



Full wwPDB EM Validation Report ⓘ

Apr 29, 2026 – 02:07 am BST

PDB ID : 9RSS / pdb_00009rss
EMDB ID : EMD-54223
Title : Cryo-EM structure of the Target of Rapamycin Complex 2 (TORC2) with the Avo1 PH domain
Authors : Tafur, L.; Zou, L.; Loewith, R.
Deposited on : 2025-07-01
Resolution : 3.01 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

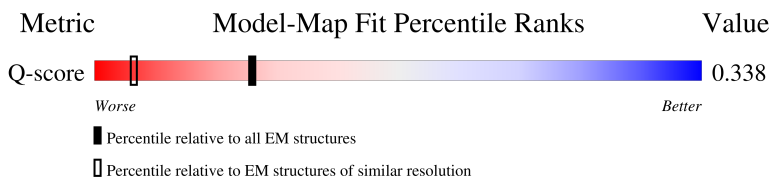
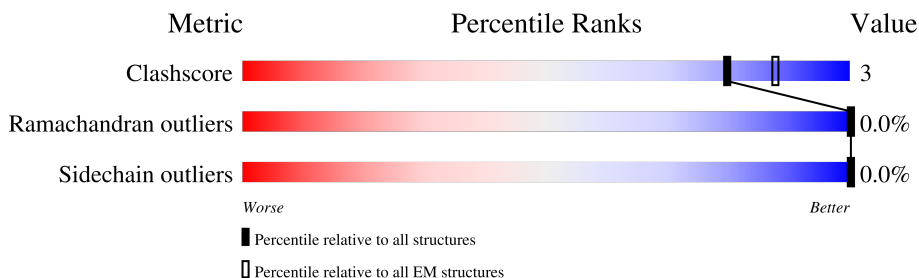
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.01 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13882 (2.51 - 3.51)

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	B	303	 5% 89% 10%
1	I	303	 5% 89% 10%
2	A	2474	 5% 85% 7% 8%
2	F	2474	 5% 85% 7% 8%

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Mol	Chain	Length	Quality of chain
3	C	1430	<div><div><div></div><div></div><div></div></div><div>69%5%26%</div></div>
3	J	1430	<div><div><div></div><div></div><div></div></div><div>69%5%26%</div></div>
4	D	426	<div><div><div></div><div></div><div></div></div><div>41%.56%</div></div>
4	K	426	<div><div><div></div><div></div><div></div></div><div>41%.56%</div></div>
5	E	543	<div><div><div></div><div></div><div></div></div><div>36%.60%</div></div>
5	L	543	<div><div><div></div><div></div><div></div></div><div>36%.60%</div></div>
6	G	1176	<div><div><div></div><div></div><div></div></div><div>15%.83%</div></div>
6	M	1176	<div><div><div></div><div></div><div></div></div><div>15%.83%</div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 68304 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 Target of rapamycin complex subunit LST8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	302	Total	C	N	O	S	0	0
			2386	1476	435	464	11		
1	I	302	Total	C	N	O	S	0	0
			2386	1476	435	464	11		

- Molecule 2 is a protein called Serine/threonine-protein kinase TOR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	2268	Total	C	N	O	S	0	0
			18184	11658	3108	3333	85		
2	F	2268	Total	C	N	O	S	0	0
			18184	11658	3108	3333	85		

- Molecule 3 is a protein called Target of rapamycin complex 2 subunit TSC11.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	1059	Total	C	N	O	S	0	0
			8627	5559	1450	1571	47		
3	J	1059	Total	C	N	O	S	0	0
			8627	5559	1450	1571	47		

- Molecule 4 is a protein called Target of rapamycin complex 2 subunit AVO2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	189	Total	C	N	O	S	0	0
			1518	969	270	267	12		
4	K	189	Total	C	N	O	S	0	0
			1518	969	270	267	12		

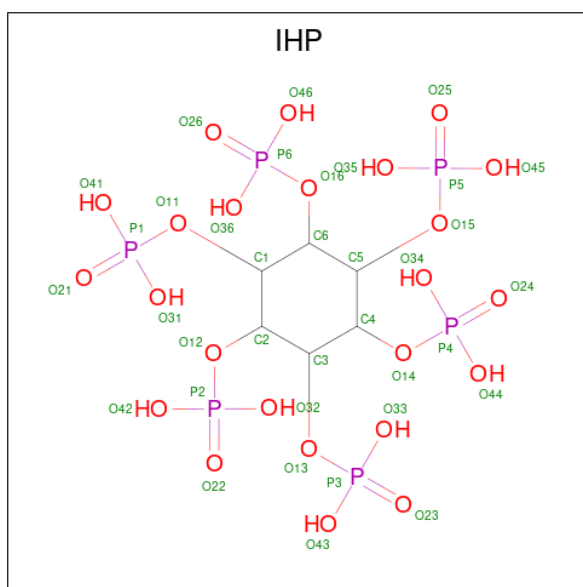
- Molecule 5 is a protein called Target of rapamycin complex 2 subunit BIT61.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	215	Total	C	N	O	S	0	0
			1776	1146	297	324	9		
5	L	215	Total	C	N	O	S	0	0
			1776	1146	297	324	9		

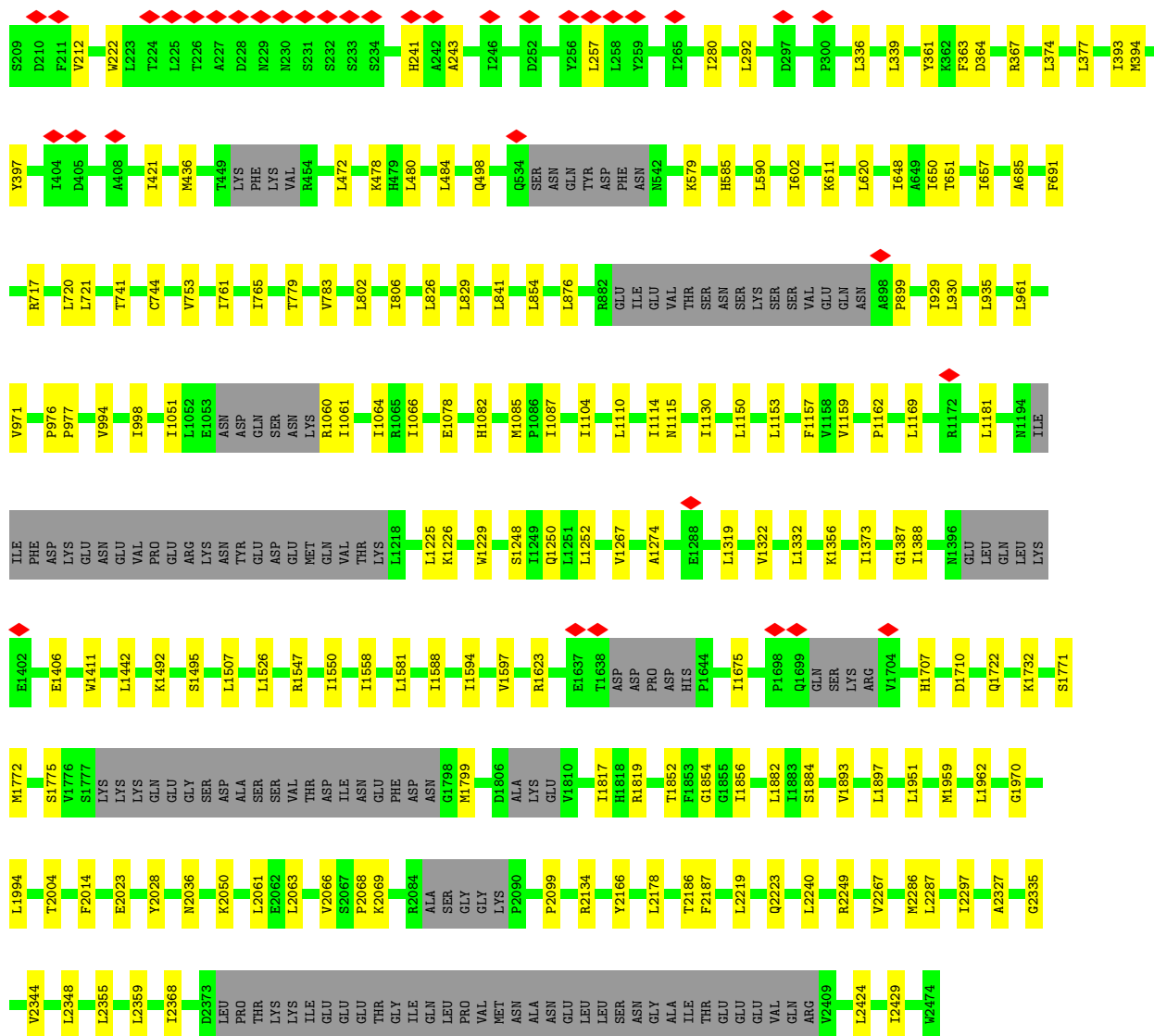
- Molecule 6 is a protein called Target of rapamycin complex 2 subunit AVO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	196	Total	C	N	O	S	0	0
			1625	1040	288	288	9		
6	M	196	Total	C	N	O	S	0	0
			1625	1040	288	288	9		

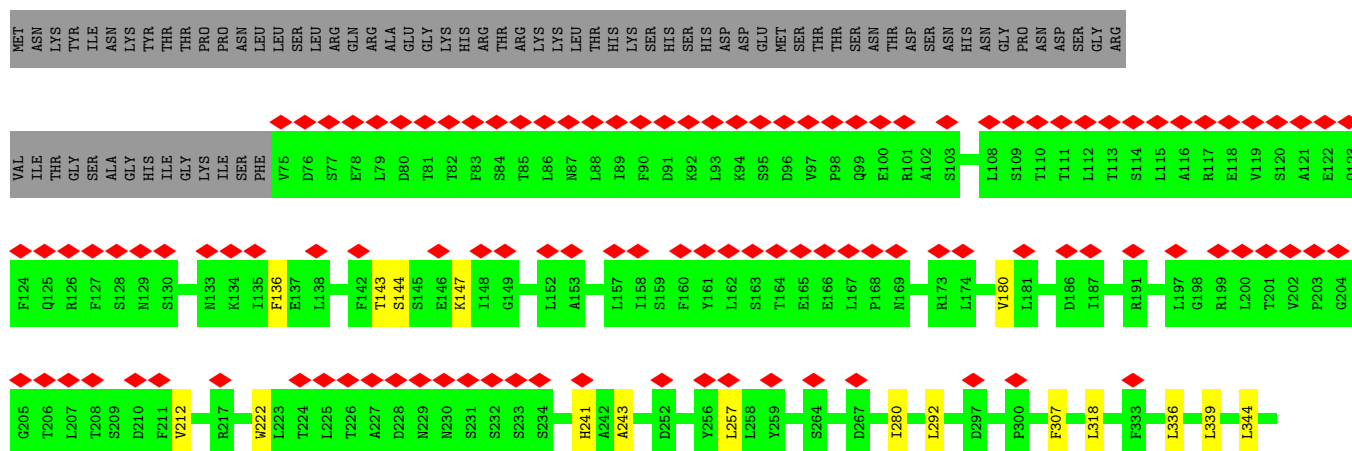
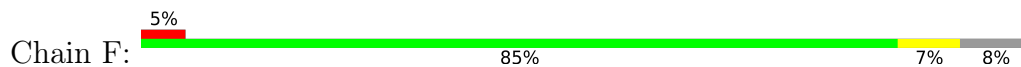
- Molecule 7 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).

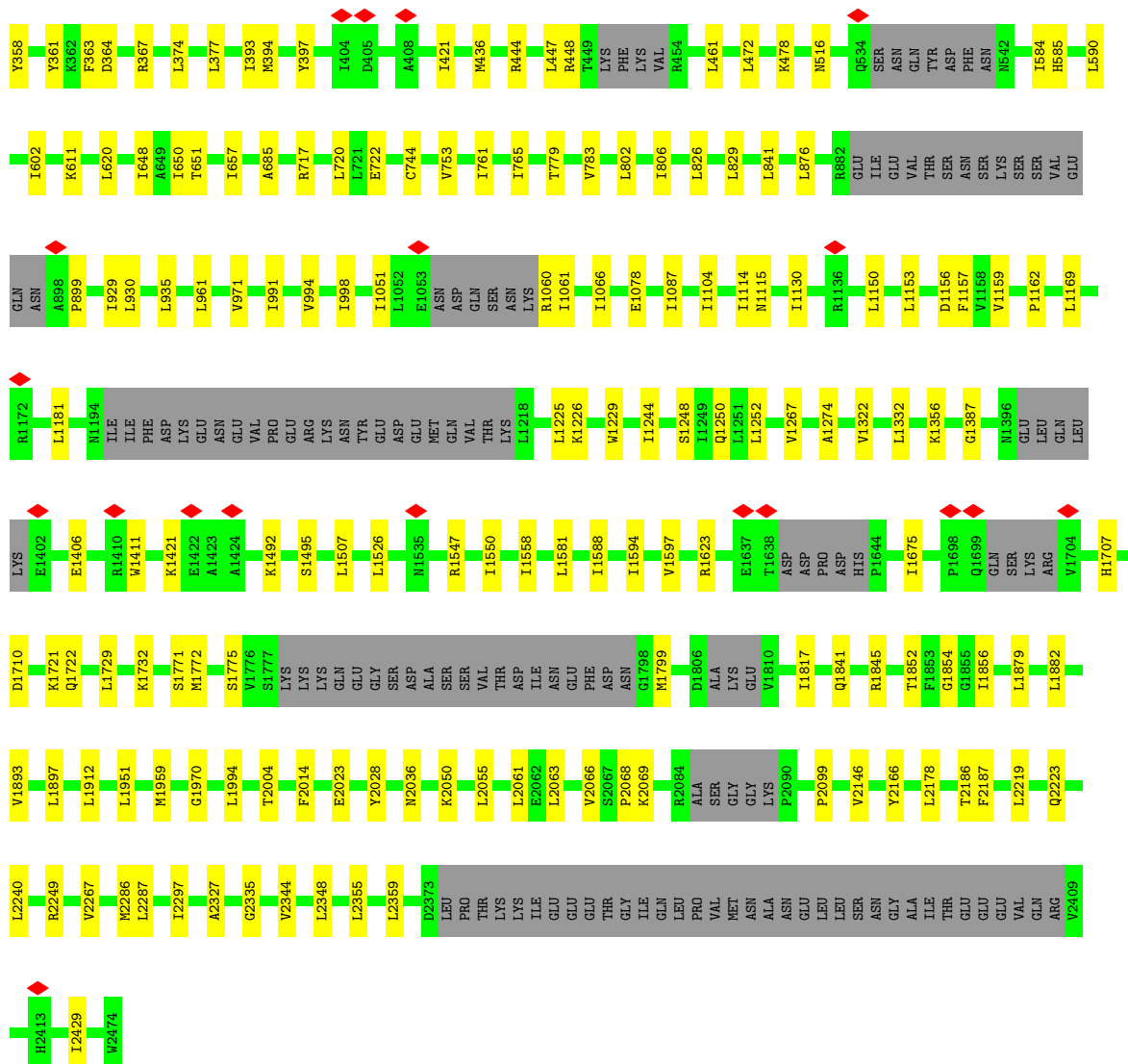


Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	O	P	0
			36	6	24	6	
7	F	1	Total	C	O	P	0
			36	6	24	6	



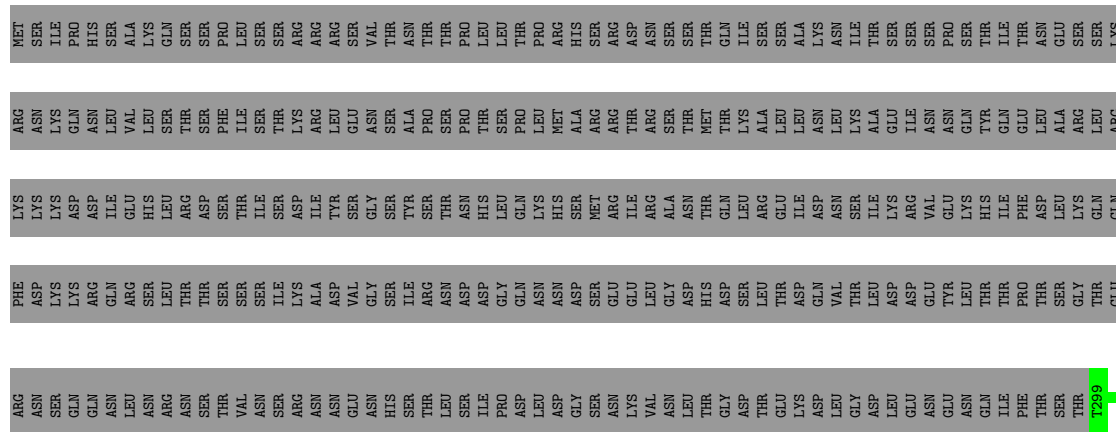
• Molecule 2: Serine/threonine-protein kinase TOR2

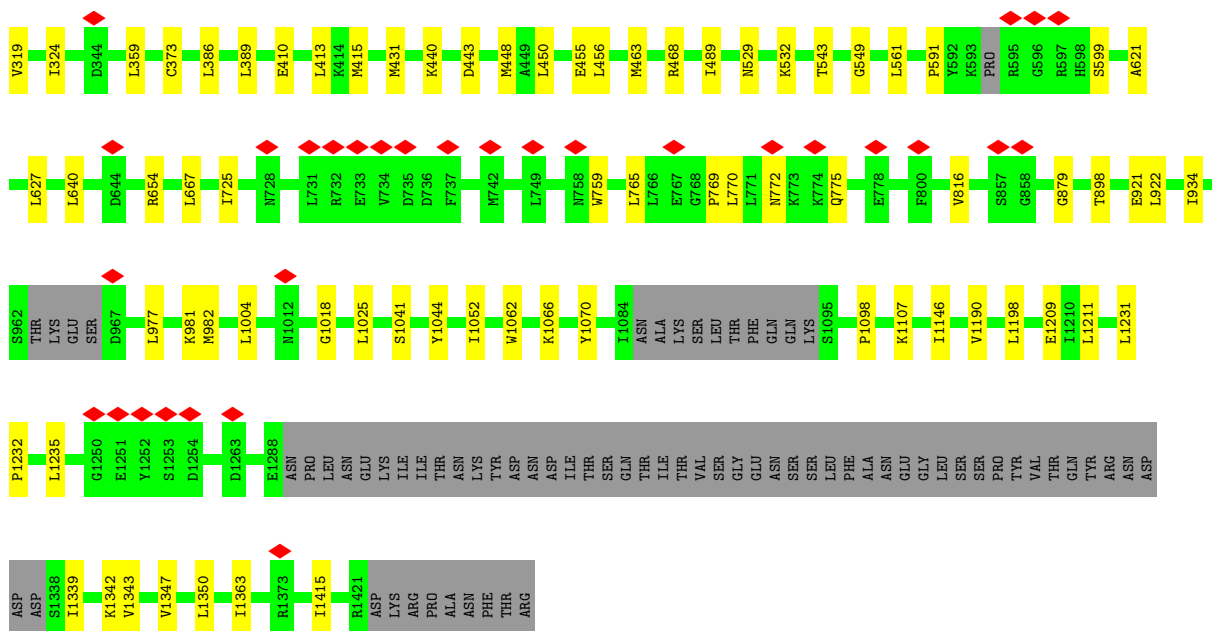




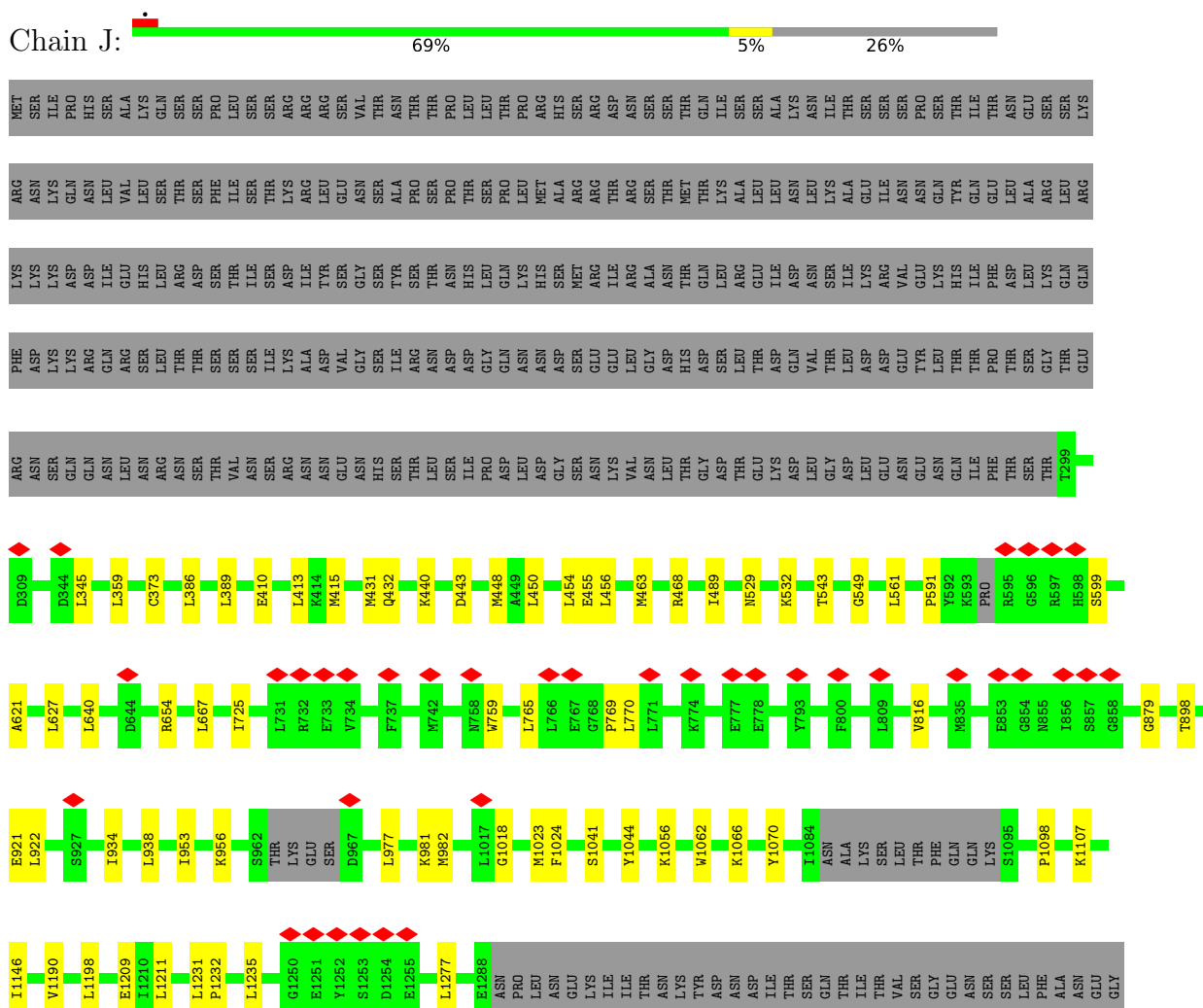
• Molecule 3: Target of rapamycin complex 2 subunit TSC11

Chain C: 69% 5% 26%





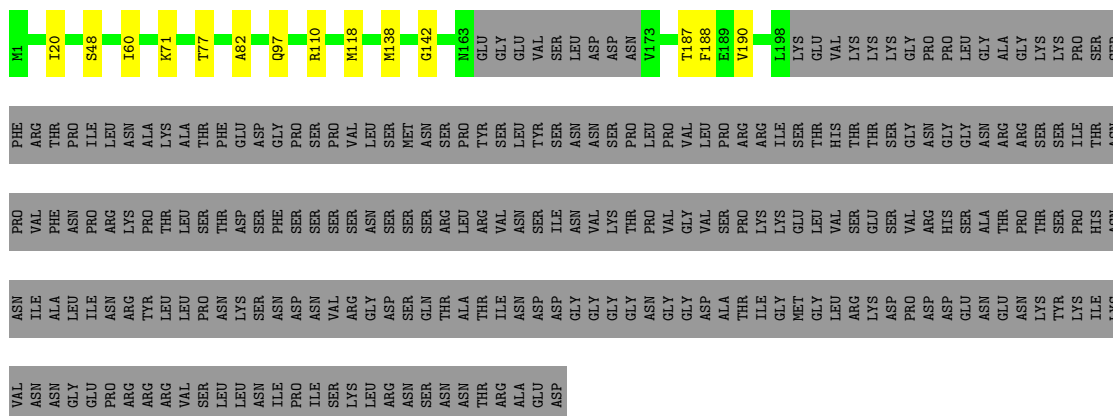
- Molecule 3: Target of rapamycin complex 2 subunit TSC11





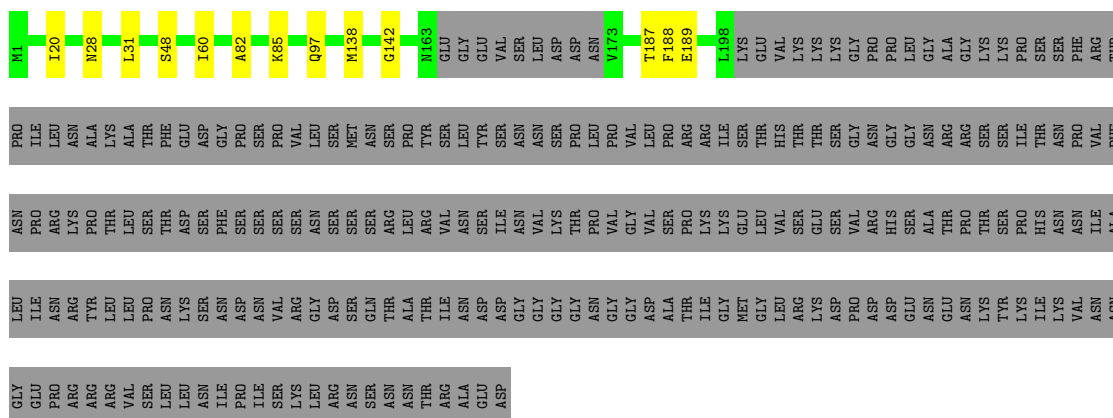
● Molecule 4: Target of rapamycin complex 2 subunit AVO2

Chain D: 41% 56%



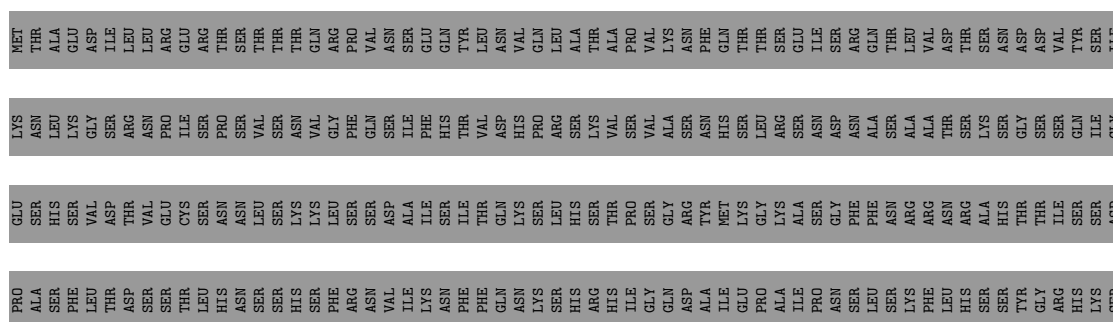
● Molecule 4: Target of rapamycin complex 2 subunit AVO2

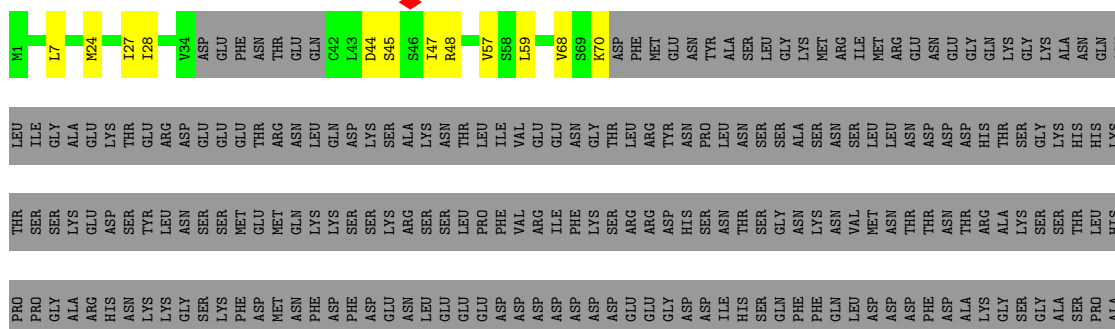
Chain K: 41% 56%



● Molecule 5: Target of rapamycin complex 2 subunit BIT61

Chain E: 36% 60%





R1073	GLY	PRO	ALA	GLY	ASP	PHE	LYS	ARG	ALA	PHE	LEU	GLY	LEU	GLY	ASP	LEU	GLY	ASP	THR	SER
R1074	GLY	THR	LEU	THR	SER	ALA	THR	THR	SER	VAL	GLU	THR	GLU	GLU	ASP	THR	GLU	ASP	THR	SER
Q1075	ALA	LEU	VAL	ASP	VAL	PHE	ASN	THR	THR	VAL	ALA	VAL	GLU	GLU	ASN	THR	GLU	ASP	HIS	ALA
K1082	GLY	PRO	GLY	ILE	LEU	CYS	LYS	ASN	THR	VAL	THR	THR	GLU	GLU	SER	THR	GLU	ASP	PRO	GLY
A1088	GLY	ASN	LYS	LYS	LYS	LYS	THR	VAL	SER	THR	MET	THR	GLU	GLU	ASN	THR	GLU	ASP	ILE	ALA
Y1095	PHE	SER	TYR	ASN	VAL	VAL	ASP	ASP	ASN	ASN	MET	MET	GLU	GLU	ASN	THR	GLU	ASP	ASN	GLY
Y1096	PHE	LEU	ILE	ASN	VAL	VAL	LYS	VAL	VAL	VAL	PRO	PRO	GLU	GLU	LYS	SER	THR	LYS	THR	GLY
E1100	ASN	ALA	LYS	SER	GLU	GLU	LYS	GLU	ASP	ASP	THR	TYR	GLU	GLU	ASN	VAL	THR	ASP	ASN	LYS
G1101	ASN	ASP	ASN	ILE	LYS	LYS	LYS	ASP	ASP	THR	THR	PHE	GLU	GLU	SER	VAL	THR	ASP	ASN	GLY
R1102	SER	GLY	THR	ASP	GLN	SER	PHE	PHE	THR	PHE	GLU	THR	GLU	GLU	LYS	VAL	THR	LEU	ASN	LYS
I1103	LYS	GLY	VAL	VAL	ASN	GLU	VAL	VAL	GLU	GLU	GLU	VAL	GLU	GLU	ARG	ARG	THR	GLY	ASN	PHE
H1104	SER	ALA	VAL	THR	GLU	ILE	CYS	GLY	GLY	ASP	THR	THR	GLU	GLU	ILE	ALA	THR	GLU	THR	GLY
W1105	LEU	ALA	LEU	TYR	GLU	GLU	ASP	ASP	THR	THR	THR	THR	GLU	GLU	SER	ARG	THR	GLU	ASN	MET
H1106	HIS	ALA	ASP	LEU	THR	THR	LYS	LYS	ARG	THR	THR	THR	GLU	GLU	LYS	ARG	THR	GLU	THR	ASN
D1107	GLY	ILE	ILE	VAL	PRO	PRO	VAL	VAL	THR	ILE	VAL	VAL	GLU	GLU	LYS	THR	VAL	THR	THR	THR
N1108	THR	PRO	ILE	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	GLU	GLU	THR	THR	VAL	THR	THR	THR
V1109	LEU	ASN	LYS	VAL	ASN	PHE	ASN	GLU	ASP	ASP	THR	TYR	GLU	GLU	LYS	THR	ASP	THR	THR	GLY
K1110	GLN	THR	VAL	ASN	GLU	GLU	ASN	THR	THR	GLU	LEU	THR	GLU	GLU	LEU	ASP	ALA	THR	THR	GLY
T1111	PHE	THR	VAL	ASN	THR	GLU	ASN	GLU	SER	ILE	THR	SER	GLU	GLU	LYS	THR	ALA	THR	THR	GLY
K1112	HIS	LYS	GLU	PRO	THR	GLY	LYS	GLU	LYS	PRO	THR	SER	GLU	GLU	THR	THR	VAL	THR	THR	GLY
R1127	ASN	VAL	LEU	LYS	GLY	GLY	MET	MET	LYS	ASN	THR	TYR	GLU	GLU	ASN	THR	THR	THR	THR	GLY
V1128	ARG	LYS	THR	LYS	THR	THR	THR	ILE	GLN	ILE	THR	THR	GLU	GLU	ASN	THR	THR	THR	THR	GLY
P1129	SER	ALA	LYS	ALA	ASP	THR	LYS	ALA	VAL	LYS	THR	THR	GLU	GLU	ASN	THR	THR	THR	THR	GLY
E1130	GLN	LYS	LYS	ILE	THR	THR	THR	ILE	VAL	ILE	THR	THR	GLU	GLU	ASN	THR	THR	THR	THR	GLY
H1131	THR	ILE	ILE	ARG	SER	SER	ILE	ARG	ALA	ILE	THR	THR	GLU	GLU	ASN	THR	THR	THR	THR	GLY
V1136	MET	SER	SER	SER	THR	THR	VAL	ALA	VAL	VAL	LEU	THR	GLU	GLU	ASN	THR	THR	THR	THR	GLY
R1137	HIS	LYS	THR	HIS	ASP	THR	VAL	THR	LEU	VAL	ALA	THR	GLU	GLU	ASN	THR	THR	THR	THR	GLY
E1139	THR	LYS	TYR	LEU	THR	THR	LYS	THR	LEU	THR	ALA	THR	GLU	GLU	ASN	THR	THR	THR	THR	GLY
R1138	PRO	LYS	LYS	GLU	GLY	GLY	LYS	LYS	THR	ASP	ASN	THR	GLU	GLU	ASN	THR	THR	THR	THR	GLY
E1139	ASP	GLY	LEU	LYS	THR	THR	THR	THR	THR	ASP	ASN	THR	GLU	GLU	ASN	THR	THR	THR	THR	GLY
I1144	GLY	PRO	GLY	GLY	THR	THR	THR	THR	THR	THR	THR	THR	GLU	GLU	ASN	THR	THR	THR	THR	GLY
K1145	GLY	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
R1146	ASN	THR	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
A1151	PHE	GLN	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER
V1152	GLN	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
K1176	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
A1065	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
K1070	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51729	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.971	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.061	Depositor
Map size (Å)	464.896, 464.896, 464.896	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.908, 0.908, 0.908	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: IHP

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	B	0.12	0/2442	0.33	0/3327
1	I	0.12	0/2442	0.33	0/3327
2	A	0.16	0/18548	0.32	0/25113
2	F	0.16	0/18548	0.33	0/25113
3	C	0.14	0/8785	0.30	0/11831
3	J	0.13	0/8785	0.30	0/11831
4	D	0.15	0/1550	0.31	0/2095
4	K	0.15	0/1550	0.31	0/2095
5	E	0.13	0/1806	0.30	0/2440
5	L	0.14	0/1806	0.29	0/2440
6	G	0.15	0/1657	0.30	0/2227
6	M	0.15	0/1657	0.31	0/2227
All	All	0.15	0/69576	0.32	0/94066

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2386	0	2276	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	2386	0	2276	17	0
2	A	18184	0	18527	107	0
2	F	18184	0	18527	103	0
3	C	8627	0	8804	42	0
3	J	8627	0	8804	46	0
4	D	1518	0	1537	8	0
4	K	1518	0	1537	8	0
5	E	1776	0	1794	10	0
5	L	1776	0	1794	10	0
6	G	1625	0	1669	12	0
6	M	1625	0	1669	16	0
7	A	36	0	6	0	0
7	F	36	0	6	0	0
All	All	68304	0	69226	373	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 3.

All (373) 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)
2:F:1492:LYS:HB2	2:F:1495:SER:HB3	1.71	0.72
2:A:1492:LYS:HB2	2:A:1495:SER:HB3	1.71	0.72
3:C:450:LEU:HD21	3:C:489:ILE:HD11	1.76	0.68
3:J:450:LEU:HD21	3:J:489:ILE:HD11	1.76	0.67
3:C:759:TRP:HB3	3:C:816:VAL:HG21	1.79	0.65
2:F:602:ILE:HG23	2:F:648:ILE:HD12	1.80	0.62
3:J:759:TRP:HB3	3:J:816:VAL:HG21	1.80	0.62
2:A:602:ILE:HG23	2:A:648:ILE:HD12	1.81	0.61
3:J:1041:SER:HB2	3:J:1107:LYS:HD2	1.82	0.61
3:C:1041:SER:HB2	3:C:1107:LYS:HD2	1.83	0.61
2:F:650:ILE:HG13	2:F:651:THR:HG23	1.83	0.61
2:A:650:ILE:HG13	2:A:651:THR:HG23	1.82	0.60
3:C:591:PRO:HB2	3:C:599:SER:HB2	1.82	0.59
2:F:744:CYS:HB2	2:F:783:VAL:HG22	1.84	0.59
3:C:898:THR:HG21	5:E:345:LYS:HG2	1.84	0.59
3:J:898:THR:HG21	5:L:345:LYS:HG2	1.84	0.59
5:L:333:LEU:HA	5:L:337:GLN:HB3	1.84	0.59
2:A:744:CYS:HB2	2:A:783:VAL:HG22	1.85	0.58
5:E:333:LEU:HA	5:E:337:GLN:HB3	1.85	0.58
2:A:1970:GLY:HA3	2:A:1994:LEU:HD11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:45:SER:HA	6:G:48:ARG:HD2	1.85	0.58
1:I:255:ASP:HB3	1:I:298:VAL:HG12	1.86	0.57
2:A:961:LEU:HD11	2:A:994:VAL:HG21	1.87	0.57
2:F:1970:GLY:HA3	2:F:1994:LEU:HD11	1.87	0.57
5:L:367:HIS:HB3	5:L:372:ARG:HG2	1.86	0.57
2:F:611:LYS:HB2	2:F:657:ILE:HG12	1.87	0.57
3:C:373:CYS:HB3	3:C:415:MET:HE1	1.86	0.57
6:M:1088:ALA:HB3	6:M:1095:TYR:HB2	1.87	0.56
2:A:841:LEU:HG	2:A:876:LEU:HD11	1.87	0.56
5:E:367:HIS:HB3	5:E:372:ARG:HG2	1.87	0.56
2:F:336:LEU:HA	2:F:339:LEU:HD12	1.87	0.56
2:F:361:TYR:HD1	2:F:363:PHE:H	1.51	0.56
1:B:255:ASP:HB3	1:B:298:VAL:HG12	1.86	0.56
1:I:115:HIS:HD2	1:I:117:ALA:HB3	1.70	0.56
5:E:470:ASP:HA	5:E:474:LEU:HD12	1.86	0.56
6:M:57:VAL:HG12	6:M:59:LEU:H	1.70	0.56
6:G:57:VAL:HG12	6:G:59:LEU:H	1.70	0.56
3:J:373:CYS:HB3	3:J:415:MET:HE1	1.88	0.56
3:C:1209:GLU:HG3	4:K:20:ILE:HG23	1.88	0.55
2:A:611:LYS:HB2	2:A:657:ILE:HG12	1.87	0.55
2:F:961:LEU:HD11	2:F:994:VAL:HG21	1.88	0.55
6:M:45:SER:HA	6:M:48:ARG:HD2	1.88	0.55
2:A:361:TYR:HD1	2:A:363:PHE:H	1.52	0.55
2:F:841:LEU:HG	2:F:876:LEU:HD11	1.87	0.55
5:L:470:ASP:HA	5:L:474:LEU:HD12	1.88	0.54
2:F:212:VAL:HG21	2:F:257:LEU:HD13	1.89	0.54
2:F:2359:LEU:HD13	2:F:2429:ILE:HD13	1.89	0.54
1:B:115:HIS:HD2	1:B:117:ALA:HB3	1.73	0.54
1:B:37:ARG:H	1:B:50:ALA:HB3	1.73	0.54
1:B:55:VAL:HG21	1:B:92:THR:HG21	1.88	0.54
2:A:212:VAL:HG21	2:A:257:LEU:HD13	1.88	0.54
2:F:1225:LEU:HD23	2:F:1250:GLN:HG3	1.89	0.54
4:D:20:ILE:HG23	3:J:1209:GLU:HG3	1.89	0.54
3:C:1062:TRP:HA	3:C:1066:LYS:HB2	1.90	0.54
1:I:55:VAL:HG21	1:I:92:THR:HG21	1.89	0.53
2:A:2359:LEU:HD13	2:A:2429:ILE:HD13	1.89	0.53
2:F:806:ILE:HG21	2:F:826:LEU:HB2	1.90	0.53
2:F:2219:LEU:HD13	2:F:2223:GLN:HB3	1.90	0.53
4:K:48:SER:HB3	4:K:82:ALA:HB2	1.91	0.53
2:A:1817:ILE:HD13	2:A:1856:ILE:HG12	1.90	0.53
6:G:1088:ALA:HB3	6:G:1095:TYR:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2348:LEU:HD22	2:A:2355:LEU:HD11	1.91	0.53
2:F:1248:SER:HB3	2:F:1274:ALA:HB1	1.91	0.53
2:A:2187:PHE:HE1	2:A:2287:LEU:HB2	1.74	0.52
2:A:1225:LEU:HD23	2:A:1250:GLN:HG3	1.91	0.52
2:F:1817:ILE:HD13	2:F:1856:ILE:HG12	1.92	0.52
3:J:1198:LEU:HD22	3:J:1211:LEU:HD21	1.92	0.52
1:I:37:ARG:H	1:I:50:ALA:HB3	1.74	0.52
2:F:2348:LEU:HD22	2:F:2355:LEU:HD11	1.91	0.52
2:A:806:ILE:HG21	2:A:826:LEU:HB2	1.91	0.52
2:A:1248:SER:HB3	2:A:1274:ALA:HB1	1.90	0.52
2:A:1799:MET:HA	2:A:1852:THR:HG21	1.91	0.52
3:C:1146:ILE:HD12	3:C:1190:VAL:HG21	1.92	0.52
2:A:2219:LEU:HD13	2:A:2223:GLN:HB3	1.91	0.52
2:F:144:SER:HA	2:F:147:LYS:HD2	1.92	0.52
3:J:561:LEU:HD21	3:J:627:LEU:HD23	1.91	0.52
3:C:561:LEU:HD21	3:C:627:LEU:HD23	1.92	0.51
3:J:1062:TRP:HA	3:J:1066:LYS:HB2	1.91	0.51
2:A:2286:MET:HE2	2:A:2297:ILE:HD13	1.93	0.51
3:C:1198:LEU:HD22	3:C:1211:LEU:HD21	1.92	0.51
2:F:374:LEU:HA	2:F:377:LEU:HD12	1.91	0.51
2:A:1153:LEU:HD12	2:A:1157:PHE:HD1	1.75	0.51
2:A:364:ASP:HA	2:A:367:ARG:HE	1.76	0.51
2:A:1162:PRO:HB3	3:C:725:ILE:HG21	1.92	0.51
2:F:2187:PHE:HE1	2:F:2287:LEU:HB2	1.75	0.51
2:A:374:LEU:HA	2:A:377:LEU:HD12	1.92	0.51
5:L:469:ARG:HD2	5:L:532:ILE:HG13	1.92	0.51
2:F:292:LEU:HB3	2:F:339:LEU:HD11	1.93	0.51
2:A:2267:VAL:HG22	2:A:2344:VAL:HG21	1.93	0.51
2:F:436:MET:HG3	2:F:472:LEU:HD21	1.93	0.51
2:F:720:LEU:HD21	2:F:761:ILE:HD11	1.93	0.51
2:A:1085:MET:HE1	2:A:1110:LEU:HD13	1.92	0.51
2:F:364:ASP:HA	2:F:367:ARG:HE	1.76	0.51
2:F:1162:PRO:HB3	3:J:725:ILE:HG21	1.92	0.51
2:F:1322:VAL:HG22	2:F:1332:LEU:HD12	1.93	0.51
1:B:264:TYR:HB3	1:B:276:LEU:HD11	1.93	0.50
1:B:230:THR:HG22	1:B:247:ASP:HB3	1.94	0.50
1:I:20:LEU:HD11	6:M:643:MET:HB3	1.91	0.50
3:J:1146:ILE:HD12	3:J:1190:VAL:HG21	1.93	0.50
3:J:454:LEU:HD12	6:M:14:PHE:HZ	1.76	0.50
2:F:1799:MET:HA	2:F:1852:THR:HG21	1.92	0.50
2:F:2267:VAL:HG22	2:F:2344:VAL:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2061:LEU:HB3	2:A:2066:VAL:HG21	1.94	0.50
2:F:1153:LEU:HD12	2:F:1157:PHE:HD1	1.75	0.50
1:I:6:VAL:HG12	1:I:38:LEU:HD13	1.92	0.50
3:J:440:LYS:HB3	3:J:443:ASP:HB2	1.94	0.50
6:M:68:VAL:HG22	6:M:70:LYS:H	1.77	0.50
2:A:585:HIS:HB2	2:A:620:LEU:HD21	1.93	0.50
2:F:1051:ILE:HD11	2:F:1066:ILE:HD11	1.94	0.49
2:A:144:SER:HA	2:A:147:LYS:HD2	1.95	0.49
4:D:48:SER:HB3	4:D:82:ALA:HB2	1.94	0.49
2:F:2023:GLU:HB3	3:J:468:ARG:HH22	1.75	0.49
2:A:1322:VAL:HG22	2:A:1332:LEU:HD12	1.93	0.49
1:B:5:LEU:HD13	1:B:300:LEU:HD13	1.95	0.49
2:F:2286:MET:HE2	2:F:2297:ILE:HD13	1.95	0.49
2:A:136:PHE:HE1	2:A:180:VAL:HG11	1.78	0.49
3:C:440:LYS:HB3	3:C:443:ASP:HB2	1.95	0.49
4:K:187:THR:HG22	4:K:189:GLU:H	1.77	0.49
2:F:516:ASN:HA	2:F:584:ILE:HD11	1.95	0.49
5:E:469:ARG:HD2	5:E:532:ILE:HG13	1.95	0.49
2:F:585:HIS:HB2	2:F:620:LEU:HD21	1.95	0.49
2:A:2023:GLU:HB3	3:C:468:ARG:HH22	1.76	0.49
2:A:436:MET:HG3	2:A:472:LEU:HD21	1.94	0.48
1:I:264:TYR:HB3	1:I:276:LEU:HD11	1.95	0.48
2:A:899:PRO:HB3	2:A:2249:ARG:HD3	1.95	0.48
1:B:275:ARG:HG2	1:B:287:GLN:HG3	1.95	0.48
2:A:1951:LEU:HD11	2:A:2069:LYS:HB3	1.95	0.48
5:L:297:LEU:HD23	5:L:300:LEU:HD22	1.96	0.48
2:F:1150:LEU:HD22	2:F:1181:LEU:HB3	1.94	0.48
2:A:1150:LEU:HD22	2:A:1181:LEU:HB3	1.94	0.48
5:E:297:LEU:HD23	5:E:300:LEU:HD22	1.95	0.48
2:A:2004:THR:HG23	2:A:2068:PRO:HD3	1.96	0.48
3:J:621:ALA:HB1	3:J:1231:LEU:HD11	1.96	0.47
1:I:181:GLY:HA2	1:I:210:ILE:HG13	1.97	0.47
2:F:650:ILE:HG22	2:F:685:ALA:HB2	1.96	0.47
2:F:136:PHE:HE1	2:F:180:VAL:HG11	1.78	0.47
1:I:5:LEU:HD13	1:I:300:LEU:HD13	1.95	0.47
2:A:1051:ILE:HD11	2:A:1066:ILE:HD11	1.95	0.47
2:F:899:PRO:HB3	2:F:2249:ARG:HD3	1.97	0.47
2:F:929:ILE:HG23	2:F:935:LEU:HD13	1.96	0.47
2:F:2004:THR:HG23	2:F:2068:PRO:HD3	1.97	0.47
6:G:68:VAL:HG22	6:G:70:LYS:H	1.78	0.47
3:J:1232:PRO:HG2	3:J:1235:LEU:HD23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1707:HIS:HB3	2:F:1710:ASP:HB2	1.96	0.47
2:F:2061:LEU:HB3	2:F:2066:VAL:HG21	1.96	0.47
3:J:529:ASN:HB3	3:J:532:LYS:HB3	1.97	0.47
2:A:1707:HIS:HB3	2:A:1710:ASP:HB2	1.96	0.47
6:G:24:MET:HB3	6:G:28:ILE:HD12	1.97	0.47
3:J:1343:VAL:HG13	3:J:1363:ILE:HD11	1.97	0.46
2:A:1387:GLY:HA3	2:A:2335:GLY:HA2	1.98	0.46
2:A:1882:LEU:HD22	2:A:1897:LEU:HD11	1.96	0.46
2:A:2014:PHE:HE1	2:A:2050:LYS:HD2	1.80	0.46
2:A:292:LEU:HB3	2:A:339:LEU:HD11	1.96	0.46
1:I:89:TRP:HZ3	6:M:623:LEU:H	1.62	0.46
3:C:1232:PRO:HG2	3:C:1235:LEU:HD23	1.97	0.46
2:A:720:LEU:HD21	2:A:761:ILE:HD11	1.96	0.46
1:I:251:ARG:HB3	1:I:270:SER:HB2	1.98	0.46
2:F:1951:LEU:HD11	2:F:2069:LYS:HB3	1.98	0.46
1:I:230:THR:HG22	1:I:247:ASP:HB3	1.97	0.46
2:A:2028:TYR:HB2	2:A:2036:ASN:HB2	1.97	0.46
2:F:2014:PHE:HE1	2:F:2050:LYS:HD2	1.80	0.46
1:B:167:MET:HE2	1:B:174:LEU:HD13	1.96	0.46
2:A:241:HIS:CG	2:A:280:ILE:HG12	2.51	0.46
2:F:1526:LEU:HD21	2:F:1547:ARG:HB3	1.97	0.46
2:F:2028:TYR:HB2	2:F:2036:ASN:HB2	1.97	0.46
1:B:181:GLY:HA2	1:B:210:ILE:HG13	1.99	0.45
1:I:167:MET:HE2	1:I:174:LEU:HD13	1.98	0.45
2:A:929:ILE:HG23	2:A:935:LEU:HD13	1.97	0.45
2:A:1526:LEU:HD21	2:A:1547:ARG:HB3	1.97	0.45
2:F:1882:LEU:HD22	2:F:1897:LEU:HD11	1.98	0.45
2:F:2240:LEU:HB3	2:F:2327:ALA:HB2	1.98	0.45
2:A:1356:LYS:HD3	2:A:1356:LYS:HA	1.84	0.45
2:A:393:ILE:HG22	2:A:394:MET:HE2	1.98	0.45
3:C:621:ALA:HB1	3:C:1231:LEU:HD11	1.98	0.45
2:F:241:HIS:CG	2:F:280:ILE:HG12	2.51	0.45
6:M:24:MET:HB3	6:M:28:ILE:HD12	1.99	0.45
2:A:1819:ARG:HH21	3:J:1277:LEU:HD23	1.82	0.45
6:M:628:THR:O	6:M:629:ASP:C	2.60	0.45
3:C:455:GLU:HG2	6:G:7:LEU:HG	1.99	0.45
1:B:251:ARG:HB3	1:B:270:SER:HB2	1.99	0.45
3:C:765:LEU:HA	3:C:769:PRO:HD2	1.99	0.45
2:F:447:LEU:HG	2:F:461:LEU:HD13	1.99	0.45
1:B:138:GLY:HA2	1:B:162:LEU:HG	1.99	0.45
2:A:1319:LEU:HD23	2:A:1319:LEU:HA	1.87	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1078:GLU:HG3	2:F:1115:ASN:H	1.82	0.45
3:J:1018:GLY:HA3	3:J:1044:TYR:HE2	1.82	0.45
6:M:44:ASP:HB3	6:M:47:ILE:HG12	1.99	0.45
1:B:9:GLY:HA2	1:B:296:VAL:HG22	1.97	0.45
1:B:89:TRP:HZ3	6:G:623:LEU:H	1.62	0.45
1:I:26:ARG:HH12	1:I:60:ILE:HA	1.82	0.45
3:C:529:ASN:HB3	3:C:532:LYS:HB3	1.99	0.45
2:A:498:GLN:HE22	2:A:579:LYS:HE2	1.82	0.44
4:D:71:LYS:HG2	4:D:77:THR:HG22	1.99	0.44
6:G:44:ASP:HB3	6:G:47:ILE:HG12	1.98	0.44
2:F:1087:ILE:HD12	2:F:1087:ILE:HA	1.89	0.44
4:K:138:MET:HB3	4:K:142:GLY:HA2	1.99	0.44
2:A:1078:GLU:HG3	2:A:1115:ASN:H	1.82	0.44
3:C:431:MET:HE1	3:C:456:LEU:HD22	1.99	0.44
2:A:1252:LEU:HD12	2:A:1267:VAL:HG21	1.99	0.44
3:C:640:LEU:HD13	3:C:654:ARG:HG2	1.99	0.44
2:A:2063:LEU:HB2	2:A:2099:PRO:HA	2.00	0.44
2:F:1356:LYS:HA	2:F:1356:LYS:HD3	1.82	0.44
2:A:1406:GLU:HG3	2:A:1411:TRP:CH2	2.53	0.44
3:C:922:LEU:HD12	3:C:934:ILE:HD13	1.99	0.44
2:F:1104:ILE:HD11	2:F:1130:ILE:HD13	1.99	0.44
3:C:1343:VAL:HG13	3:C:1363:ILE:HD11	1.99	0.44
3:J:345:LEU:HD23	3:J:345:LEU:HA	1.90	0.44
2:A:2166:TYR:HE2	2:A:2178:LEU:HD22	1.82	0.44
3:C:879:GLY:HA3	3:C:921:GLU:HB3	2.00	0.44
6:G:1138:ARG:HD3	6:G:1138:ARG:HA	1.79	0.44
4:K:85:LYS:HA	4:K:85:LYS:HD3	1.84	0.44
2:A:1078:GLU:HA	2:A:1114:ILE:HG23	2.00	0.44
3:J:455:GLU:HG2	6:M:7:LEU:HG	1.99	0.44
2:A:2240:LEU:HB3	2:A:2327:ALA:HB2	1.99	0.44
4:D:187:THR:HG22	4:D:190:VAL:H	1.83	0.44
5:E:315:LEU:HD11	5:E:359:LEU:HD22	2.00	0.44
2:F:222:TRP:HE3	2:F:243:ALA:HB2	1.83	0.44
2:F:2166:TYR:HE2	2:F:2178:LEU:HD22	1.82	0.43
3:J:1023:MET:HG3	3:J:1024:PHE:CD1	2.53	0.43
2:F:779:THR:O	2:F:783:VAL:HG23	2.18	0.43
3:J:591:PRO:HB2	3:J:599:SER:HB2	1.99	0.43
3:J:765:LEU:HA	3:J:769:PRO:HD2	1.99	0.43
2:A:976:PRO:HA	2:A:977:PRO:HD3	1.91	0.43
3:J:431:MET:HE1	3:J:456:LEU:HD22	2.00	0.43
2:A:397:TYR:HB3	2:A:421:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:802:LEU:HD13	2:A:829:LEU:HD11	2.00	0.43
2:A:1104:ILE:HD11	2:A:1130:ILE:HD13	1.99	0.43
2:F:1078:GLU:HA	2:F:1114:ILE:HG23	2.00	0.43
2:F:397:TYR:HB3	2:F:421:ILE:HD11	1.99	0.43
2:F:1406:GLU:HG3	2:F:1411:TRP:CH2	2.54	0.43
3:C:413:LEU:HD21	3:C:448:MET:HB3	1.99	0.43
3:C:621:ALA:HB2	3:C:667:LEU:HB3	2.00	0.43
6:G:1096:ILE:HD12	6:G:1112:LYS:HB2	2.01	0.43
2:F:1387:GLY:HA3	2:F:2335:GLY:HA2	2.00	0.43
2:F:1879:LEU:HD11	2:F:1912:LEU:HD21	2.00	0.43
2:F:2186:THR:HG22	2:F:2286:MET:HG2	2.01	0.43
3:J:765:LEU:HG	3:J:770:LEU:HG	2.01	0.43
3:J:982:MET:HE2	3:J:982:MET:HB2	1.96	0.43
2:A:590:LEU:HB2	2:A:620:LEU:HD22	2.01	0.43
3:J:922:LEU:HD12	3:J:934:ILE:HD13	2.00	0.43
1:B:26:ARG:HH12	1:B:60:ILE:HA	1.83	0.43
1:I:232:ARG:HG2	1:I:245:THR:HG23	2.01	0.43
3:J:410:GLU:HG2	6:M:27:ILE:HD11	2.00	0.43
3:J:621:ALA:HB2	3:J:667:LEU:HB3	2.01	0.43
2:A:717:ARG:HG3	2:A:753:VAL:HG13	2.01	0.43
2:A:854:LEU:HD23	2:A:854:LEU:HA	1.91	0.43
2:A:1771:SER:O	2:A:1775:SER:HB2	2.18	0.43
3:C:977:LEU:HG	3:C:981:LYS:HD2	2.01	0.43
3:C:1018:GLY:HA3	3:C:1044:TYR:HE2	1.84	0.43
2:A:478:LYS:HD3	4:D:188:PHE:CE1	2.54	0.43
2:A:779:THR:O	2:A:783:VAL:HG23	2.19	0.43
2:A:1507:LEU:HD21	2:A:1558:ILE:HG12	2.01	0.43
3:C:772:ASN:HB3	3:C:775:GLN:HB2	2.01	0.43
3:C:982:MET:HE2	3:C:982:MET:HB2	1.96	0.43
3:J:1347:VAL:HA	3:J:1350:LEU:HD12	2.00	0.43
4:K:28:ASN:HB3	4:K:31:LEU:HD13	2.00	0.43
6:M:622:ILE:HG22	6:M:624:ILE:HG13	2.01	0.43
6:M:1096:ILE:HD12	6:M:1112:LYS:HB2	2.01	0.43
2:A:1581:LEU:HD13	2:A:1594:ILE:HG21	2.01	0.42
2:A:1732:LYS:HE2	2:A:1732:LYS:HB2	1.89	0.42
2:A:2178:LEU:HD23	2:A:2178:LEU:HA	1.86	0.42
3:C:1070:TYR:HE1	3:C:1098:PRO:HB2	1.83	0.42
2:F:336:LEU:HB3	2:F:344:LEU:HD11	2.01	0.42
2:F:2063:LEU:HB2	2:F:2099:PRO:HA	2.01	0.42
4:K:60:ILE:HG21	4:K:97:GLN:HG2	2.02	0.42
2:A:1252:LEU:HD23	2:A:1252:LEU:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1854:GLY:HA3	2:A:1893:VAL:HG22	2.00	0.42
3:J:386:LEU:HD23	3:J:389:LEU:HD12	2.01	0.42
5:L:315:LEU:HD11	5:L:359:LEU:HD22	2.00	0.42
3:C:543:THR:O	3:C:549:GLY:HA3	2.20	0.42
3:C:765:LEU:HG	3:C:770:LEU:HG	2.00	0.42
5:E:406:LEU:HB3	5:E:512:LEU:HD11	2.00	0.42
2:F:802:LEU:HD13	2:F:829:LEU:HD11	2.02	0.42
3:J:431:MET:HE3	3:J:463:MET:HB3	2.01	0.42
5:L:415:ILE:O	5:L:419:GLU:HB2	2.19	0.42
2:A:480:LEU:HA	2:A:484:LEU:HB3	2.01	0.42
2:F:1550:ILE:HG23	2:F:1597:VAL:HG21	2.01	0.42
2:F:1675:ILE:HA	2:F:1722:GLN:HE21	1.85	0.42
3:J:934:ILE:HD12	3:J:934:ILE:HA	1.91	0.42
2:A:1060:ARG:HB3	2:A:1061:ILE:H	1.60	0.42
3:C:410:GLU:HG2	6:G:27:ILE:HD11	2.01	0.42
4:D:138:MET:HB3	4:D:142:GLY:HA2	2.00	0.42
2:F:1721:LYS:HA	2:F:1721:LYS:HD3	1.84	0.42
6:M:1138:ARG:HA	6:M:1138:ARG:HD3	1.78	0.42
2:A:1064:ILE:HD12	2:A:1064:ILE:HA	1.91	0.42
2:A:1159:VAL:HG11	2:F:650:ILE:HD11	2.02	0.42
2:A:1588:ILE:HG21	2:A:1623:ARG:CZ	2.50	0.42
2:A:1772:MET:HE3	2:A:1772:MET:HB3	1.96	0.42
3:C:1025:LEU:HB3	3:C:1052:ILE:HD13	2.01	0.42
2:F:1581:LEU:HD13	2:F:1594:ILE:HG21	2.01	0.42
2:A:222:TRP:HE3	2:A:243:ALA:HB2	1.84	0.42
2:A:650:ILE:HG22	2:A:685:ALA:HB2	2.01	0.42
2:A:1087:ILE:HD12	2:A:1087:ILE:HA	1.90	0.42
6:G:622:ILE:HG22	6:G:624:ILE:HG13	2.02	0.42
2:F:393:ILE:HG22	2:F:394:MET:HE2	2.02	0.42
2:F:1772:MET:HE3	2:F:1772:MET:HB3	1.96	0.42
2:A:2186:THR:HG22	2:A:2286:MET:HG2	2.02	0.41
2:F:717:ARG:HG3	2:F:753:VAL:HG13	2.01	0.41
2:A:650:ILE:HD11	2:F:1159:VAL:HG11	2.02	0.41
2:A:721:LEU:HD23	2:A:721:LEU:HA	1.91	0.41
2:A:1675:ILE:HA	2:A:1722:GLN:HE21	1.85	0.41
2:F:1771:SER:O	2:F:1775:SER:HB2	2.20	0.41
5:L:406:LEU:HB3	5:L:512:LEU:HD11	2.01	0.41
2:A:761:ILE:HG23	2:A:765:ILE:HD12	2.01	0.41
3:C:431:MET:HE3	3:C:463:MET:HB3	2.02	0.41
3:C:1347:VAL:HA	3:C:1350:LEU:HD12	2.01	0.41
2:F:1169:LEU:HD23	2:F:1169:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:406:LEU:HD12	5:L:498:GLN:HG2	2.02	0.41
2:A:1884:SER:HB2	2:A:2134:ARG:NH2	2.36	0.41
2:A:998:ILE:HD12	2:A:998:ILE:HA	1.96	0.41
2:A:1226:LYS:HA	2:A:1229:TRP:CE2	2.55	0.41
3:C:359:LEU:HD11	3:C:1415:ILE:HD12	2.03	0.41
2:F:444:ARG:HD3	2:F:448:ARG:HH22	1.86	0.41
2:F:1421:LYS:HA	2:F:1421:LYS:HD3	1.82	0.41
2:F:1854:GLY:HA3	2:F:1893:VAL:HG22	2.02	0.41
3:J:413:LEU:HD21	3:J:448:MET:HB3	2.02	0.41
3:J:640:LEU:HD13	3:J:654:ARG:HG2	2.02	0.41
2:A:336:LEU:HA	2:A:339:LEU:HD12	2.01	0.41
3:C:1004:LEU:HD23	3:C:1004:LEU:HA	1.94	0.41
2:F:590:LEU:HB2	2:F:620:LEU:HD22	2.03	0.41
3:J:1070:TYR:HE1	3:J:1098:PRO:HB2	1.85	0.41
2:A:1550:ILE:HG23	2:A:1597:VAL:HG21	2.02	0.41
2:A:1959:MET:HG2	2:A:2066:VAL:HG12	2.01	0.41
2:A:1962:LEU:HD23	2:A:1962:LEU:HA	1.91	0.41
2:F:1252:LEU:HD12	2:F:1267:VAL:HG21	2.02	0.41
2:F:1841:GLN:O	2:F:1845:ARG:HG2	2.21	0.41
2:F:1959:MET:HG2	2:F:2066:VAL:HG12	2.01	0.41
3:J:359:LEU:HD11	3:J:1415:ILE:HD12	2.03	0.41
3:J:938:LEU:HD11	3:J:953:ILE:HD13	2.03	0.41
2:A:364:ASP:HA	2:A:367:ARG:HG3	2.03	0.41
2:A:602:ILE:HD13	2:A:602:ILE:HA	1.91	0.41
2:A:2134:ARG:HB3	2:A:2368:ILE:HD11	2.02	0.41
5:E:406:LEU:HD12	5:E:498:GLN:HG2	2.03	0.41
5:E:460:ILE:HD13	5:E:460:ILE:HA	1.93	0.41
2:F:318:LEU:HD23	2:F:318:LEU:HA	1.94	0.41
2:F:1060:ARG:HB3	2:F:1061:ILE:H	1.59	0.41
2:F:1226:LYS:HA	2:F:1229:TRP:CE2	2.56	0.41
3:J:432:GLN:HB3	3:J:1392:ARG:HG3	2.02	0.41
3:J:879:GLY:HA3	3:J:921:GLU:HB3	2.03	0.41
3:J:1056:LYS:HB2	3:J:1056:LYS:HE2	1.85	0.41
6:M:52:MET:HE2	6:M:52:MET:HB3	1.89	0.41
1:I:258:PHE:HE1	1:I:279:LEU:HD11	1.87	0.41
2:A:691:PHE:HZ	2:A:741:THR:HB	1.86	0.41
3:J:956:LYS:HD3	3:J:956:LYS:HA	1.96	0.41
2:A:1169:LEU:HD23	2:A:1169:LEU:HA	1.92	0.40
2:A:1373:ILE:HG12	2:A:1388:ILE:HG23	2.02	0.40
2:F:1588:ILE:HG21	2:F:1623:ARG:CZ	2.50	0.40
2:F:1732:LYS:HE2	2:F:1732:LYS:HB2	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:930:LEU:HD22	2:A:971:VAL:HG21	2.03	0.40
3:C:386:LEU:HD23	3:C:389:LEU:HD12	2.04	0.40
4:D:110:ARG:NE	4:D:118:MET:HE1	2.36	0.40
2:F:358:TYR:HB3	2:F:361:TYR:HD2	1.85	0.40
2:F:761:ILE:HG23	2:F:765:ILE:HD12	2.03	0.40
2:F:1507:LEU:HD21	2:F:1558:ILE:HG12	2.03	0.40
2:A:1442:LEU:HD23	2:A:1442:LEU:HA	1.95	0.40
2:F:930:LEU:HD22	2:F:971:VAL:HG21	2.04	0.40
2:F:1153:LEU:HB3	2:F:1156:ASP:HB2	2.04	0.40
2:F:2055:LEU:HD23	2:F:2055:LEU:HA	1.90	0.40
2:F:1729:LEU:HD23	2:F:1729:LEU:HA	1.90	0.40
1:B:258:PHE:HE1	1:B:279:LEU:HD11	1.85	0.40
1:I:90:MET:HE2	1:I:90:MET:HB3	1.98	0.40
2:A:1082:HIS:CE1	2:F:722:GLU:HG2	2.56	0.40
2:A:2424:LEU:HD23	2:A:2424:LEU:HA	1.92	0.40
3:C:319:VAL:HG23	3:C:324:ILE:HD11	2.04	0.40
3:C:1339:ILE:HD12	3:C:1342:LYS:HB2	2.04	0.40
4:D:60:ILE:HG21	4:D:97:GLN:HG2	2.03	0.40
2:F:292:LEU:HD22	2:F:307:PHE:HE1	1.85	0.40
2:F:478:LYS:HD3	4:K:188:PHE:CE1	2.56	0.40
2:F:991:ILE:HG12	2:F:998:ILE:HG12	2.03	0.40
2:F:1244:ILE:HD12	2:F:1244:ILE:HA	1.92	0.40
2:F:2146:VAL:HG13	2:F:2348:LEU:HD21	2.03	0.40
3:J:543:THR:O	3:J:549:GLY:HA3	2.20	0.40
3:J:977:LEU:HG	3:J:981:LYS:HD2	2.02	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	B	300/303 (99%)	281 (94%)	19 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	300/303 (99%)	284 (95%)	16 (5%)	0	100	100
2	A	2242/2474 (91%)	2199 (98%)	43 (2%)	0	100	100
2	F	2242/2474 (91%)	2194 (98%)	48 (2%)	0	100	100
3	C	1049/1430 (73%)	1030 (98%)	19 (2%)	0	100	100
3	J	1049/1430 (73%)	1030 (98%)	19 (2%)	0	100	100
4	D	185/426 (43%)	178 (96%)	7 (4%)	0	100	100
4	K	185/426 (43%)	179 (97%)	6 (3%)	0	100	100
5	E	205/543 (38%)	200 (98%)	4 (2%)	1 (0%)	24	59
5	L	205/543 (38%)	201 (98%)	3 (2%)	1 (0%)	24	59
6	G	186/1176 (16%)	179 (96%)	7 (4%)	0	100	100
6	M	186/1176 (16%)	178 (96%)	8 (4%)	0	100	100
All	All	8334/12704 (66%)	8133 (98%)	199 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	504	VAL
5	L	504	VAL

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	B	266/267 (100%)	266 (100%)	0	100	100
1	I	266/267 (100%)	266 (100%)	0	100	100
2	A	2031/2219 (92%)	2030 (100%)	1 (0%)	100	100
2	F	2031/2219 (92%)	2030 (100%)	1 (0%)	100	100
3	C	970/1320 (74%)	970 (100%)	0	100	100
3	J	970/1320 (74%)	970 (100%)	0	100	100
4	D	168/378 (44%)	168 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	K	168/378 (44%)	168 (100%)	0	100	100
5	E	203/499 (41%)	203 (100%)	0	100	100
5	L	203/499 (41%)	203 (100%)	0	100	100
6	G	185/1066 (17%)	185 (100%)	0	100	100
6	M	185/1066 (17%)	185 (100%)	0	100	100
All	All	7646/11498 (66%)	7644 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	143	THR
2	F	143	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	148	ASN
1	B	221	HIS
1	I	66	ASN
1	I	148	ASN
1	I	163	GLN
1	I	221	HIS
2	A	305	GLN
2	A	407	ASN
2	A	486	ASN
2	A	498	GLN
2	A	565	ASN
2	A	668	ASN
2	A	815	ASN
2	A	828	GLN
2	A	1082	HIS
2	A	1152	GLN
2	A	1250	GLN
2	A	1667	GLN
2	A	1673	GLN
2	A	1861	GLN
2	A	2036	ASN
2	A	2065	HIS
2	A	2206	HIS

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Mol	Chain	Res	Type
2	A	2296	HIS
3	C	356	ASN
3	C	569	GLN
3	C	608	GLN
3	C	758	ASN
3	C	775	GLN
3	C	895	ASN
3	C	905	GLN
3	C	1002	GLN
3	C	1184	ASN
3	C	1217	ASN
3	C	1223	GLN
3	C	1233	ASN
4	D	17	ASN
5	E	320	ASN
5	E	498	GLN
5	E	529	GLN
6	G	1067	HIS
6	G	1075	GLN
6	G	1081	ASN
6	G	1115	HIS
2	F	305	GLN
2	F	486	ASN
2	F	565	ASN
2	F	726	GLN
2	F	828	GLN
2	F	924	HIS
2	F	1082	HIS
2	F	1152	GLN
2	F	1188	ASN
2	F	1250	GLN
2	F	1667	GLN
2	F	1673	GLN
2	F	1861	GLN
2	F	2036	ASN
2	F	2065	HIS
2	F	2206	HIS
2	F	2296	HIS
2	F	2351	ASN
3	J	356	ASN
3	J	548	ASN
3	J	569	GLN

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Mol	Chain	Res	Type
3	J	666	ASN
3	J	758	ASN
3	J	905	GLN
3	J	1002	GLN
3	J	1184	ASN
3	J	1217	ASN
3	J	1223	GLN
3	J	1233	ASN
4	K	17	ASN
5	L	320	ASN
5	L	498	GLN
5	L	529	GLN
6	M	1067	HIS
6	M	1075	GLN
6	M	1081	ASN
6	M	1115	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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
7	IHP	F	2501	-	36,36,36	1.89	6 (16%)	54,60,60	0.98	2 (3%)
7	IHP	A	2501	-	36,36,36	1.89	6 (16%)	54,60,60	0.98	2 (3%)

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
7	IHP	F	2501	-	-	5/30/54/54	0/1/1/1
7	IHP	A	2501	-	-	5/30/54/54	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2501	IHP	P2-O12	4.54	1.67	1.59
7	F	2501	IHP	P5-O15	4.53	1.67	1.59
7	F	2501	IHP	P2-O12	4.52	1.67	1.59
7	A	2501	IHP	P5-O15	4.52	1.67	1.59
7	A	2501	IHP	P6-O16	4.27	1.67	1.59
7	F	2501	IHP	P6-O16	4.22	1.67	1.59
7	F	2501	IHP	P4-O14	4.11	1.67	1.59
7	A	2501	IHP	P1-O11	4.06	1.67	1.59
7	A	2501	IHP	P4-O14	4.05	1.67	1.59
7	F	2501	IHP	P1-O11	4.03	1.66	1.59
7	A	2501	IHP	P3-O13	4.03	1.66	1.59
7	F	2501	IHP	P3-O13	3.99	1.66	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	2501	IHP	C5-C6-C1	-2.35	105.27	110.41
7	A	2501	IHP	C5-C6-C1	-2.35	105.27	110.41
7	F	2501	IHP	O11-C1-C2	2.23	113.94	108.69
7	A	2501	IHP	O11-C1-C2	2.22	113.93	108.69

There are no chirality outliers.

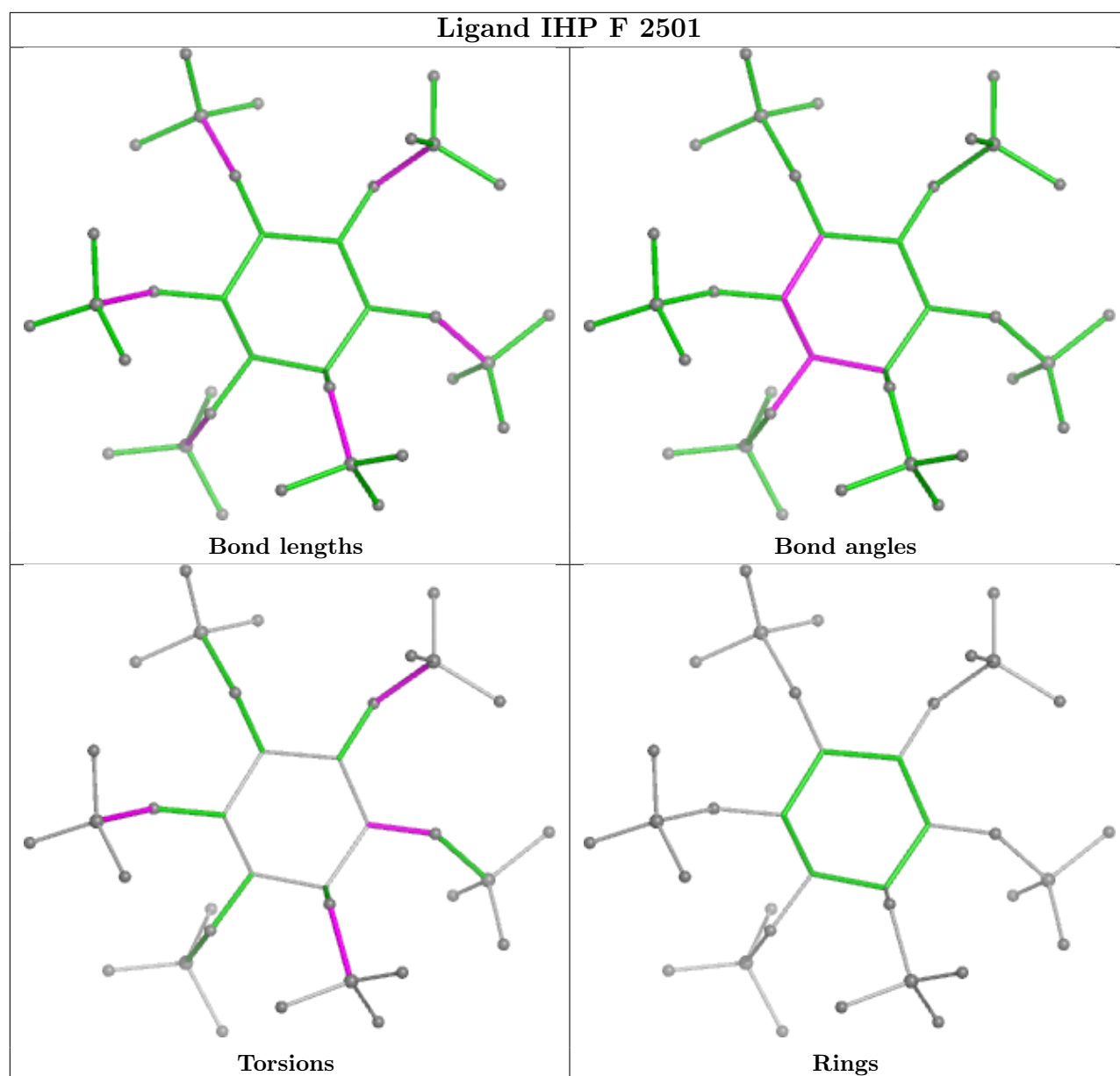
All (10) torsion outliers are listed below:

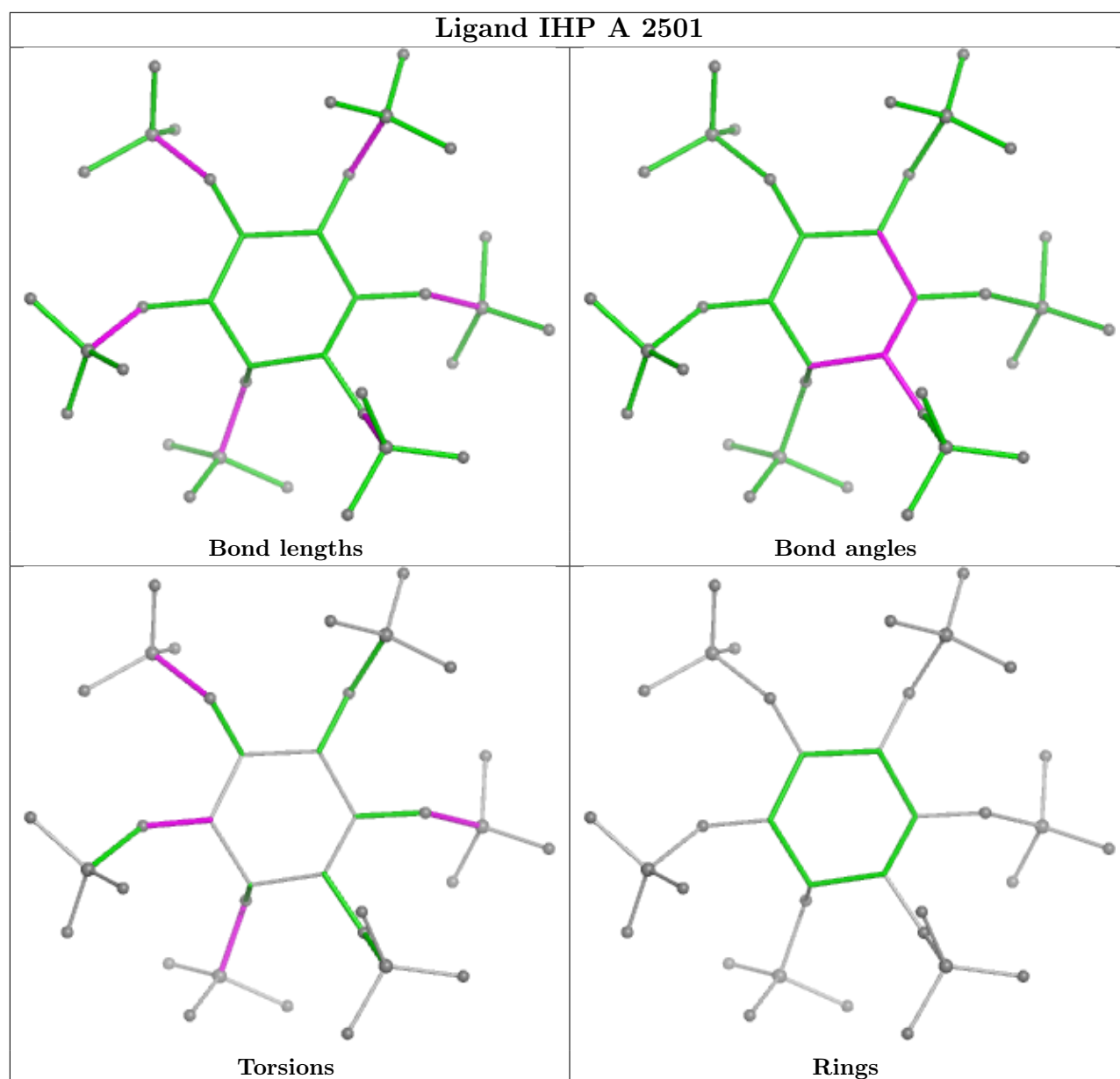
Mol	Chain	Res	Type	Atoms
7	A	2501	IHP	C2-O12-P2-O22
7	A	2501	IHP	C6-O16-P6-O26
7	F	2501	IHP	C2-O12-P2-O22
7	F	2501	IHP	C6-O16-P6-O26
7	A	2501	IHP	C6-O16-P6-O36
7	A	2501	IHP	C2-C3-O13-P3
7	F	2501	IHP	C2-C3-O13-P3
7	A	2501	IHP	C4-O14-P4-O34
7	F	2501	IHP	C4-O14-P4-O34
7	F	2501	IHP	C6-O16-P6-O36

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

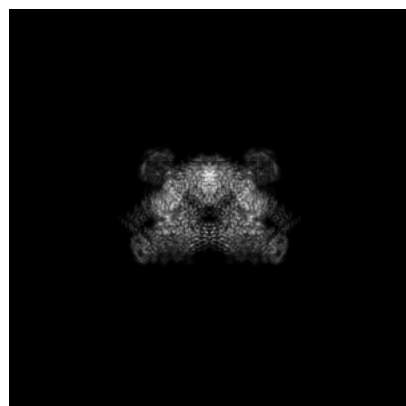
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54223. These allow visual inspection of the internal detail of the map and identification of artifacts.

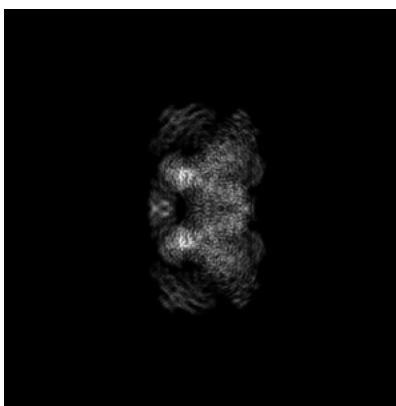
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

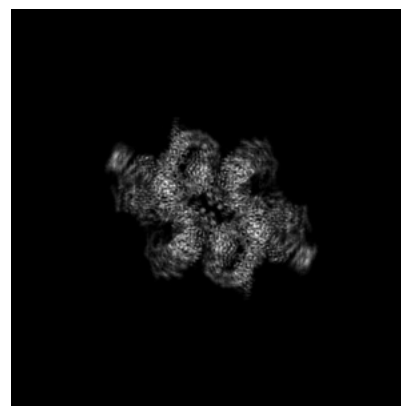
6.1.1 Primary map



X

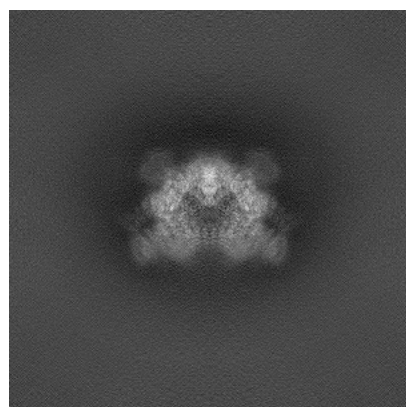


Y

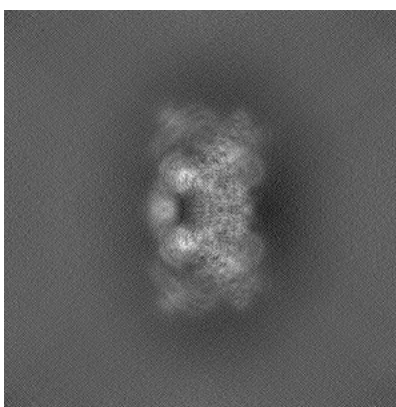


Z

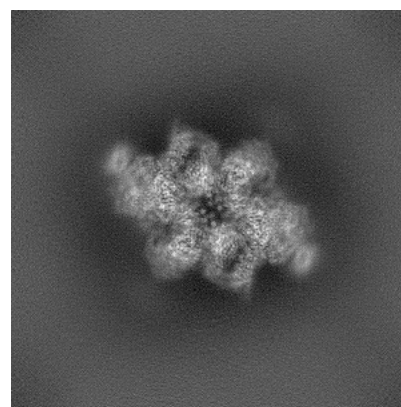
6.1.2 Raw map



X



Y

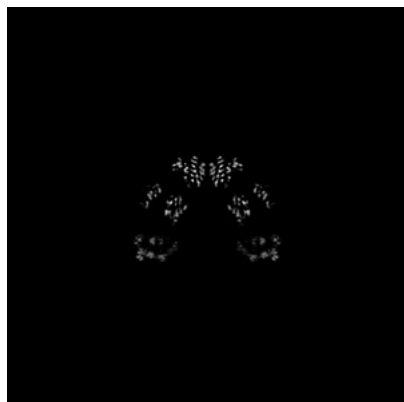


Z

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

6.2 Central slices [i](#)

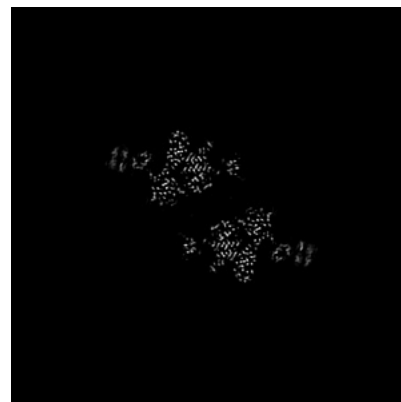
6.2.1 Primary map



X Index: 256

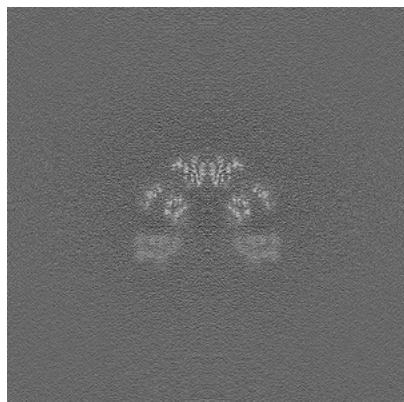


Y Index: 256

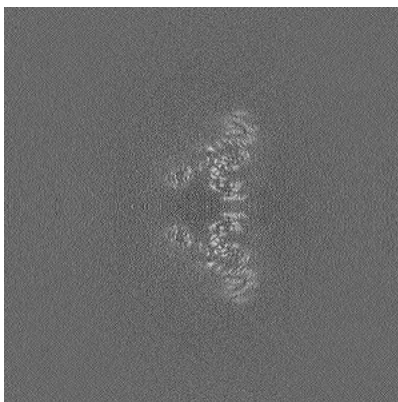


Z Index: 256

6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

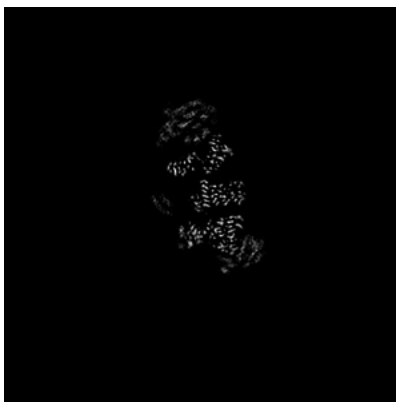
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

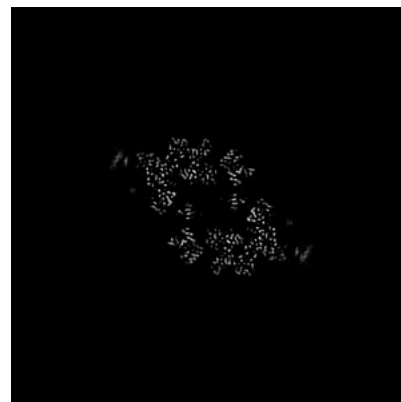
6.3.1 Primary map



X Index: 209

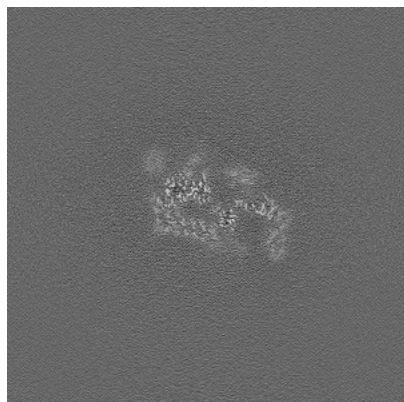


Y Index: 206

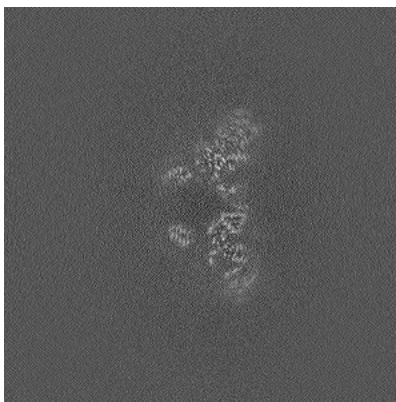


Z Index: 263

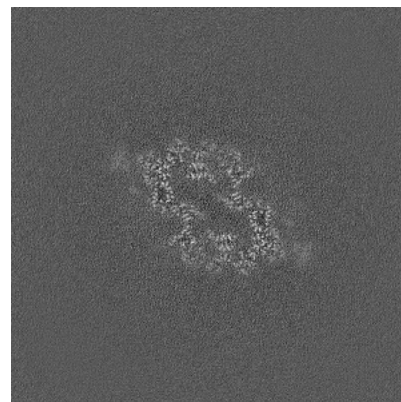
6.3.2 Raw map



X Index: 224



Y Index: 252

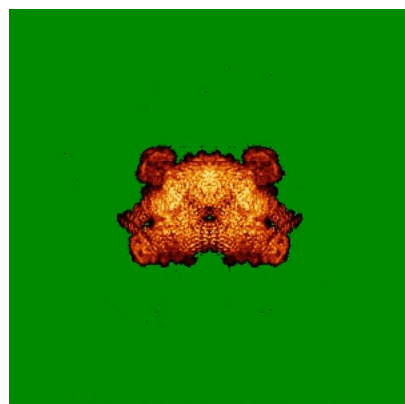


Z Index: 267

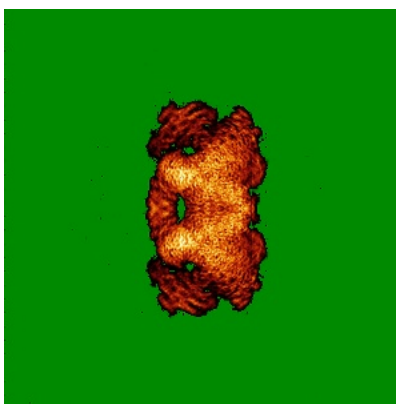
The images above show the largest variance slices of the map in three orthogonal directions.

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

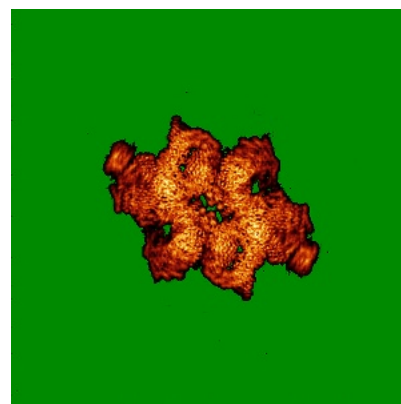
6.4.1 Primary map



X

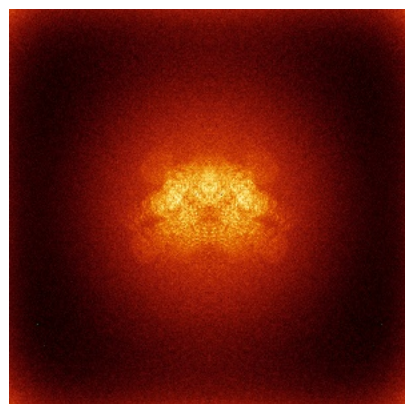


Y

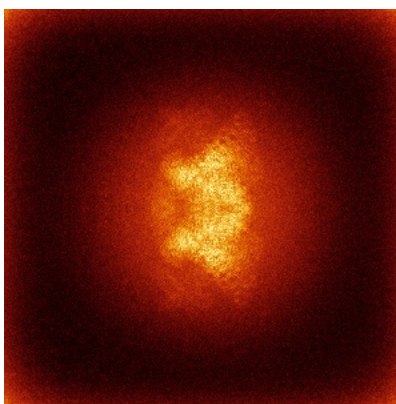


Z

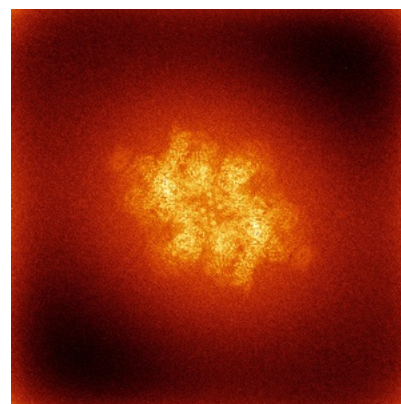
6.4.2 Raw map



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.

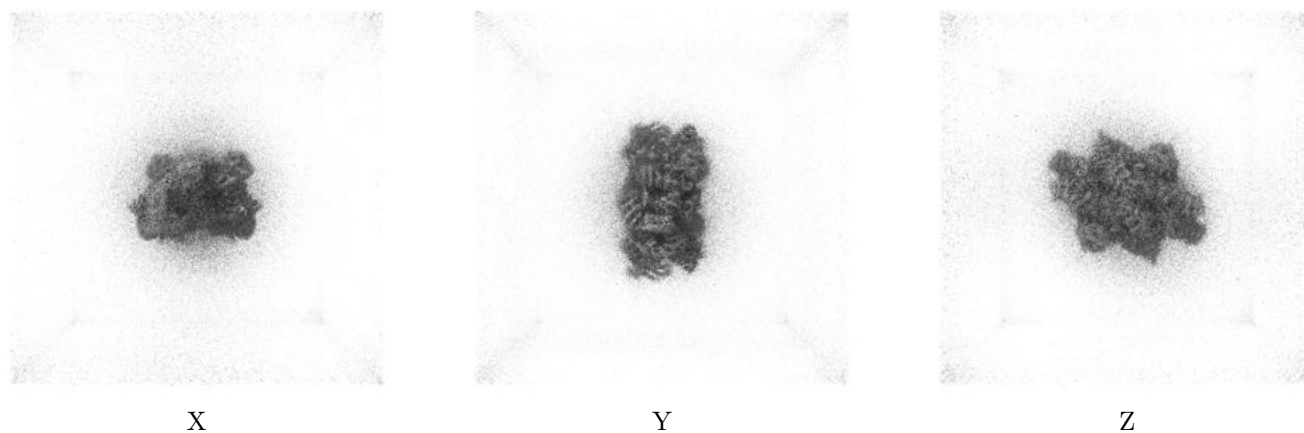
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.061. 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.

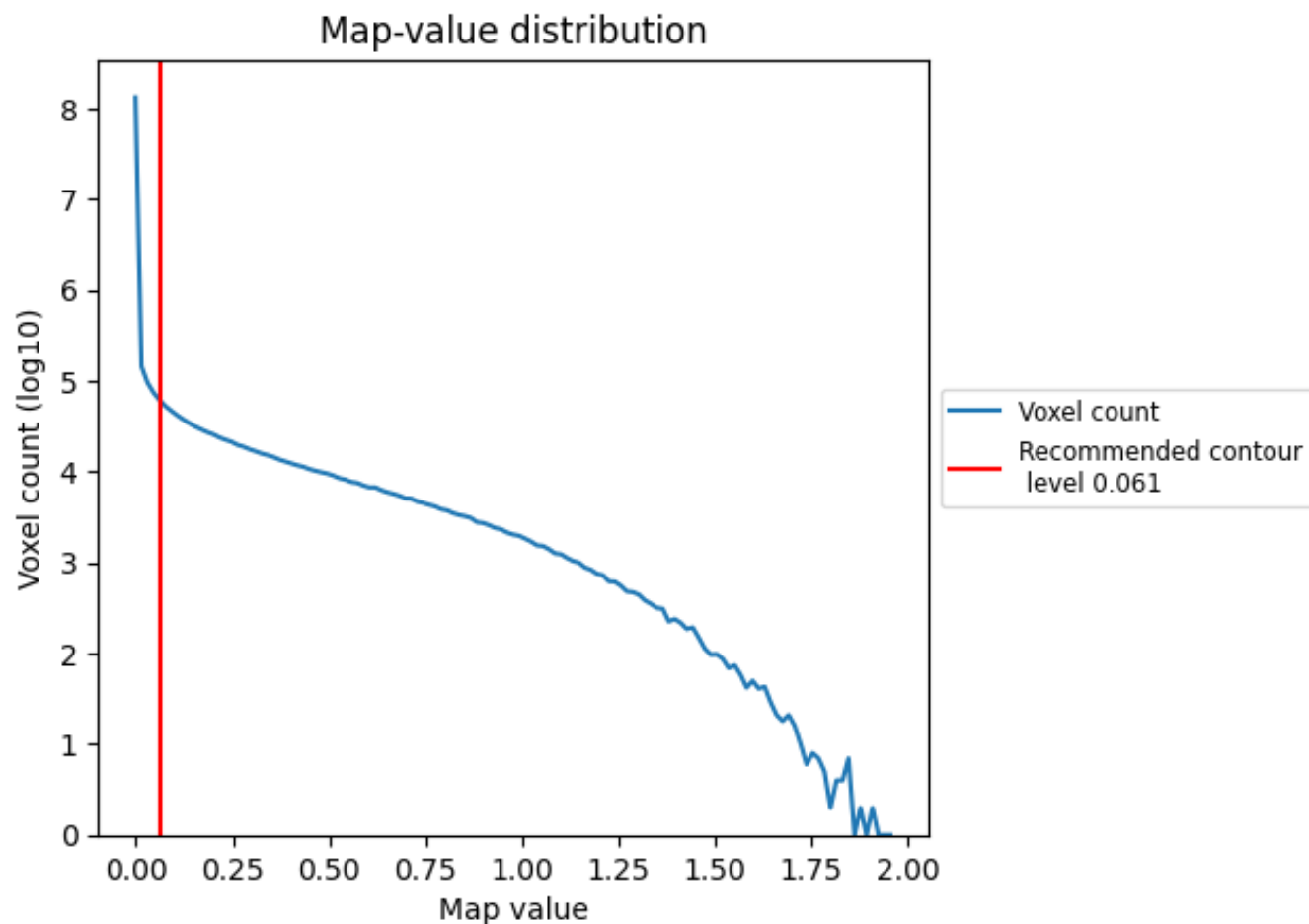
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

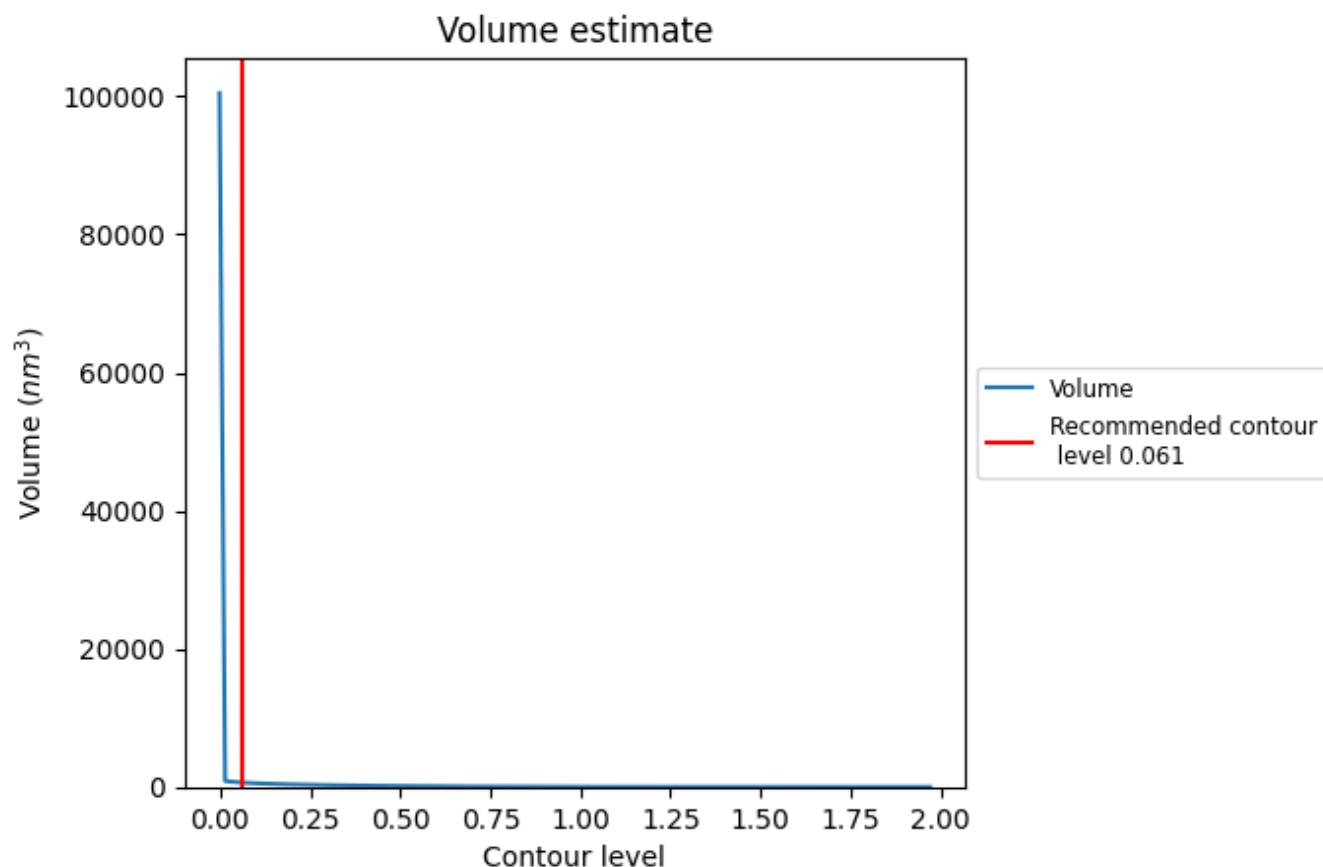
This section contains the results of statistical analysis of the map.

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.

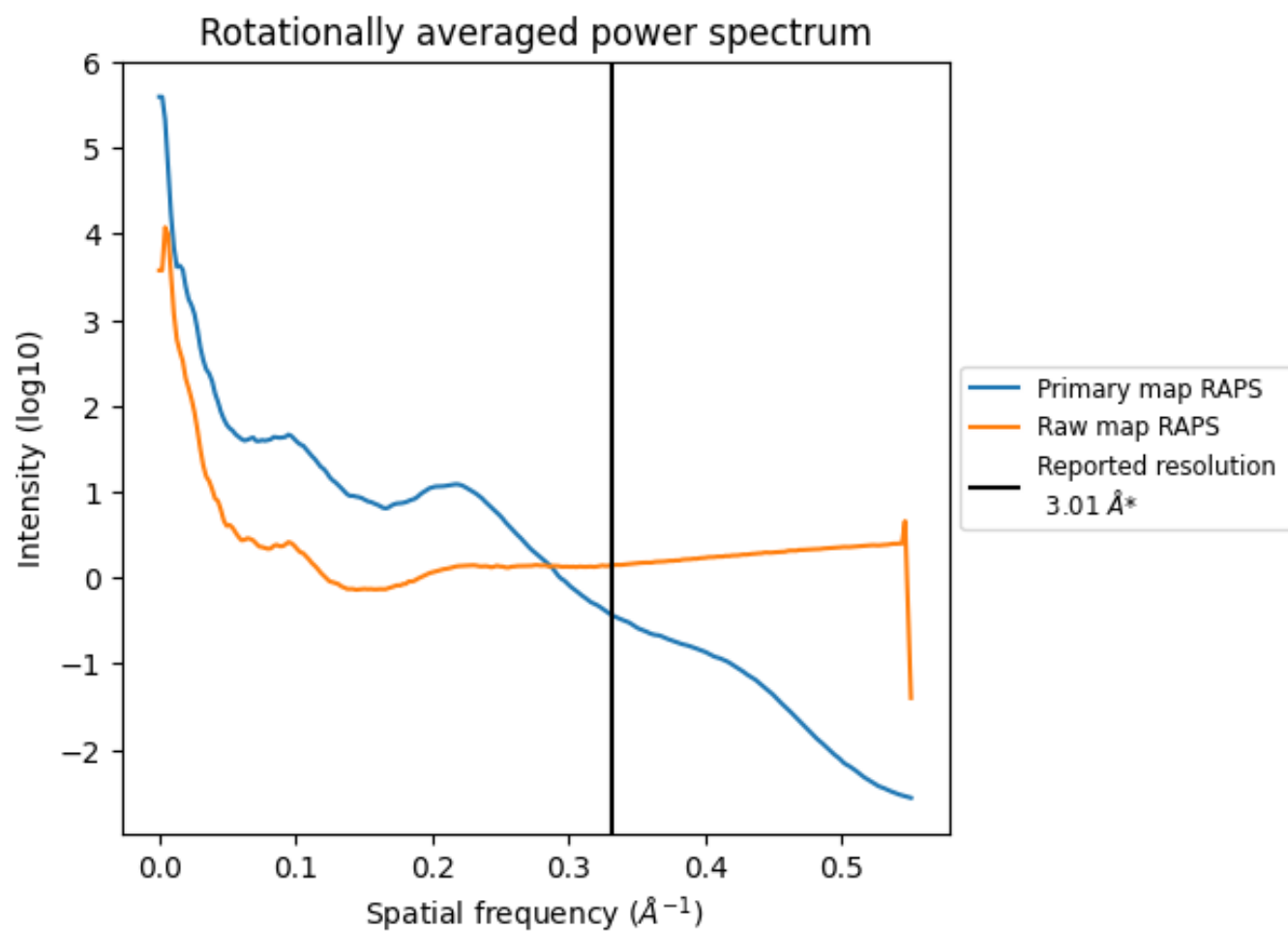
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 638 nm^3 ; this corresponds to an approximate mass of 576 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 ⓘ

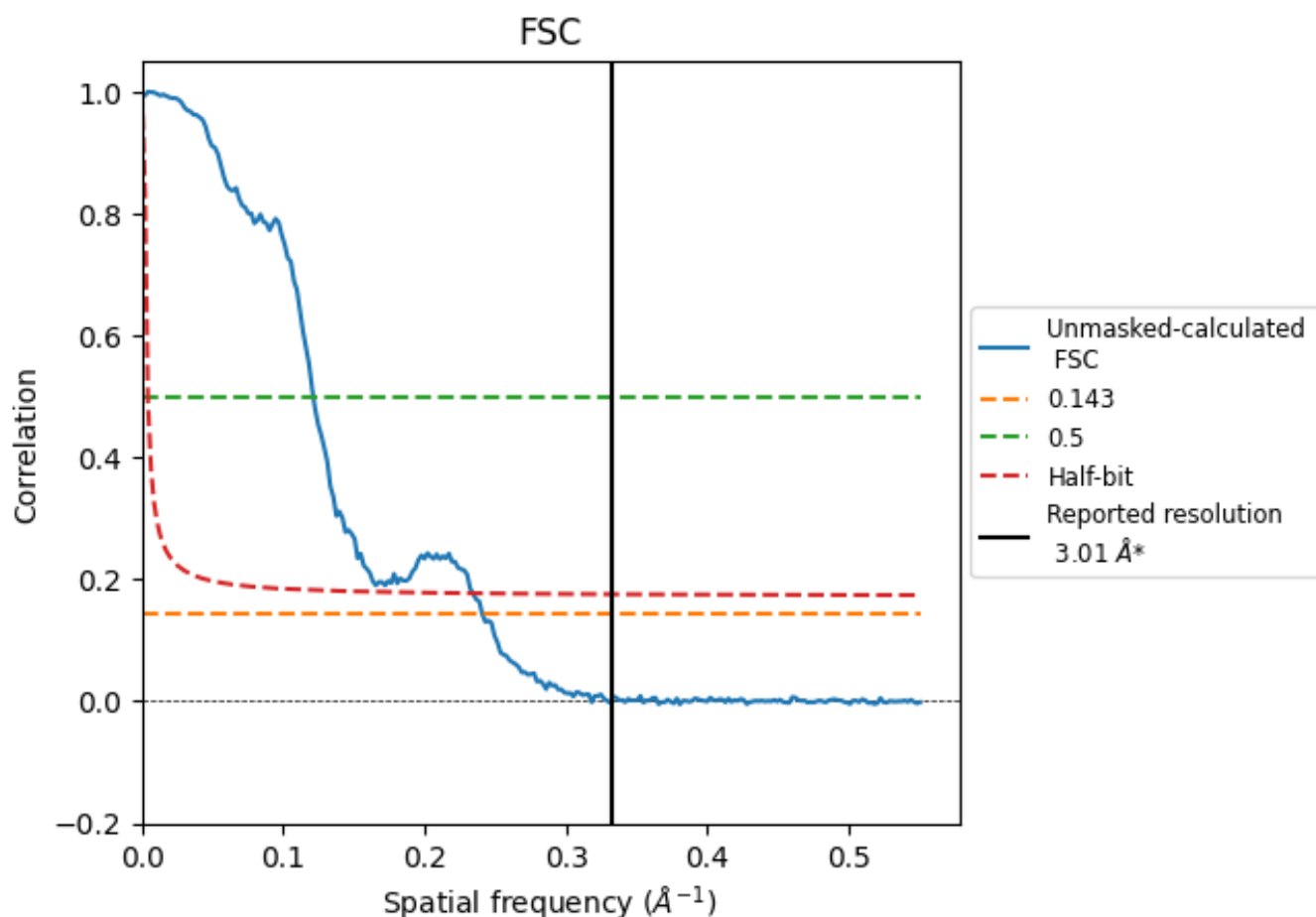


*Reported resolution corresponds to spatial frequency of 0.332 \AA^{-1}

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 0.332 Å⁻¹

8.2 Resolution estimates [i](#)

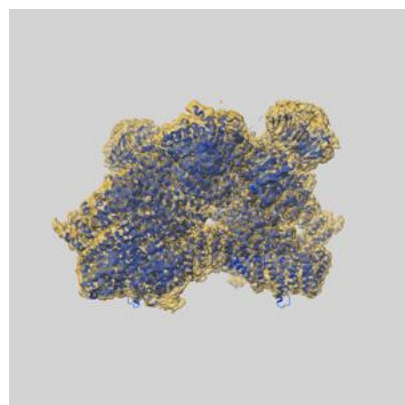
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.01	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.15	8.25	4.27

*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 4.15 differs from the reported value 3.01 by more than 10 %

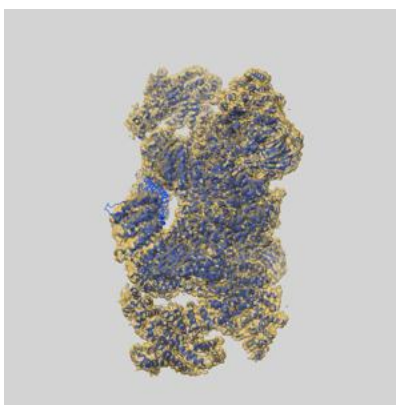
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54223 and PDB model 9RSS. Per-residue inclusion information can be found in section [3](#) on page [6](#).

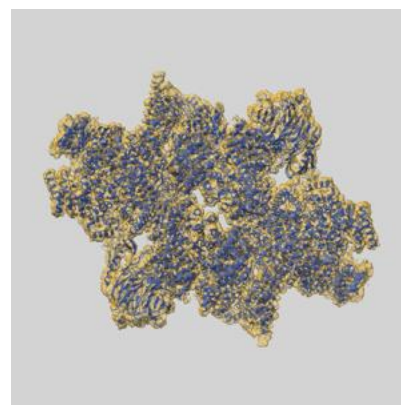
9.1 Map-model overlay [i](#)



X



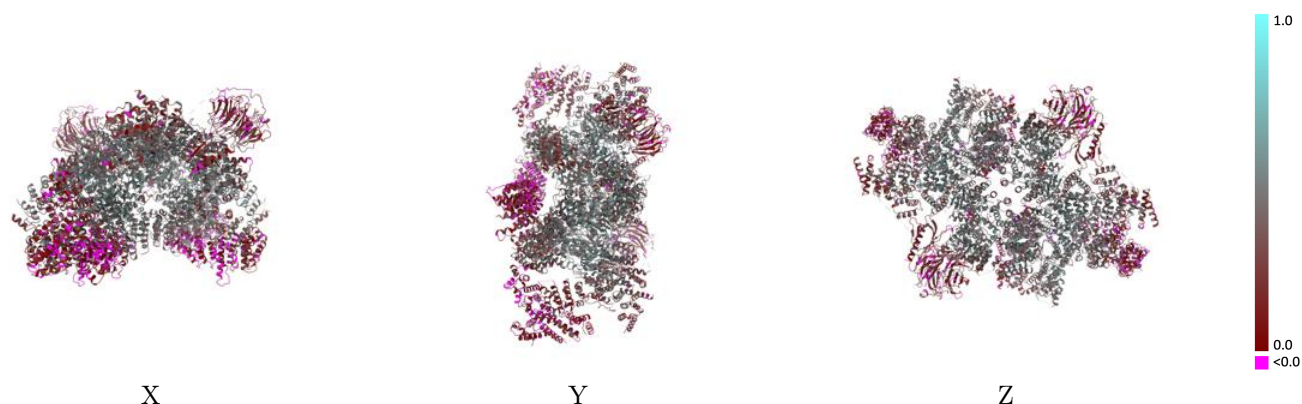
Y



Z

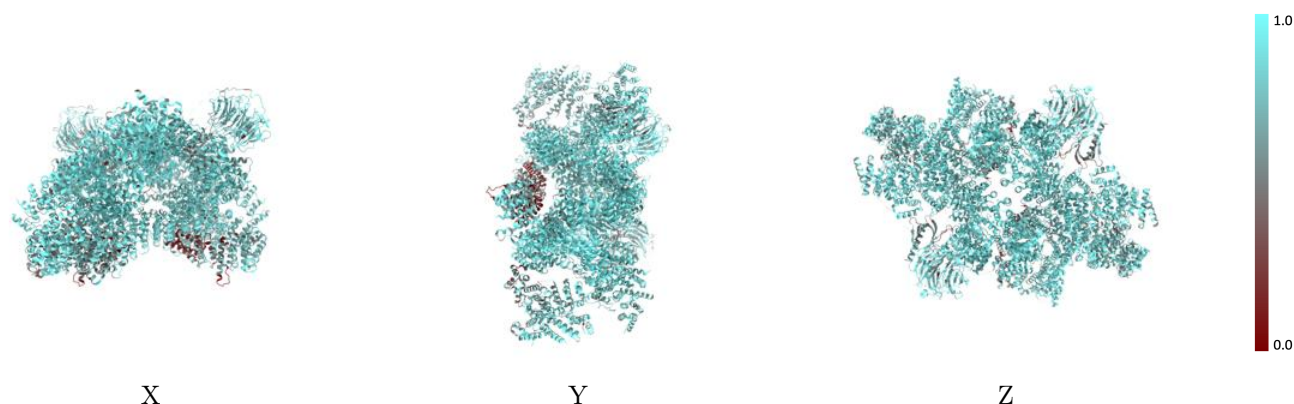
The images above show the 3D surface view of the map at the recommended contour level 0.061 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



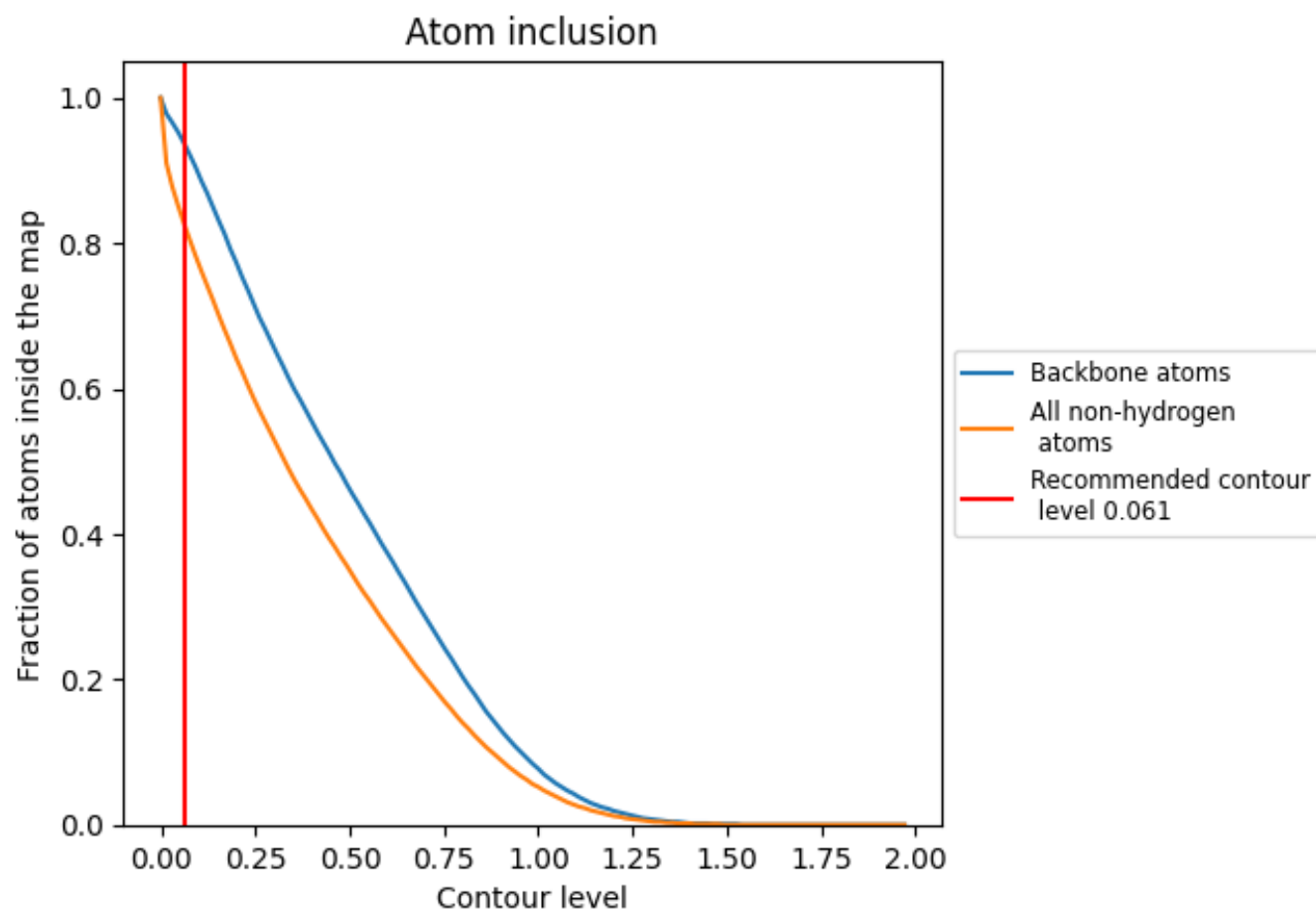
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.061).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.061) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8260</div>	<div><div></div>0.3380</div>
A	<div><div></div>0.8440</div>	<div><div></div>0.3810</div>
B	<div><div></div>0.8040</div>	<div><div></div>0.2070</div>
C	<div><div></div>0.8190</div>	<div><div></div>0.3270</div>
D	<div><div></div>0.9190</div>	<div><div></div>0.4620</div>
E	<div><div></div>0.7720</div>	<div><div></div>0.1250</div>
F	<div><div></div>0.8440</div>	<div><div></div>0.3820</div>
G	<div><div></div>0.6670</div>	<div><div></div>0.2200</div>
I	<div><div></div>0.8020</div>	<div><div></div>0.2130</div>
J	<div><div></div>0.8190</div>	<div><div></div>0.3250</div>
K	<div><div></div>0.9200</div>	<div><div></div>0.4630</div>
L	<div><div></div>0.7750</div>	<div><div></div>0.1210</div>
M	<div><div></div>0.6630</div>	<div><div></div>0.2250</div>

1.0

0.0

<0.0