Full wwPDB EM Validation Report

Sep 22, 2025 – 01:38 pm BST

PDB ID	:	9Q9H / pdb_00009q9h
EMDB ID	:	EMD-52959
Title	:	Cryo-EM structure of human Mre11-Rad50 complex bound to DNA
Authors	:	Cui, H.J.; Lammens, K.; Hopfner, K.P.; Fan, Y.L.; Kuybu, F.
Deposited on	:	2025-02-26
Resolution	:	3.11 Å(reported)
Based on initial model	:	.

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:

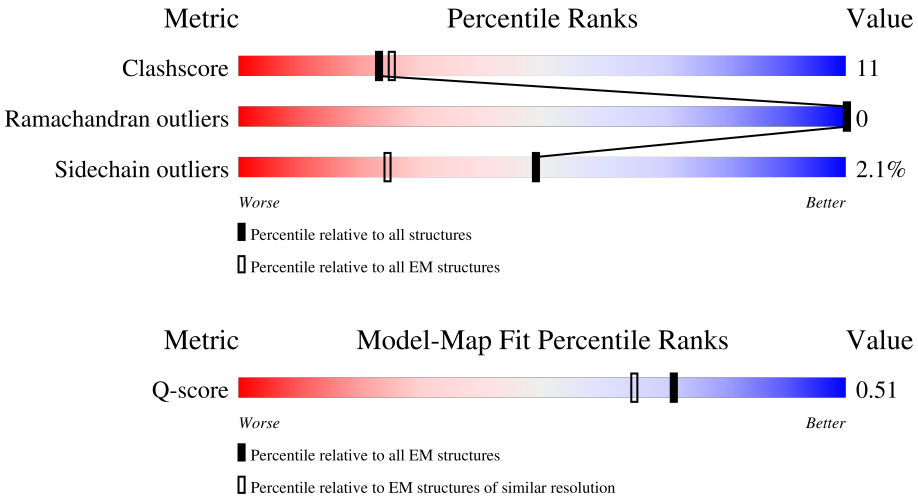
EMDB validation analysis	:	0.0.1.dev129
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up 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)	:	2.46

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 3.11 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14465 (2.61 - 3.61)

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 <=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	1312	27% 10% 63%
1	B	1312	26% 10% 63%
2	D	738	51% 13% 35%
2	E	738	50% 15% 35%

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Mol	Chain	Length	Quality of chain
3	P	50	32% 18% 50%
4	T	50	24% 24% 50%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	BEF	B	1403	-	-	X	-
7	BEF	B	1404	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 16786 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 DNA repair protein RAD50.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	487	Total	C	N	O	S	0	0
			3936	2469	695	748	24		
1	B	487	Total	C	N	O	S	0	0
			3938	2473	691	750	24		

- Molecule 2 is a protein called Double-strand break repair protein MRE11.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	479	Total	C	N	O	S	0	0
			3908	2483	683	726	16		
2	E	479	Total	C	N	O	S	0	0
			3906	2483	681	726	16		

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	709	SER	-	expression tag	UNP P49959
D	710	GLY	-	expression tag	UNP P49959
D	711	GLY	-	expression tag	UNP P49959
D	712	SER	-	expression tag	UNP P49959
D	713	LEU	-	expression tag	UNP P49959
D	714	GLU	-	expression tag	UNP P49959
D	715	VAL	-	expression tag	UNP P49959
D	716	LEU	-	expression tag	UNP P49959
D	717	PHE	-	expression tag	UNP P49959
D	718	GLN	-	expression tag	UNP P49959
D	719	GLY	-	expression tag	UNP P49959
D	720	PRO	-	expression tag	UNP P49959
D	721	ASP	-	expression tag	UNP P49959
D	722	TYR	-	expression tag	UNP P49959
D	723	LYS	-	expression tag	UNP P49959
D	724	ASP	-	expression tag	UNP P49959
D	725	ASP	-	expression tag	UNP P49959

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Chain	Residue	Modelled	Actual	Comment	Reference
D	726	ASP	-	expression tag	UNP P49959
D	727	ASP	-	expression tag	UNP P49959
D	728	LYS	-	expression tag	UNP P49959
D	729	GLY	-	expression tag	UNP P49959
D	730	THR	-	expression tag	UNP P49959
D	731	ASP	-	expression tag	UNP P49959
D	732	TYR	-	expression tag	UNP P49959
D	733	LYS	-	expression tag	UNP P49959
D	734	ASP	-	expression tag	UNP P49959
D	735	ASP	-	expression tag	UNP P49959
D	736	ASP	-	expression tag	UNP P49959
D	737	ASP	-	expression tag	UNP P49959
D	738	LYS	-	expression tag	UNP P49959
E	709	SER	-	expression tag	UNP P49959
E	710	GLY	-	expression tag	UNP P49959
E	711	GLY	-	expression tag	UNP P49959
E	712	SER	-	expression tag	UNP P49959
E	713	LEU	-	expression tag	UNP P49959
E	714	GLU	-	expression tag	UNP P49959
E	715	VAL	-	expression tag	UNP P49959
E	716	LEU	-	expression tag	UNP P49959
E	717	PHE	-	expression tag	UNP P49959
E	718	GLN	-	expression tag	UNP P49959
E	719	GLY	-	expression tag	UNP P49959
E	720	PRO	-	expression tag	UNP P49959
E	721	ASP	-	expression tag	UNP P49959
E	722	TYR	-	expression tag	UNP P49959
E	723	LYS	-	expression tag	UNP P49959
E	724	ASP	-	expression tag	UNP P49959
E	725	ASP	-	expression tag	UNP P49959
E	726	ASP	-	expression tag	UNP P49959
E	727	ASP	-	expression tag	UNP P49959
E	728	LYS	-	expression tag	UNP P49959
E	729	GLY	-	expression tag	UNP P49959
E	730	THR	-	expression tag	UNP P49959
E	731	ASP	-	expression tag	UNP P49959
E	732	TYR	-	expression tag	UNP P49959
E	733	LYS	-	expression tag	UNP P49959
E	734	ASP	-	expression tag	UNP P49959
E	735	ASP	-	expression tag	UNP P49959
E	736	ASP	-	expression tag	UNP P49959
E	737	ASP	-	expression tag	UNP P49959

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Chain	Residue	Modelled	Actual	Comment	Reference
E	738	LYS	-	expression tag	UNP P49959

- Molecule 3 is a DNA chain called DNA (50-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	P	25	500	250	50	175	25	0	0

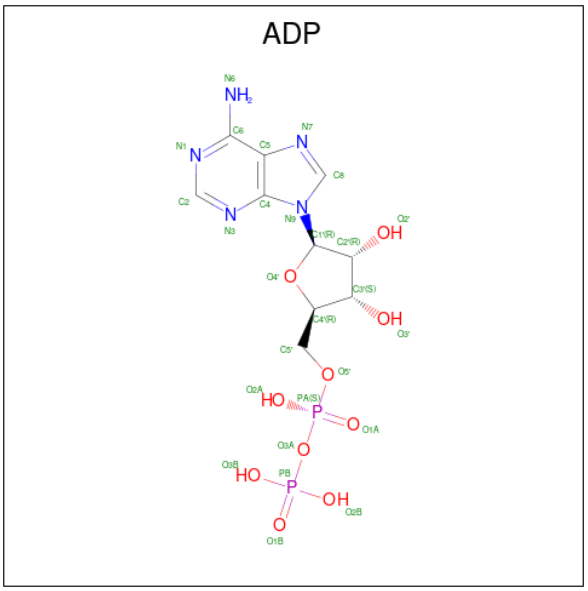
- Molecule 4 is a DNA chain called DNA (50-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	T	25	525	250	125	125	25	0	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

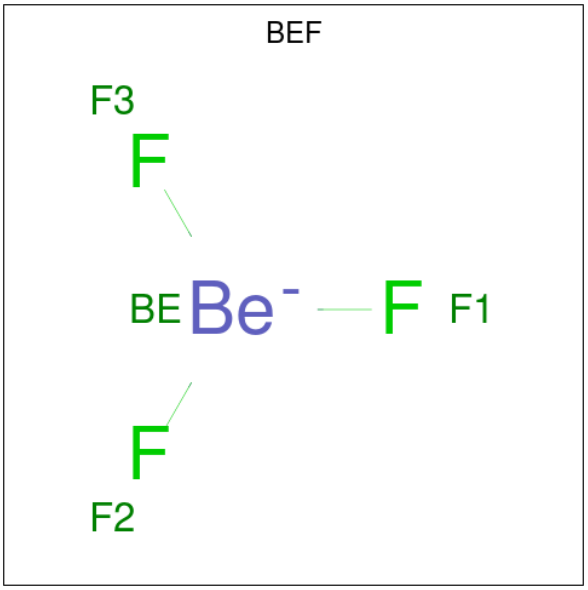
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
5	A	1	1	1	0
5	B	1	1	1	0

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
6	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 7 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
7	B	1	Total	Be	F		0
			4	1	3		
7	B	1	Total	Be	F		0
			4	1	3		

- Molecule 8 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
8	D	2	Total	Mn	0
			2	2	
8	E	2	Total	Mn	0
			2	2	

- Molecule 9 is water.

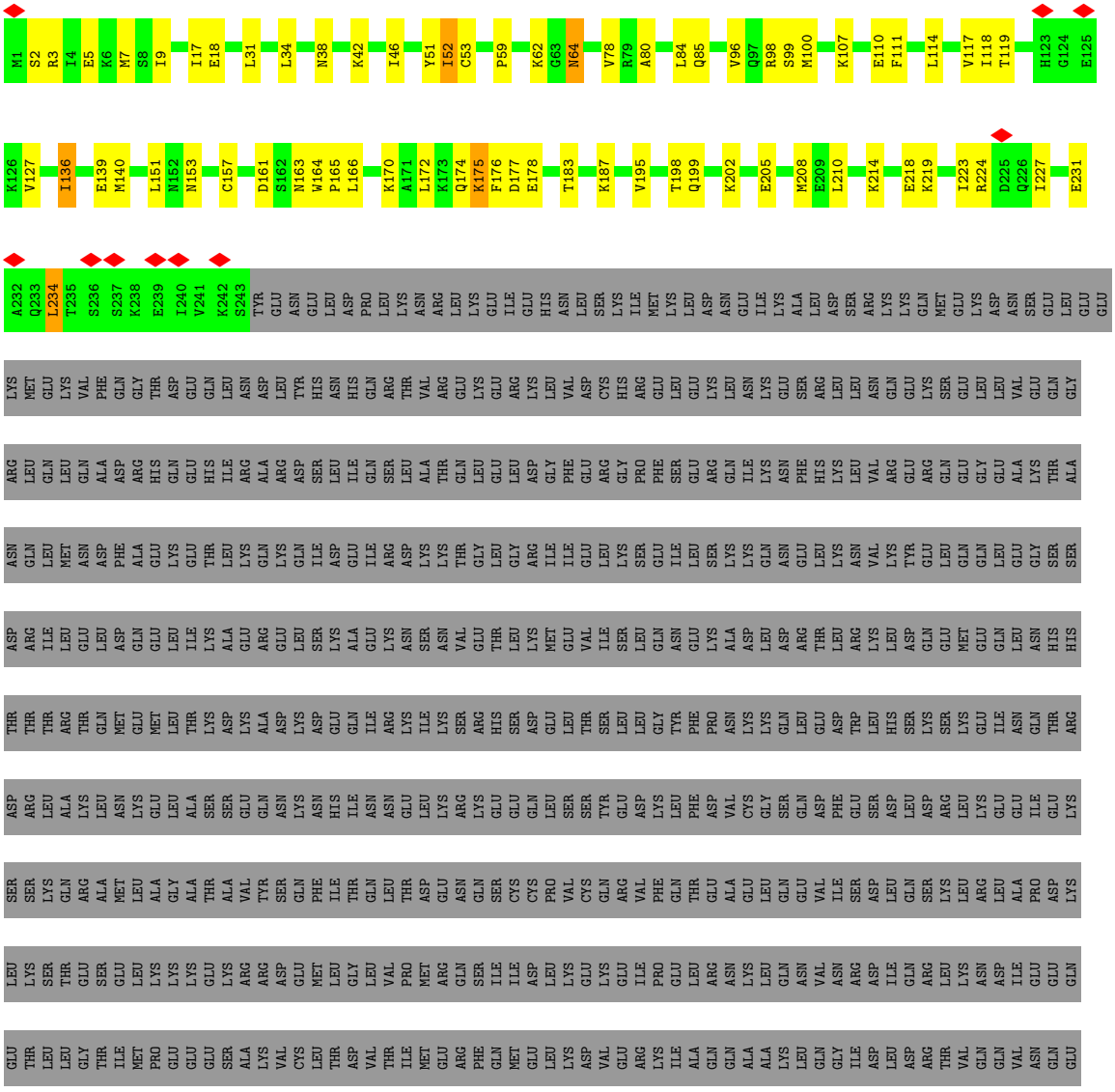
Mol	Chain	Residues	Atoms	AltConf
9	A	2	Total O 2 2	0
9	B	2	Total O 2 2	0
9	E	1	Total O 1 1	0

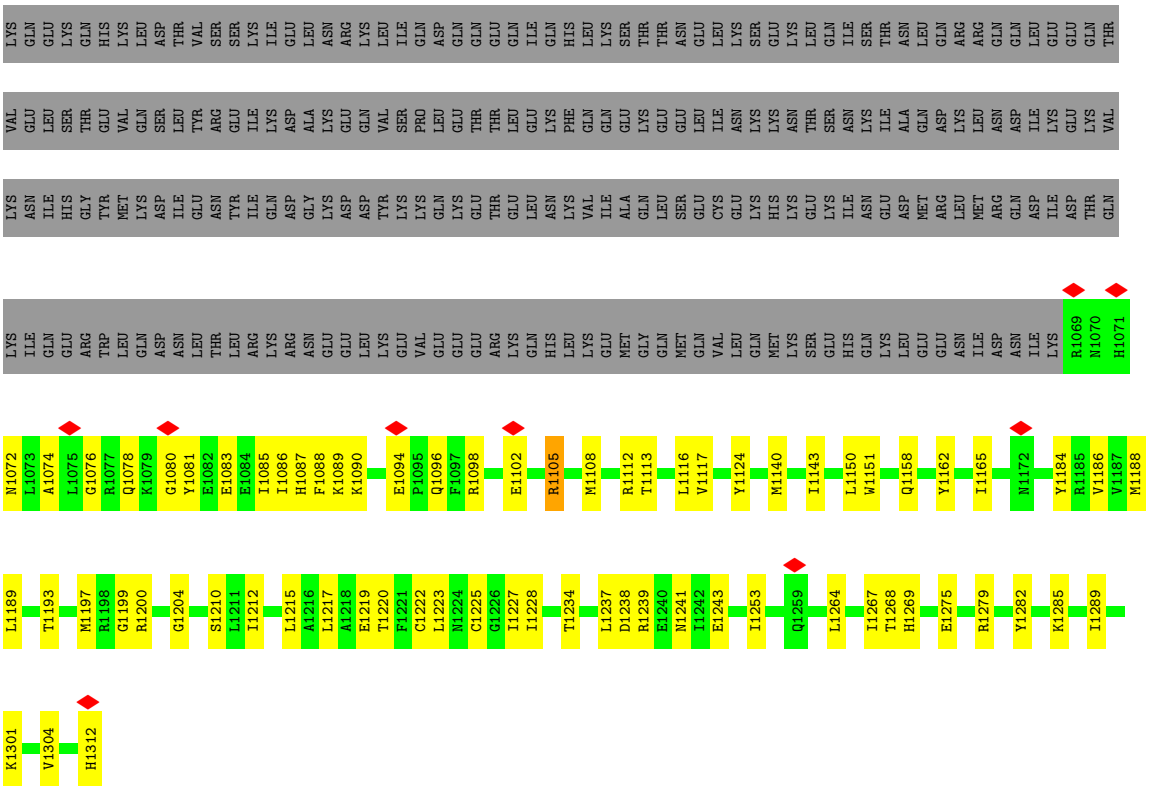
3 Residue-property plots (i)

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

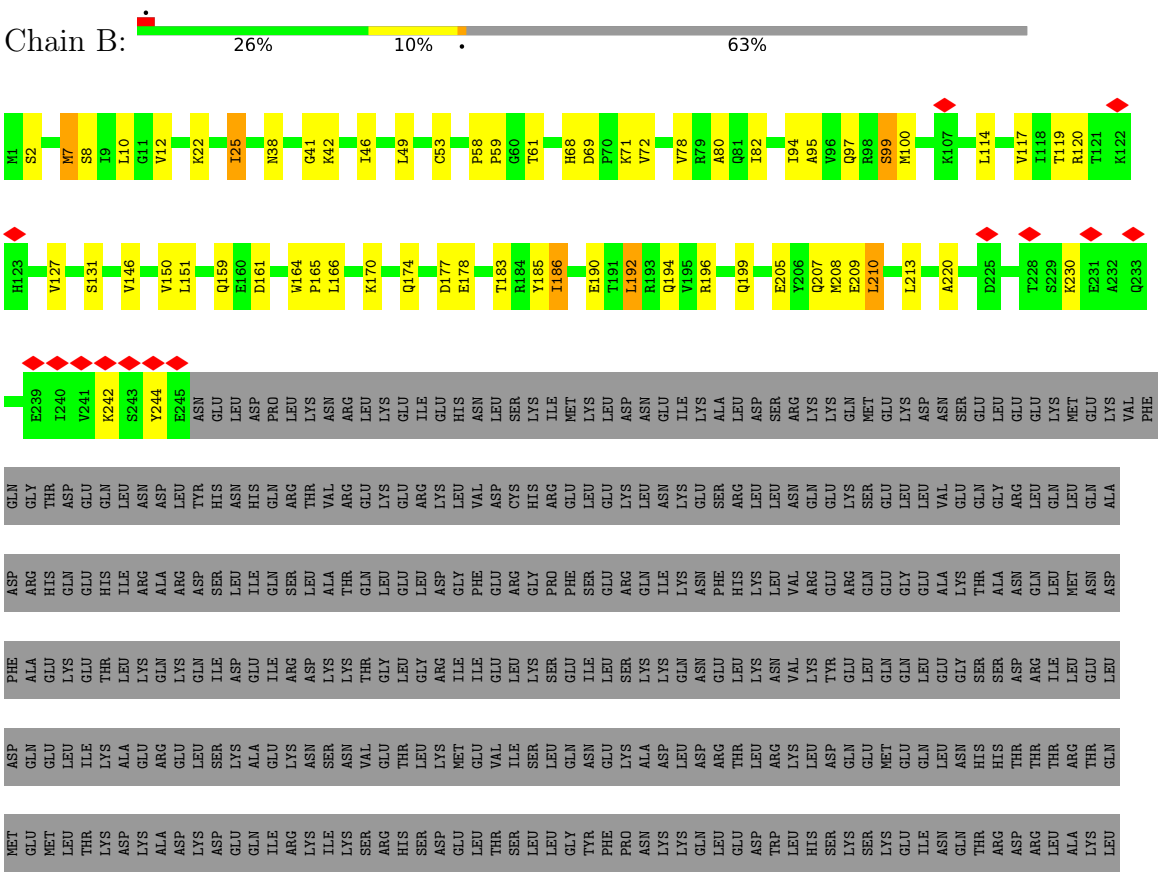
- Molecule 1: DNA repair protein RAD50

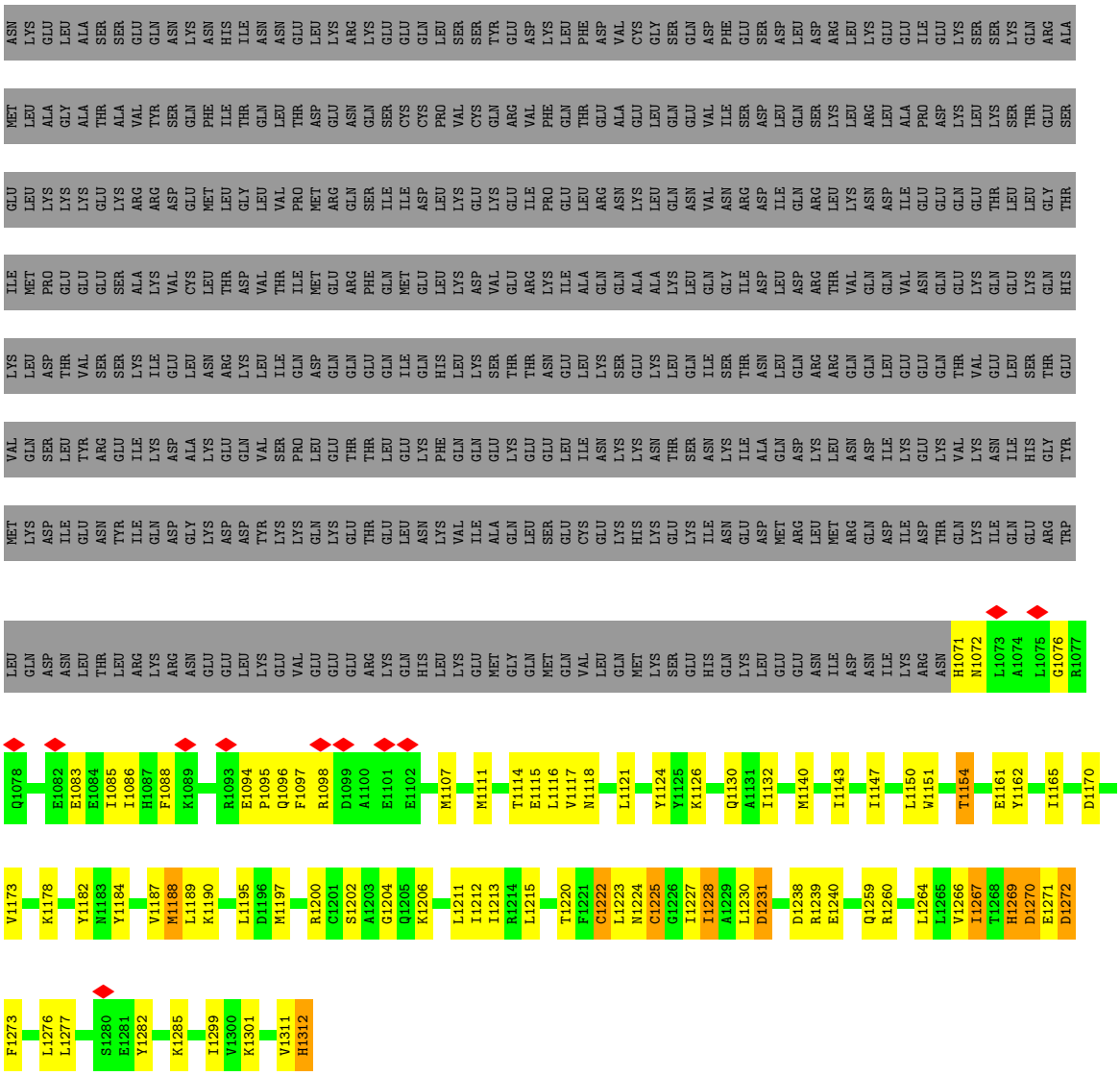
Chain A:





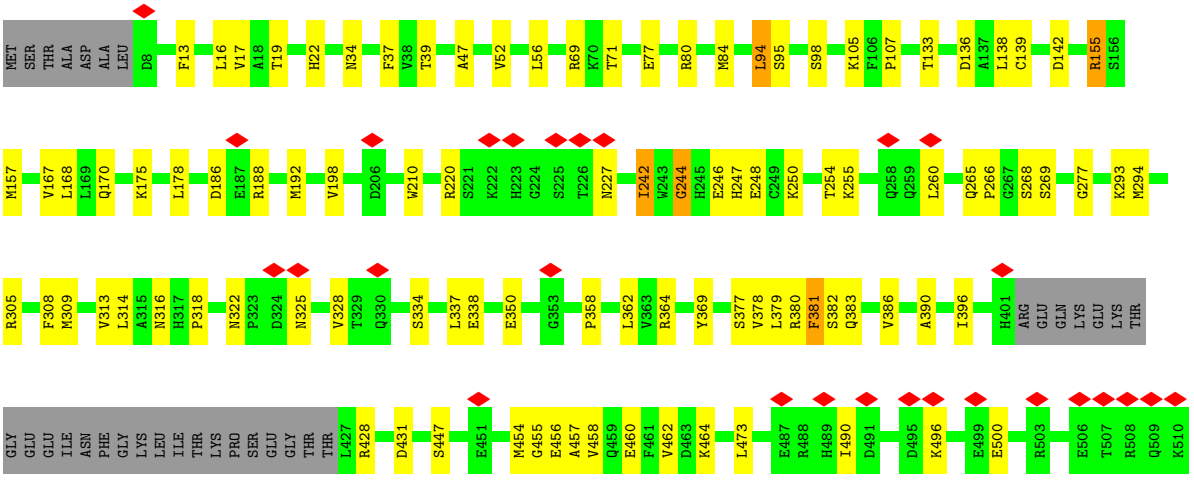
• Molecule 1: DNA repair protein RAD50

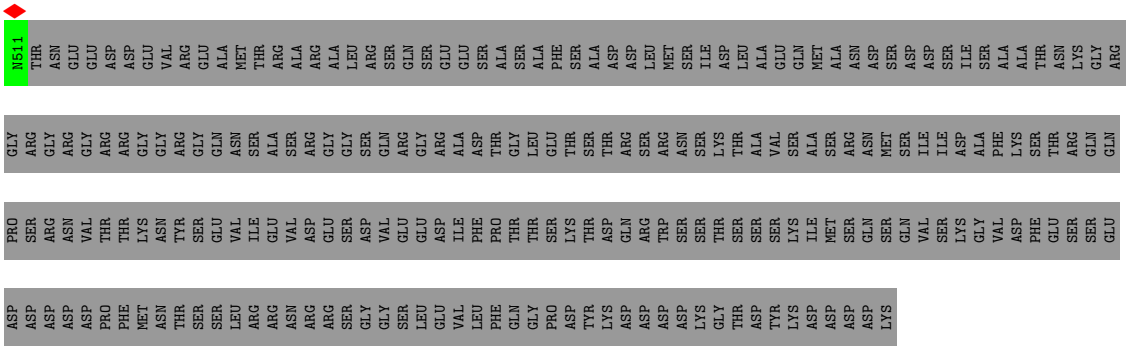




• Molecule 2: Double-strand break repair protein MRE11

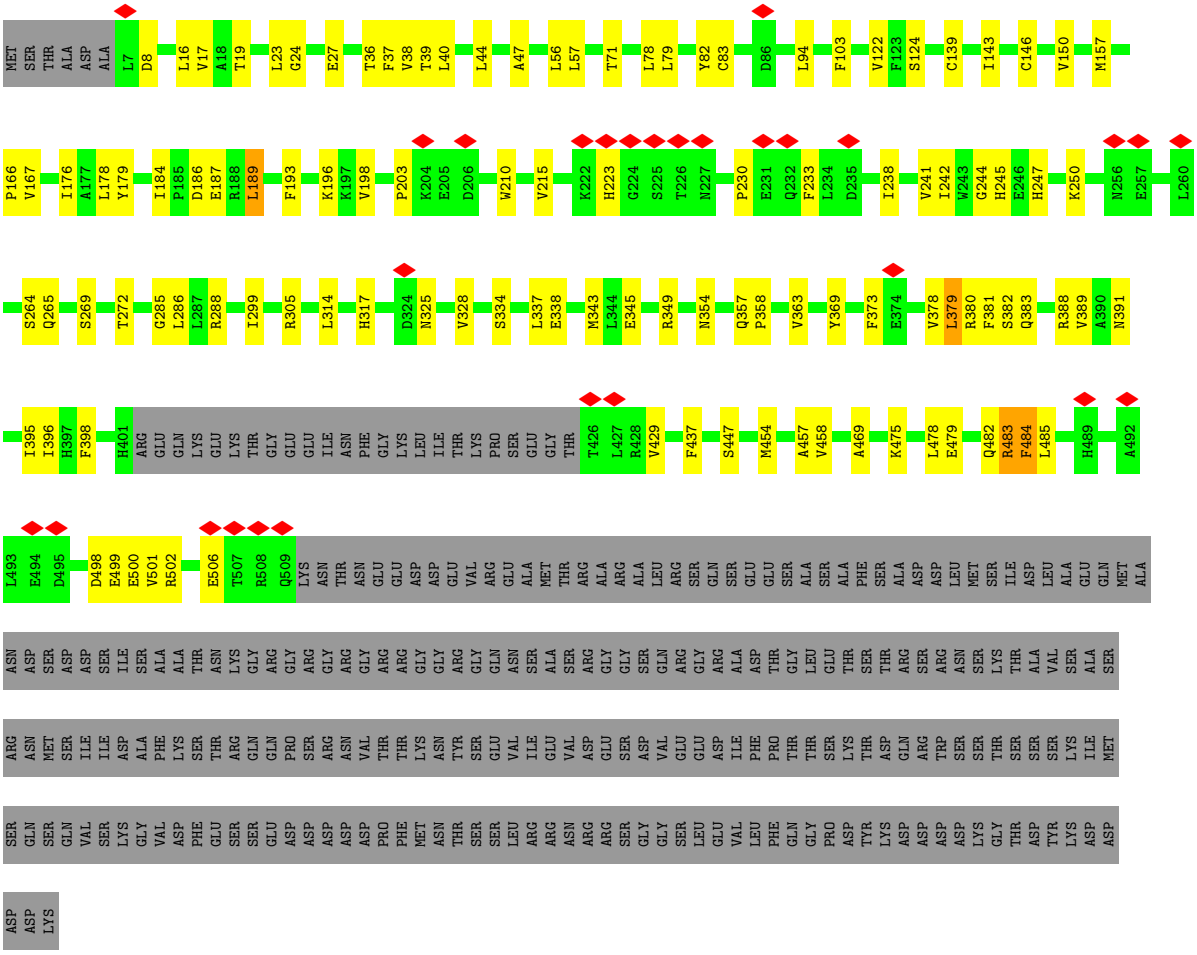
Chain D:





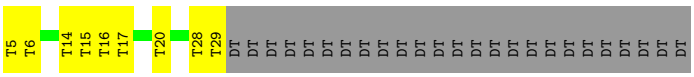
• Molecule 2: Double-strand break repair protein MRE11

Chain E:



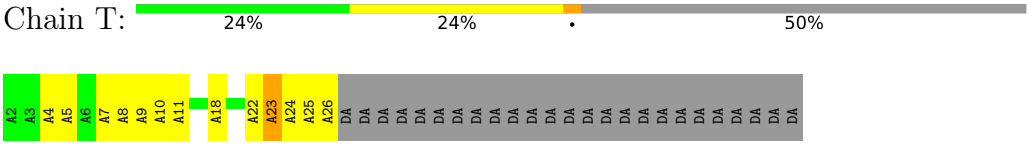
• Molecule 3: DNA (50-MER)

Chain P:



• Molecule 4: DNA (50-MER)

Chain T:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	95397	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 ($e^-/Å^2$)	42.38	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.844	Depositor
Minimum map value	-3.281	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.095	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	377.64, 377.64, 377.64	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.049, 1.049, 1.049	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, BEF, MN

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	0.37	2/3988 (0.1%)	0.59	7/5344 (0.1%)
1	B	0.36	1/3991 (0.0%)	0.59	9/5349 (0.2%)
2	D	0.35	2/3991 (0.1%)	0.50	7/5379 (0.1%)
2	E	0.35	0/3989	0.59	6/5378 (0.1%)
3	P	0.23	0/549	0.54	0/846
4	T	0.47	0/599	0.93	3/921 (0.3%)
All	All	0.36	5/17107 (0.0%)	0.59	32/23217 (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	1
1	B	0	1
2	D	0	2
2	E	0	3
All	All	0	7

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	293	LYS	C-N	7.42	1.43	1.33
1	A	1184	TYR	CA-C	-5.55	1.46	1.52
2	D	294	MET	C-N	5.50	1.40	1.33
1	A	2	SER	CA-CB	-5.46	1.44	1.53
1	B	1267	ILE	C-O	-5.36	1.18	1.24

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1222	CYS	CB-CA-C	-12.26	91.19	111.41
1	A	177	ASP	N-CA-C	-8.73	101.73	114.39
2	E	38	VAL	N-CA-C	-8.72	104.31	111.81
1	B	1228	ILE	N-CA-C	-8.61	95.99	107.88
1	B	1312	HIS	CA-CB-CG	7.99	121.79	113.80
1	A	178	GLU	N-CA-C	-7.60	104.53	113.88
1	A	3	ARG	CB-CA-C	-7.57	98.03	110.14
1	B	1225	CYS	CB-CA-C	-7.27	101.70	112.09
1	B	1272	ASP	N-CA-C	-7.05	104.81	113.41
2	E	383	GLN	N-CA-C	-6.93	104.63	113.23
1	A	175	LYS	N-CA-C	-6.73	105.36	113.97
1	A	1222	CYS	CB-CA-C	-6.47	101.94	112.03
2	E	379	LEU	N-CA-C	-6.42	105.27	113.23
2	D	456	GLU	N-CA-C	-6.38	105.53	113.38
2	E	245	HIS	CB-CA-C	-6.10	101.42	111.36
2	D	244	GLY	N-CA-C	6.04	127.49	113.18
2	D	242	ILE	CA-C-O	-5.87	115.71	121.58
2	D	378	VAL	N-CA-C	-5.67	104.62	112.50
4	T	18	DA	O3'-P-O5'	-5.66	95.51	104.00
1	B	1228	ILE	CA-C-O	-5.63	116.23	120.96
1	A	1219	GLU	CB-CA-C	-5.60	101.33	110.85
4	T	23	DA	O3'-P-O5'	-5.51	95.73	104.00
2	D	293	LYS	O-C-N	5.38	129.63	123.29
1	B	210	LEU	N-CA-C	-5.33	105.56	111.36
1	A	187	LYS	N-CA-C	-5.26	105.63	111.36
1	B	1267	ILE	CA-C-O	-5.13	115.19	121.04
4	T	7	DA	O3'-P-O5'	-5.13	96.31	104.00
2	E	186	ASP	CA-C-N	-5.10	112.20	120.71
2	E	186	ASP	C-N-CA	-5.10	112.20	120.71
2	D	382	SER	N-CA-C	-5.08	107.63	113.88
1	B	1269	HIS	CA-CB-CG	5.06	118.86	113.80
2	D	381	PHE	N-CA-C	-5.00	106.60	113.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1105	ARG	Sidechain
1	B	196	ARG	Sidechain
2	D	155	ARG	Sidechain
2	D	380	ARG	Sidechain
2	E	380	ARG	Sidechain
2	E	388	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	E	483	ARG	Sidechain

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	3936	0	4015	109	0
1	B	3938	0	4011	118	0
2	D	3908	0	3867	71	0
2	E	3906	0	3866	80	0
3	P	500	0	301	5	0
4	T	525	0	276	7	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	27	0	12	4	0
6	B	27	0	12	3	0
7	B	8	0	0	5	0
8	D	2	0	0	0	0
8	E	2	0	0	0	0
9	A	2	0	0	0	0
9	B	2	0	0	0	0
9	E	1	0	0	0	0
All	All	16786	0	16360	358	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 11.

All (358) 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:D:19:THR:HG21	2:D:244:GLY:HA2	1.33	1.05
1:A:1094:GLU:O	1:A:1098:ARG:HG3	1.63	0.97
2:E:94:LEU:HD12	2:E:94:LEU:O	1.63	0.96
1:A:1228:ILE:HG23	1:A:1264:LEU:HD12	1.49	0.93
1:B:1161:GLU:HA	2:D:379:LEU:CD1	2.01	0.90
1:A:110:GLU:HG2	1:A:111:PHE:H	1.32	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:GLU:HA	1:B:208:MET:HE3	1.54	0.90
1:B:1161:GLU:HA	2:D:379:LEU:HD12	1.52	0.89
1:B:1202:SER:OG	7:B:1403:BEF:F2	1.81	0.88
2:D:19:THR:CG2	2:D:244:GLY:HA2	2.05	0.86
1:A:59:PRO:HG3	1:A:161:ASP:HB2	1.59	0.85
1:A:1204:GLY:N	7:B:1404:BEF:F2	1.99	0.85
1:A:1199:GLY:O	1:B:61:THR:HG21	1.79	0.82
1:B:1115:GLU:HA	1:B:1118:ASN:HD22	1.44	0.82
2:E:37:PHE:HZ	2:E:71:THR:HG22	1.45	0.81
1:A:1228:ILE:HG23	1:A:1264:LEU:CD1	2.14	0.78
1:A:1225:CYS:SG	1:A:1227:ILE:HD12	2.23	0.77
1:B:199:GLN:HB3	1:B:1118:ASN:OD1	1.84	0.77
1:B:1188:MET:HE2	1:B:1200:ARG:HD2	1.68	0.76
2:E:37:PHE:CZ	2:E:71:THR:HG22	2.22	0.75
1:B:1188:MET:HE3	1:B:1190:LYS:HD2	1.68	0.74
1:A:110:GLU:HG2	1:A:111:PHE:N	2.02	0.74
1:A:1072:ASN:HB2	1:B:1072:ASN:HB2	1.70	0.74
2:E:23:LEU:HD23	2:E:36:THR:HG22	1.70	0.73
1:B:1161:GLU:OE2	2:D:377:SER:HA	1.89	0.73
1:B:95:ALA:HB3	1:B:119:THR:HB	1.70	0.73
1:B:1204:GLY:N	7:B:1403:BEF:F2	2.11	0.72
2:D:250:LYS:HB2	2:D:265:GLN:HB3	1.70	0.72
1:B:159:GLN:HG3	1:B:1231:ASP:HB3	1.71	0.71
2:E:23:LEU:HA	2:E:36:THR:HG21	1.73	0.71
1:B:1161:GLU:CA	2:D:379:LEU:HD12	2.20	0.70
2:D:460:GLU:HA	2:D:464:LYS:HD3	1.72	0.70
1:A:1074:ALA:O	1:A:1078:GLN:HG2	1.92	0.70
2:D:305:ARG:HB3	2:D:358:PRO:HG2	1.74	0.69
1:A:110:GLU:CG	1:A:111:PHE:H	2.06	0.69
1:A:1140:MET:HE2	1:A:1165:ILE:HB	1.75	0.69
2:E:23:LEU:CD2	2:E:36:THR:HG22	2.23	0.68
2:E:23:LEU:HD11	2:E:40:LEU:HD22	1.77	0.65
1:B:1211:LEU:HD11	1:B:1230:LEU:HD22	1.79	0.65
2:E:378:VAL:HG13	2:E:396:ILE:HB	1.79	0.65
2:E:94:LEU:O	2:E:94:LEU:CD1	2.41	0.65
2:E:389:VAL:HG22	2:E:391:ASN:H	1.60	0.65
1:B:1161:GLU:HA	2:D:379:LEU:HD11	1.78	0.65
1:A:62:LYS:HD2	1:A:64:ASN:HD21	1.61	0.64
1:A:118:ILE:HD11	1:A:136:ILE:HD13	1.80	0.64
2:E:24:GLY:HA3	2:E:71:THR:HG21	1.79	0.64
2:D:337:LEU:HG	2:D:381:PHE:HE1	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:23:LEU:HD23	2:E:36:THR:CG2	2.29	0.63
1:B:1264:LEU:O	1:B:1266:VAL:HG23	1.99	0.63
2:E:24:GLY:CA	2:E:71:THR:HG21	2.29	0.63
1:A:170:LYS:O	1:A:174:GLN:HG3	1.99	0.62
1:B:1150:LEU:HB3	1:B:1212:ILE:HD12	1.81	0.62
2:D:383:GLN:HA	2:D:386:VAL:HG23	1.81	0.62
1:A:1094:GLU:C	1:A:1098:ARG:HG3	2.24	0.62
2:E:325:ASN:HB3	2:E:328:VAL:HB	1.80	0.62
1:B:1114:THR:O	1:B:1118:ASN:ND2	2.33	0.62
2:E:27:GLU:OE1	2:E:71:THR:HG23	1.99	0.61
2:E:250:LYS:HB2	2:E:265:GLN:HB3	1.81	0.61
1:A:1200:ARG:HB2	6:B:1402:ADP:N7	2.13	0.61
2:D:16:LEU:HD13	2:D:47:ALA:HB2	1.82	0.61
2:E:378:VAL:HG22	2:E:398:PHE:HE2	1.64	0.61
1:B:208:MET:HG3	1:B:209:GLU:OE2	2.01	0.61
3:P:5:DT:H1'	3:P:6:DT:H5'	1.83	0.61
1:A:1223:LEU:HD12	1:A:1223:LEU:C	2.26	0.60
1:A:214:LYS:O	1:A:218:GLU:HG2	2.02	0.59
2:D:255:LYS:HD2	2:D:260:LEU:HD12	1.83	0.59
1:A:1228:ILE:CG2	1:A:1264:LEU:HD12	2.28	0.59
2:D:334:SER:O	2:D:338:GLU:HG2	2.02	0.59
2:E:286:LEU:HD22	2:E:299:ILE:HD11	1.85	0.59
1:A:1188:MET:HB3	1:A:1197:MET:HG2	1.84	0.59
1:B:2:SER:HB3	1:B:1224:ASN:O	2.03	0.59
2:E:122:VAL:HB	2:E:150:VAL:HG22	1.85	0.59
1:B:199:GLN:HE22	1:B:1117:VAL:HG12	1.67	0.59
2:D:142:ASP:OD2	2:D:155:ARG:NH2	2.36	0.58
1:A:1228:ILE:CG2	1:A:1264:LEU:CD1	2.82	0.58
1:B:199:GLN:CB	1:B:1118:ASN:OD1	2.50	0.58
2:E:8:ASP:OD1	2:E:288:ARG:NH1	2.36	0.58
2:E:354:ASN:HD21	2:E:357:GLN:HG3	1.67	0.58
1:B:199:GLN:NE2	1:B:1118:ASN:OD1	2.31	0.58
1:B:210:LEU:HA	1:B:1107:MET:HE1	1.86	0.57
2:D:313:VAL:HB	2:D:316:ASN:HB2	1.86	0.57
1:A:1165:ILE:HG12	1:A:1186:VAL:HG22	1.87	0.57
1:B:166:LEU:HD21	1:B:1197:MET:HG2	1.87	0.57
1:B:1187:VAL:HG23	1:B:1189:LEU:CD1	2.35	0.57
1:B:1264:LEU:O	1:B:1264:LEU:HG	2.04	0.57
2:D:94:LEU:HD13	2:D:210:TRP:HH2	1.70	0.56
2:E:499:GLU:HA	2:E:502:ARG:HH12	1.70	0.56
1:A:53:CYS:HB3	1:A:151:LEU:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1234:THR:HA	1:A:1237:LEU:HD12	1.86	0.56
1:B:53:CYS:HB3	1:B:151:LEU:HD13	1.87	0.56
1:B:1094:GLU:HG3	1:B:1096:GLN:H	1.71	0.56
1:B:1147:ILE:HD13	1:B:1213:ILE:HD13	1.88	0.56
2:E:167:VAL:HB	2:E:178:LEU:HB3	1.88	0.55
1:A:1199:GLY:O	1:B:61:THR:CG2	2.51	0.55
2:D:69:ARG:HG3	2:E:143:ILE:HD11	1.87	0.55
2:E:184:ILE:HB	2:E:189:LEU:HD23	1.87	0.55
1:B:1143:ILE:HG22	1:B:1220:THR:OG1	2.07	0.55
1:B:1272:ASP:O	1:B:1276:LEU:HG	2.07	0.55
1:A:1285:LYS:HD3	1:A:1301:LYS:HD3	1.89	0.55
2:D:490:ILE:HD13	2:D:500:GLU:OE2	2.08	0.55
1:B:1225:CYS:SG	1:B:1227:ILE:HD12	2.47	0.54
2:D:98:SER:HA	2:D:107:PRO:HB2	1.89	0.54
1:B:1140:MET:SD	1:B:1143:ILE:HD11	2.47	0.54
2:D:139:CYS:SG	2:D:142:ASP:CG	2.91	0.54
2:D:457:ALA:HB2	2:D:473:LEU:HD13	1.90	0.54
1:A:231:GLU:HA	1:A:1085:ILE:HD11	1.89	0.53
2:D:19:THR:HB	2:D:266:PRO:HB2	1.90	0.53
2:D:383:GLN:HA	2:D:386:VAL:CG2	2.38	0.53
2:D:188:ARG:O	2:D:192:MET:HG3	2.08	0.53
1:A:1090:LYS:HE3	1:A:1090:LYS:HA	1.90	0.53
1:B:146:VAL:HG11	1:B:1225:CYS:HB2	1.91	0.53
1:A:1239:ARG:HB2	1:B:1312:HIS:HB3	1.91	0.53
2:D:105:LYS:H	2:D:105:LYS:HD2	1.74	0.53
2:D:155:ARG:HD3	2:D:157:MET:HE3	1.89	0.52
6:A:1402:ADP:O2B	7:B:1403:BEF:F3	2.17	0.52
2:D:167:VAL:HG13	2:D:178:LEU:HB3	1.92	0.52
1:A:1076:GLY:HA3	1:B:1076:GLY:HA3	1.91	0.52
2:E:16:LEU:HD22	2:E:47:ALA:HB2	1.92	0.52
1:B:41:GLY:HA2	6:B:1402:ADP:O1A	2.09	0.52
1:B:146:VAL:CG1	1:B:1225:CYS:HB2	2.40	0.52
2:D:186:ASP:HB3	2:D:227:ASN:HA	1.91	0.52
2:D:247:HIS:ND1	2:D:268:SER:HB3	2.25	0.51
1:B:1143:ILE:CG2	1:B:1220:THR:HG21	2.40	0.51
1:B:94:ILE:HD11	1:B:120:ARG:HH21	1.75	0.51
1:A:153:ASN:OD1	1:A:175:LYS:NZ	2.42	0.51
2:E:389:VAL:HG11	2:E:395:ILE:HD11	1.93	0.51
2:E:475:LYS:HG2	2:E:479:GLU:OE2	2.11	0.51
1:B:1215:LEU:HD23	1:B:1228:ILE:CD1	2.41	0.51
2:D:362:LEU:HD23	2:D:390:ALA:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:56:LEU:HD11	2:E:215:VAL:HG21	1.91	0.51
1:A:1143:ILE:HD11	1:A:1220:THR:HG21	1.93	0.51
1:B:190:GLU:O	1:B:194:GLN:HG2	2.11	0.51
1:A:1080:GLY:O	1:A:1083:GLU:HG2	2.11	0.51
2:D:454:MET:O	2:D:457:ALA:N	2.42	0.51
1:A:1102:GLU:HG3	1:A:1105:ARG:HH21	1.76	0.51
1:B:7:MET:HB3	1:B:25:ILE:HG23	1.92	0.51
2:E:17:VAL:HB	2:E:285:GLY:HA3	1.92	0.51
6:A:1402:ADP:C8	1:B:1200:ARG:O	2.64	0.50
1:B:59:PRO:HG2	1:B:161:ASP:HB2	1.92	0.50
1:B:1165:ILE:HD11	1:B:1213:ILE:HD12	1.93	0.50
2:D:95:SER:HB3	2:D:168:LEU:HG	1.92	0.50
1:A:1304:VAL:HG13	1:A:1304:VAL:O	2.11	0.50
2:E:230:PRO:HD2	2:E:233:PHE:CD2	2.46	0.50
1:A:1124:TYR:CE2	2:E:454:MET:HB3	2.47	0.50
1:A:1096:GLN:CD	1:A:1096:GLN:H	2.19	0.50
1:A:1239:ARG:O	1:A:1243:GLU:HG3	2.11	0.50
1:B:207:GLN:HG2	1:B:1111:MET:HE2	1.94	0.49
2:E:193:PHE:CD1	2:E:198:VAL:HG11	2.47	0.49
2:E:498:ASP:HA	2:E:501:VAL:HG12	1.94	0.49
1:A:219:LYS:O	1:A:223:ILE:HG23	2.12	0.49
1:B:1121:LEU:CD2	2:D:454:MET:HE1	2.42	0.49
2:D:16:LEU:HD13	2:D:47:ALA:CA	2.42	0.49
1:A:7:MET:HE3	1:A:9:ILE:HD11	1.93	0.49
1:A:1151:TRP:HA	1:A:1212:ILE:HD13	1.94	0.49
2:E:57:LEU:HB2	2:E:124:SER:HB2	1.93	0.49
2:D:322:ASN:HB3	2:D:325:ASN:HB2	1.93	0.49
4:T:22:DA:H1'	4:T:23:DA:H5'	1.93	0.49
2:E:314:LEU:HD12	2:E:369:TYR:HB3	1.95	0.49
1:B:1115:GLU:HA	1:B:1118:ASN:ND2	2.22	0.49
2:D:39:THR:HG21	2:D:269:SER:HB3	1.95	0.49
1:A:46:ILE:HD11	1:A:1267:ILE:HD11	1.95	0.49
1:A:118:ILE:HD12	1:A:139:GLU:HG2	1.95	0.49
1:A:172:LEU:HD11	1:A:176:PHE:HE2	1.78	0.49
2:D:309:MET:HB2	2:D:364:ARG:HB3	1.95	0.49
2:E:79:LEU:O	2:E:83:CYS:HB3	2.12	0.49
2:E:485:LEU:CD2	2:E:500:GLU:HG2	2.43	0.48
3:P:28:DT:H2'	3:P:29:DT:H71	1.95	0.48
1:B:25:ILE:HB	1:B:1299:ILE:HG21	1.94	0.48
2:D:175:LYS:HB3	2:D:210:TRP:CE3	2.49	0.48
2:E:187:GLU:HA	2:E:187:GLU:OE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:378:VAL:CG1	2:E:396:ILE:HB	2.42	0.48
1:A:210:LEU:HD21	1:A:1108:MET:SD	2.53	0.48
1:A:227:ILE:HG12	1:A:1088:PHE:HB3	1.94	0.48
1:A:1113:THR:HG22	2:E:478:LEU:HD22	1.95	0.48
1:B:1161:GLU:CA	2:D:379:LEU:CD1	2.83	0.48
2:D:248:GLU:HG3	2:D:277:GLY:O	2.13	0.48
2:E:103:PHE:HZ	2:E:157:MET:HA	1.78	0.48
1:B:174:GLN:O	1:B:178:GLU:HG2	2.14	0.48
1:A:164:TRP:CG	1:A:165:PRO:HD3	2.49	0.48
1:B:210:LEU:CD1	1:B:1107:MET:HE1	2.44	0.47
1:A:1116:LEU:HD22	2:E:447:SER:HB3	1.95	0.47
1:A:52:ILE:HG21	1:A:84:LEU:HB3	1.95	0.47
1:A:1113:THR:HG22	2:E:478:LEU:CD2	2.44	0.47
1:B:1126:LYS:O	1:B:1130:GLN:HG2	2.13	0.47
2:D:381:PHE:CE2	2:D:396:ILE:HG13	2.49	0.47
1:A:17:ILE:HG22	1:A:78:VAL:HG13	1.97	0.47
1:B:1271:GLU:HG3	1:B:1311:VAL:HG21	1.96	0.47
2:D:77:GLU:HG2	2:E:146:CYS:SG	2.54	0.47
1:A:1151:TRP:CD1	1:A:1162:TYR:HA	2.50	0.47
1:A:1158:GLN:HB3	2:E:379:LEU:HD22	1.96	0.47
1:B:7:MET:HE1	1:B:49:LEU:HG	1.97	0.47
1:B:205:GLU:O	1:B:208:MET:HG2	2.13	0.47
2:E:345:GLU:O	2:E:349:ARG:HG3	2.14	0.47
1:A:7:MET:HB2	1:A:84:LEU:HD12	1.96	0.47
1:A:1162:TYR:CE1	1:A:1189:LEU:HD13	2.50	0.47
2:D:325:ASN:ND2	2:D:328:VAL:HG23	2.29	0.47
2:D:458:VAL:O	2:D:462:VAL:HG13	2.15	0.47
2:D:37:PHE:HZ	2:D:71:THR:HG22	1.80	0.47
2:E:369:TYR:HE1	2:E:398:PHE:HB3	1.80	0.47
4:T:4:DA:H2"	4:T:5:DA:OP2	2.14	0.47
2:D:16:LEU:HB2	2:D:52:VAL:HG11	1.97	0.46
2:E:40:LEU:HD23	2:E:78:LEU:HD12	1.97	0.46
2:E:382:SER:HB2	2:E:395:ILE:HD12	1.97	0.46
1:B:244:TYR:CG	1:B:1071:HIS:HB3	2.50	0.46
1:B:1143:ILE:HG22	1:B:1220:THR:HG21	1.98	0.46
3:P:16:DT:H2"	3:P:17:DT:H72	1.97	0.46
1:A:53:CYS:HA	1:A:140:MET:HE2	1.96	0.46
2:E:44:LEU:HB3	2:E:82:TYR:CD2	2.50	0.46
2:E:305:ARG:HG3	2:E:358:PRO:HG2	1.97	0.46
1:A:5:GLU:HB2	1:A:85:GLN:O	2.16	0.46
1:A:1083:GLU:HA	1:A:1086:ILE:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:LEU:HD13	1:B:1206:LYS:HG3	1.97	0.46
2:E:369:TYR:HB2	2:E:373:PHE:HB2	1.98	0.46
1:A:234:LEU:HD13	1:A:1085:ILE:HD12	1.98	0.46
2:D:16:LEU:HD13	2:D:47:ALA:CB	2.45	0.46
2:E:23:LEU:HA	2:E:36:THR:CG2	2.43	0.46
2:E:457:ALA:HB1	2:E:469:ALA:O	2.16	0.46
4:T:10:DA:H2"	4:T:11:DA:C8	2.50	0.46
1:B:1150:LEU:O	1:B:1154:THR:HG23	2.16	0.46
2:D:490:ILE:HD11	2:D:496:LYS:HE2	1.97	0.46
1:A:157:CYS:SG	1:A:161:ASP:O	2.74	0.46
1:B:10:LEU:HD13	1:B:22:LYS:HB2	1.97	0.46
1:B:1270:ASP:OD1	1:B:1273:PHE:HB3	2.16	0.46
1:A:80:ALA:HB3	1:A:100:MET:HG2	1.97	0.45
6:A:1402:ADP:N7	1:B:1200:ARG:HB2	2.31	0.45
1:B:1228:ILE:HG23	1:B:1264:LEU:HD12	1.97	0.45
1:B:1083:GLU:O	1:B:1086:ILE:HG13	2.15	0.45
2:D:337:LEU:HG	2:D:381:PHE:CE1	2.47	0.45
2:E:19:THR:HG21	2:E:244:GLY:HA2	1.96	0.45
2:E:242:ILE:HD13	2:E:264:SER:HB3	1.99	0.45
1:A:42:LYS:HE3	1:A:1269:HIS:CE1	2.52	0.45
1:B:80:ALA:HB3	1:B:100:MET:HE3	1.98	0.45
2:D:314:LEU:HD12	2:D:369:TYR:HB3	1.99	0.45
1:B:192:LEU:HD21	2:D:454:MET:HE3	1.99	0.45
1:A:1237:LEU:HD22	1:A:1241:ASN:HB3	1.99	0.45
1:B:242:LYS:HD2	1:B:242:LYS:HA	1.78	0.45
2:D:22:HIS:NE2	2:D:247:HIS:HE1	2.14	0.45
2:E:334:SER:O	2:E:338:GLU:HG2	2.17	0.45
1:B:1116:LEU:HD22	2:D:447:SER:HB3	1.97	0.45
1:B:1277:LEU:HD23	1:B:1277:LEU:HA	1.83	0.45
2:E:196:LYS:HB3	2:E:196:LYS:HE3	1.73	0.45
1:A:195:VAL:O	1:A:199:GLN:HG2	2.16	0.44
2:D:17:VAL:HG12	2:D:56:LEU:HB3	1.99	0.44
2:E:343:MET:HE3	2:E:363:VAL:CG2	2.47	0.44
1:A:1253:ILE:HD11	1:A:1264:LEU:HD22	1.99	0.44
2:E:499:GLU:HA	2:E:502:ARG:NH1	2.32	0.44
1:B:150:VAL:HG11	1:B:1222:CYS:SG	2.57	0.44
1:B:164:TRP:CG	1:B:165:PRO:HD3	2.52	0.44
1:A:31:LEU:HD12	1:A:31:LEU:HA	1.88	0.44
1:B:1178:LYS:HE2	1:B:1178:LYS:HB3	1.82	0.44
2:E:238:ILE:HG21	2:E:241:VAL:HG22	1.99	0.44
2:E:502:ARG:O	2:E:506:GLU:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:THR:O	1:A:202:LYS:HG2	2.18	0.44
1:B:12:VAL:HG21	1:B:82:ILE:HD11	1.98	0.44
1:B:186:ILE:HG22	1:B:1132:ILE:HD13	2.00	0.44
2:D:94:LEU:HD11	2:D:170:GLN:HB2	2.00	0.44
1:A:117:VAL:HG12	1:A:119:THR:H	1.83	0.44
1:A:1228:ILE:HG23	1:A:1228:ILE:O	2.18	0.44
1:B:46:ILE:HD11	1:B:1267:ILE:HD11	2.00	0.44
2:D:455:GLY:HA2	2:D:458:VAL:HG12	1.99	0.44
1:A:1215:LEU:HD23	1:A:1228:ILE:CD1	2.48	0.44
2:E:24:GLY:HA2	2:E:71:THR:HG21	2.00	0.44
1:A:1204:GLY:HA3	1:B:38:ASN:ND2	2.32	0.44
1:B:1211:LEU:HD11	1:B:1230:LEU:CD2	2.47	0.44
2:D:325:ASN:HB3	2:D:328:VAL:HB	2.00	0.44
1:B:183:THR:O	1:B:186:ILE:HG13	2.18	0.43
1:A:223:ILE:HG13	1:A:224:ARG:N	2.33	0.43
1:A:1124:TYR:HE2	2:E:454:MET:HB3	1.84	0.43
1:B:7:MET:HG3	1:B:8:SER:N	2.33	0.43
2:D:155:ARG:HG3	2:D:155:ARG:HH11	1.83	0.43
4:T:8:DA:H5'	4:T:8:DA:C8	2.54	0.43
1:A:1279:ARG:O	1:A:1282:TYR:CZ	2.72	0.43
3:P:14:DT:H2"	3:P:15:DT:C5	2.53	0.43
2:E:39:THR:HG21	2:E:269:SER:HB3	1.99	0.43
4:T:8:DA:H2"	4:T:9:DA:OP2	2.17	0.43
2:E:483:ARG:O	2:E:484:PHE:C	2.61	0.43
1:B:230:LYS:HD3	1:B:230:LYS:HA	1.76	0.43
1:A:163:ASN:HA	1:A:1210:SER:OG	2.19	0.43
1:A:1193:THR:CG2	1:B:72:VAL:HG22	2.49	0.43
1:B:99:SER:HB2	1:B:114:LEU:HB2	2.01	0.43
1:B:1285:LYS:HD2	1:B:1301:LYS:HG2	2.00	0.43
2:D:34:ASN:HA	2:D:37:PHE:HD2	1.84	0.43
1:A:34:LEU:HB2	1:A:1267:ILE:HG12	2.01	0.43
1:A:1238:ASP:HB3	1:B:1269:HIS:CE1	2.54	0.43
1:A:1268:THR:OG1	1:A:1269:HIS:N	2.52	0.43
1:B:58:PRO:HG2	1:B:61:THR:OG1	2.19	0.43
1:B:177:ASP:OD2	1:B:186:ILE:HG12	2.19	0.43
1:B:38:ASN:ND2	7:B:1404:BEF:F1	2.42	0.42
1:B:170:LYS:HD3	1:B:1182:TYR:CE2	2.55	0.42
1:A:205:GLU:O	1:A:208:MET:HG2	2.19	0.42
1:A:1113:THR:HG21	2:E:482:GLN:HG3	2.02	0.42
4:T:24:DA:H4'	4:T:25:DA:OP1	2.20	0.42
1:A:99:SER:HB2	1:A:114:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1094:GLU:HB3	1:A:1096:GLN:OE1	2.19	0.42
1:A:107:LYS:HE2	1:A:107:LYS:HB2	1.82	0.42
4:T:25:DA:H2"	4:T:26:DA:O5'	2.19	0.42
1:B:42:LYS:N	6:B:1402:ADP:O1B	2.48	0.42
2:E:166:PRO:HB3	2:E:179:TYR:CE1	2.55	0.42
1:A:1124:TYR:HD2	2:E:454:MET:HG2	1.85	0.42
1:A:1225:CYS:HG	1:A:1227:ILE:HD12	1.81	0.42
1:B:1095:PRO:HA	1:B:1098:ARG:HG2	2.02	0.42
2:D:168:LEU:HB3	2:D:210:TRP:CH2	2.55	0.42
2:D:381:PHE:CD2	2:D:396:ILE:HG13	2.55	0.42
1:B:1259:GLN:HE21	1:B:1260:ARG:HH12	1.68	0.42
2:E:381:PHE:CE1	2:E:396:ILE:HD11	2.54	0.42
1:A:42:LYS:HB2	1:A:42:LYS:HE2	1.84	0.42
1:B:185:TYR:CZ	2:D:462:VAL:HG21	2.55	0.42
1:B:1085:ILE:HD13	1:B:1085:ILE:HA	1.84	0.42
1:B:1151:TRP:CD1	1:B:1162:TYR:HA	2.54	0.42
1:B:1161:GLU:HG3	1:B:1162:TYR:HD2	1.85	0.42
2:D:308:PHE:HZ	2:D:350:GLU:OE1	2.03	0.42
1:A:1140:MET:HE3	1:A:1140:MET:HA	2.02	0.42
1:A:1089:LYS:HE3	1:A:1089:LYS:HB2	1.96	0.41
1:A:1193:THR:HG21	1:B:72:VAL:HG22	2.02	0.41
2:D:136:ASP:HB3	2:D:138:LEU:HD23	2.00	0.41
1:B:1170:ASP:HB3	1:B:1173:VAL:HB	2.01	0.41
1:A:227:ILE:CG1	1:A:1088:PHE:HB3	2.50	0.41
1:A:1124:TYR:CD2	2:E:454:MET:HG2	2.55	0.41
1:B:210:LEU:HA	1:B:1107:MET:CE	2.50	0.41
2:D:220:ARG:HB3	2:D:246:GLU:HG3	2.03	0.41
2:E:203:PRO:HG2	2:E:210:TRP:CD1	2.56	0.41
1:B:97:GLN:HB3	1:B:117:VAL:HG22	2.02	0.41
2:E:498:ASP:O	2:E:501:VAL:HG12	2.20	0.41
1:A:1150:LEU:HB3	1:A:1212:ILE:HG23	2.02	0.41
2:D:80:ARG:HA	2:D:84:MET:HG3	2.01	0.41
1:A:176:PHE:HE1	1:A:1217:LEU:HD21	1.86	0.41
2:D:69:ARG:HD2	2:E:139:CYS:C	2.46	0.41
1:A:42:LYS:HG2	1:A:1289:ILE:HD13	2.02	0.41
1:B:69:ASP:OD2	1:B:71:LYS:HB2	2.20	0.41
1:B:210:LEU:HD13	1:B:1107:MET:HE1	2.03	0.41
1:B:1188:MET:HG3	1:B:1195:LEU:HB2	2.02	0.41
2:E:363:VAL:HG12	2:E:389:VAL:CG2	2.50	0.41
2:E:437:PHE:HE2	2:E:458:VAL:HG11	1.86	0.41
1:A:51:TYR:CE2	1:A:98:ARG:HD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:316:ASN:C	2:D:318:PRO:HD3	2.46	0.41
1:A:42:LYS:N	6:A:1402:ADP:O1B	2.54	0.41
1:A:18:GLU:H	1:A:18:GLU:HG2	1.61	0.40
1:A:1312:HIS:HA	1:B:1239:ARG:HG3	2.03	0.40
1:B:68:HIS:HB3	1:B:78:VAL:HG11	2.02	0.40
1:B:213:LEU:HD12	1:B:1107:MET:HE2	2.03	0.40
1:A:110:GLU:CG	1:A:111:PHE:N	2.70	0.40
1:A:234:LEU:HB2	1:A:1081:TYR:HB3	2.04	0.40
1:A:1087:HIS:CD2	1:B:1088:PHE:HZ	2.39	0.40
2:E:193:PHE:CE1	2:E:198:VAL:HG11	2.56	0.40
2:E:247:HIS:HE1	2:E:272:THR:HG21	1.86	0.40
1:A:210:LEU:HD12	1:A:210:LEU:HA	1.93	0.40
3:P:20:DT:H6	3:P:20:DT:H2'	1.74	0.40
1:B:1140:MET:HE2	1:B:1140:MET:HB2	1.80	0.40
2:E:24:GLY:HA2	2:E:71:THR:CG2	2.51	0.40
1:A:118:ILE:O	1:A:118:ILE:HG22	2.22	0.40
1:A:166:LEU:HD11	1:A:1197:MET:HB3	2.04	0.40
1:A:1112:ARG:HA	1:A:1112:ARG:HD2	1.81	0.40
1:B:220:ALA:HB2	1:B:1097:PHE:HB2	2.04	0.40
1:B:1124:TYR:HD1	1:B:1124:TYR:HA	1.79	0.40
1:B:1238:ASP:OD1	1:B:1240:GLU:HG2	2.22	0.40
1:B:1271:GLU:O	1:B:1271:GLU:HG2	2.20	0.40
1:B:1312:HIS:OXT	1:B:1312:HIS:ND1	2.54	0.40
2:D:428:ARG:NH2	2:D:431:ASP:OD2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	483/1312 (37%)	456 (94%)	27 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	483/1312 (37%)	472 (98%)	11 (2%)	0	100	100
2	D	475/738 (64%)	462 (97%)	13 (3%)	0	100	100
2	E	475/738 (64%)	445 (94%)	30 (6%)	0	100	100
All	All	1916/4100 (47%)	1835 (96%)	81 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	440/1222 (36%)	430 (98%)	10 (2%)	45	68
1	B	440/1222 (36%)	426 (97%)	14 (3%)	34	61
2	D	436/659 (66%)	430 (99%)	6 (1%)	62	79
2	E	436/659 (66%)	429 (98%)	7 (2%)	58	77
All	All	1752/3762 (47%)	1715 (98%)	37 (2%)	49	71

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	52	ILE
1	A	64	ASN
1	A	96	VAL
1	A	127	VAL
1	A	136	ILE
1	A	183	THR
1	A	234	LEU
1	A	1117	VAL
1	A	1275	GLU
1	B	7	MET
1	B	25	ILE
1	B	99	SER

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Mol	Chain	Res	Type
1	B	127	VAL
1	B	131	SER
1	B	186	ILE
1	B	192	LEU
1	B	1154	THR
1	B	1184	TYR
1	B	1188	MET
1	B	1223	LEU
1	B	1231	ASP
1	B	1270	ASP
1	B	1282	TYR
2	D	13	PHE
2	D	94	LEU
2	D	133	THR
2	D	198	VAL
2	D	242	ILE
2	D	254	THR
2	E	176	ILE
2	E	189	LEU
2	E	223	HIS
2	E	317	HIS
2	E	337	LEU
2	E	429	VAL
2	E	484	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	1312	HIS
1	B	199	GLN
2	D	48	GLN
2	D	223	HIS
2	E	22	HIS
2	E	50	ASN
2	E	247	HIS
2	E	443	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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	ADP	B	1402	5	24,29,29	0.94	1 (4%)	29,45,45	0.97	1 (3%)
6	ADP	A	1402	5	24,29,29	0.94	1 (4%)	29,45,45	0.91	1 (3%)
7	BEF	B	1404	-	0,3,3	-	-	-		
7	BEF	B	1403	-	0,3,3	-	-	-		

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
6	ADP	B	1402	5	-	3/12/32/32	0/3/3/3
6	ADP	A	1402	5	-	3/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1402	ADP	C8-N7	-2.27	1.30	1.34
6	B	1402	ADP	C8-N7	-2.15	1.30	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1402	ADP	C5-C6-N6	2.17	123.65	120.35
6	A	1402	ADP	C5-C6-N6	2.08	123.52	120.35

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1402	ADP	C5'-O5'-PA-O2A
6	A	1402	ADP	C5'-O5'-PA-O3A
6	B	1402	ADP	C5'-O5'-PA-O3A
6	A	1402	ADP	O4'-C4'-C5'-O5'
6	B	1402	ADP	C5'-O5'-PA-O2A
6	B	1402	ADP	O4'-C4'-C5'-O5'

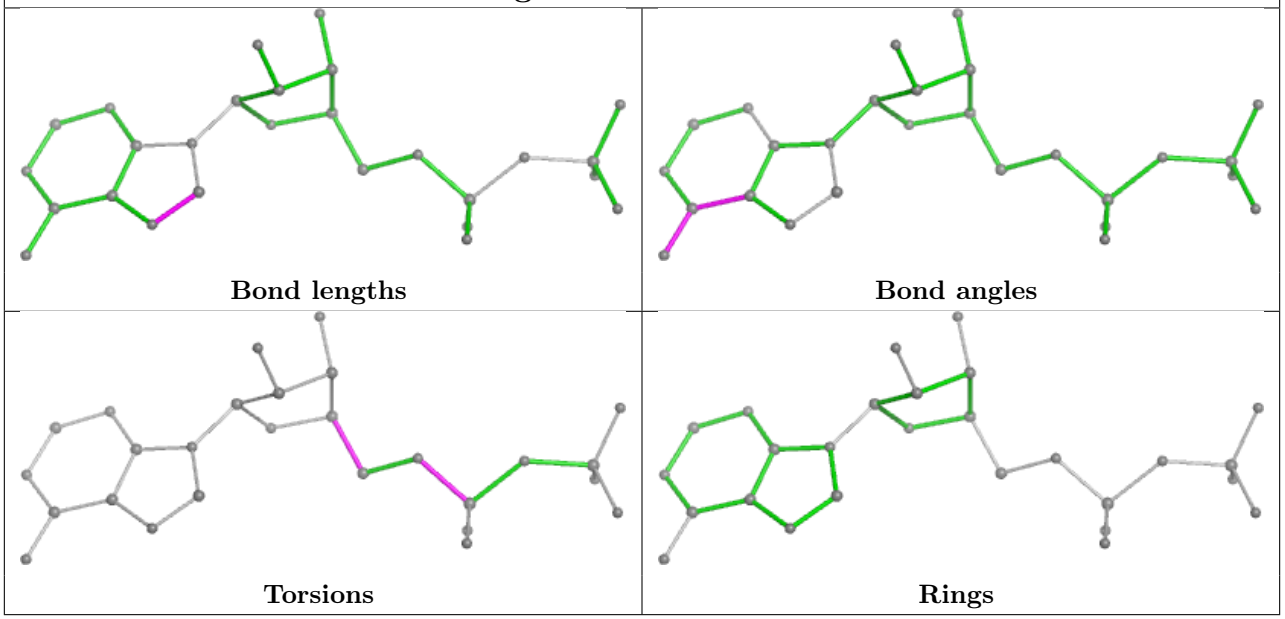
There are no ring outliers.

4 monomers are involved in 11 short contacts:

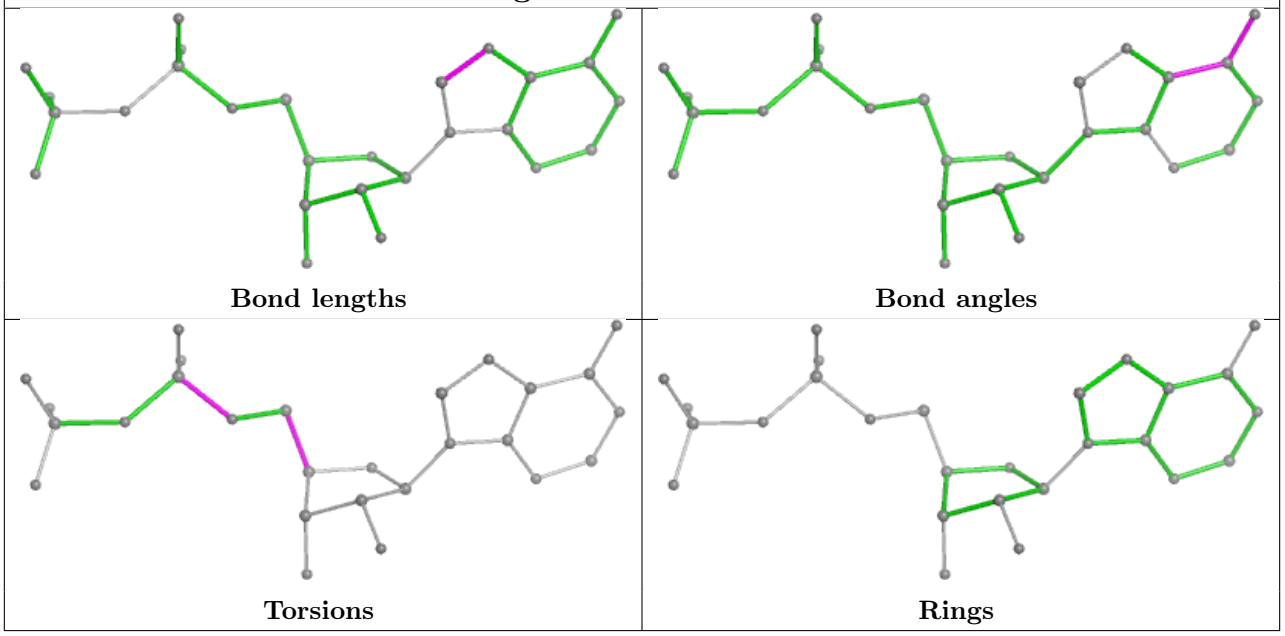
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1402	ADP	3	0
6	A	1402	ADP	4	0
7	B	1404	BEF	2	0
7	B	1403	BEF	3	0

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

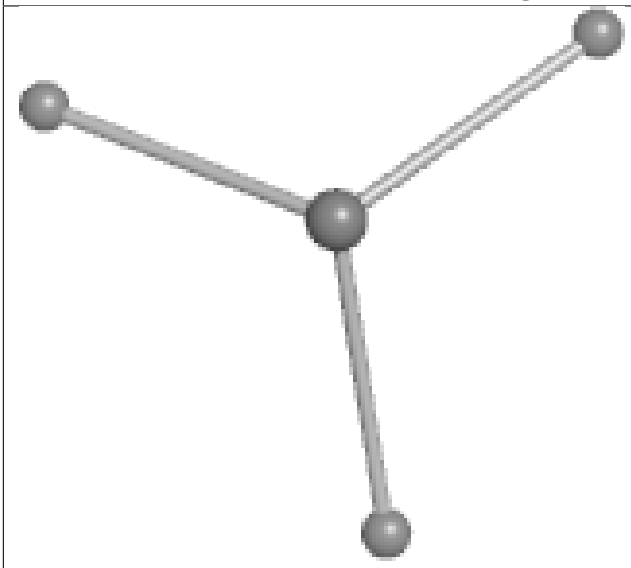
Ligand ADP B 1402



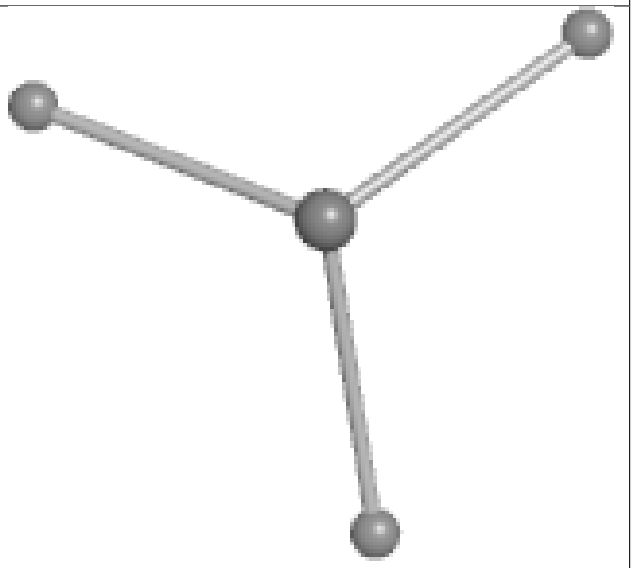
Ligand ADP A 1402



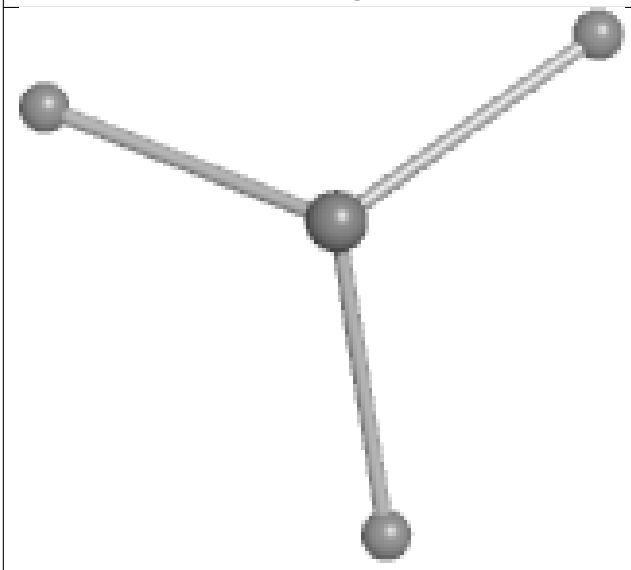
Ligand BEF B 1404



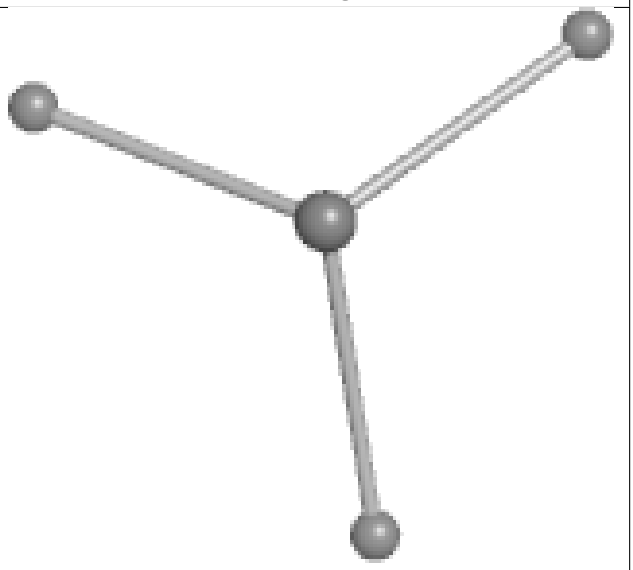
Bond lengths



Bond angles

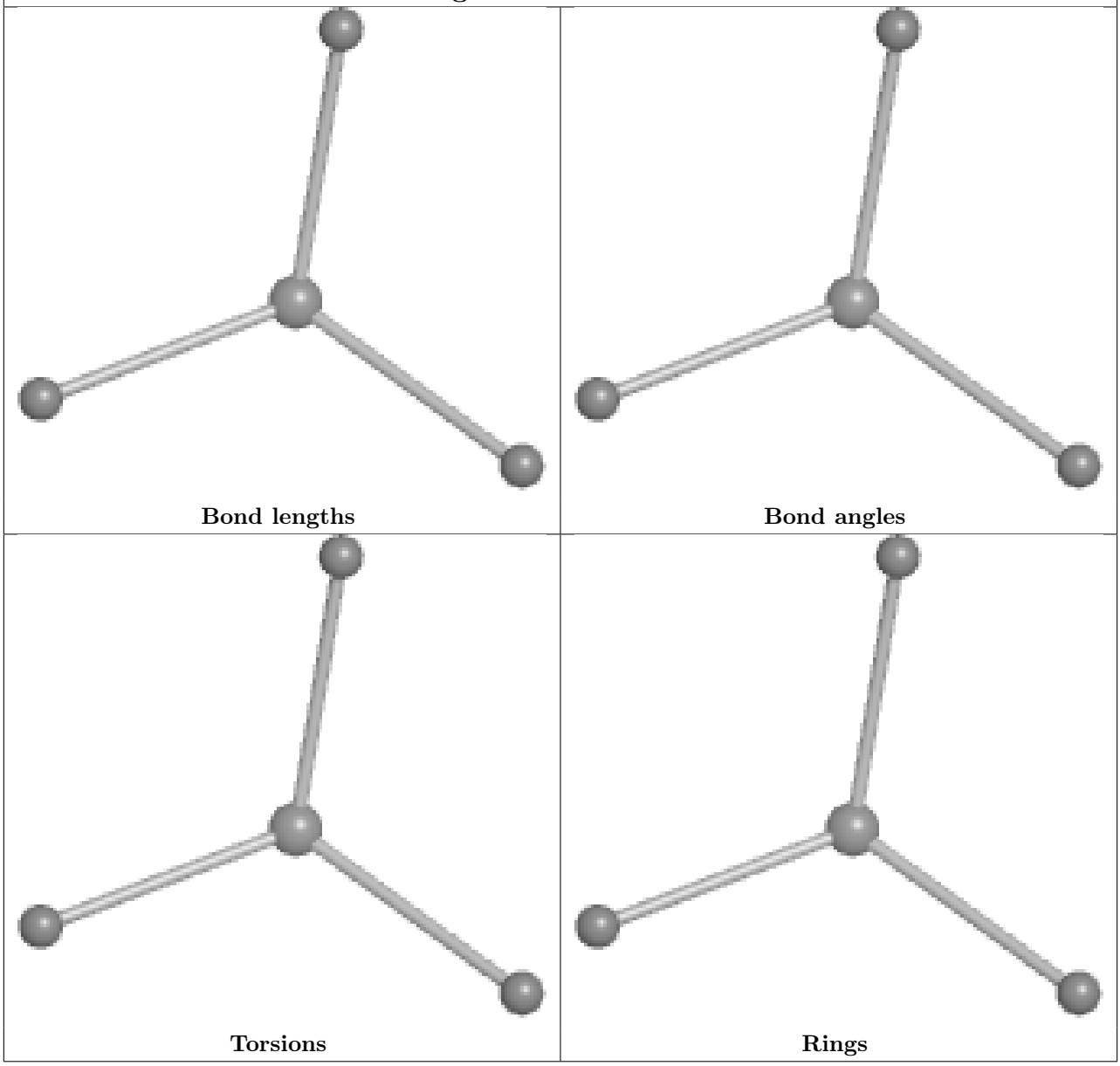


Torsions



Rings

Ligand BEF B 1403



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.

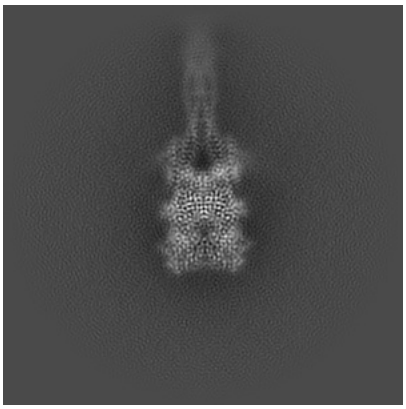
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-52959. These allow visual inspection of the internal detail of the map and identification of artifacts.

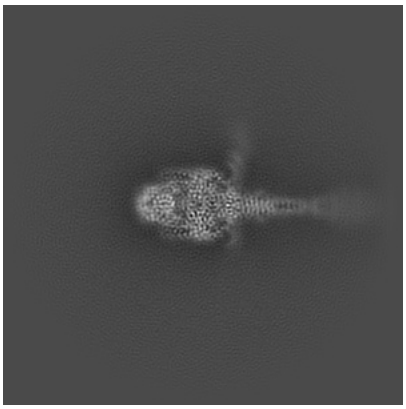
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

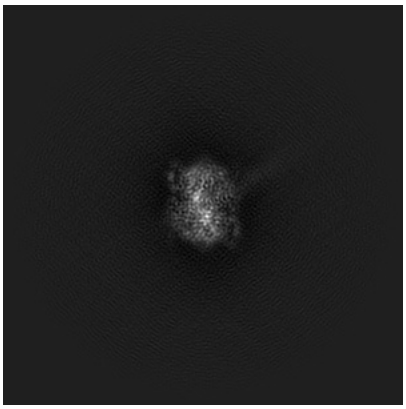
6.1.1 Primary map



X

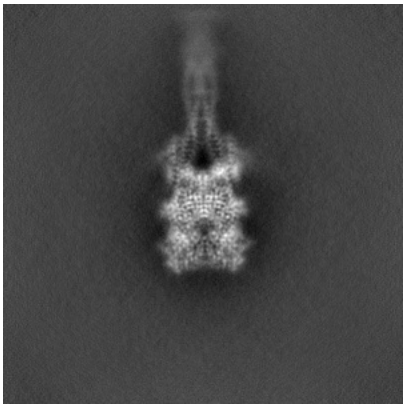


Y

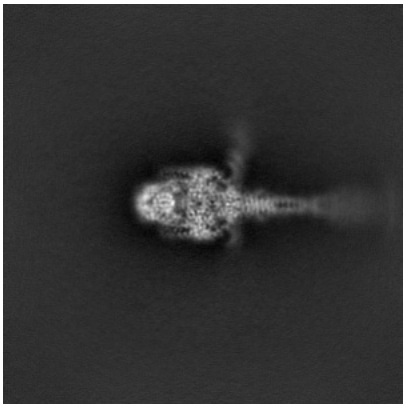


Z

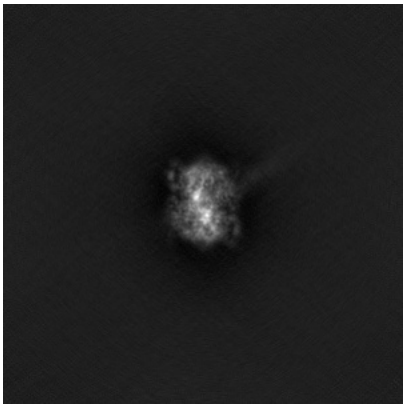
6.1.2 Raw map



X



Y

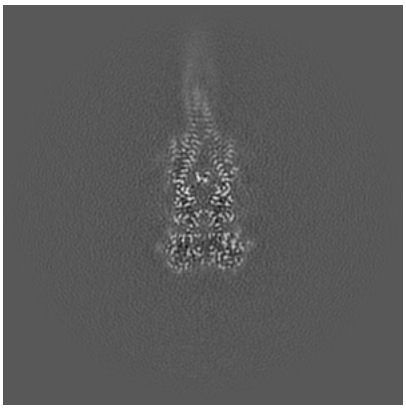


Z

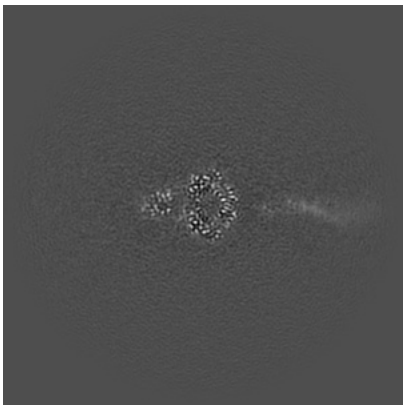
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

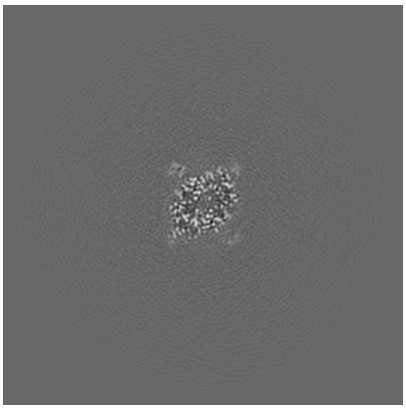
6.2.1 Primary map



X Index: 180

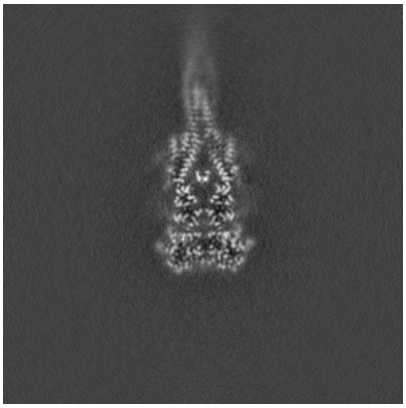


Y Index: 180

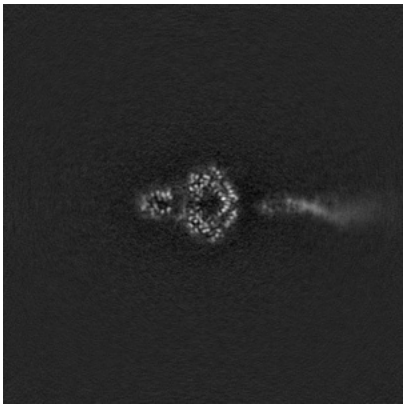


Z Index: 180

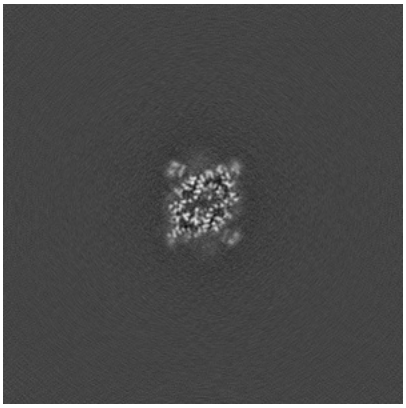
6.2.2 Raw map



X Index: 180



Y Index: 180

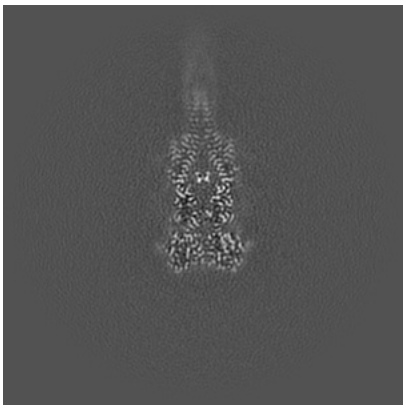


Z Index: 180

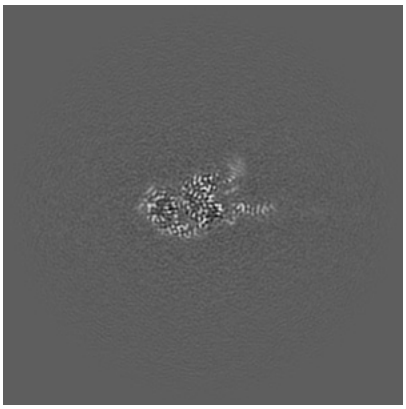
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

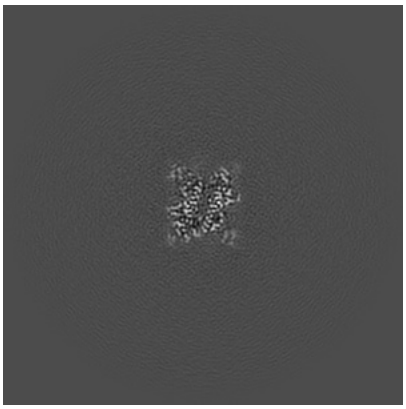
6.3.1 Primary map



X Index: 179

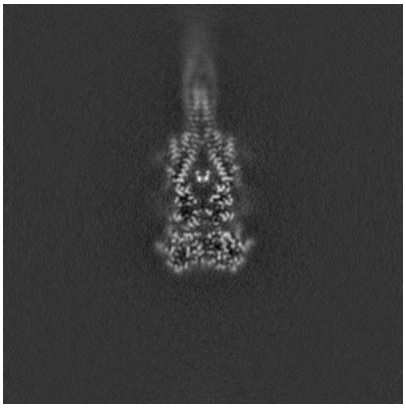


Y Index: 194

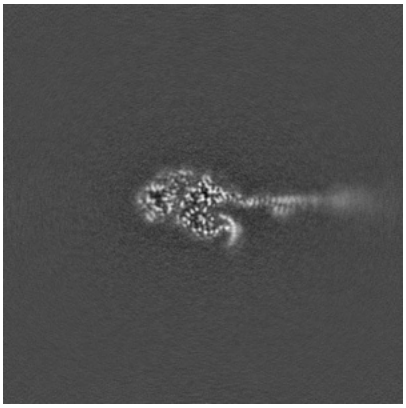


Z Index: 178

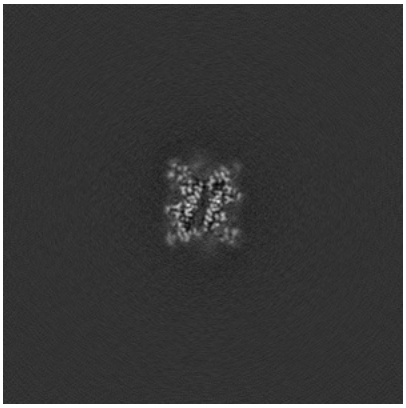
6.3.2 Raw map



X Index: 179



Y Index: 169

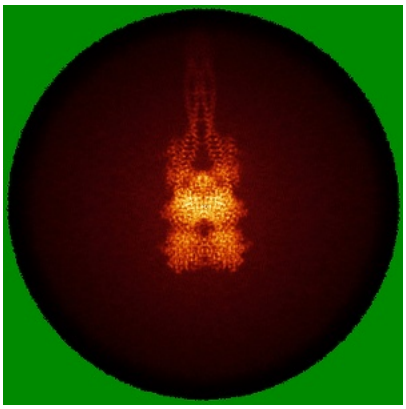


Z Index: 177

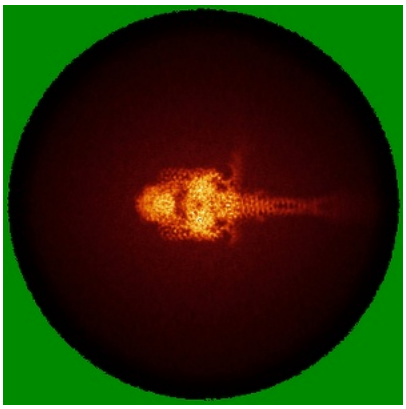
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

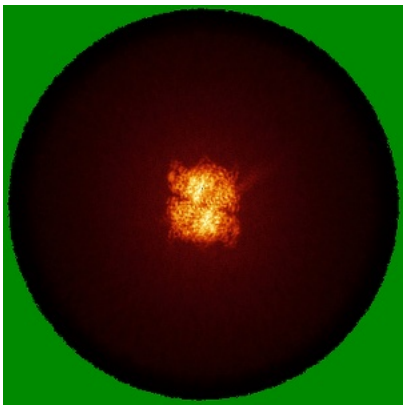
6.4.1 Primary map



X

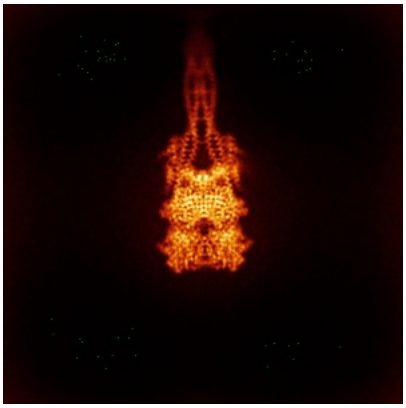


Y

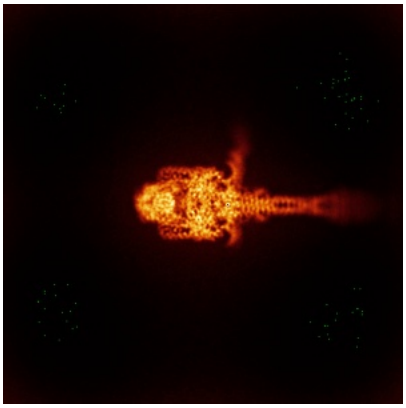


Z

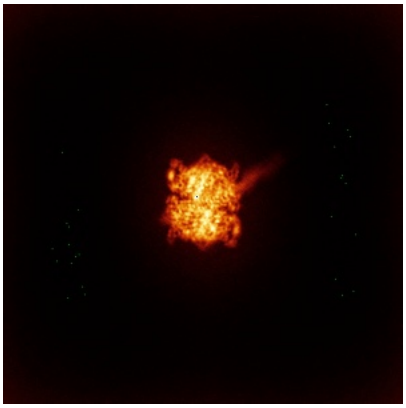
6.4.2 Raw map



X



Y



Z

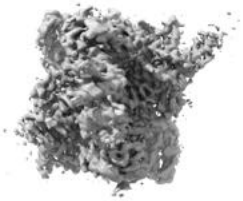
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.6. 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

X

Y

Z

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.

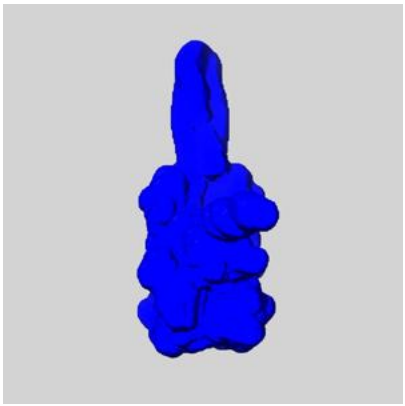
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

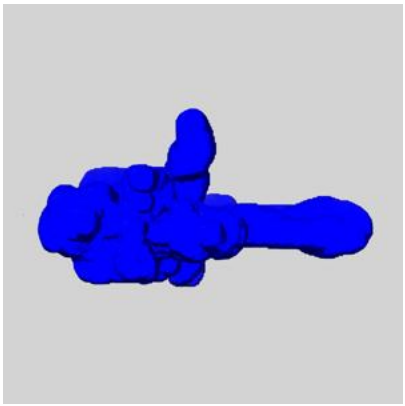
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

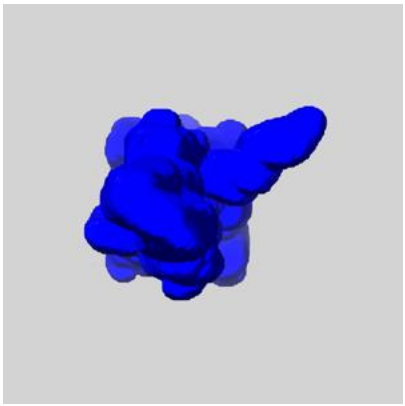
6.6.1 emd_52959_msk_1.map (i)



X



Y

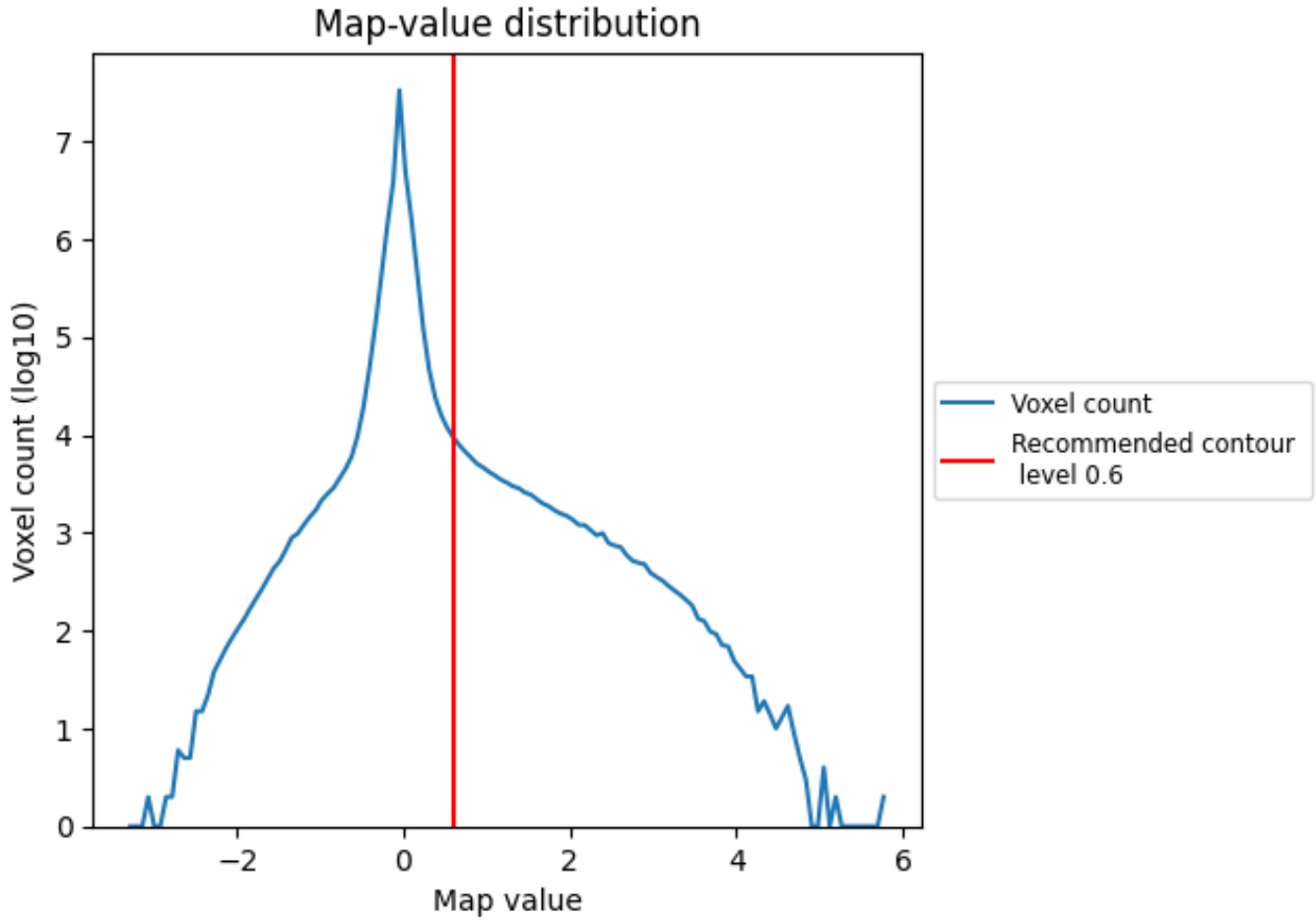


Z

7 Map analysis

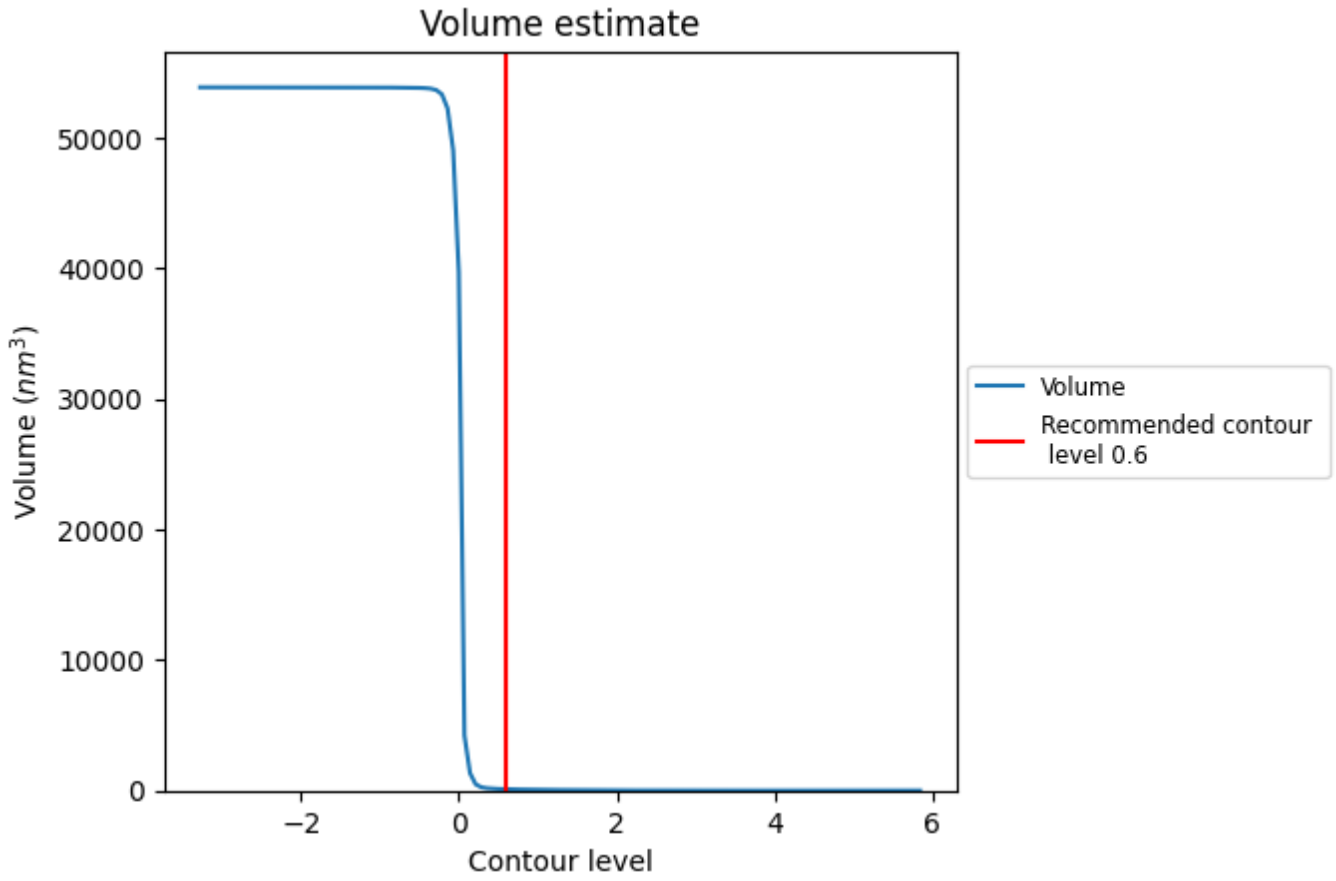
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

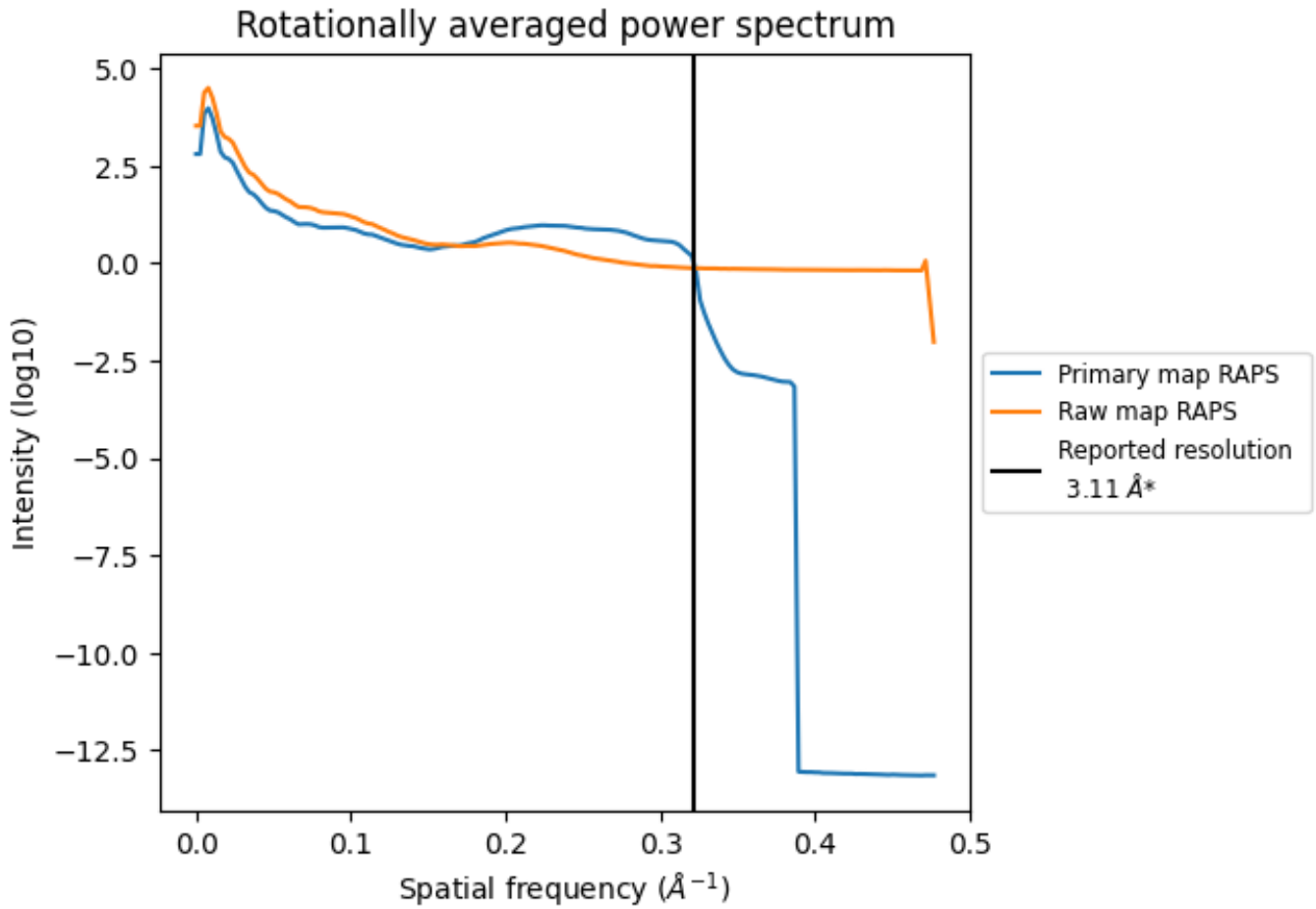
7.2 Volume estimate



The volume at the recommended contour level is 104 nm^3; this corresponds to an approximate mass of 94 kDa.

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

7.3 Rotationally averaged power spectrum (i)

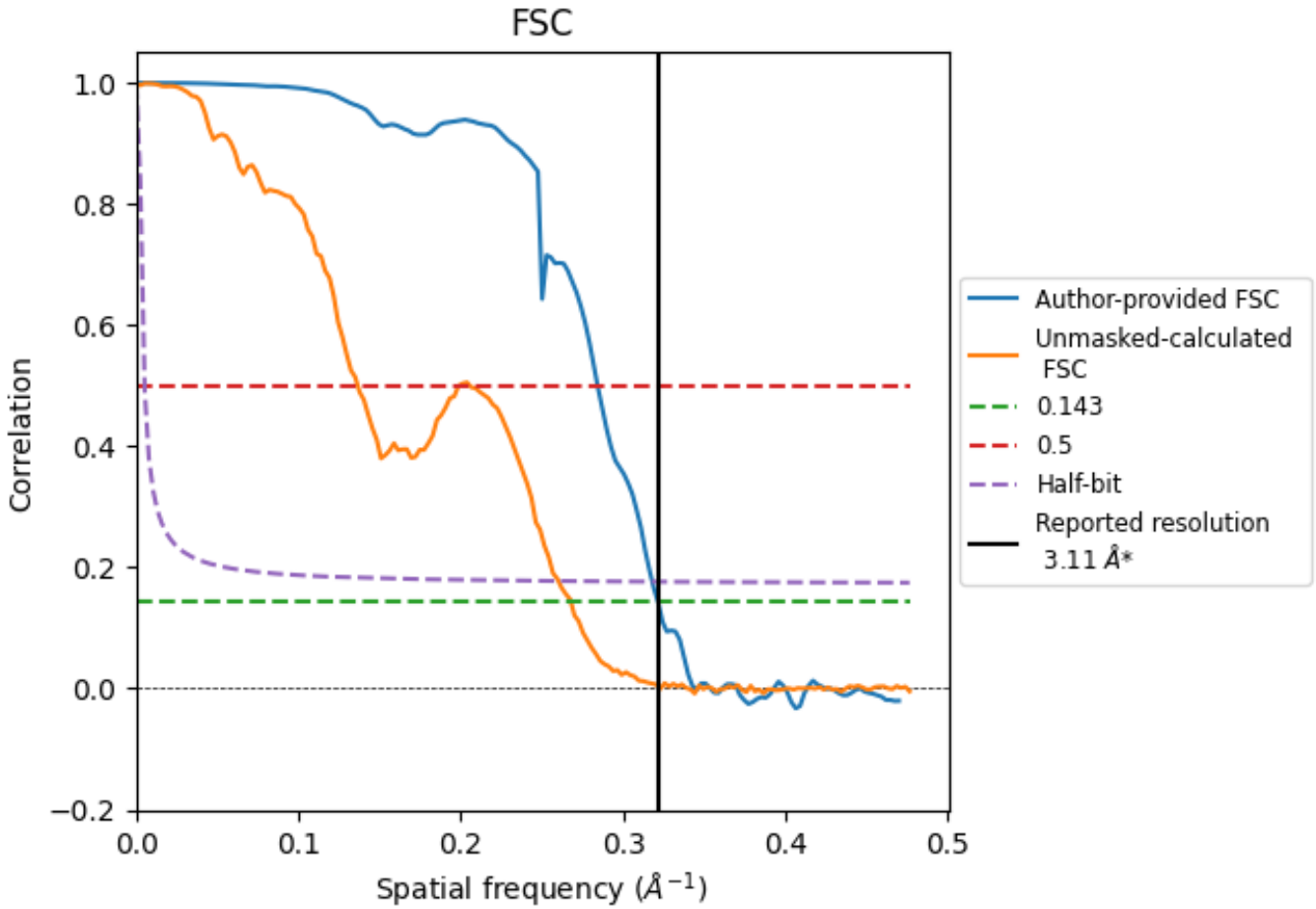


*Reported resolution corresponds to spatial frequency of 0.322 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.322 Å^{-1}

8.2 Resolution estimates (i)

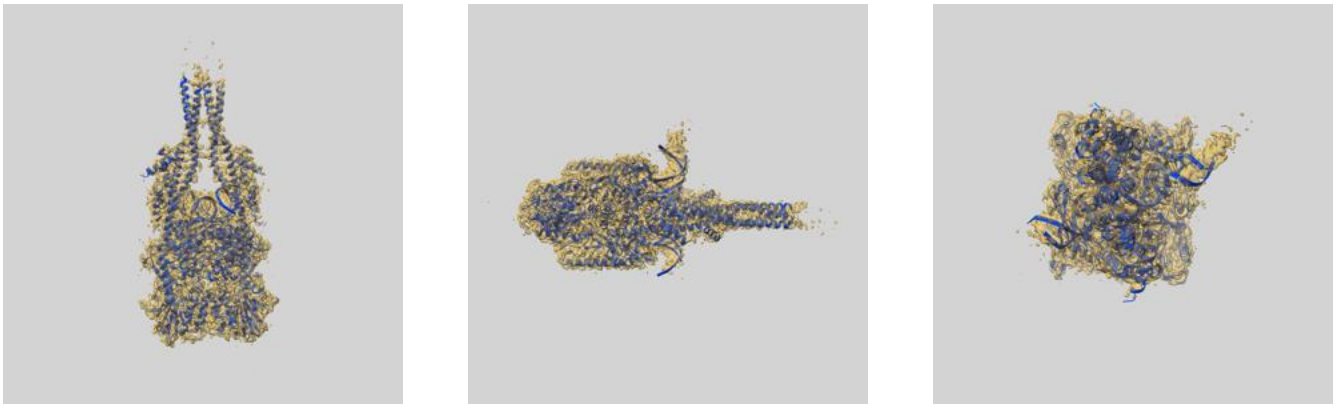
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.11	-	-
Author-provided FSC curve	3.11	3.52	3.14
Unmasked-calculated*	3.73	7.32	3.84

*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 3.73 differs from the reported value 3.11 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-52959 and PDB model 9Q9H. Per-residue inclusion information can be found in section 3 on page 9.

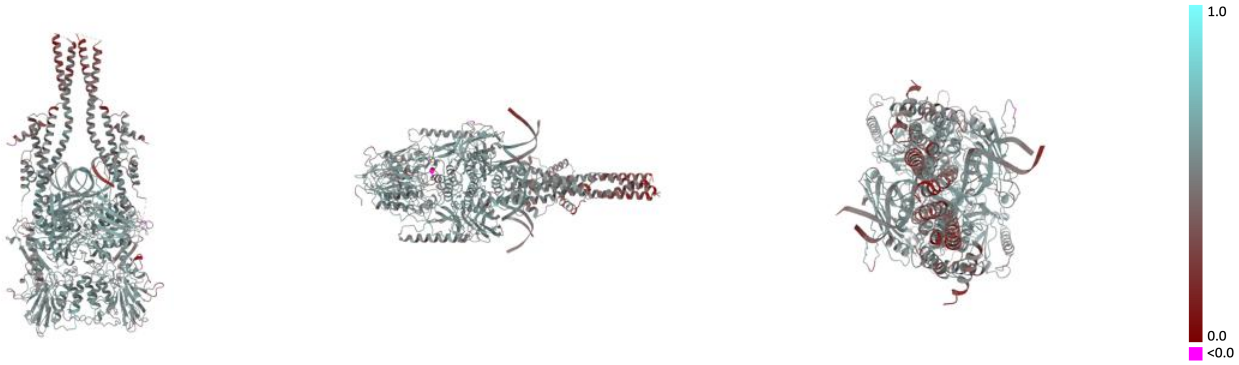
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.6 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.

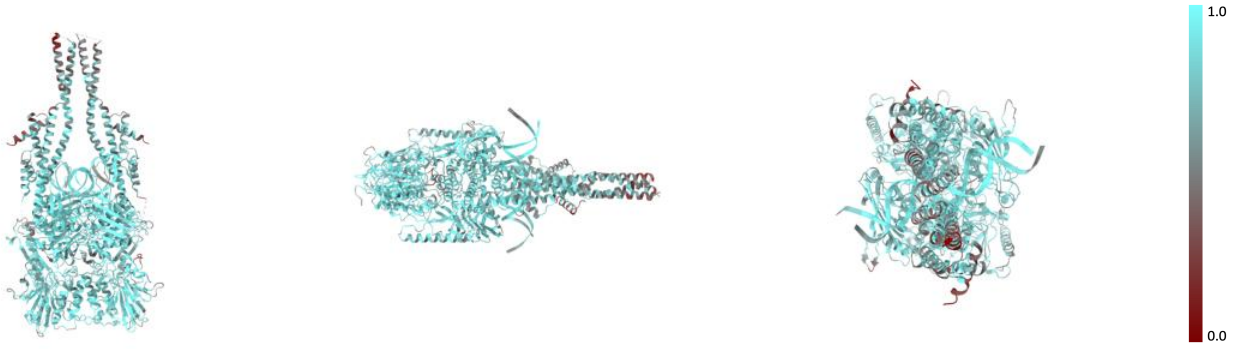
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

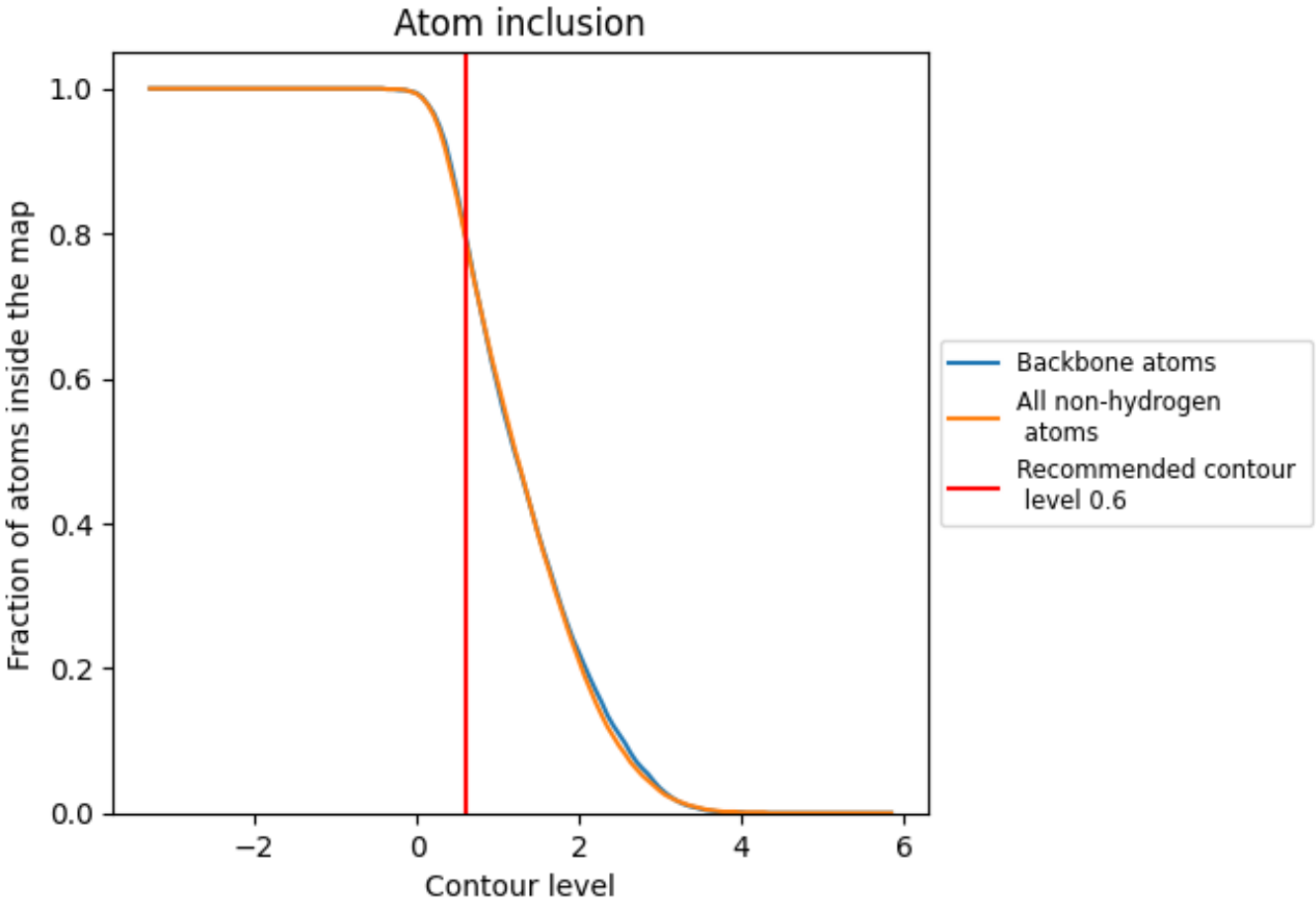
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.6).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 79% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7940	0.5100
A	0.8020	0.5110
B	0.8120	0.5190
D	0.7690	0.5090
E	0.7900	0.5020
P	0.8220	0.4640
T	0.9090	0.5300