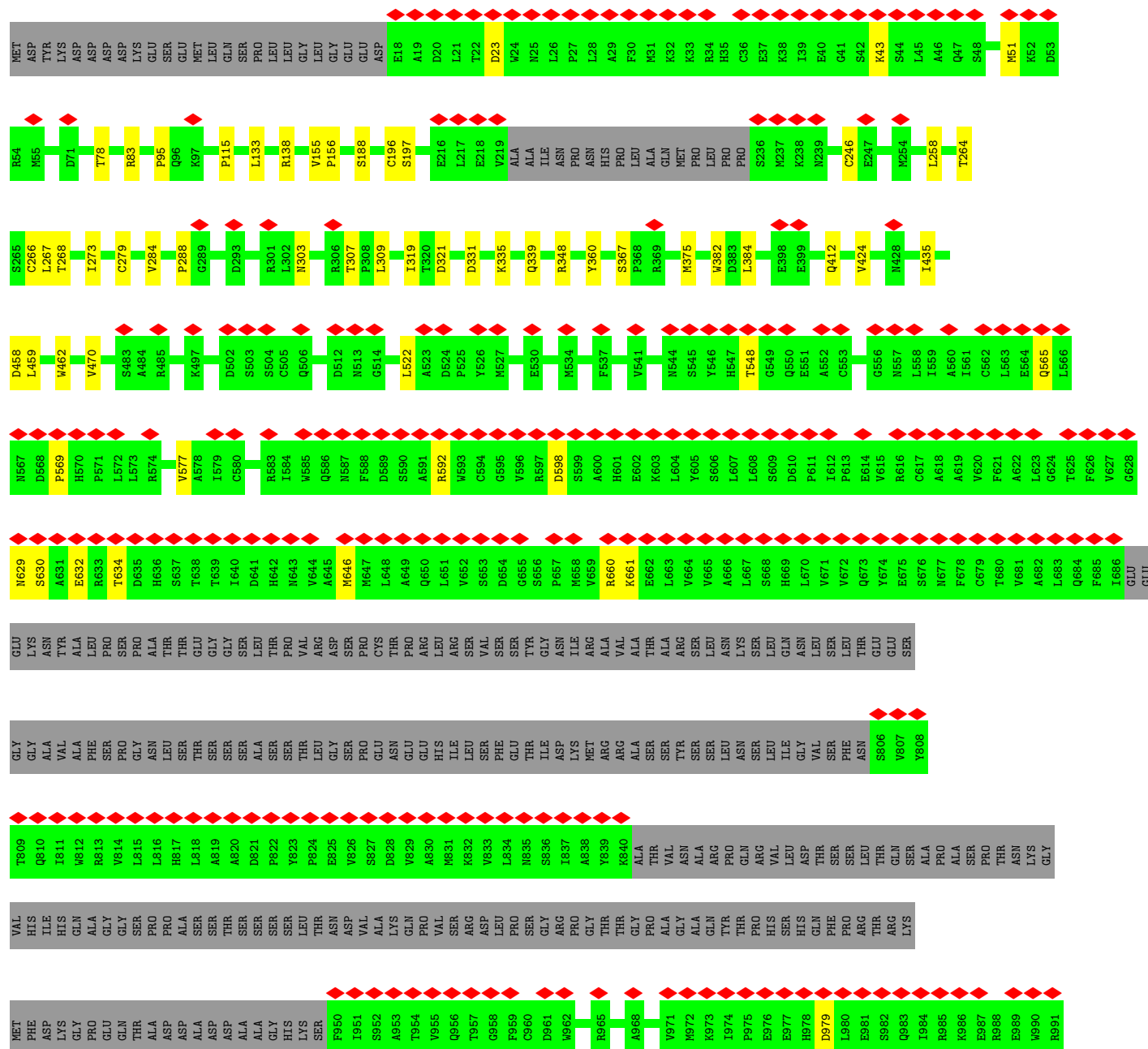
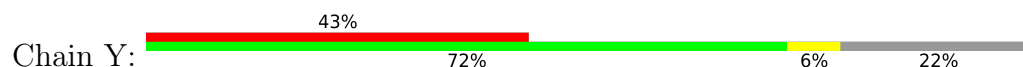


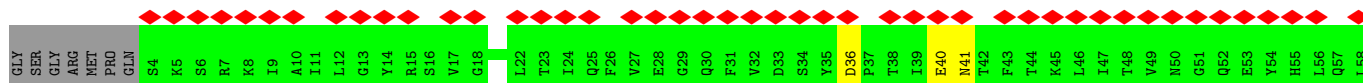


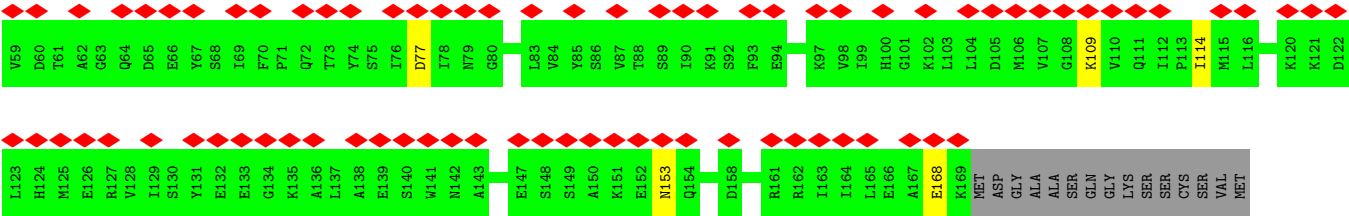
L1180	I1181	V1182	A1183	G1184	L1185	G1186	D1187	G1188	S1189	I1190	R1191	V1192	Y1193	D1194	R1195	R1196	A1197	L1198	L1199	S1200	E1201	C1202	R1203	V1204	M1205	T1206	Y1207	R1208	E1209	H1210	T1211	A1212	V1213	V1214	V1215	K1216	A1217	S1218	L1219	Q1220	K1221	R1222	P1223	D1224	G1225	H1226	I1227	V1228	S1229	V1230	S1231	V1232	C1233	G1234	D1235	V1236	R1237	I1238	F1239																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
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F1060	H1061	M1062	G1063	M1064	P1065	R1066	T1067	T1068	R1069	V1070	T1071	A1072	M1073	E1074	Y1075	L1076	M1077	G1078	Q1079	D1080	C1081	S1082	L1083	L1084	L1085	T1086	A1087	T1088	D1089	D1090	G1091	A1092	I1093	R1094	V1095	W1096	K1097	M1098	F1099	A1100	D1101	L1102	E1103	K1104	M1105	P1106	E1107	M1108	V1109	T1110	A1111	W1112	Q1113	G1114	L1115	S1116	ASP	MET	LEU																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
R1000	Q1001	A1002	Q1003	Q1004	V1005	I1006	Q1007	K1008	G1009	I1010	T1011	R1012	L1013	D1014	D1015	Q1016	I1017	F1018	L1019	M1020	R1021	M1022	P1023	G1024	V1025	P1026	S1027	V1028	V1029	K1030	F1031	H1032	P1033	F1034	T1035	P1036	C1037	I1038	A1039	V1040	A1041	D1042	K1043	D1044	S1045	I1046	C1047	F1048	W1049	D1050	W1051	N995	S996	R997	V998	R999																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
ALA	ASP	ASP	ALA	ASP	ALA	ALA	GLY	HIS	LYS	SER	F950	I951	S952	A953	T954	V955	Q956	T957	G958	F959	C960	D961	W962	R965	Y966	F967	A968	V971	M972	K973	I974	P975	E976	E977	H978	D979	L980	S981	S982	Q983	I984	R985	K986	E987	R988	E989	W990	R991	F992	L993	R994	N995	S996	R997	V998	R999																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
PRO	PRO	ALA	SER	THR	SER	SER	ALA	THR	LEU	THR	ASN	ASP	VAL	ALA	LYS	GLN	PRO	VAL	ARG	ASP	LEU	PRO	SER	GLY	ARG	PRO	GLY	THR	THR	THR	GLN	VAL	THR	ASP	THR	SER	LEU	THR	GLN	ARG	THR	THR	LYS	MET	PHE	ASP	LYS	GLY	PRO	GLN	THR	THR	GLY	GLY	SER																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
L818	A819	A820	D821	P822	Y823	P824	E825	V826	S827	D828	V829	M831	K832	V833	L834	N835	S836	I837	A838	Y839	K840	ALA	THR	VAL	ASN	ALA	ALA	ARG	PRO	GLN	VAL	THR	ASP	THR	SER	LEU	THR	GLN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR</



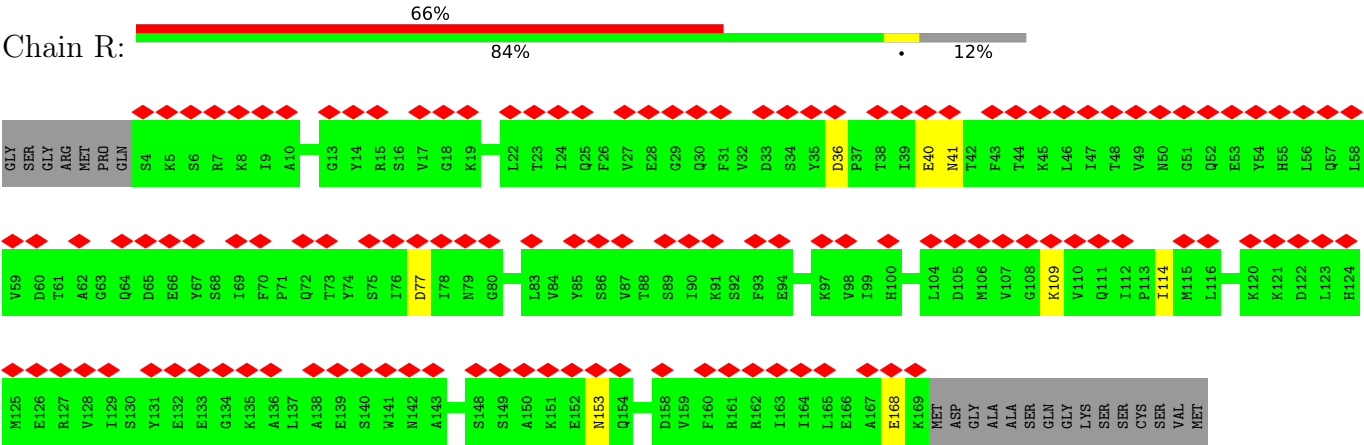
- Molecule 3: Regulatory-associated protein of mTOR,Regulatory-associated protein of mTOR







• Molecule 5: GTP-binding protein Rheb



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	198237	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 ($e^-/\text{\AA}^2$)	56	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.167	Depositor
Minimum map value	-0.086	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	497.6444, 497.6444, 497.6444	wwPDB
Map dimensions	374, 374, 374	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3306, 1.3306, 1.3306	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.59	0/17599	0.84	17/23827 (0.1%)
1	B	0.59	0/17599	0.84	17/23827 (0.1%)
2	D	0.56	0/2514	0.78	2/3426 (0.1%)
2	E	0.56	0/2514	0.78	2/3426 (0.1%)
3	W	0.55	0/8584	0.78	4/11677 (0.0%)
3	Y	0.55	0/8584	0.78	4/11677 (0.0%)
4	X	0.62	0/68	0.70	0/89
4	Z	0.62	0/68	0.70	0/89
5	R	0.59	0/1340	0.73	0/1809
5	S	0.59	0/1340	0.73	0/1809
All	All	0.57	0/60210	0.81	46/81656 (0.1%)

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	5
1	B	0	5
2	D	0	1
2	E	0	1
3	Y	0	2
5	R	0	2
5	S	0	2
All	All	0	18

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1743	LEU	CA-CB-CG	6.48	130.20	115.30
1	A	1743	LEU	CA-CB-CG	6.46	130.17	115.30
1	A	2138	LEU	CA-CB-CG	6.10	129.33	115.30
1	B	2138	LEU	CA-CB-CG	5.96	129.01	115.30
1	B	1273	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	B	2193	ARG	NE-CZ-NH1	5.63	123.12	120.30
3	W	660	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	1273	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	B	1039	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	A	2193	ARG	NE-CZ-NH1	5.52	123.06	120.30
3	W	1000	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	1616	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	1039	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	1339	ARG	NE-CZ-NH1	5.50	123.05	120.30
3	Y	660	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	1339	ARG	NE-CZ-NH1	5.49	123.04	120.30
2	D	48	LEU	CA-CB-CG	5.47	127.89	115.30
2	E	48	LEU	CA-CB-CG	5.44	127.81	115.30
3	Y	1222	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	1482	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	B	1161	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	A	957	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	1616	ARG	NE-CZ-NH1	5.37	122.98	120.30
3	Y	1000	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	B	151	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	1161	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	628	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	628	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	1482	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	2086	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	2086	ARG	NE-CZ-NH1	5.32	122.96	120.30
3	W	1222	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	B	957	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	A	151	ARG	NE-CZ-NH1	5.29	122.95	120.30
2	E	117	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	2397	ARG	NE-CZ-NH1	5.24	122.92	120.30
2	D	117	ARG	NE-CZ-NH1	5.24	122.92	120.30
3	W	348	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	1585	ARG	NE-CZ-NH1	5.18	122.89	120.30
3	Y	348	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	1568	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	1585	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	A	1568	ARG	NE-CZ-NH1	5.11	122.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2397	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	B	1568	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	B	1568	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1377	ASP	Peptide
1	A	197	ALA	Peptide
1	A	878	GLN	Peptide
1	A	894	LEU	Peptide
1	A	941	LEU	Peptide
1	B	1377	ASP	Peptide
1	B	197	ALA	Peptide
1	B	878	GLN	Peptide
1	B	894	LEU	Peptide
1	B	941	LEU	Peptide
2	D	251	ASN	Peptide
2	E	251	ASN	Peptide
5	R	114	ILE	Peptide
5	R	77	ASP	Peptide
5	S	114	ILE	Peptide
5	S	77	ASP	Peptide
3	Y	196	CYS	Peptide
3	Y	458	ASP	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	17538	17859	17553	38	0
1	B	17538	17859	17553	41	0
2	D	2456	2353	2341	5	0
2	E	2456	2353	2341	6	0
3	W	8385	8406	8374	19	0
3	Y	8385	8406	8374	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	X	68	58	57	0	0
4	Z	68	58	57	0	0
5	R	1318	1339	1334	0	0
5	S	1318	1339	1333	0	0
6	A	31	12	12	0	0
6	B	31	12	12	0	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
7	R	1	0	0	0	0
7	S	1	0	0	0	0
8	R	32	12	12	0	0
8	S	32	12	12	0	0
All	All	59662	60078	59365	121	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 1.

All (121) 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:B:190:PHE:CZ	1:B:194:ILE:HD11	2.32	0.64
1:A:190:PHE:CZ	1:A:194:ILE:HD11	2.32	0.64
1:A:1970:GLN:HE21	1:A:1970:GLN:HA	1.63	0.63
1:B:1970:GLN:HE21	1:B:1970:GLN:HA	1.64	0.63
1:B:964:LEU:HD13	1:B:968:HIS:CD2	2.35	0.62
1:A:964:LEU:HD13	1:A:968:HIS:CD2	2.35	0.61
1:A:1898:ASN:HD21	1:A:2211:ASN:HD21	1.53	0.57
1:B:1898:ASN:HD21	1:B:2211:ASN:HD21	1.53	0.56
1:A:1020:VAL:HG22	1:A:1027:ILE:HD13	1.87	0.56
1:A:2246:LEU:HD21	1:A:2383:LEU:HD21	1.88	0.56
3:W:424:VAL:HG22	3:W:459:LEU:HD22	1.88	0.56
1:B:2246:LEU:HD21	1:B:2383:LEU:HD21	1.88	0.56
1:B:1020:VAL:HG22	1:B:1027:ILE:HD13	1.87	0.55
3:Y:424:VAL:HG22	3:Y:459:LEU:HD22	1.88	0.55
1:B:2431:LEU:HD13	1:B:2500:ILE:HD13	1.89	0.55
1:A:2431:LEU:HD13	1:A:2500:ILE:HD13	1.89	0.54
1:B:964:LEU:HD22	1:B:968:HIS:HA	1.93	0.50
1:A:964:LEU:HD22	1:A:968:HIS:HA	1.94	0.50
1:B:1579:ALA:HB2	1:B:1586:ALA:HB2	1.94	0.50
3:Y:412:GLN:HG2	3:Y:435:ILE:HD13	1.94	0.50
1:A:442:VAL:HG22	1:A:492:ALA:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:VAL:HG22	1:B:492:ALA:HB2	1.94	0.49
3:W:412:GLN:HG2	3:W:435:ILE:HD13	1.94	0.49
2:E:284:TYR:HB3	2:E:296:LEU:HD11	1.95	0.49
3:W:258:LEU:HD11	3:W:360:TYR:CE2	2.48	0.49
1:A:442:VAL:HA	1:A:492:ALA:HB1	1.95	0.48
1:A:1579:ALA:HB2	1:A:1586:ALA:HB2	1.94	0.48
2:D:284:TYR:HB3	2:D:296:LEU:HD11	1.96	0.48
3:Y:279:CYS:HA	3:Y:284:VAL:HG21	1.95	0.48
1:B:1416:LEU:HA	1:B:1419:ILE:HG22	1.96	0.48
3:Y:258:LEU:HD11	3:Y:360:TYR:CE2	2.49	0.48
1:A:1939:ILE:HG23	1:A:1943:ILE:HD13	1.96	0.48
3:W:279:CYS:HA	3:W:284:VAL:HG21	1.94	0.48
1:B:1939:ILE:HG23	1:B:1943:ILE:HD13	1.96	0.48
1:A:1416:LEU:HA	1:A:1419:ILE:HG22	1.96	0.47
3:W:266:CYS:HA	3:W:273:ILE:HD11	1.95	0.47
1:A:2140:VAL:HG13	1:A:2174:LEU:HD12	1.97	0.47
1:B:2140:VAL:HG13	1:B:2174:LEU:HD12	1.97	0.47
3:Y:266:CYS:HA	3:Y:273:ILE:HD11	1.97	0.47
1:B:442:VAL:HA	1:B:492:ALA:HB1	1.95	0.47
3:Y:1252:ILE:HG22	3:Y:1253:VAL:HG23	1.98	0.46
3:W:522:LEU:O	3:W:565:GLN:NE2	2.48	0.46
3:Y:522:LEU:O	3:Y:565:GLN:NE2	2.48	0.46
3:W:1252:ILE:HG22	3:W:1253:VAL:HG23	1.98	0.46
3:W:592:ARG:NH1	3:W:629:ASN:O	2.48	0.46
1:B:2140:VAL:HG11	1:B:2182:PHE:HD2	1.81	0.46
1:B:990:LEU:HD11	1:B:1023:VAL:HG13	1.98	0.45
1:A:2140:VAL:HG11	1:A:2182:PHE:HD2	1.81	0.45
3:W:155:VAL:HB	3:W:156:PRO:HD2	1.98	0.45
1:B:2142:GLY:HA3	1:B:2228:ILE:HD11	1.99	0.45
1:A:990:LEU:HD11	1:A:1023:VAL:HG13	1.98	0.45
1:A:1740:LYS:HA	1:A:1743:LEU:HB3	1.99	0.45
3:Y:592:ARG:NH1	3:Y:629:ASN:O	2.48	0.45
1:A:2142:GLY:HA3	1:A:2228:ILE:HD11	1.99	0.45
3:Y:155:VAL:HB	3:Y:156:PRO:HD2	1.98	0.44
1:B:1740:LYS:HA	1:B:1743:LEU:HB3	1.98	0.44
1:B:1600:GLU:HA	1:B:1603:ILE:HD12	2.00	0.44
1:A:959:PHE:HA	1:A:964:LEU:HD11	2.00	0.44
1:A:1557:PHE:CD1	1:A:1603:ILE:HG23	2.53	0.44
1:B:1557:PHE:CD1	1:B:1603:ILE:HG23	2.53	0.44
1:A:2321:THR:HG23	1:A:2387:MET:SD	2.58	0.44
2:D:109:ALA:HB2	2:D:131:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:109:ALA:HB2	2:E:131:ILE:HD13	2.00	0.44
1:A:1600:GLU:HA	1:A:1603:ILE:HD12	2.00	0.43
1:A:2117:GLN:HE22	3:W:96:GLN:HB3	1.83	0.43
1:B:2321:THR:HG23	1:B:2387:MET:SD	2.58	0.43
1:A:1157:HIS:HB2	1:A:1158:PRO:HD3	2.01	0.43
1:B:1575:LEU:HG	1:B:1589:ALA:HB1	2.01	0.43
1:B:2282:GLN:HE21	2:E:316:VAL:HG11	1.83	0.43
3:Y:319:ILE:HD13	3:Y:382:TRP:HB2	2.00	0.43
1:B:1157:HIS:HB2	1:B:1158:PRO:HD3	2.01	0.43
3:Y:1220:GLN:OE1	3:Y:1222:ARG:NH1	2.52	0.43
1:B:959:PHE:HA	1:B:964:LEU:HD11	2.00	0.43
3:W:1252:ILE:HG21	3:W:1270:CYS:SG	2.59	0.42
3:W:23:ASP:HB3	3:W:992:PHE:CD2	2.54	0.42
3:Y:23:ASP:HB3	3:Y:992:PHE:CD2	2.54	0.42
3:Y:1252:ILE:HG21	3:Y:1270:CYS:SG	2.59	0.42
3:Y:1252:ILE:HG23	3:Y:1280:TYR:CE2	2.54	0.42
1:A:1575:LEU:HG	1:A:1589:ALA:HB1	2.01	0.42
3:W:319:ILE:HD13	3:W:382:TRP:HB2	2.02	0.42
3:W:1220:GLN:OE1	3:W:1222:ARG:NH1	2.52	0.42
3:W:1159:GLN:HE22	3:W:1195:ARG:HB2	1.84	0.42
1:A:760:LEU:HD13	1:A:768:ILE:HD11	2.01	0.42
1:A:2384:THR:HA	1:A:2387:MET:HE3	2.01	0.42
1:B:2160:LEU:HD22	1:B:2172:LEU:HA	2.02	0.42
1:A:1322:PHE:CD2	1:A:1360:LEU:HD21	2.55	0.42
1:A:990:LEU:HD21	1:A:1023:VAL:HG21	2.02	0.41
3:W:1252:ILE:HG23	3:W:1280:TYR:CE2	2.54	0.41
1:B:630:LEU:HD11	1:B:655:VAL:HG11	2.02	0.41
1:B:1322:PHE:CD2	1:B:1360:LEU:HD21	2.55	0.41
1:B:1970:GLN:HE21	1:B:1970:GLN:CA	2.28	0.41
1:B:2254:ARG:HD2	1:B:2261:LEU:HD12	2.02	0.41
3:Y:1159:GLN:HE22	3:Y:1195:ARG:HB2	1.84	0.41
1:B:958:ILE:O	1:B:960:ARG:N	2.50	0.41
3:Y:1079:GLN:HE22	3:Y:1133:GLN:HE21	1.67	0.41
1:A:2277:HIS:O	2:D:44:GLN:NE2	2.54	0.41
3:W:439:VAL:HG13	3:W:445:HIS:HB2	2.02	0.41
1:B:2378:ARG:HB2	1:B:2545:TRP:CH2	2.55	0.41
1:B:2277:HIS:O	2:E:44:GLN:NE2	2.52	0.41
1:A:731:ARG:HD2	3:Y:384:LEU:HD13	2.03	0.41
1:A:1396:ALA:HB3	1:A:1419:ILE:HD11	2.02	0.41
1:A:2254:ARG:HD2	1:A:2261:LEU:HD12	2.02	0.41
1:B:2424:ASP:O	1:B:2428:ASN:ND2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:760:LEU:HD13	1:B:768:ILE:HD11	2.02	0.41
1:A:1930:ILE:HD11	1:A:1934:THR:HG21	2.03	0.41
1:A:2160:LEU:HD22	1:A:2172:LEU:HA	2.03	0.41
2:D:146:GLY:HA3	2:D:173:ILE:HD11	2.03	0.41
1:B:990:LEU:HD21	1:B:1023:VAL:HG21	2.03	0.41
1:B:1396:ALA:HB3	1:B:1419:ILE:HD11	2.02	0.41
1:A:2282:GLN:HE21	2:D:316:VAL:HG11	1.86	0.41
1:B:852:GLY:HA3	1:B:1618:ILE:HG12	2.02	0.41
1:B:2170:ARG:HD2	1:B:2170:ARG:N	2.36	0.41
2:E:146:GLY:HA3	2:E:173:ILE:HD11	2.03	0.41
3:W:1079:GLN:HE22	3:W:1133:GLN:HE21	1.68	0.40
3:Y:264:THR:O	3:Y:268:THR:HG22	2.21	0.40
1:B:2245:THR:HA	1:B:2345:MET:HB3	2.04	0.40
1:A:1970:GLN:HE21	1:A:1970:GLN:CA	2.28	0.40
3:W:264:THR:O	3:W:268:THR:HG22	2.22	0.40
1:A:2378:ARG:HB2	1:A:2545:TRP:CH2	2.57	0.40
1:B:2052:GLU:HG2	1:B:2053:PRO:HD3	2.03	0.40
2:E:103:GLY:CA	2:E:134:VAL:HG21	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	2124/2549 (83%)	1934 (91%)	170 (8%)	20 (1%)	17	54
1	B	2124/2549 (83%)	1933 (91%)	171 (8%)	20 (1%)	17	54
2	D	315/326 (97%)	263 (84%)	50 (16%)	2 (1%)	25	62
2	E	315/326 (97%)	263 (84%)	50 (16%)	2 (1%)	25	62
3	W	1038/1343 (77%)	936 (90%)	89 (9%)	13 (1%)	12	46
3	Y	1038/1343 (77%)	934 (90%)	91 (9%)	13 (1%)	12	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	X	6/122 (5%)	5 (83%)	1 (17%)	0	100	100
4	Z	6/122 (5%)	5 (83%)	1 (17%)	0	100	100
5	R	164/188 (87%)	152 (93%)	11 (7%)	1 (1%)	25	62
5	S	164/188 (87%)	152 (93%)	11 (7%)	1 (1%)	25	62
All	All	7294/9056 (80%)	6577 (90%)	645 (9%)	72 (1%)	20	52

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	959	PHE
1	A	1444	GLU
1	A	1766	GLU
3	W	1115	LEU
3	W	1212	ALA
1	B	959	PHE
1	B	1444	GLU
1	B	1766	GLU
3	Y	1115	LEU
3	Y	1212	ALA
1	A	598	SER
1	A	810	GLY
1	A	864	LEU
1	A	1375	ARG
1	A	1555	ASP
1	A	1648	GLU
3	W	979	ASP
1	B	598	SER
1	B	810	GLY
1	B	864	LEU
1	B	1375	ARG
1	B	1555	ASP
1	B	1648	GLU
3	Y	979	ASP
1	A	2308	PRO
1	A	2338	ASP
1	A	2357	ASP
1	A	2376	PRO
2	D	75	PRO
2	D	323	SER
3	W	1203	ARG
3	W	1213	TRP

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Mol	Chain	Res	Type
1	B	2308	PRO
1	B	2338	ASP
1	B	2357	ASP
1	B	2376	PRO
2	E	75	PRO
2	E	323	SER
3	Y	1203	ARG
3	Y	1213	TRP
1	A	612	ASN
3	W	303	ASN
3	W	632	GLU
3	W	634	THR
3	W	1202	CYS
5	S	40	GLU
1	B	612	ASN
3	Y	303	ASN
3	Y	632	GLU
3	Y	634	THR
3	Y	1202	CYS
5	R	40	GLU
1	A	613	SER
1	A	1108	ASP
1	A	2189	HIS
1	B	613	SER
1	B	1108	ASP
1	B	2189	HIS
3	Y	630	SER
3	W	43	LYS
3	W	630	SER
3	Y	43	LYS
1	A	1407	GLY
3	W	1263	PRO
1	B	1407	GLY
3	Y	1263	PRO
1	A	787	ASP
3	W	569	PRO
1	B	787	ASP
3	Y	569	PRO
1	A	463	LEU
1	B	463	LEU

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	1881/2166 (87%)	1800 (96%)	81 (4%)	29	61
1	B	1881/2166 (87%)	1801 (96%)	80 (4%)	29	61
2	D	269/276 (98%)	262 (97%)	7 (3%)	46	74
2	E	269/276 (98%)	262 (97%)	7 (3%)	46	74
3	W	928/1171 (79%)	893 (96%)	35 (4%)	33	64
3	Y	928/1171 (79%)	893 (96%)	35 (4%)	33	64
4	X	8/104 (8%)	7 (88%)	1 (12%)	4	21
4	Z	8/104 (8%)	7 (88%)	1 (12%)	4	21
5	R	147/163 (90%)	142 (97%)	5 (3%)	37	68
5	S	147/163 (90%)	142 (97%)	5 (3%)	37	68
All	All	6466/7760 (83%)	6209 (96%)	257 (4%)	35	63

All (257) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	ARG
1	A	214	ARG
1	A	415	ASP
1	A	514	SER
1	A	592	PHE
1	A	610	PHE
1	A	665	THR
1	A	670	ASP
1	A	702	ASP
1	A	712	ILE
1	A	732	LYS
1	A	760	LEU
1	A	781	LEU
1	A	805	LEU
1	A	807	GLN
1	A	818	ASP

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Mol	Chain	Res	Type
1	A	821	PHE
1	A	838	GLN
1	A	861	TYR
1	A	895	ASP
1	A	934	MET
1	A	944	ASP
1	A	996	THR
1	A	1039	ARG
1	A	1048	ILE
1	A	1054	LEU
1	A	1097	LEU
1	A	1114	LEU
1	A	1183	GLN
1	A	1199	LEU
1	A	1207	GLN
1	A	1287	LEU
1	A	1337	LEU
1	A	1350	ILE
1	A	1377	ASP
1	A	1395	LYS
1	A	1402	LEU
1	A	1423	LEU
1	A	1565	ASP
1	A	1594	HIS
1	A	1606	LYS
1	A	1701	MET
1	A	1702	LYS
1	A	1710	LYS
1	A	1740	LYS
1	A	1764	ILE
1	A	1780	THR
1	A	1877	LEU
1	A	1881	THR
1	A	1895	SER
1	A	1899	ASN
1	A	1901	GLN
1	A	1948	THR
1	A	1956	LEU
1	A	1963	ASP
1	A	1970	GLN
1	A	1973	ILE
1	A	1988	HIS

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Mol	Chain	Res	Type
1	A	2005	LEU
1	A	2074	TYR
1	A	2077	ASP
1	A	2090	LYS
1	A	2120	SER
1	A	2138	LEU
1	A	2173	THR
1	A	2195	ASP
1	A	2223	GLN
1	A	2233	ASN
1	A	2244	ASP
1	A	2303	LEU
1	A	2340	HIS
1	A	2353	ILE
1	A	2354	LEU
1	A	2367	THR
1	A	2378	ARG
1	A	2381	ARG
1	A	2408	ARG
1	A	2409	GLU
1	A	2413	SER
1	A	2503	ARG
1	A	2514	SER
2	D	159	THR
2	D	162	ASN
2	D	164	GLN
2	D	238	CYS
2	D	242	GLN
2	D	290	SER
2	D	298	CYS
3	W	51	MET
3	W	78	THR
3	W	83	ARG
3	W	95	PRO
3	W	115	PRO
3	W	133	LEU
3	W	138	ARG
3	W	188	SER
3	W	197	SER
3	W	246	CYS
3	W	267	LEU
3	W	288	PRO

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Mol	Chain	Res	Type
3	W	307	THR
3	W	309	LEU
3	W	321	ASP
3	W	331	ASP
3	W	335	LYS
3	W	339	GLN
3	W	367	SER
3	W	375	MET
3	W	462	TRP
3	W	470	VAL
3	W	548	THR
3	W	577	VAL
3	W	598	ASP
3	W	646	MET
3	W	661	LYS
3	W	1011	THR
3	W	1014	ASP
3	W	1021	ARG
3	W	1058	ASP
3	W	1069	ARG
3	W	1105	ASN
3	W	1139	MET
3	W	1208	ARG
4	X	111	GLU
5	S	36	ASP
5	S	41	ASN
5	S	109	LYS
5	S	153	ASN
5	S	168	GLU
1	B	173	ARG
1	B	214	ARG
1	B	415	ASP
1	B	514	SER
1	B	592	PHE
1	B	610	PHE
1	B	665	THR
1	B	670	ASP
1	B	702	ASP
1	B	712	ILE
1	B	732	LYS
1	B	760	LEU
1	B	781	LEU

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Mol	Chain	Res	Type
1	B	805	LEU
1	B	807	GLN
1	B	818	ASP
1	B	821	PHE
1	B	838	GLN
1	B	861	TYR
1	B	895	ASP
1	B	934	MET
1	B	944	ASP
1	B	1039	ARG
1	B	1048	ILE
1	B	1054	LEU
1	B	1097	LEU
1	B	1114	LEU
1	B	1183	GLN
1	B	1199	LEU
1	B	1207	GLN
1	B	1287	LEU
1	B	1337	LEU
1	B	1350	ILE
1	B	1377	ASP
1	B	1395	LYS
1	B	1402	LEU
1	B	1423	LEU
1	B	1565	ASP
1	B	1594	HIS
1	B	1606	LYS
1	B	1701	MET
1	B	1702	LYS
1	B	1710	LYS
1	B	1740	LYS
1	B	1764	ILE
1	B	1780	THR
1	B	1877	LEU
1	B	1881	THR
1	B	1895	SER
1	B	1899	ASN
1	B	1901	GLN
1	B	1948	THR
1	B	1956	LEU
1	B	1963	ASP
1	B	1970	GLN

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Mol	Chain	Res	Type
1	B	1973	ILE
1	B	1988	HIS
1	B	2005	LEU
1	B	2074	TYR
1	B	2077	ASP
1	B	2090	LYS
1	B	2120	SER
1	B	2138	LEU
1	B	2173	THR
1	B	2195	ASP
1	B	2223	GLN
1	B	2233	ASN
1	B	2244	ASP
1	B	2303	LEU
1	B	2340	HIS
1	B	2354	LEU
1	B	2367	THR
1	B	2378	ARG
1	B	2381	ARG
1	B	2408	ARG
1	B	2409	GLU
1	B	2413	SER
1	B	2503	ARG
1	B	2514	SER
1	B	2539	CYS
2	E	159	THR
2	E	162	ASN
2	E	164	GLN
2	E	238	CYS
2	E	242	GLN
2	E	290	SER
2	E	298	CYS
3	Y	51	MET
3	Y	78	THR
3	Y	83	ARG
3	Y	95	PRO
3	Y	115	PRO
3	Y	133	LEU
3	Y	138	ARG
3	Y	188	SER
3	Y	197	SER
3	Y	246	CYS

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Mol	Chain	Res	Type
3	Y	267	LEU
3	Y	288	PRO
3	Y	307	THR
3	Y	309	LEU
3	Y	321	ASP
3	Y	331	ASP
3	Y	335	LYS
3	Y	339	GLN
3	Y	367	SER
3	Y	375	MET
3	Y	462	TRP
3	Y	470	VAL
3	Y	548	THR
3	Y	577	VAL
3	Y	598	ASP
3	Y	646	MET
3	Y	661	LYS
3	Y	1011	THR
3	Y	1014	ASP
3	Y	1021	ARG
3	Y	1058	ASP
3	Y	1069	ARG
3	Y	1105	ASN
3	Y	1139	MET
3	Y	1208	ARG
4	Z	111	GLU
5	R	36	ASP
5	R	41	ASN
5	R	109	LYS
5	R	153	ASN
5	R	168	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	389	GLN
1	A	807	GLN
1	A	940	ASN
1	A	1421	ASN
1	A	1496	GLN
1	A	1741	GLN
1	A	1898	ASN

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Mol	Chain	Res	Type
1	A	1941	GLN
1	A	1970	GLN
1	A	1989	ASN
1	A	2117	GLN
1	A	2200	GLN
1	A	2277	HIS
2	D	28	GLN
2	D	39	GLN
2	D	132	ASN
2	D	148	GLN
3	W	112	ASN
3	W	151	ASN
3	W	242	GLN
3	W	513	ASN
3	W	565	GLN
3	W	587	ASN
3	W	677	ASN
3	W	995	ASN
3	W	1159	GLN
3	W	1233	ASN
5	S	41	ASN
5	S	153	ASN
1	B	807	GLN
1	B	940	ASN
1	B	1421	ASN
1	B	1496	GLN
1	B	1741	GLN
1	B	1898	ASN
1	B	1941	GLN
1	B	1970	GLN
1	B	1989	ASN
1	B	2117	GLN
1	B	2200	GLN
1	B	2277	HIS
2	E	28	GLN
2	E	39	GLN
2	E	132	ASN
2	E	148	GLN
3	Y	112	ASN
3	Y	151	ASN
3	Y	242	GLN
3	Y	513	ASN

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Mol	Chain	Res	Type
3	Y	565	GLN
3	Y	677	ASN
3	Y	995	ASN
3	Y	1159	GLN
3	Y	1233	ASN
5	R	41	ASN
5	R	153	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	ATP	A	3000	7	26,33,33	1.49	3 (11%)	31,52,52	1.77	7 (22%)
6	ATP	B	3000	7	26,33,33	1.59	5 (19%)	31,52,52	1.89	8 (25%)
8	GTP	S	201	7	26,34,34	0.84	0	32,54,54	1.37	5 (15%)
8	GTP	R	201	7	26,34,34	0.85	0	32,54,54	1.36	5 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ATP	A	3000	7	-	0/18/38/38	0/3/3/3
6	ATP	B	3000	7	-	0/18/38/38	0/3/3/3
8	GTP	S	201	7	-	3/18/38/38	0/3/3/3
8	GTP	R	201	7	-	4/18/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	3000	ATP	C5-C4	4.24	1.52	1.40
6	B	3000	ATP	C2-N3	4.06	1.38	1.32
6	B	3000	ATP	C5-C4	3.92	1.51	1.40
6	A	3000	ATP	C2-N1	3.47	1.40	1.33
6	A	3000	ATP	C2'-C1'	2.30	1.57	1.53
6	B	3000	ATP	C2-N1	2.15	1.37	1.33
6	B	3000	ATP	C2'-C1'	2.14	1.57	1.53
6	B	3000	ATP	O4'-C1'	-2.03	1.38	1.41

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	3000	ATP	C3'-C2'-C1'	4.38	107.57	100.98
6	B	3000	ATP	O4'-C4'-C3'	4.32	113.66	105.11
6	A	3000	ATP	C3'-C2'-C1'	3.85	106.78	100.98
8	S	201	GTP	PA-O3A-PB	-3.30	121.50	132.83
6	A	3000	ATP	PB-O3B-PG	-3.24	121.70	132.83
6	A	3000	ATP	C2-N1-C6	3.21	124.25	118.75
6	B	3000	ATP	PB-O3B-PG	-3.10	122.18	132.83
6	A	3000	ATP	N6-C6-N1	3.10	125.00	118.57
8	R	201	GTP	PA-O3A-PB	-3.08	122.26	132.83
6	A	3000	ATP	C5-C6-N1	-3.03	113.49	120.35
8	S	201	GTP	PB-O3B-PG	-2.78	123.29	132.83
6	B	3000	ATP	N3-C2-N1	-2.75	124.38	128.68
6	B	3000	ATP	N6-C6-N1	2.74	124.26	118.57
6	B	3000	ATP	C2'-C3'-C4'	-2.66	97.47	102.64
8	R	201	GTP	PB-O3B-PG	-2.66	123.70	132.83
6	A	3000	ATP	O4'-C4'-C3'	2.62	110.31	105.11
8	S	201	GTP	C5-C6-N1	2.59	118.52	113.95
8	R	201	GTP	C5-C6-N1	2.59	118.52	113.95
6	A	3000	ATP	N3-C2-N1	-2.48	124.80	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	R	201	GTP	O6-C6-C5	-2.37	119.75	124.37
6	B	3000	ATP	C2-N1-C6	2.32	122.72	118.75
8	R	201	GTP	C8-N7-C5	2.24	107.26	102.99
8	S	201	GTP	C8-N7-C5	2.24	107.25	102.99
8	S	201	GTP	O6-C6-C5	-2.22	120.04	124.37
6	B	3000	ATP	C5-C6-N1	-2.09	115.62	120.35

There are no chirality outliers.

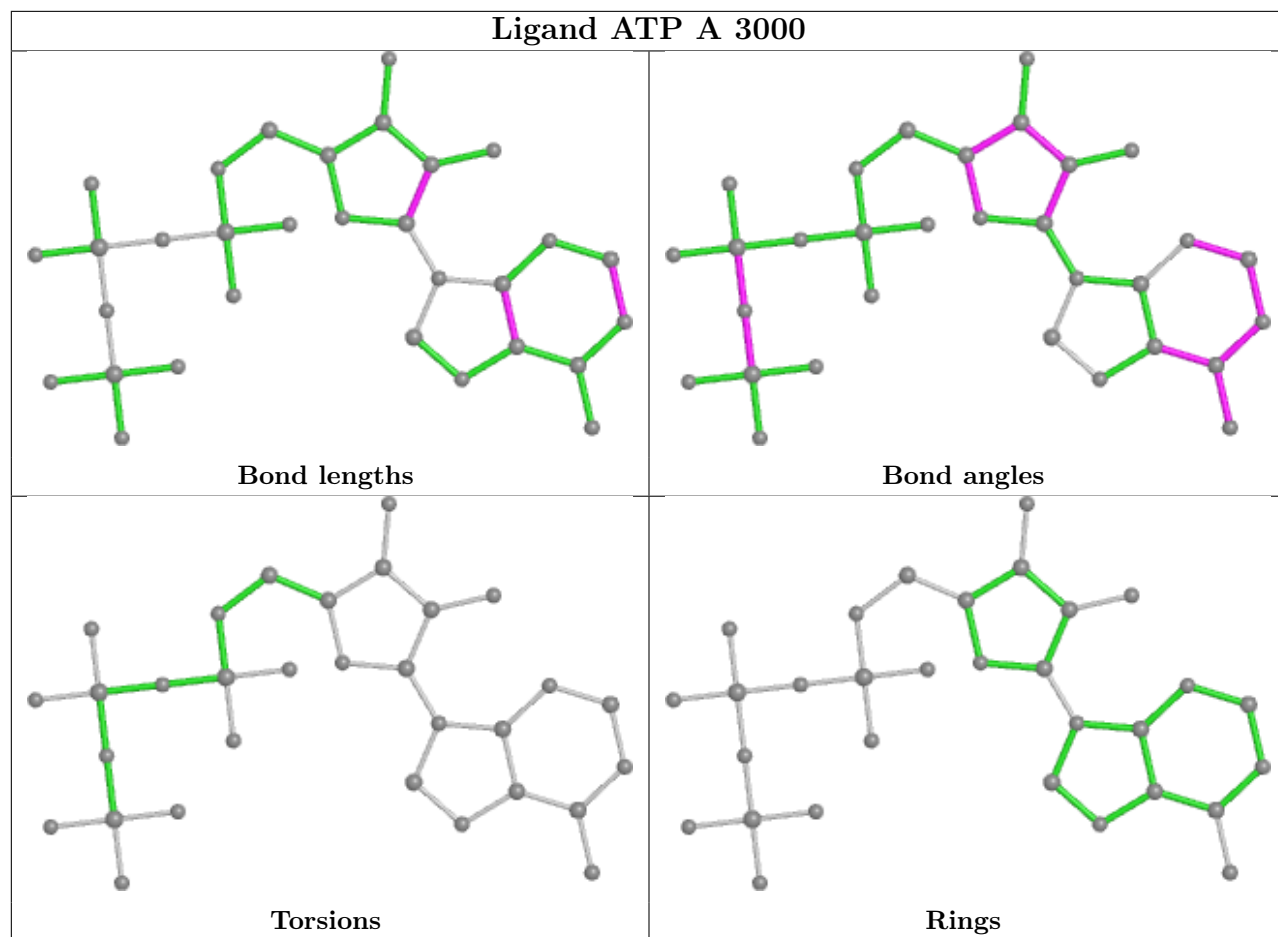
All (7) torsion outliers are listed below:

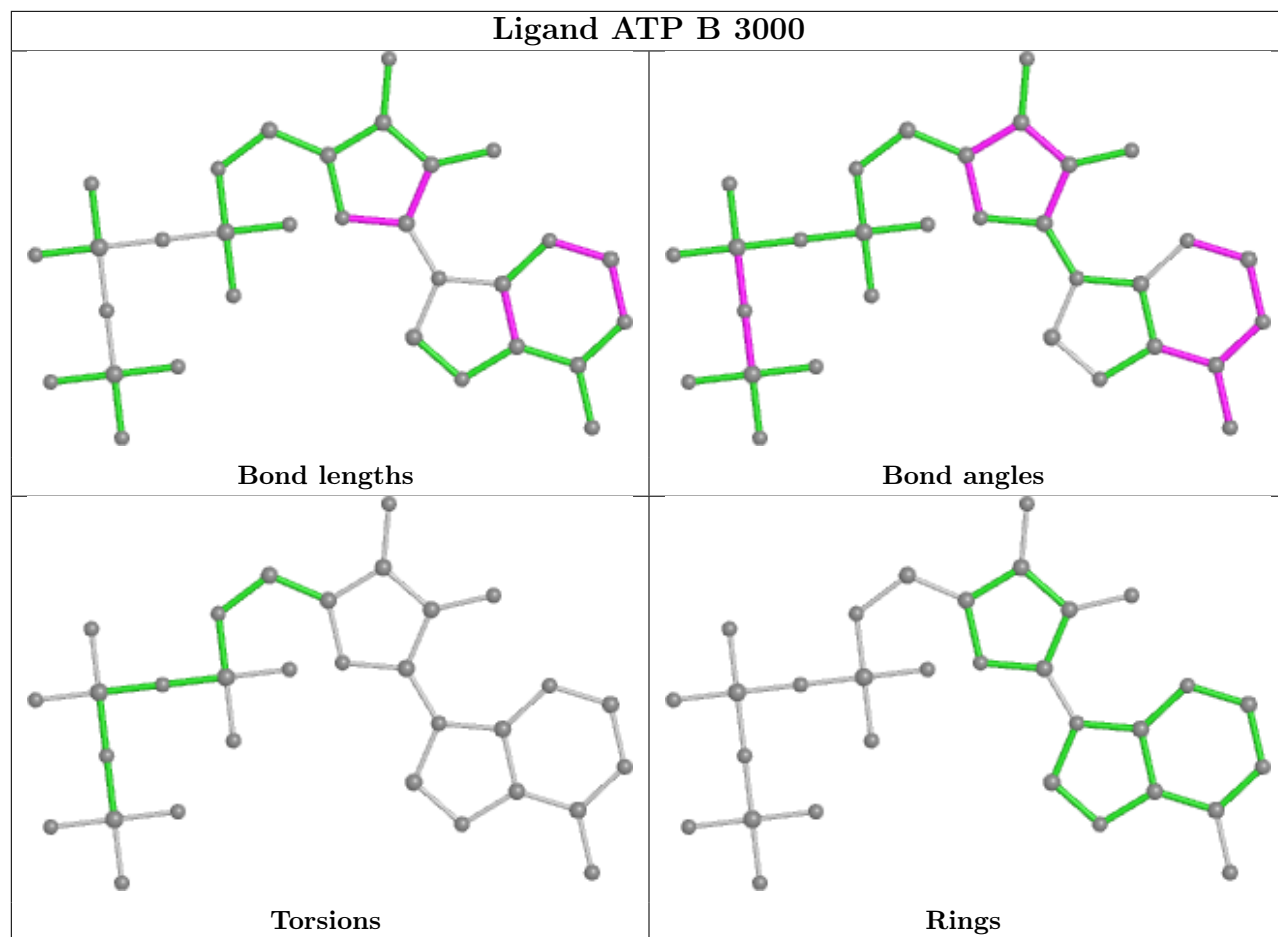
Mol	Chain	Res	Type	Atoms
8	S	201	GTP	PB-O3A-PA-O1A
8	R	201	GTP	PB-O3A-PA-O1A
8	S	201	GTP	PB-O3A-PA-O2A
8	S	201	GTP	C4'-C5'-O5'-PA
8	R	201	GTP	C4'-C5'-O5'-PA
8	R	201	GTP	PB-O3A-PA-O2A
8	R	201	GTP	C5'-O5'-PA-O1A

There are no ring outliers.

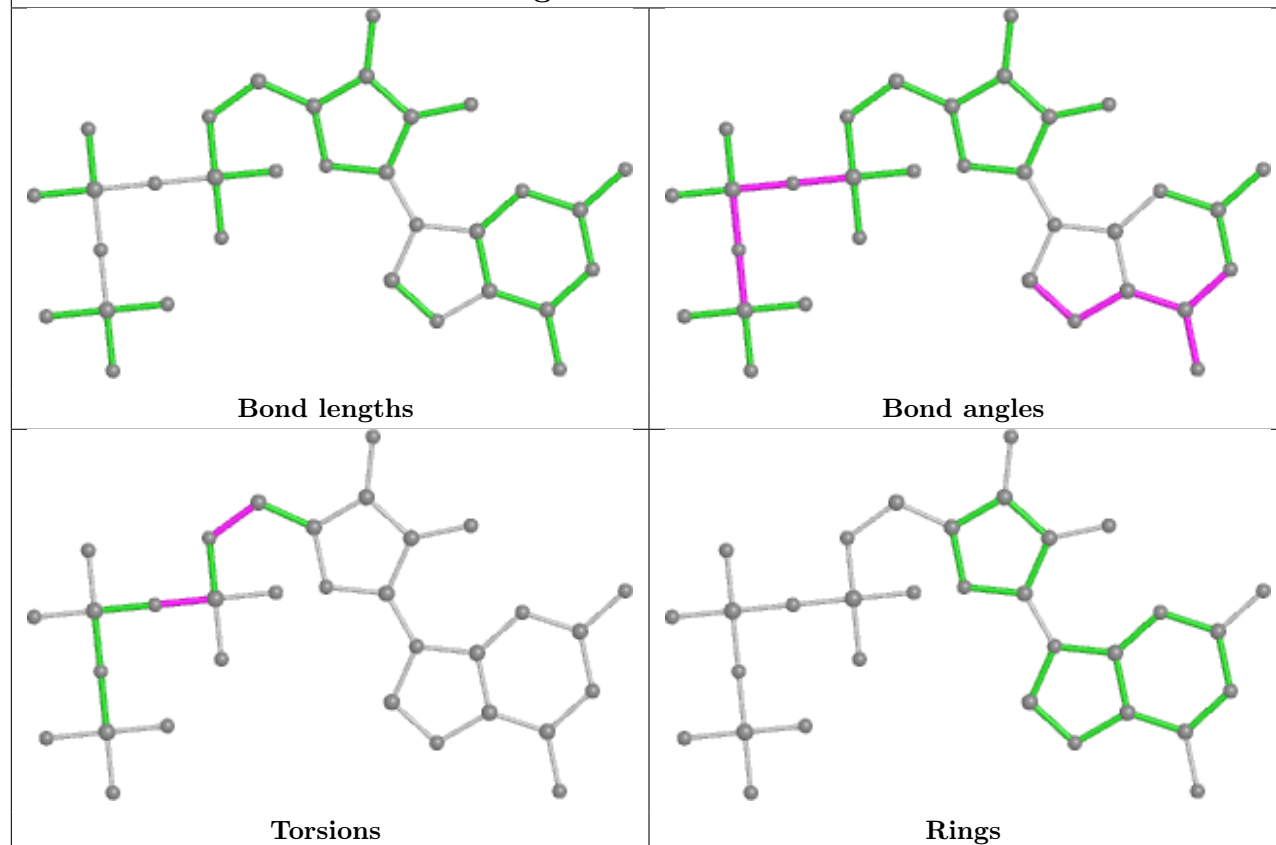
No monomer is involved in short contacts.

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.

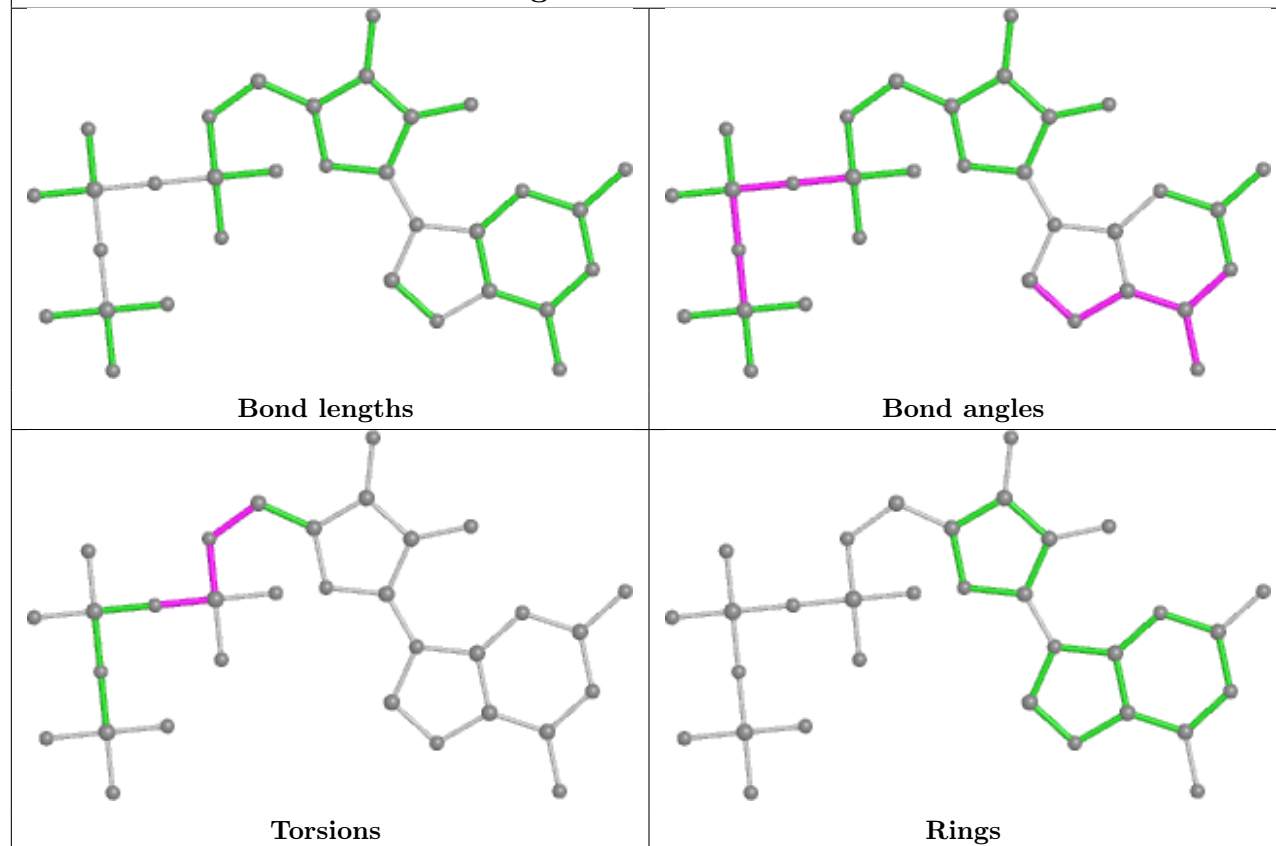




Ligand GTP S 201



Ligand GTP R 201



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
3	Y	1
3	W	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Y	40:GLU	C	41:GLY	N	3.34
1	W	40:GLU	C	41:GLY	N	3.22

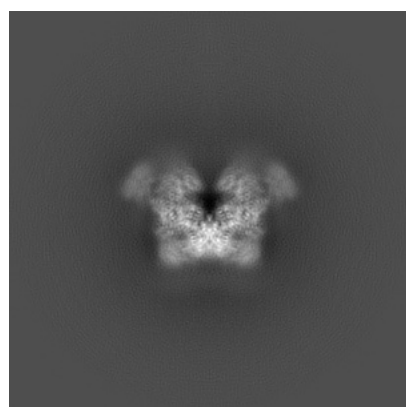
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7086. These allow visual inspection of the internal detail of the map and identification of artifacts.

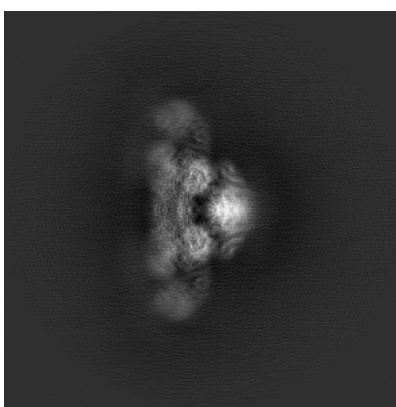
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

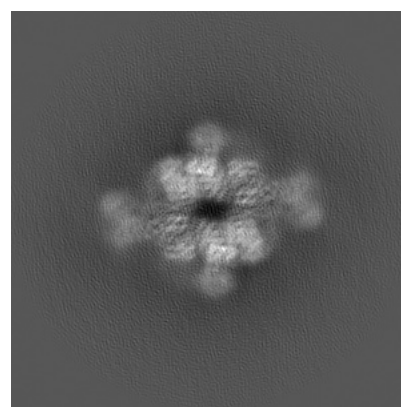
6.1.1 Primary map



X



Y

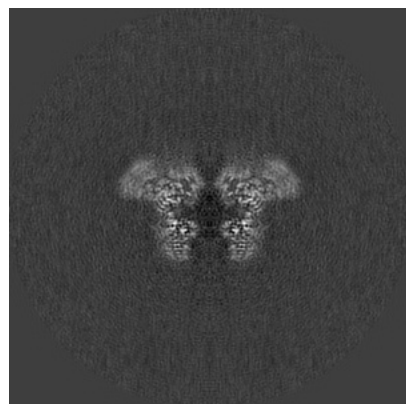


Z

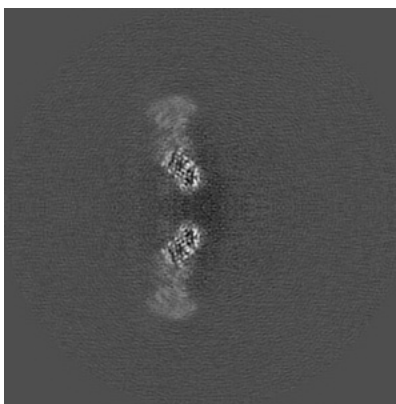
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

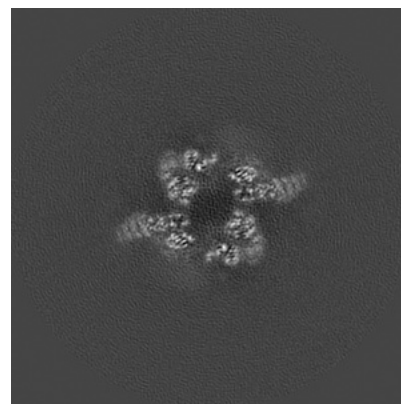
6.2.1 Primary map



X Index: 187



Y Index: 187

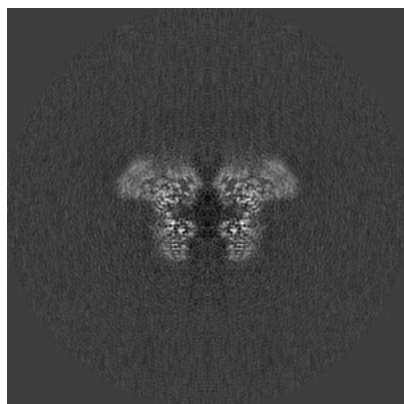


Z Index: 187

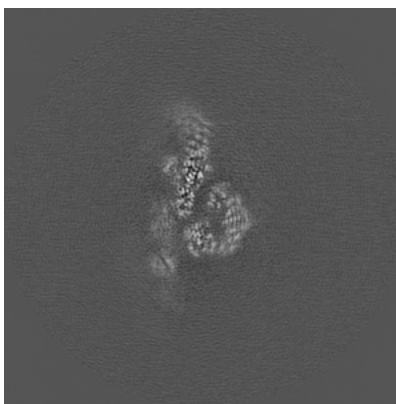
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

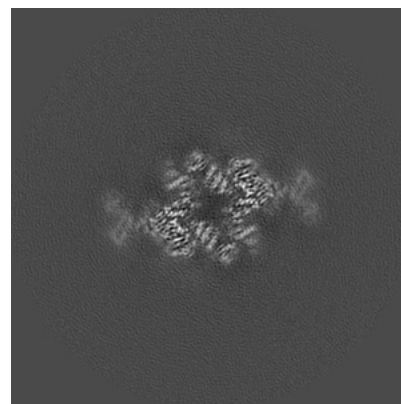
6.3.1 Primary map



X Index: 187



Y Index: 207



Z Index: 174

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

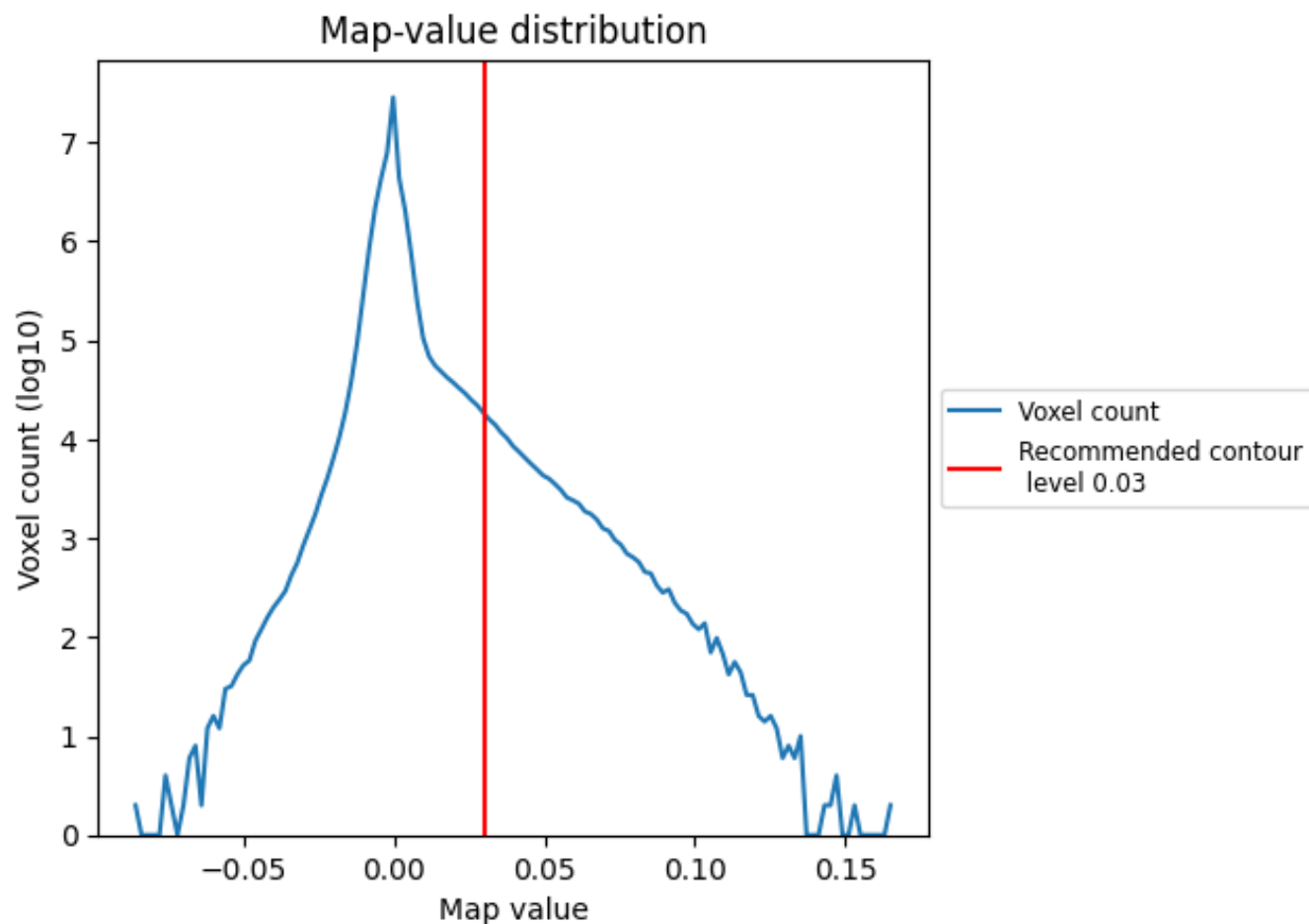
6.5 Mask visualisation

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

7 Map analysis [i](#)

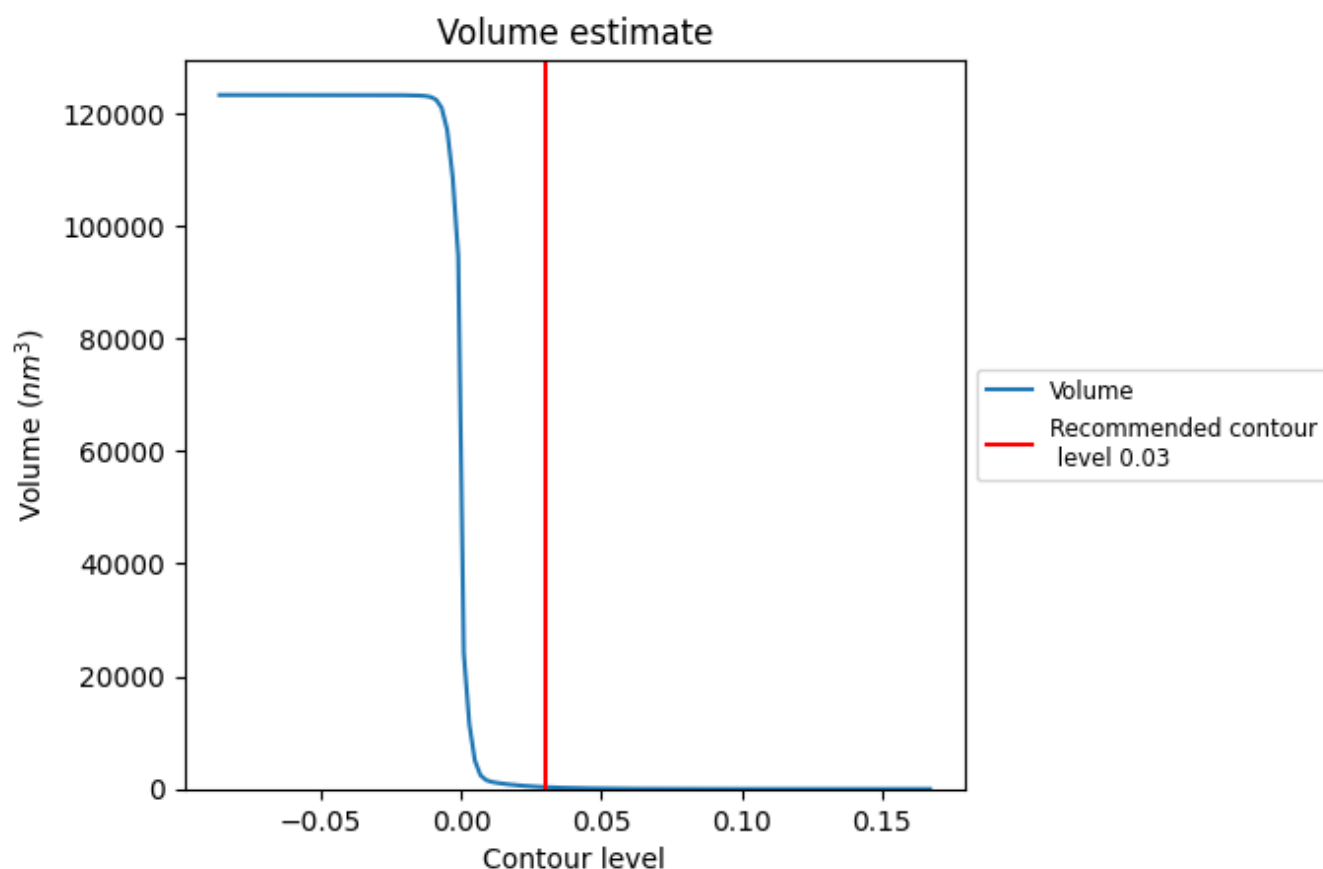
This section contains the results of statistical analysis of the map.

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.

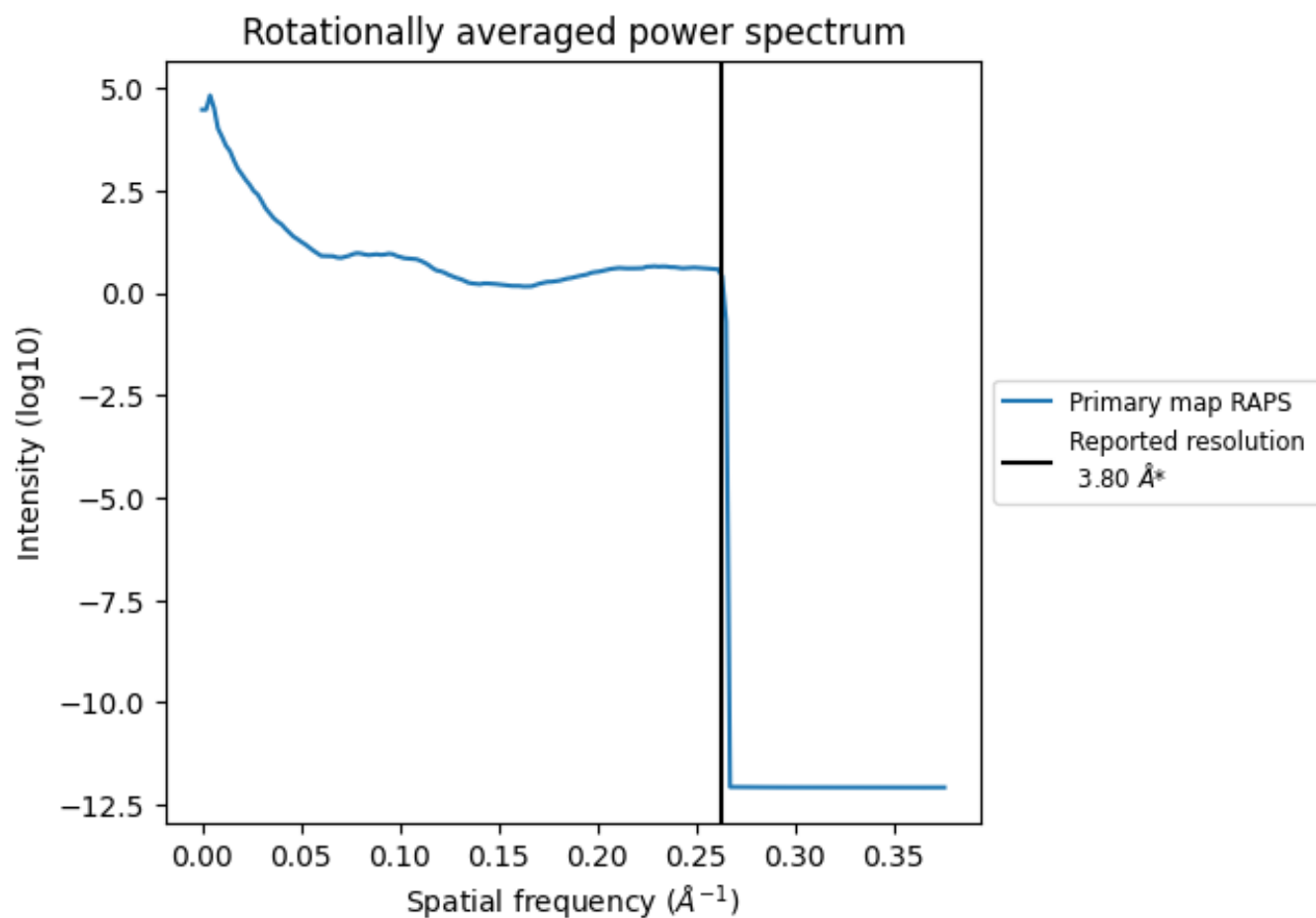
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 320 nm³; this corresponds to an approximate mass of 289 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 0.263 Å⁻¹

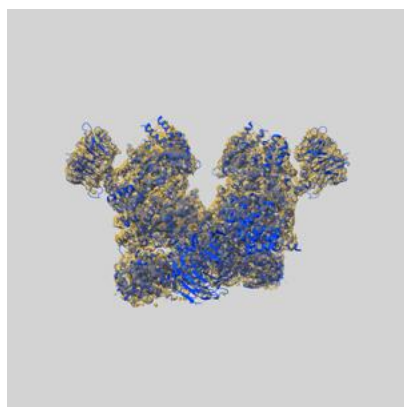
8 Fourier-Shell correlation

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

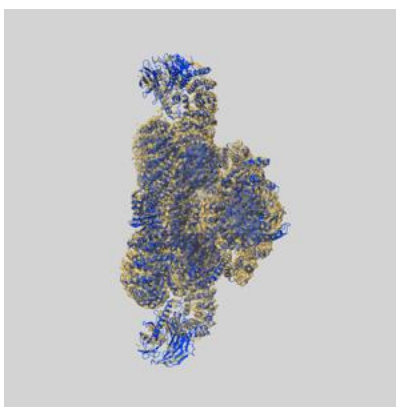
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7086 and PDB model 6BCU. Per-residue inclusion information can be found in section [3](#) on page [8](#).

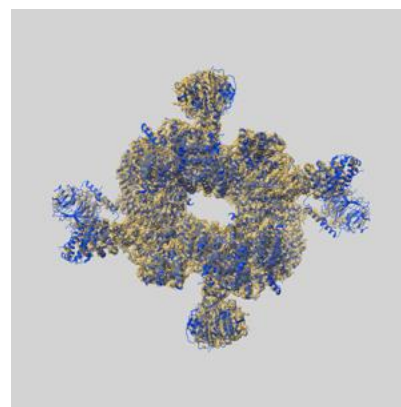
9.1 Map-model overlay [i](#)



X



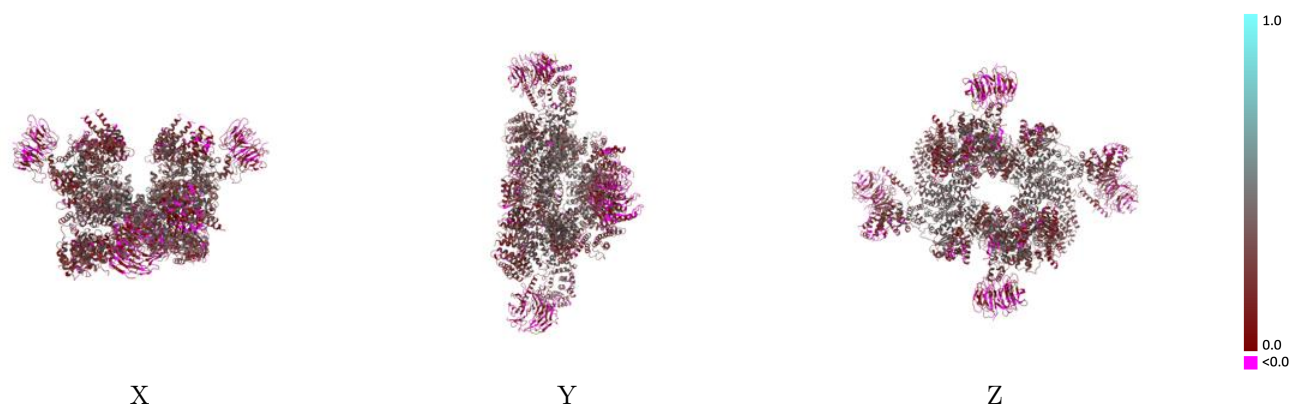
Y



Z

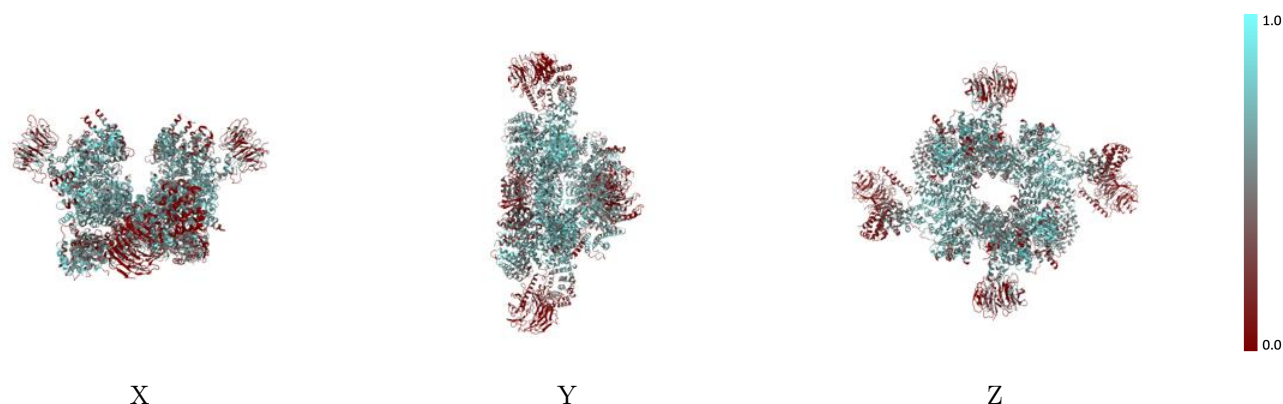
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



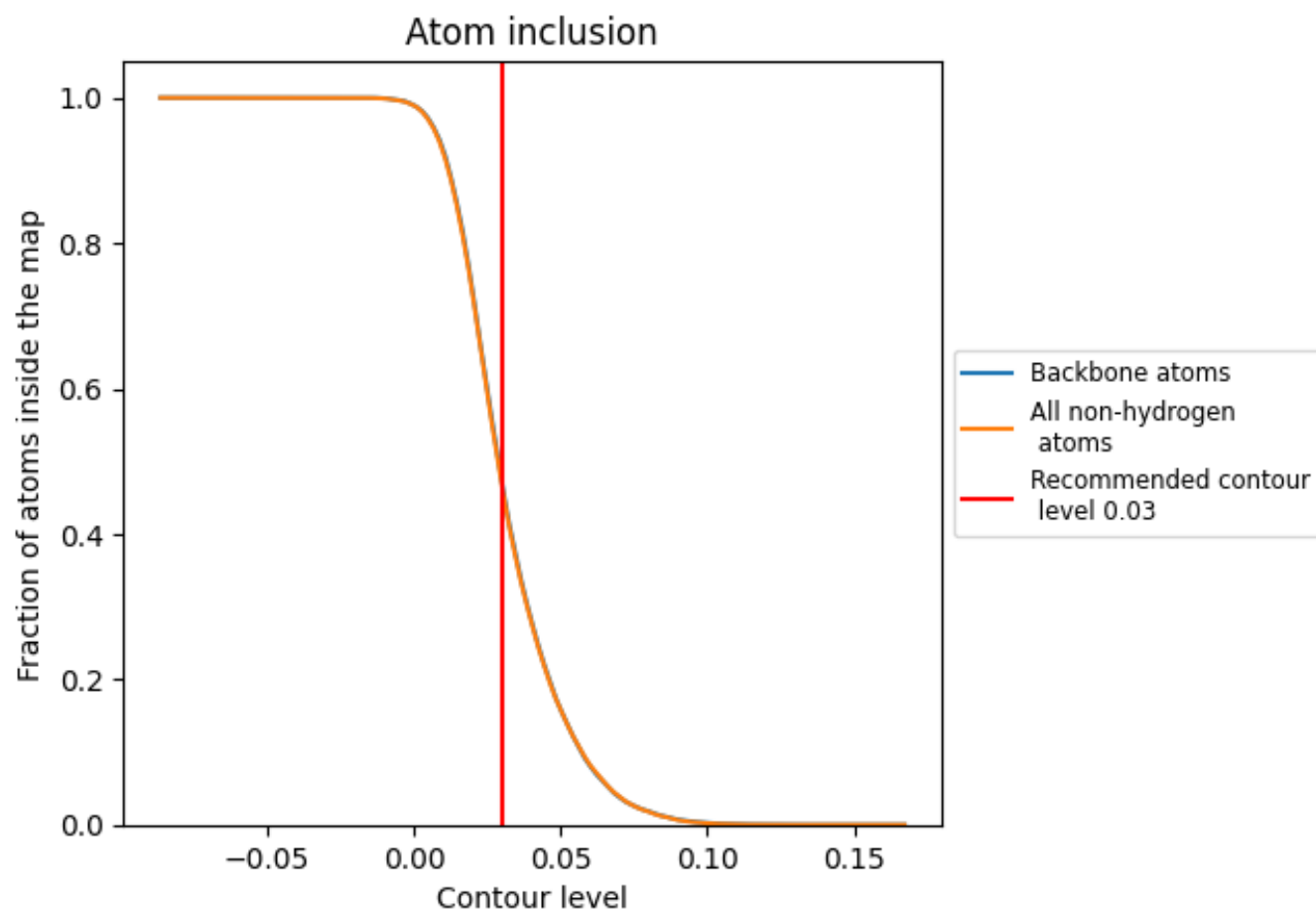
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 47% of all backbone atoms, 47% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4677	<div></div> 0.2500
A	<div></div> 0.5790	<div></div> 0.2870
B	<div></div> 0.5805	<div></div> 0.2870
D	<div></div> 0.2592	<div></div> 0.0710
E	<div></div> 0.2592	<div></div> 0.0680
R	<div></div> 0.2545	<div></div> 0.2150
S	<div></div> 0.2568	<div></div> 0.2230
W	<div></div> 0.3742	<div></div> 0.2280
X	<div></div> 0.4706	<div></div> 0.3660
Y	<div></div> 0.3706	<div></div> 0.2270
Z	<div></div> 0.5000	<div></div> 0.3750

1.0

0.0

<0.0