Full wwPDB EM Validation Report ⓘ

Aug 26, 2024 – 02:05 PM EDT

PDB ID	:	8TWA
EMDB ID	:	EMD-41664
Title	:	Cryo-EM structure of S. cerevisiae Ctf18-RFC-PCNA-PolE-DNA complex
Authors	:	Yuan, Z.; Georgescu, R.; O'Donnell, M.; Li, H.
Deposited on	:	2023-08-20
Resolution	:	4.10 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:

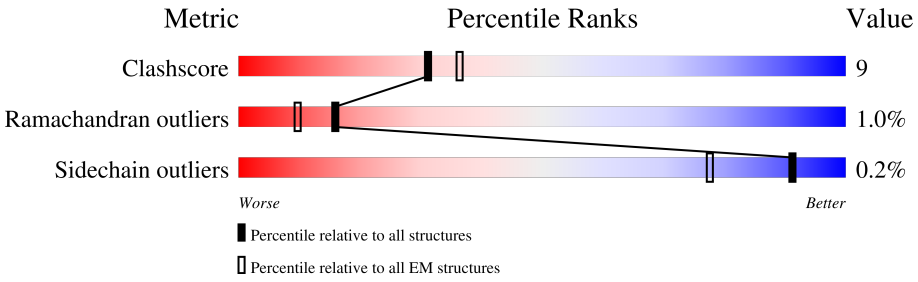
EMDB validation analysis	:	0.0.1.dev112
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	C	26	73% 27%
2	P	9	22% 56% 22%
3	T	15	20% 33% 60% 7%
4	E	2222	42% 7% 49%
5	D	132	25% 78% 21%
6	B	380	8% 33% 11% 55%
7	4	319	78% 21%
8	3	327	83% 17%

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Mol	Chain	Length	Quality of chain
9	2	340	
10	5	354	
11	1	741	
12	X	258	
12	Y	258	
12	Z	258	

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
13	SF4	E	2301	-	-	X	-
16	ADP	5	401	-	-	X	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 31914 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 Chromosome transmission fidelity protein 18.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	C	26	Total	C	N	O	0	0
			206	132	37	37		

- Molecule 2 is a DNA chain called Primer DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	9	Total	C	N	O	P	0	0
			183	88	29	57	9		

- Molecule 3 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	15	Total	C	N	O	P	0	0
			303	147	54	88	14		

- Molecule 4 is a protein called DNA polymerase epsilon catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	1123	Total	C	N	O	S	0	0
			8868	5642	1499	1686	41		

- Molecule 5 is a protein called Chromosome transmission fidelity protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	132	Total	C	N	O	S	0	0
			1014	642	171	194	7		

- Molecule 6 is a protein called Sister chromatid cohesion protein DCC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	171	Total	C	N	O	S	0	0
			1362	868	229	259	6		

- Molecule 7 is a protein called Replication factor C subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	4	319	Total	C	N	O	S	0	0
			2457	1545	440	460	12		

- Molecule 8 is a protein called Replication factor C subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	3	327	Total	C	N	O	S	0	0
			2563	1613	446	496	8		

- Molecule 9 is a protein called Replication factor C subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	2	340	Total	C	N	O	S	0	0
			2675	1690	461	514	10		

- Molecule 10 is a protein called Replication factor C subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	5	335	Total	C	N	O	S	0	0
			2613	1658	452	487	16		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	1	MET	-	initiating methionine	UNP P38251
5	2	SER	-	expression tag	UNP P38251
5	3	LEU	-	expression tag	UNP P38251
5	354	ASP	-	expression tag	UNP P38251

- Molecule 11 is a protein called Chromosome transmission fidelity protein 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1	457	Total	C	N	O	S	0	0
			3576	2274	630	658	14		

- Molecule 12 is a protein called Proliferating cell nuclear antigen.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	X	258	Total	C	N	O	S	0	0
			2003	1275	314	404	10		

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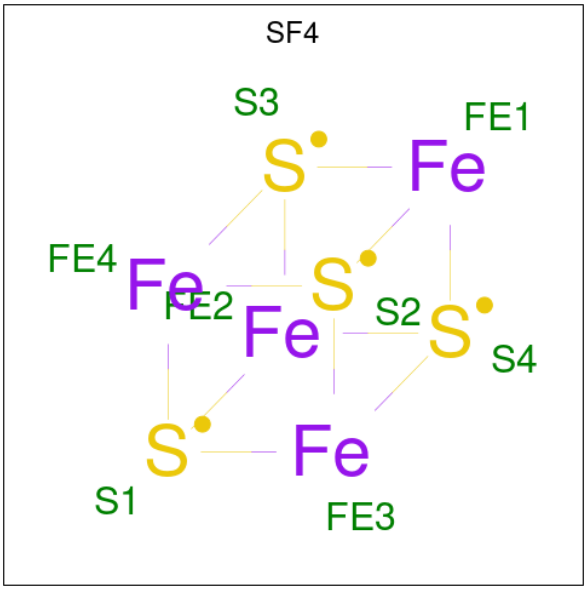
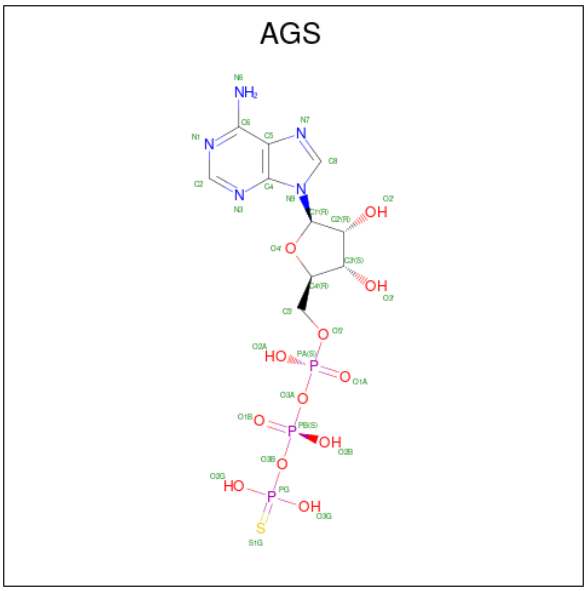
Mol	Chain	Residues	Atoms					AltConf	Trace
12	Y	258	Total	C	N	O	S	0	0
			1997	1272	316	401	8		
12	Z	254	Total	C	N	O	S	0	0
			1963	1258	308	387	10		

- Molecule 13 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
13	E	1	Total	Fe	S	0
			8	4	4	

- Molecule 14 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).

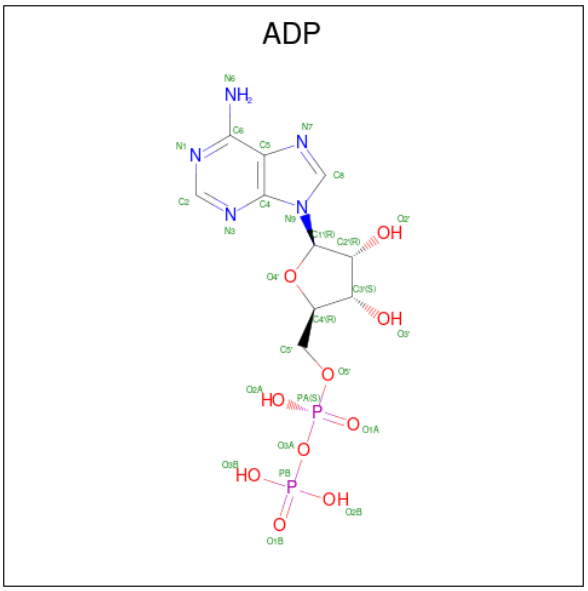


Mol	Chain	Residues	Atoms						AltConf
14	4	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
14	3	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
14	2	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
15	4	1	Total	Mg	0
			1	1	
15	3	1	Total	Mg	0
			1	1	
15	2	1	Total	Mg	0
			1	1	

- Molecule 16 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



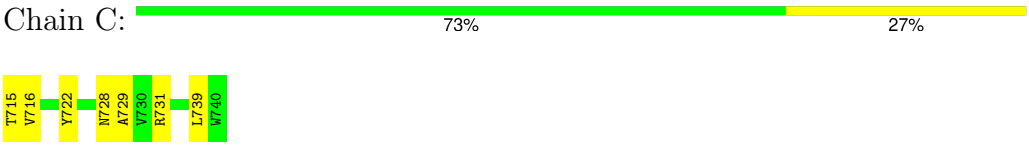
Mol	Chain	Residues	Atoms					AltConf
16	5	1	Total	C	N	O	P	0
			27	10	5	10	2	

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.

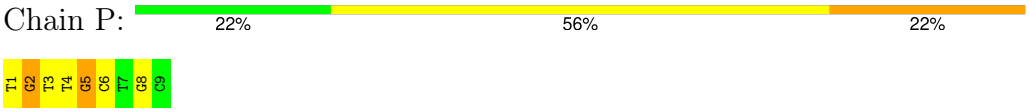
• Molecule 1: Chromosome transmission fidelity protein 18

Chain C:



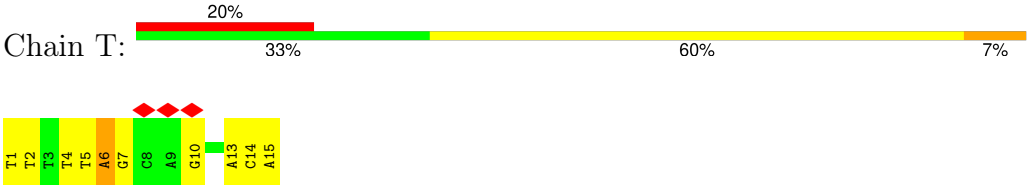
• Molecule 2: Primer DNA

Chain P:



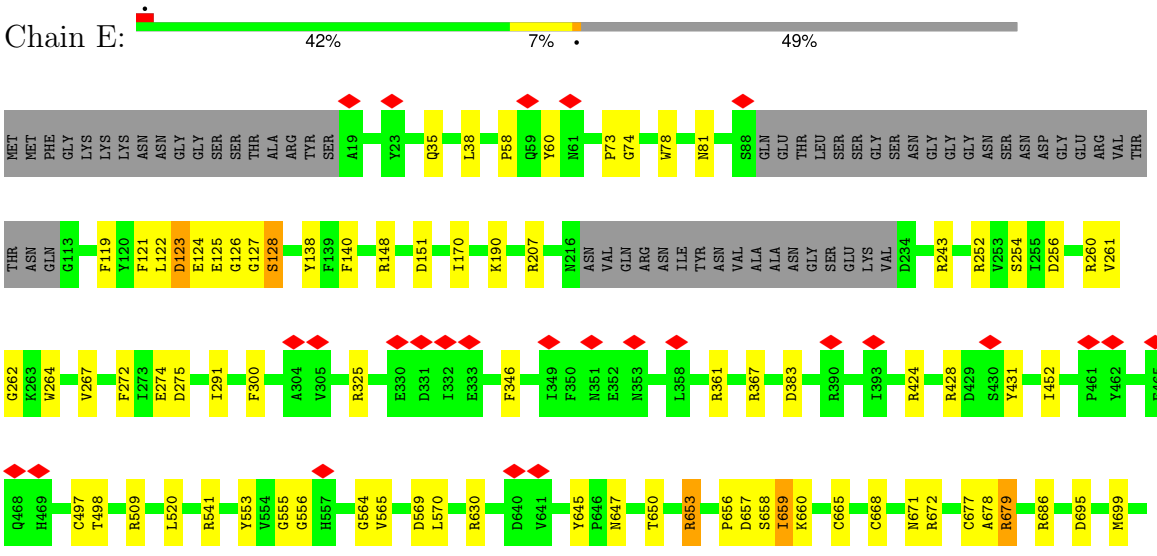
• Molecule 3: Template DNA

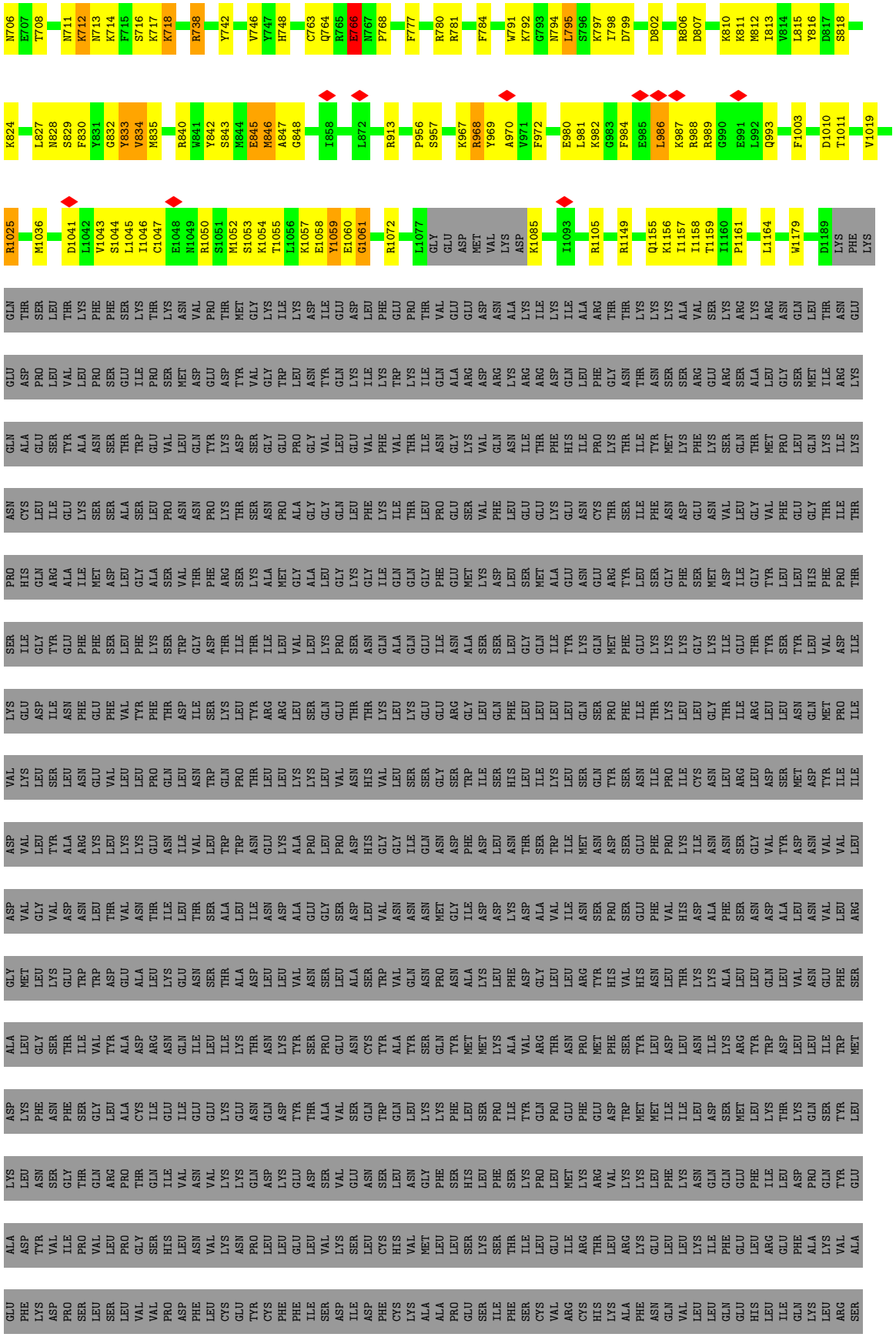
Chain T:

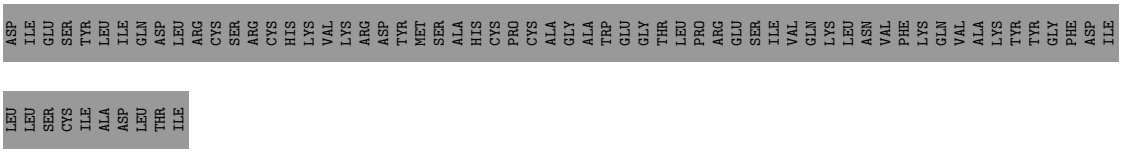


• Molecule 4: DNA polymerase epsilon catalytic subunit A

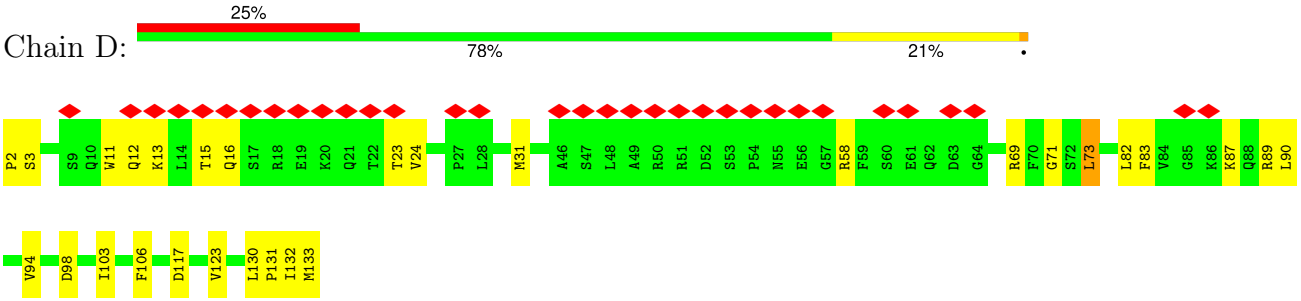
Chain E:



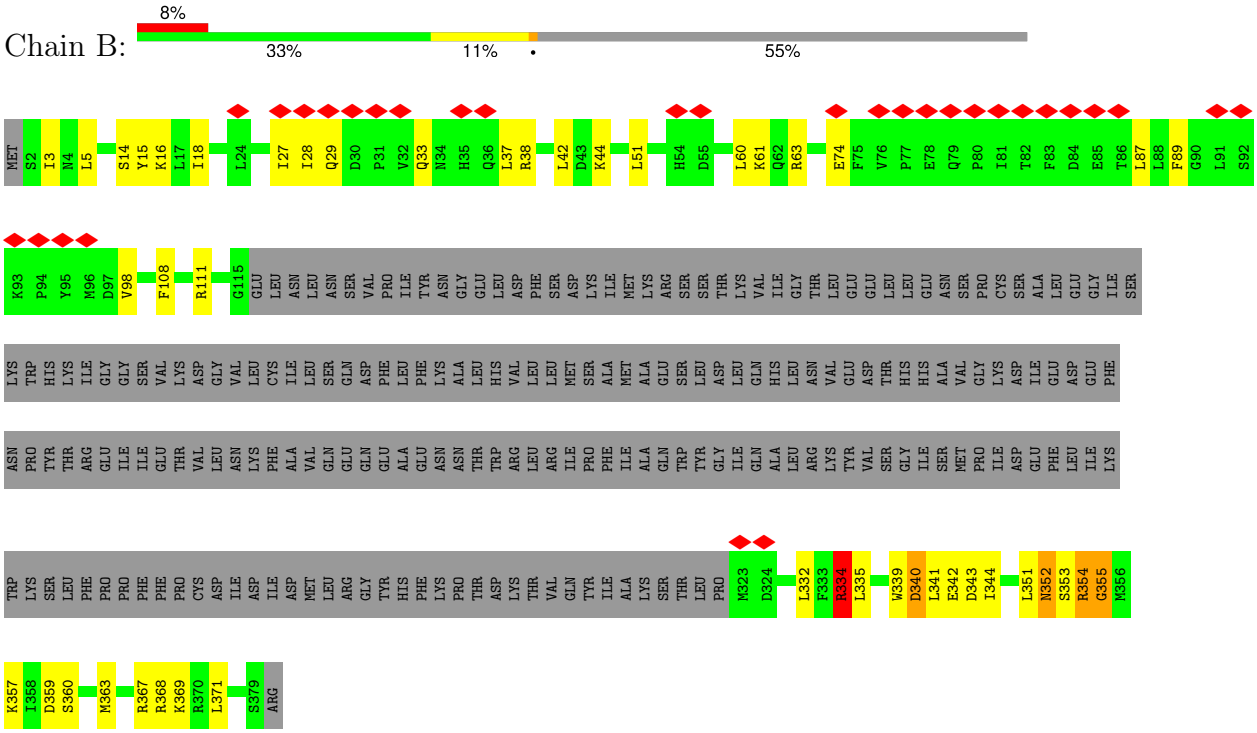

N706 E707 T708 N711 K712 N713 K714 F715 S716 K717 K718 R738 Y742 V746 Y747 H748 C763 Q764 R765 E766 N767 P768 F777 R780 R781 F784 W791 K792 G793 N794 L795 S796 K797 I798 D799 D802 R806 D807 K810 K811 M812 I813 V814 L815 Y816 D817 S818
K824 L827 N828 S829 F830 Y831 G832 Y833 V834 M835 R840 W841 Y842 S843 M844 E845 M846 A847 G848 I858 L872 R913 P956 S957 K967 R968 Y969 A970 V971 F972 E980 L981 K982 G983 F984 E985 L986 K987 R988 R989 G990 E991 L992 Q993 F1003 D1010 T1011 V1019
R1025 M1036 D1041 L1042 V1043 S1044 L1045 I1046 C1047 E1048 M1049 R1050 S1051 M1052 S1053 K1054 T1055 L1056 K1057 E1058 Y1059 E1060 G1061 R1072 L1077 GLY GLU ASP MET VAL LYS ASP K1085 I1093 R1105 R1149 Q1155 K1156 I1157 I1158 T1159 I1160 P1161 L1164 W1179 D1189 LYS PHE LYS



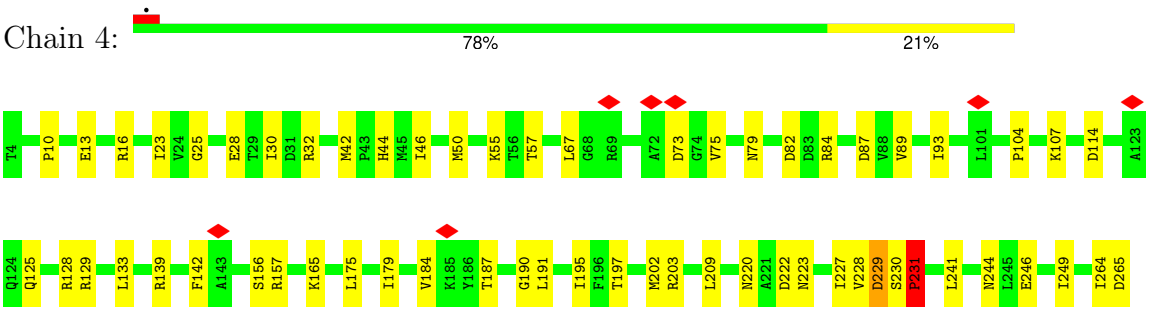
• Molecule 5: Chromosome transmission fidelity protein 8

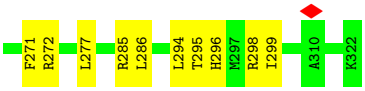


• Molecule 6: Sister chromatid cohesion protein DCC1

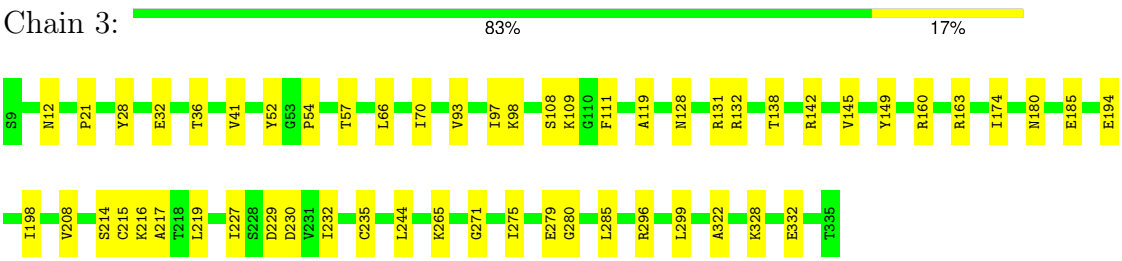


• Molecule 7: Replication factor C subunit 4

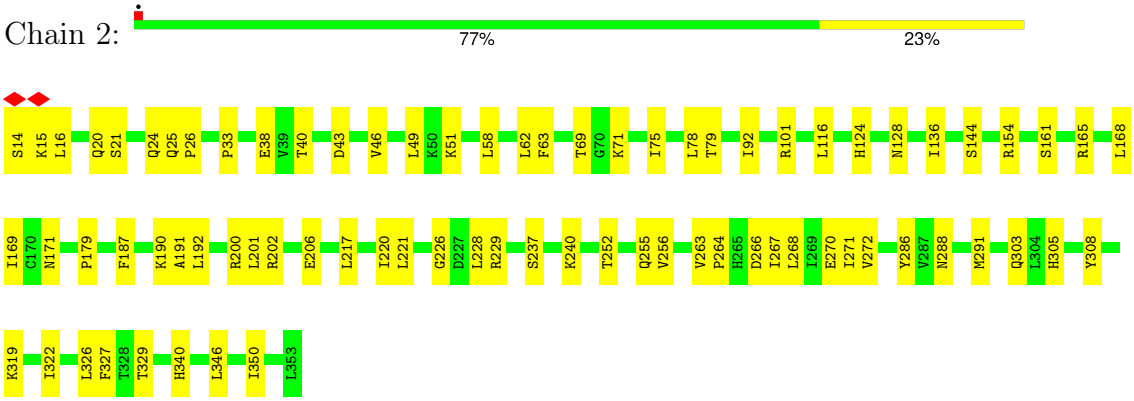




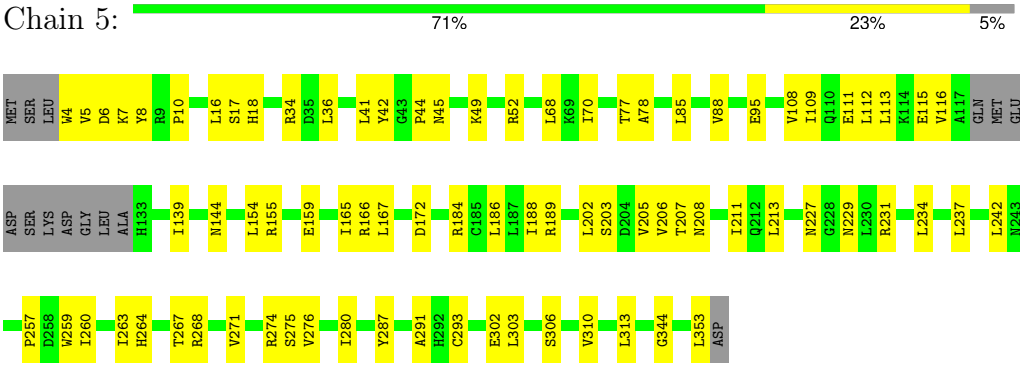
• Molecule 8: Replication factor C subunit 3



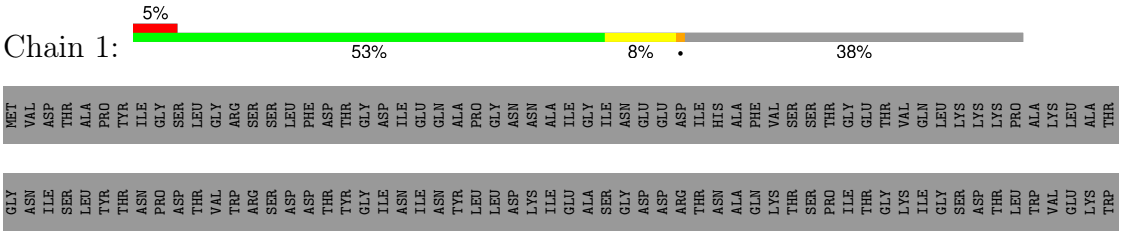
• Molecule 9: Replication factor C subunit 2

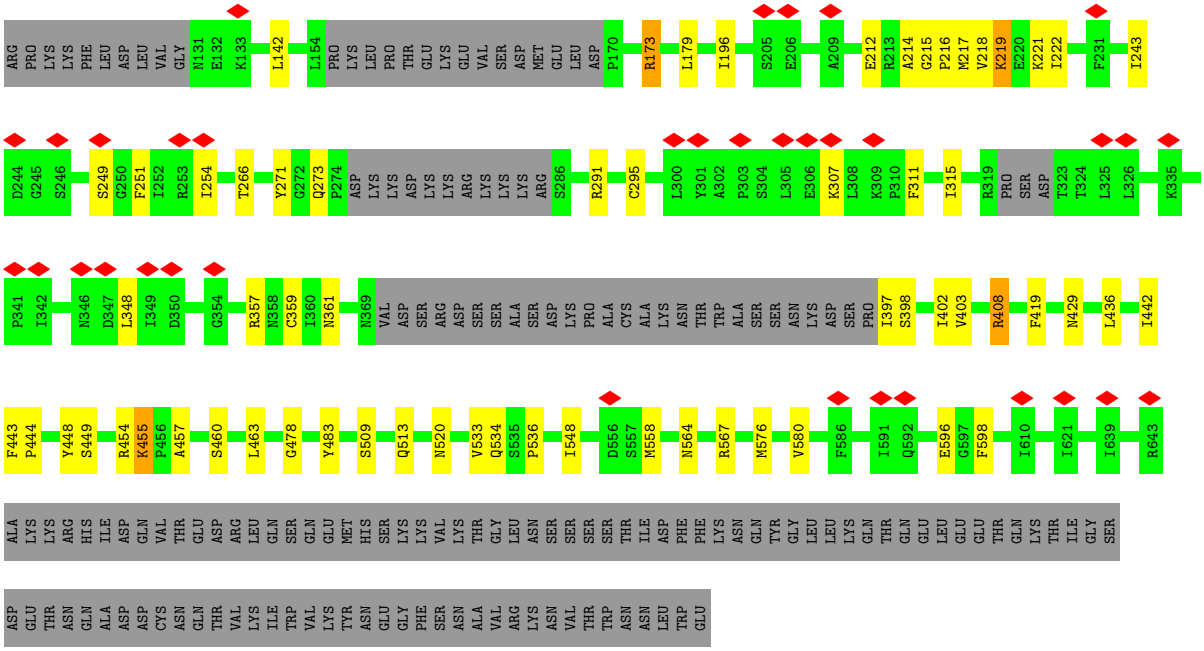


• Molecule 10: Replication factor C subunit 5



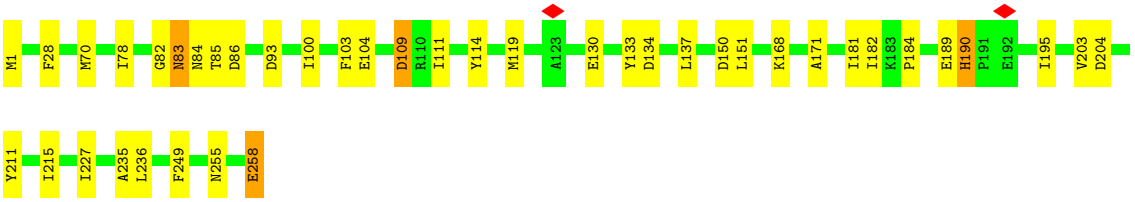
• Molecule 11: Chromosome transmission fidelity protein 18





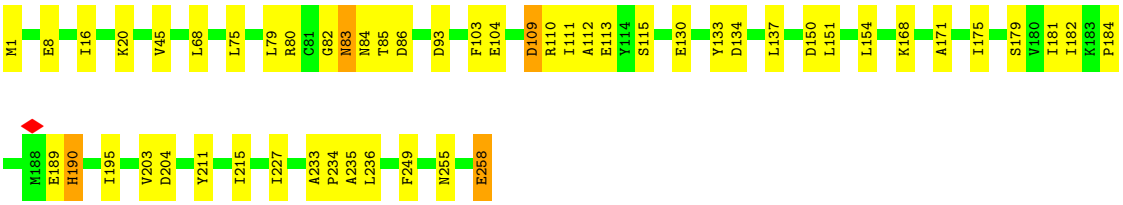
• Molecule 12: Proliferating cell nuclear antigen

Chain X:



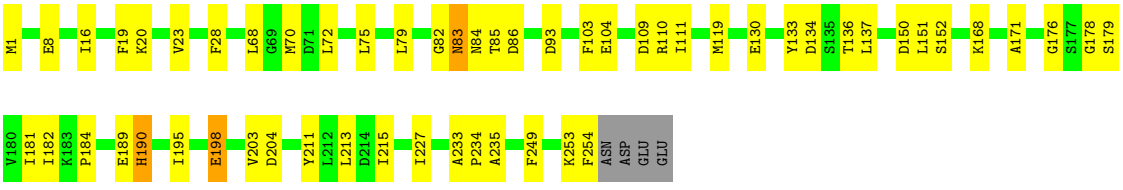
• Molecule 12: Proliferating cell nuclear antigen

Chain Y:



• Molecule 12: Proliferating cell nuclear antigen

Chain Z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87643	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.963	Depositor
Minimum map value	-0.430	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.144	Depositor
Map size (Å)	298.08002, 298.08002, 298.08002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82800007, 0.82800007, 0.82800007	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, AGS, MG, SF4

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	C	0.42	0/211	0.61	0/289
2	P	1.37	3/203 (1.5%)	1.13	0/311
3	T	1.41	1/339 (0.3%)	1.01	1/521 (0.2%)
4	E	0.70	1/9065 (0.0%)	0.98	30/12275 (0.2%)
5	D	0.36	0/1030	0.76	1/1387 (0.1%)
6	B	0.56	2/1387 (0.1%)	1.15	10/1871 (0.5%)
7	4	0.27	0/2491	0.41	0/3365
8	3	0.24	0/2602	0.39	0/3521
9	2	0.24	0/2720	0.38	0/3679
10	5	0.24	0/2650	0.39	0/3587
11	1	0.61	0/3639	0.85	4/4921 (0.1%)
12	X	0.63	2/2033 (0.1%)	0.82	1/2745 (0.0%)
12	Y	0.64	2/2026 (0.1%)	0.83	2/2737 (0.1%)
12	Z	0.59	0/1993	0.80	1/2692 (0.0%)
All	All	0.57	11/32389 (0.0%)	0.79	50/43901 (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
4	E	0	5
6	B	0	2
7	4	0	1
11	1	0	1
All	All	0	9

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	354	ARG	C-N	11.80	1.54	1.33
4	E	766	GLU	C-N	9.65	1.56	1.34
2	P	2	DG	C1'-N9	-7.70	1.36	1.47
12	Y	258	GLU	C-O	7.44	1.37	1.23
2	P	8	DG	C1'-N9	-7.42	1.36	1.47
12	X	258	GLU	C-O	7.32	1.37	1.23
12	Y	258	GLU	C-OXT	-7.28	1.09	1.23
12	X	258	GLU	C-OXT	-7.20	1.09	1.23
2	P	5	DG	C1'-N9	-5.64	1.39	1.47
6	B	355	GLY	C-N	-5.63	1.21	1.34
3	T	6	DA	C1'-N9	-5.51	1.39	1.47

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	334	ARG	O-C-N	-32.70	70.38	122.70
11	1	173	ARG	NE-CZ-NH1	11.99	126.30	120.30
6	B	334	ARG	CA-C-N	11.32	142.10	117.20
4	E	325	ARG	NE-CZ-NH1	10.16	125.38	120.30
11	1	173	ARG	NE-CZ-NH2	-9.93	115.33	120.30
4	E	913	ARG	NE-CZ-NH1	9.45	125.02	120.30
4	E	672	ARG	NE-CZ-NH2	-9.14	115.73	120.30
4	E	361	ARG	NE-CZ-NH1	9.01	124.80	120.30
6	B	87	LEU	CA-CB-CG	9.00	136.00	115.30
4	E	672	ARG	NE-CZ-NH1	8.98	124.79	120.30
4	E	243	ARG	NE-CZ-NH1	8.90	124.75	120.30
4	E	361	ARG	NE-CZ-NH2	-8.53	116.03	120.30
11	1	291	ARG	NE-CZ-NH1	8.25	124.42	120.30
4	E	738	ARG	NE-CZ-NH1	7.71	124.16	120.30
4	E	1105	ARG	NE-CZ-NH2	7.29	123.95	120.30
5	D	73	LEU	CA-CB-CG	7.26	132.00	115.30
11	1	408	ARG	NE-CZ-NH1	7.26	123.93	120.30
4	E	424	ARG	NE-CZ-NH1	7.11	123.86	120.30
12	Y	68	LEU	CA-CB-CG	7.11	131.65	115.30
12	Z	68	LEU	CA-CB-CG	7.05	131.51	115.30
4	E	968	ARG	NE-CZ-NH2	6.94	123.77	120.30
4	E	766	GLU	O-C-N	-6.90	111.66	122.70
4	E	252	ARG	NE-CZ-NH1	6.82	123.71	120.30
4	E	1072	ARG	NE-CZ-NH1	6.80	123.70	120.30
4	E	148	ARG	NE-CZ-NH1	6.75	123.67	120.30
6	B	334	ARG	C-N-CA	6.59	138.18	121.70
6	B	352	ASN	O-C-N	6.47	133.05	122.70
4	E	367	ARG	NE-CZ-NH2	6.25	123.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	42	LEU	CA-CB-CG	6.13	129.40	115.30
4	E	1025	ARG	NE-CZ-NH1	6.04	123.32	120.30
4	E	679	ARG	NE-CZ-NH1	6.02	123.31	120.30
4	E	645	TYR	CB-CG-CD2	-5.95	117.43	121.00
4	E	1149	ARG	NE-CZ-NH1	5.93	123.27	120.30
6	B	37	LEU	CA-CB-CG	5.87	128.80	115.30
4	E	1050	ARG	NE-CZ-NH1	5.85	123.23	120.30
4	E	1059	TYR	CA-CB-CG	-5.83	102.32	113.40
4	E	653	ARG	NE-CZ-NH1	5.81	123.21	120.30
4	E	428	ARG	NE-CZ-NH1	5.75	123.18	120.30
6	B	352	ASN	CA-C-N	-5.72	104.62	117.20
6	B	371	LEU	CA-CB-CG	5.65	128.29	115.30
4	E	541	ARG	NE-CZ-NH1	5.52	123.06	120.30
6	B	355	GLY	C-N-CA	-5.42	108.16	121.70
12	Y	258	GLU	CA-C-O	-5.40	108.77	120.10
4	E	1105	ARG	NH1-CZ-NH2	-5.36	113.51	119.40
4	E	151	ASP	CB-CG-OD1	5.33	123.10	118.30
12	X	258	GLU	CA-C-O	-5.33	108.91	120.10
4	E	989	ARG	NE-CZ-NH1	5.26	122.93	120.30
3	T	10	DG	C3'-C2'-C1'	-5.10	96.38	102.50
4	E	272	PHE	CB-CG-CD2	-5.05	117.26	120.80
4	E	207	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	1	408	ARG	Sidechain
7	4	272	ARG	Sidechain
6	B	334	ARG	Mainchain
6	B	355	GLY	Mainchain
4	E	123	ASP	Mainchain
4	E	509	ARG	Sidechain
4	E	630	ARG	Sidechain
4	E	766	GLU	Mainchain
4	E	81	ASN	Mainchain

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	C	206	0	183	8	0
2	P	183	0	102	6	0
3	T	303	0	172	15	0
4	E	8868	0	8504	149	0
5	D	1014	0	1007	28	0
6	B	1362	0	1357	34	0
7	4	2457	0	2496	55	0
8	3	2563	0	2577	41	0
9	2	2675	0	2701	55	0
10	5	2613	0	2709	66	0
11	1	3576	0	3538	56	0
12	X	2003	0	1977	34	0
12	Y	1997	0	1979	48	0
12	Z	1963	0	1958	47	0
13	E	8	0	0	6	0
14	2	31	0	12	3	0
14	3	31	0	12	2	0
14	4	31	0	12	3	0
15	2	1	0	0	0	0
15	3	1	0	0	0	0
15	4	1	0	0	0	0
16	5	27	0	12	9	0
All	All	31914	0	31308	542	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 9.

All (542) 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)
4:E:706:ASN:CB	11:1:311:PHE:CE1	2.39	1.06
7:4:156:SER:O	11:1:361:ASN:CB	2.08	1.02
10:5:5:VAL:HG13	16:5:401:ADP:O3'	1.58	1.01
12:X:109:ASP:O	12:Y:181:ILE:O	1.77	1.01
9:2:40:THR:HG21	9:2:200:ARG:HB2	1.43	1.00
4:E:713:ASN:HB3	4:E:716:SER:HB2	1.41	0.98
12:Y:236:LEU:HD12	12:Y:249:PHE:CE2	1.99	0.96
12:X:236:LEU:HD13	12:X:249:PHE:CE2	2.01	0.96
4:E:656:PRO:HB3	4:E:843:SER:HB2	1.46	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:X:82:GLY:O	12:X:86:ASP:HB2	1.77	0.85
7:4:229:ASP:HB2	8:3:163:ARG:HH21	1.42	0.85
4:E:706:ASN:CB	11:1:311:PHE:CZ	2.59	0.84
12:Y:82:GLY:O	12:Y:86:ASP:HB2	1.76	0.84
4:E:834:VAL:HG12	4:E:834:VAL:O	1.76	0.83
3:T:5:DT:H4'	4:E:835:MET:CB	2.08	0.83
9:2:288:ASN:HD21	10:5:227:ASN:HD21	1.27	0.82
12:X:236:LEU:HD13	12:X:249:PHE:CZ	2.17	0.79
4:E:60:TYR:CB	4:E:73:PRO:HG3	2.13	0.79
8:3:41:VAL:HG21	8:3:66:LEU:HD11	1.64	0.79
4:E:1054:LYS:HA	4:E:1085:LYS:CB	2.13	0.79
12:Z:137:LEU:HD11	12:Z:227:ILE:HD12	1.65	0.78
4:E:714:LYS:HA	11:1:596:GLU:O	1.84	0.78
12:X:137:LEU:HD11	12:X:227:ILE:HD12	1.66	0.77
12:Y:137:LEU:HD11	12:Y:227:ILE:HD12	1.66	0.77
2:P:2:DG:H2'	2:P:3:DT:H71	1.67	0.76
7:4:197:THR:HG22	7:4:231:PRO:HD3	1.66	0.76
10:5:4:TRP:HD1	10:5:6:ASP:H	1.32	0.76
12:Z:23:VAL:O	12:Z:72:LEU:HD23	1.85	0.76
9:2:252:THR:OG1	9:2:255:GLN:HG3	1.85	0.75
4:E:671:ASN:HB2	13:E:2301:SF4:S3	2.26	0.75
12:Y:104:GLU:HG2	12:Y:111:ILE:HG12	1.68	0.75
12:X:104:GLU:HG2	12:X:111:ILE:HG12	1.68	0.75
12:Z:104:GLU:HG2	12:Z:111:ILE:HG12	1.68	0.74
8:3:174:ILE:HD11	8:3:208:VAL:HG21	1.69	0.74
9:2:263:VAL:H	9:2:303:GLN:HE22	1.33	0.73
4:E:845:GLU:O	4:E:847:ALA:N	2.21	0.73
7:4:265:ASP:OD2	8:3:52:TYR:OH	2.05	0.73
4:E:784:PHE:CD1	4:E:816:TYR:HD1	2.07	0.73
1:C:722:TYR:H	4:E:1041:ASP:CB	2.01	0.73
3:T:4:DT:O2	4:E:832:GLY:HA3	1.90	0.72
4:E:827:LEU:HA	4:E:830:PHE:HD2	1.55	0.71
4:E:834:VAL:O	4:E:834:VAL:CG1	2.38	0.70
4:E:261:VAL:HB	4:E:497:CYS:HB3	1.72	0.70
4:E:784:PHE:CD1	4:E:816:TYR:CD1	2.79	0.70
4:E:665:CYS:HA	13:E:2301:SF4:S2	2.30	0.70
4:E:784:PHE:HD1	4:E:816:TYR:CD1	2.09	0.69
12:Z:136:THR:HB	12:Z:198:GLU:HG2	1.74	0.69
12:Y:75:LEU:HG	12:Y:79:LEU:HD11	1.74	0.69
12:Z:75:LEU:HG	12:Z:79:LEU:HD11	1.74	0.69
12:Y:83:ASN:ND2	12:Y:110:ARG:HH22	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:75:LEU:O	12:Z:79:LEU:HG	1.93	0.69
12:Z:83:ASN:ND2	12:Z:110:ARG:HH22	1.90	0.69
5:D:103:ILE:HD11	6:B:15:TYR:HB3	1.75	0.69
12:Y:75:LEU:O	12:Y:79:LEU:HG	1.93	0.68
7:4:296:HIS:HD1	11:1:483:TYR:HE2	1.38	0.68
8:3:229:ASP:OD1	8:3:230:ASP:N	2.25	0.68
12:Y:236:LEU:HD12	12:Y:249:PHE:HE2	1.55	0.68
7:4:203:ARG:HE	14:4:401:AGS:H5'1	1.60	0.67
8:3:229:ASP:OD1	8:3:230:ASP:OD1	2.12	0.67
12:X:1:MET:HG2	12:X:93:ASP:HA	1.78	0.66
11:1:454:ARG:O	11:1:457:ALA:N	2.28	0.66
7:4:82:ASP:OD1	8:3:98:LYS:NZ	2.29	0.66
12:Z:1:MET:HG2	12:Z:93:ASP:HA	1.78	0.65
4:E:781:ARG:HE	4:E:824:LYS:HB2	1.61	0.65
4:E:124:GLU:O	4:E:126:GLY:N	2.30	0.65
4:E:38:LEU:HG	11:1:567:ARG:HE	1.61	0.65
8:3:271:GLY:HA3	9:2:190:LYS:HD3	1.79	0.65
12:Y:1:MET:HG2	12:Y:93:ASP:HA	1.78	0.64
3:T:1:DT:H4'	3:T:2:DT:OP1	1.97	0.64
4:E:986:LEU:O	4:E:988:ARG:N	2.30	0.64
4:E:677:CYS:O	4:E:764:GLN:HG2	1.98	0.64
4:E:1155:GLN:HA	4:E:1159:THR:OG1	1.98	0.63
7:4:13:GLU:HG3	8:3:138:THR:HG21	1.79	0.63
4:E:845:GLU:O	4:E:848:GLY:N	2.29	0.63
7:4:46:ILE:HG12	7:4:142:PHE:HB2	1.80	0.63
7:4:229:ASP:CB	8:3:163:ARG:HH21	2.09	0.63
10:5:45:ASN:O	10:5:229:ASN:ND2	2.32	0.63
4:E:125:GLU:C	6:B:368:ARG:O	2.37	0.63
6:B:332:LEU:O	6:B:339:TRP:NE1	2.32	0.63
11:1:243:ILE:HD13	11:1:295:CYS:HB3	1.81	0.63
12:X:82:GLY:C	12:X:84:ASN:H	2.03	0.62
7:4:286:LEU:HD21	11:1:419:PHE:HZ	1.64	0.62
7:4:227:ILE:HG23	7:4:228:VAL:HG23	1.82	0.62
5:D:15:THR:HG21	6:B:29:GLN:HE22	1.64	0.62
9:2:192:LEU:HD12	9:2:228:LEU:HB2	1.82	0.62
12:Z:82:GLY:C	12:Z:84:ASN:H	2.03	0.61
12:Y:82:GLY:C	12:Y:84:ASN:H	2.03	0.61
10:5:10:PRO:HG2	16:5:401:ADP:C6	2.35	0.61
3:T:7:DG:H21	4:E:967:LYS:HD2	1.65	0.61
7:4:84:ARG:NH1	7:4:114:ASP:O	2.33	0.61
10:5:4:TRP:HB3	10:5:7:LYS:HG2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:5:205:VAL:HG21	10:5:234:LEU:HD21	1.82	0.61
4:E:738:ARG:HB3	4:E:742:TYR:CE2	2.36	0.61
7:4:175:LEU:HD22	7:4:209:LEU:HD22	1.84	0.60
10:5:274:ARG:O	10:5:274:ARG:HG3	2.01	0.60
8:3:285:LEU:HD13	8:3:299:LEU:HD21	1.84	0.60
4:E:986:LEU:C	4:E:988:ARG:H	2.06	0.60
10:5:68:LEU:HD11	11:1:536:PRO:HA	1.84	0.60
6:B:341:LEU:O	6:B:344:ILE:N	2.34	0.59
7:4:156:SER:OG	11:1:357:ARG:HD2	2.02	0.59
8:3:12:ASN:O	9:2:165:ARG:NH2	2.35	0.59
4:E:35:GLN:OE1	11:1:564:ASN:HB3	2.02	0.59
7:4:67:LEU:HD12	7:4:75:VAL:HG23	1.84	0.59
2:P:5:DG:H2"	2:P:6:DC:H5'	1.84	0.59
4:E:711:ASN:C	4:E:713:ASN:H	2.06	0.59
5:D:12:GLN:NE2	6:B:28:ILE:O	2.36	0.59
4:E:1059:TYR:C	4:E:1061:GLY:N	2.54	0.59
4:E:300:PHE:CB	4:E:1085:LYS:N	2.66	0.58
4:E:657:ASP:O	4:E:766:GLU:HG2	2.02	0.58
7:4:128:ARG:HE	7:4:157:ARG:HH21	1.49	0.58
12:Y:82:GLY:HA2	12:Y:103:PHE:CD2	2.38	0.58
10:5:36:LEU:O	10:5:166:ARG:NH1	2.36	0.58
6:B:351:LEU:O	6:B:352:ASN:OD1	2.21	0.58
2:P:1:DT:OP1	4:E:1179:TRP:HZ2	1.86	0.58
10:5:344:GLY:HA3	11:1:460:SER:CB	2.33	0.58
12:Z:82:GLY:HA2	12:Z:103:PHE:CD2	2.38	0.58
4:E:658:SER:O	4:E:659:ILE:C	2.41	0.58
11:1:173:ARG:HH22	11:1:266:THR:CG2	2.17	0.58
7:4:57:THR:HG21	14:4:401:AGS:H3'	1.86	0.58
4:E:656:PRO:HB3	4:E:843:SER:CB	2.30	0.57
12:Y:45:VAL:HG11	12:Y:258:GLU:HB2	1.86	0.57
12:Y:203:VAL:HG12	12:Y:204:ASP:N	2.19	0.57
1:C:731:ARG:HH21	6:B:61:LYS:HG3	1.69	0.57
1:C:715:THR:HG23	1:C:716:VAL:HG23	1.86	0.57
10:5:244:ASN:HD22	10:5:248:LEU:HA	1.69	0.57
12:Z:203:VAL:HG12	12:Z:204:ASP:N	2.19	0.57
6:B:341:LEU:C	6:B:343:ASP:N	2.58	0.57
12:X:82:GLY:HA2	12:X:103:PHE:CD2	2.38	0.57
4:E:799:ASP:OD1	4:E:799:ASP:N	2.38	0.57
4:E:78:TRP:HE1	4:E:262:GLY:C	2.07	0.57
4:E:262:GLY:C	4:E:498:THR:HG22	2.24	0.57
8:3:185:GLU:OE1	8:3:216:LYS:NZ	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:121:PHE:C	4:E:123:ASP:N	2.50	0.56
4:E:746:VAL:HG22	11:1:271:TYR:HB3	1.85	0.56
12:Y:16:ILE:HG21	12:Y:79:LEU:HD12	1.87	0.56
4:E:829:SER:O	4:E:830:PHE:C	2.44	0.56
12:X:203:VAL:HG12	12:X:204:ASP:N	2.19	0.56
9:2:25:GLN:HG3	9:2:26:PRO:HD2	1.86	0.56
12:X:82:GLY:O	12:X:84:ASN:N	2.38	0.56
12:Z:82:GLY:C	12:Z:84:ASN:N	2.59	0.56
3:T:7:DG:OP2	4:E:686:ARG:NH1	2.33	0.56
12:Z:82:GLY:O	12:Z:84:ASN:N	2.39	0.56
12:Z:253:LYS:HG2	12:Z:254:PHE:H	1.71	0.56
10:5:16:LEU:HA	16:5:401:ADP:HN62	1.69	0.56
4:E:807:ASP:O	4:E:811:LYS:HG3	2.06	0.56
12:Y:20:LYS:HB3	12:Y:20:LYS:HZ2	1.71	0.56
12:Y:75:LEU:HG	12:Y:79:LEU:CD1	2.35	0.56
12:Z:75:LEU:HG	12:Z:79:LEU:CD1	2.35	0.56
8:3:54:PRO:HD2	8:3:57:THR:HG21	1.88	0.56
12:Z:16:ILE:HG21	12:Z:79:LEU:HD12	1.87	0.56
12:Y:82:GLY:O	12:Y:84:ASN:N	2.39	0.55
3:T:5:DT:C4'	4:E:835:MET:CB	2.82	0.55
12:X:82:GLY:C	12:X:84:ASN:N	2.59	0.55
6:B:341:LEU:O	6:B:343:ASP:N	2.39	0.55
8:3:219:LEU:HD21	8:3:227:ILE:HG12	1.88	0.55
10:5:263:ILE:O	10:5:267:THR:HG23	2.06	0.55
12:Z:20:LYS:HA	12:Z:72:LEU:HD21	1.88	0.55
10:5:41:LEU:HD13	10:5:188:ILE:HB	1.88	0.55
4:E:827:LEU:HA	4:E:830:PHE:CD2	2.38	0.55
4:E:980:GLU:O	4:E:981:LEU:HD23	2.07	0.55
7:4:125:GLN:OE1	7:4:128:ARG:NH1	2.40	0.54
10:5:70:ILE:CB	11:1:533:VAL:HG22	2.37	0.54
4:E:712:LYS:HG2	11:1:598:PHE:CZ	2.42	0.54
12:Y:82:GLY:C	12:Y:84:ASN:N	2.59	0.54
7:4:28:GLU:O	7:4:32:ARG:HG3	2.07	0.54
11:1:218:VAL:O	11:1:221:LYS:N	2.41	0.54
7:4:156:SER:OG	11:1:357:ARG:CD	2.55	0.54
3:T:6:DA:O3'	4:E:555:GLY:N	2.38	0.54
4:E:706:ASN:CB	11:1:311:PHE:HE1	2.14	0.54
3:T:7:DG:H4'	4:E:556:GLY:O	2.08	0.54
7:4:271:PHE:HB2	11:1:483:TYR:OH	2.08	0.54
4:E:708:THR:HG21	11:1:307:LYS:HG2	1.90	0.54
12:X:28:PHE:CE2	12:X:70:MET:HE3	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1059:TYR:O	4:E:1060:GLU:C	2.44	0.53
9:2:79:THR:HG22	9:2:136:ILE:HD12	1.90	0.53
10:5:267:THR:HG22	10:5:303:LEU:HD12	1.88	0.53
4:E:78:TRP:CZ2	4:E:262:GLY:HA2	2.44	0.53
9:2:319:LYS:HA	9:2:322:ILE:HG22	1.90	0.53
12:Z:28:PHE:CE2	12:Z:70:MET:HE3	2.43	0.53
4:E:125:GLU:CB	6:B:369:LYS:HA	2.38	0.53
4:E:972:PHE:CZ	4:E:1003:PHE:O	2.61	0.53
1:C:728:ASN:HD21	6:B:63:ARG:HD3	1.74	0.53
4:E:711:ASN:HD21	4:E:713:ASN:ND2	2.07	0.53
10:5:154:LEU:HD11	10:5:167:LEU:HD11	1.89	0.53
10:5:206:VAL:HG21	10:5:213:LEU:HD11	1.90	0.53
11:1:402:ILE:HD12	11:1:429:ASN:ND2	2.23	0.53
4:E:829:SER:O	4:E:832:GLY:N	2.41	0.53
5:D:89:ARG:N	5:D:130:LEU:O	2.41	0.53
4:E:738:ARG:O	4:E:742:TYR:CD2	2.62	0.53
4:E:1025:ARG:CD	5:D:89:ARG:NH2	2.71	0.53
6:B:27:ILE:HG23	6:B:33:GLN:HE22	1.73	0.53
7:4:179:ILE:HD12	7:4:184:VAL:HB	1.90	0.53
8:3:119:ALA:HB3	8:3:145:VAL:HG13	1.90	0.53
12:Z:253:LYS:O	12:Z:254:PHE:C	2.47	0.53
7:4:50:MET:O	7:4:55:LYS:NZ	2.42	0.52
9:2:69:THR:OG1	9:2:71:LYS:NZ	2.42	0.52
11:1:509:SER:O	11:1:513:GLN:HG2	2.09	0.52
1:C:729:ALA:HA	4:E:452:ILE:HD12	1.91	0.52
4:E:802:ASP:HA	4:E:806:ARG:HE	1.74	0.52
6:B:341:LEU:C	6:B:343:ASP:H	2.12	0.52
9:2:268:LEU:O	9:2:272:VAL:HG23	2.09	0.52
12:Y:211:TYR:CE2	12:Y:258:GLU:HB3	2.44	0.52
10:5:44:PRO:O	10:5:49:LYS:NZ	2.42	0.52
12:Y:80:ARG:O	12:Y:80:ARG:HG2	2.10	0.52
12:X:78:ILE:HG13	12:Y:175:ILE:HD12	1.91	0.52
4:E:1025:ARG:HD3	5:D:89:ARG:NH2	2.25	0.52
4:E:1019:VAL:CG1	4:E:1158:ILE:HG12	2.40	0.51
7:4:23:ILE:HG22	7:4:25:GLY:H	1.75	0.51
4:E:1044:SER:O	4:E:1047:CYS:HB3	2.10	0.51
4:E:658:SER:O	4:E:660:LYS:N	2.43	0.51
11:1:142:LEU:HD12	11:1:196:ILE:HG22	1.92	0.51
7:4:89:VAL:HG22	7:4:93:ILE:HD12	1.92	0.51
9:2:171:ASN:ND2	14:2:401:AGS:S1G	2.77	0.51
10:5:271:VAL:HG11	10:5:310:VAL:HG11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:5:291:ALA:O	11:1:520:ASN:ND2	2.43	0.51
4:E:291:ILE:HG12	4:E:383:ASP:OD1	2.11	0.51
5:D:106:PHE:N	6:B:14:SER:OG	2.44	0.51
7:4:295:THR:O	7:4:298:ARG:N	2.43	0.51
11:1:403:VAL:HG11	11:1:442:ILE:HD12	1.92	0.51
4:E:969:TYR:O	4:E:982:LYS:N	2.44	0.51
11:1:533:VAL:HG12	11:1:534:GLN:NE2	2.26	0.51
9:2:40:THR:HG21	9:2:200:ARG:CB	2.29	0.50
12:X:111:ILE:O	12:Y:179:SER:O	2.29	0.50
5:D:13:LYS:O	5:D:16:GLN:NE2	2.41	0.50
7:4:230:SER:O	7:4:231:PRO:C	2.49	0.50
8:3:93:VAL:HG22	8:3:97:ILE:HD12	1.92	0.50
12:Y:113:GLU:O	12:Z:178:GLY:HA2	2.10	0.50
4:E:969:TYR:H	4:E:982:LYS:CB	2.24	0.50
5:D:106:PHE:HE2	6:B:16:LYS:HD2	1.76	0.50
7:4:73:ASP:OD1	7:4:73:ASP:N	2.38	0.50
1:C:729:ALA:O	6:B:63:ARG:NH1	2.45	0.50
10:5:68:LEU:HD21	11:1:536:PRO:O	2.11	0.50
8:3:217:ALA:HA	9:2:51:LYS:HD2	1.94	0.50
8:3:194:GLU:O	8:3:198:ILE:HG12	2.12	0.50
10:5:144:ASN:HD21	10:5:172:ASP:H	1.59	0.50
4:E:712:LYS:HA	11:1:598:PHE:CE2	2.46	0.50
8:3:328:LYS:O	8:3:332:GLU:HG2	2.11	0.50
12:X:114:TYR:CE2	12:Y:154:LEU:HD21	2.46	0.50
4:E:274:GLU:HG2	4:E:275:ASP:O	2.12	0.49
10:5:17:SER:OG	16:5:401:ADP:N1	2.44	0.49
4:E:647:ASN:HA	4:E:650:THR:HG22	1.93	0.49
5:D:23:THR:OG1	5:D:24:VAL:N	2.44	0.49
10:5:16:LEU:HA	16:5:401:ADP:N6	2.27	0.49
12:Z:19:PHE:O	12:Z:72:LEU:HD21	2.12	0.49
4:E:791:TRP:HB3	4:E:813:ILE:HG12	1.93	0.49
10:5:68:LEU:HD13	10:5:88:VAL:HG13	1.93	0.49
11:1:212:GLU:HB3	11:1:218:VAL:HG21	1.94	0.49
6:B:363:MET:SD	6:B:367:ARG:HA	2.53	0.49
8:3:108:SER:OG	8:3:109:LYS:N	2.45	0.49
4:E:832:GLY:O	4:E:833:TYR:C	2.50	0.49
5:D:2:PRO:HG3	6:B:44:LYS:HG2	1.94	0.49
9:2:266:ASP:O	9:2:270:GLU:HG3	2.12	0.49
12:X:211:TYR:CE2	12:X:258:GLU:CB	2.95	0.49
7:4:13:GLU:OE2	7:4:16:ARG:NH2	2.43	0.49
10:5:203:SER:O	10:5:207:THR:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:695:ASP:O	4:E:699:MET:HG2	2.13	0.49
9:2:308:TYR:O	9:2:319:LYS:NZ	2.45	0.49
9:2:16:LEU:O	9:2:20:GLN:HG2	2.13	0.49
12:Z:152:SER:OG	12:Z:213:LEU:HD11	2.12	0.49
6:B:18:ILE:HG22	6:B:108:PHE:HB2	1.95	0.48
5:D:3:SER:HB2	6:B:38:ARG:HE	1.78	0.48
11:1:179:LEU:HD11	11:1:315:ILE:HD12	1.95	0.48
12:Z:23:VAL:HG23	12:Z:72:LEU:HD22	1.94	0.48
7:4:87:ASP:OD2	7:4:87:ASP:N	2.46	0.48
10:5:88:VAL:HB	10:5:95:GLU:HB2	1.95	0.48
3:T:4:DT:O2	4:E:832:GLY:CA	2.62	0.48
7:4:296:HIS:O	7:4:299:ILE:N	2.46	0.48
10:5:95:GLU:HG2	10:5:139:ILE:HB	1.94	0.48
4:E:708:THR:CG2	11:1:307:LYS:HG2	2.43	0.48
4:E:1058:GLU:C	4:E:1059:TYR:HD2	2.17	0.48
5:D:71:GLY:CA	5:D:83:PHE:O	2.61	0.48
9:2:271:ILE:HG12	9:2:286:TYR:HE2	1.77	0.48
4:E:38:LEU:HD21	11:1:567:ARG:HG2	1.94	0.48
7:4:220:ASN:ND2	7:4:222:ASP:H	2.12	0.48
10:5:5:VAL:CG1	16:5:401:ADP:O3'	2.48	0.48
9:2:264:PRO:HD2	9:2:267:ILE:HD12	1.95	0.48
10:5:112:LEU:O	10:5:116:VAL:HG23	2.12	0.48
12:Y:109:ASP:O	12:Z:182:ILE:HA	2.14	0.48
4:E:777:PHE:HA	4:E:780:ARG:HG2	1.96	0.47
12:Z:136:THR:HB	12:Z:198:GLU:CG	2.43	0.47
10:5:267:THR:HG21	10:5:306:SER:OG	2.14	0.47
3:T:13:DA:H2"	3:T:14:DC:C6	2.49	0.47
4:E:1157:ILE:O	4:E:1161:PRO:HG2	2.15	0.47
4:E:1059:TYR:N	4:E:1059:TYR:CD2	2.79	0.47
8:3:131:ARG:HB2	8:3:160:ARG:HE	1.78	0.47
9:2:329:THR:HG21	9:2:346:LEU:HD22	1.96	0.47
4:E:832:GLY:O	4:E:834:VAL:N	2.47	0.47
10:5:259:TRP:HZ3	10:5:302:GLU:HG3	1.78	0.47
11:1:215:GLY:N	11:1:216:PRO:HD2	2.29	0.47
7:4:165:LYS:HA	7:4:165:LYS:HD3	1.72	0.47
9:2:58:LEU:O	9:2:165:ARG:NE	2.46	0.47
12:X:114:TYR:HE2	12:Y:154:LEU:HD21	1.80	0.47
12:X:203:VAL:CG1	12:X:204:ASP:N	2.77	0.47
4:E:78:TRP:HA	4:E:264:TRP:HA	1.97	0.47
4:E:717:LYS:HD2	4:E:717:LYS:N	2.30	0.47
4:E:834:VAL:CG1	4:E:843:SER:HB3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:31:MET:HE2	5:D:123:VAL:HG22	1.97	0.47
7:4:104:PRO:HB2	7:4:107:LYS:HG2	1.96	0.47
7:4:220:ASN:HD22	7:4:222:ASP:H	1.61	0.47
10:5:257:PRO:HD2	10:5:260:ILE:HD12	1.97	0.47
7:4:229:ASP:CB	8:3:163:ARG:NH2	2.77	0.47
8:3:21:PRO:HD3	14:3:401:AGS:H2'	1.96	0.47
9:2:33:PRO:HB3	9:2:38:GLU:HB2	1.97	0.47
12:Y:203:VAL:CG1	12:Y:204:ASP:N	2.77	0.47
12:Z:203:VAL:CG1	12:Z:204:ASP:N	2.77	0.47
10:5:70:ILE:CB	11:1:533:VAL:CG2	2.93	0.46
12:Z:8:GLU:OE1	12:Z:85:THR:HA	2.15	0.46
2:P:3:DT:H2"	2:P:4:DT:O5'	2.15	0.46
7:4:79:ASN:HB3	8:3:132:ARG:HG2	1.97	0.46
1:C:739:LEU:HD22	5:D:106:PHE:CE2	2.50	0.46
4:E:1025:ARG:HD2	5:D:89:ARG:NH2	2.31	0.46
4:E:1059:TYR:HD2	4:E:1059:TYR:N	2.13	0.46
10:5:280:ILE:HG12	11:1:444:PRO:HB3	1.98	0.46
11:1:218:VAL:O	11:1:219:LYS:C	2.53	0.46
7:4:187:THR:HG23	7:4:190:GLY:H	1.81	0.46
9:2:116:LEU:HD12	12:Z:119:MET:SD	2.54	0.46
6:B:340:ASP:HB2	6:B:343:ASP:HB2	1.98	0.46
4:E:968:ARG:HA	4:E:982:LYS:CB	2.46	0.46
9:2:171:ASN:OD1	10:5:155:ARG:NH1	2.49	0.46
10:5:8:TYR:HE2	10:5:208:ASN:HD22	1.63	0.46
10:5:109:ILE:HG23	10:5:113:LEU:HD12	1.96	0.46
12:X:130:GLU:HB2	12:X:133:TYR:CE1	2.51	0.46
12:Y:8:GLU:OE1	12:Y:85:THR:HA	2.15	0.46
3:T:6:DA:H5'	4:E:553:TYR:CE2	2.51	0.46
4:E:121:PHE:O	4:E:122:LEU:C	2.51	0.46
12:X:119:MET:HE3	12:X:119:MET:HB3	1.89	0.46
7:4:277:LEU:HB3	7:4:285:ARG:HD3	1.98	0.46
10:5:116:VAL:HG12	10:5:165:ILE:HD11	1.98	0.46
12:X:189:GLU:O	12:X:190:HIS:HB2	2.16	0.46
12:Y:20:LYS:HB3	12:Y:20:LYS:NZ	2.30	0.46
4:E:784:PHE:CE1	4:E:816:TYR:CD1	3.04	0.45
4:E:957:SER:HB2	4:E:1164:LEU:CB	2.46	0.45
9:2:201:LEU:HD23	9:2:217:LEU:HB3	1.97	0.45
12:Y:83:ASN:HD21	12:Y:110:ARG:HH22	1.64	0.45
12:Z:189:GLU:O	12:Z:190:HIS:HB2	2.16	0.45
4:E:569:ASP:O	4:E:1010:ASP:O	2.34	0.45
5:D:73:LEU:HD23	6:B:5:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:4:223:ASN:O	7:4:227:ILE:HG22	2.16	0.45
4:E:717:LYS:O	4:E:718:LYS:C	2.54	0.45
7:4:42:MET:O	7:4:139:ARG:NH1	2.42	0.45
7:4:265:ASP:OD2	8:3:52:TYR:CZ	2.69	0.45
5:D:133:MET:HA	6:B:89:PHE:HE2	1.81	0.45
6:B:359:ASP:O	6:B:363:MET:HG2	2.16	0.45
10:5:267:THR:O	10:5:271:VAL:HG22	2.17	0.45
12:Y:130:GLU:HB2	12:Y:133:TYR:CE1	2.51	0.45
12:Y:189:GLU:O	12:Y:190:HIS:HB2	2.16	0.45
12:Z:130:GLU:HB2	12:Z:133:TYR:CE1	2.51	0.45
5:D:73:LEU:HB3	6:B:5:LEU:HD11	1.98	0.45
10:5:344:GLY:CA	11:1:460:SER:CB	2.94	0.45
11:1:454:ARG:O	11:1:455:LYS:C	2.55	0.45
4:E:763:CYS:SG	13:E:2301:SF4:S1	3.15	0.45
11:1:448:TYR:O	11:1:449:SER:C	2.55	0.45
12:Z:83:ASN:HD21	12:Z:110:ARG:HH22	1.63	0.45
3:T:5:DT:H5'	4:E:835:MET:O	2.16	0.45
4:E:1036:MET:CB	5:D:87:LYS:O	2.64	0.45
9:2:14:SER:OG	9:2:15:LYS:N	2.47	0.45
12:Y:20:LYS:HZ2	12:Y:20:LYS:CB	2.29	0.45
4:E:668:CYS:HB3	13:E:2301:SF4:S3	2.56	0.45
4:E:748:HIS:HE2	11:1:273:GLN:CD	2.20	0.45
5:D:11:TRP:NE1	5:D:117:ASP:OD1	2.42	0.45
4:E:1046:ILE:O	4:E:1047:CYS:C	2.55	0.45
9:2:21:SER:HA	9:2:24:GLN:HG2	1.98	0.45
10:5:202:LEU:HD22	10:5:237:LEU:HD22	1.99	0.45
12:Z:19:PHE:C	12:Z:72:LEU:HD21	2.38	0.45
4:E:678:ALA:HB2	13:E:2301:SF4:S4	2.57	0.45
7:4:286:LEU:HD21	11:1:419:PHE:CZ	2.47	0.45
12:X:184:PRO:HA	12:X:195:ILE:O	2.17	0.45
4:E:671:ASN:N	13:E:2301:SF4:S3	2.90	0.44
2:P:5:DG:H2"	2:P:6:DC:C5'	2.47	0.44
4:E:812:MET:HG3	4:E:815:LEU:HD23	1.99	0.44
9:2:220:ILE:HG12	9:2:256:VAL:HG11	1.99	0.44
3:T:14:DC:H2"	3:T:15:DA:C8	2.53	0.44
4:E:138:TYR:CG	4:E:190:LYS:HE3	2.52	0.44
11:1:215:GLY:C	11:1:254:ILE:HD11	2.38	0.44
9:2:191:ALA:HB1	9:2:226:GLY:HA3	1.99	0.44
4:E:711:ASN:C	4:E:713:ASN:N	2.70	0.44
4:E:792:LYS:HA	4:E:795:LEU:HD23	1.98	0.44
4:E:970:ALA:HB2	4:E:984:PHE:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:94:VAL:HG22	5:D:123:VAL:HG12	2.00	0.44
7:4:241:LEU:HD21	7:4:277:LEU:HD21	1.99	0.44
8:3:128:ASN:HA	8:3:131:ARG:HE	1.82	0.44
12:Y:184:PRO:HA	12:Y:195:ILE:O	2.17	0.44
12:Z:184:PRO:HA	12:Z:195:ILE:O	2.17	0.44
4:E:520:LEU:CD1	4:E:833:TYR:CE2	3.00	0.44
9:2:43:ASP:HA	9:2:46:VAL:HG22	1.99	0.44
3:T:7:DG:P	4:E:555:GLY:H	2.39	0.44
4:E:431:TYR:CG	4:E:431:TYR:O	2.71	0.44
7:4:129:ARG:HG3	7:4:133:LEU:HG	1.98	0.44
10:5:274:ARG:O	10:5:274:ARG:CG	2.66	0.44
11:1:436:LEU:HD21	11:1:463:LEU:CD2	2.48	0.44
4:E:1057:LYS:C	4:E:1059:TYR:N	2.67	0.44
8:3:28:TYR:OH	8:3:180:ASN:ND2	2.51	0.44
10:5:293:CYS:O	11:1:548:ILE:CB	2.66	0.44
11:1:576:MET:O	11:1:580:VAL:HG23	2.18	0.44
4:E:810:LYS:HA	4:E:813:ILE:HD12	2.00	0.43
4:E:812:MET:HA	4:E:815:LEU:HB3	1.99	0.43
7:4:244:ASN:ND2	7:4:246:GLU:H	2.15	0.43
11:1:222:ILE:HD11	11:1:251:PHE:CE2	2.53	0.43
12:Y:115:SER:O	12:Z:176:GLY:HA3	2.17	0.43
2:P:2:DG:H2'	2:P:3:DT:C6	2.53	0.43
4:E:956:PRO:HB3	4:E:1156:LYS:O	2.17	0.43
8:3:322:ALA:HB2	9:2:327:PHE:HB2	2.00	0.43
9:2:201:LEU:HD22	9:2:221:LEU:HG	2.00	0.43
9:2:252:THR:HG1	9:2:255:GLN:HG3	1.83	0.43
10:5:251:SER:O	10:5:251:SER:OG	2.33	0.43
4:E:845:GLU:O	4:E:846:MET:C	2.55	0.43
9:2:346:LEU:O	9:2:350:ILE:HG23	2.19	0.43
10:5:85:LEU:HD13	10:5:108:VAL:HG11	2.00	0.43
3:T:6:DA:H5'	4:E:553:TYR:CZ	2.53	0.43
10:5:313:LEU:HD22	10:5:353:LEU:HD22	2.00	0.43
12:X:151:LEU:HB3	12:X:171:ALA:HB2	2.01	0.43
12:Z:134:ASP:HB2	12:Z:203:VAL:HG21	2.00	0.43
4:E:1052:MET:HB3	4:E:1059:TYR:CZ	2.54	0.43
12:Y:134:ASP:CB	12:Y:203:VAL:CG2	2.96	0.43
12:Z:134:ASP:CB	12:Z:203:VAL:CG2	2.96	0.43
4:E:58:PRO:HD2	4:E:74:GLY:HA2	2.01	0.43
4:E:840:ARG:C	4:E:842:TYR:N	2.72	0.43
10:5:77:THR:OG1	10:5:78:ALA:N	2.51	0.43
12:X:134:ASP:CB	12:X:203:VAL:CG2	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:267:VAL:HG13	4:E:267:VAL:O	2.19	0.43
5:D:73:LEU:HD11	6:B:3:ILE:HD12	2.01	0.43
7:4:10:PRO:HD3	8:3:142:ARG:HH22	1.84	0.43
7:4:249:ILE:HD13	8:3:296:ARG:NH2	2.33	0.43
9:2:240:LYS:HE3	9:2:240:LYS:HB2	1.83	0.43
10:5:17:SER:H	16:5:401:ADP:HN62	1.65	0.43
11:1:217:MET:O	11:1:218:VAL:C	2.56	0.43
4:E:993:GLN:HB3	4:E:1045:LEU:O	2.19	0.43
11:1:173:ARG:NH2	11:1:266:THR:CG2	2.82	0.43
4:E:125:GLU:CB	6:B:368:ARG:O	2.67	0.43
5:D:58:ARG:HA	5:D:69:ARG:HE	1.84	0.43
7:4:191:LEU:O	7:4:195:ILE:HG12	2.19	0.43
8:3:70:ILE:HD13	8:3:111:PHE:HZ	1.84	0.43
9:2:154:ARG:HD3	9:2:179:PRO:HB2	1.99	0.43
7:4:202:MET:HG2	14:4:401:AGS:C4	2.48	0.42
10:5:18:HIS:CE1	10:5:52:ARG:HH21	2.37	0.42
6:B:352:ASN:C	6:B:354:ARG:H	2.22	0.42
11:1:179:LEU:HD11	11:1:315:ILE:CD1	2.49	0.42
12:X:236:LEU:CD1	12:X:249:PHE:CZ	2.96	0.42
12:Y:134:ASP:HB2	12:Y:203:VAL:HG21	2.00	0.42
8:3:132:ARG:HD2	8:3:132:ARG:HA	1.85	0.42
6:B:74:GLU:HA	6:B:98:VAL:HG12	2.01	0.42
8:3:265:LYS:HE3	8:3:265:LYS:HB2	1.85	0.42
9:2:101:ARG:NH2	9:2:144:SER:OG	2.52	0.42
10:5:159:GLU:OE1	10:5:184:ARG:NH2	2.52	0.42
4:E:845:GLU:C	4:E:847:ALA:N	2.72	0.42
5:D:89:ARG:HB2	5:D:132:ILE:HA	2.00	0.42
8:3:214:SER:HB3	8:3:235:CYS:SG	2.59	0.42
9:2:40:THR:CG2	9:2:200:ARG:HD3	2.49	0.42
4:E:565:VAL:O	4:E:565:VAL:HG13	2.19	0.42
4:E:794:ASN:HA	4:E:797:LYS:HG2	2.00	0.42
5:D:82:LEU:HD23	5:D:90:LEU:HD12	2.02	0.42
4:E:833:TYR:O	4:E:835:MET:N	2.53	0.42
6:B:51:LEU:HB2	6:B:60:LEU:HD11	2.02	0.42
6:B:357:LYS:O	6:B:360:SER:OG	2.25	0.42
9:2:49:LEU:HD13	9:2:78:LEU:HD22	2.01	0.42
9:2:161:SER:O	9:2:165:ARG:NH1	2.53	0.42
12:Y:151:LEU:HB3	12:Y:171:ALA:HB2	2.01	0.42
12:Y:182:ILE:HD12	12:Y:195:ILE:HD13	2.02	0.42
12:Z:168:LYS:HG3	12:Z:181:ILE:HG12	2.02	0.42
4:E:127:GLY:O	4:E:128:SER:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:5:42:TYR:CZ	10:5:189:ARG:HB3	2.55	0.42
4:E:834:VAL:HG13	4:E:843:SER:HB3	2.01	0.42
4:E:1158:ILE:O	4:E:1159:THR:C	2.58	0.42
6:B:28:ILE:HD13	6:B:28:ILE:HA	1.83	0.42
7:4:44:HIS:CE1	7:4:139:ARG:HA	2.55	0.42
12:Y:168:LYS:HG3	12:Y:181:ILE:HG12	2.02	0.42
12:Z:23:VAL:CG2	12:Z:72:LEU:HD22	2.50	0.42
7:4:30:ILE:HD13	7:4:30:ILE:HA	1.84	0.41
8:3:32:GLU:O	8:3:36:THR:OG1	2.29	0.41
8:3:275:ILE:O	8:3:279:GLU:HG2	2.20	0.41
12:Y:83:ASN:C	12:Y:85:THR:H	2.24	0.41
11:1:397:ILE:O	11:1:398:SER:C	2.58	0.41
11:1:443:PHE:CD1	11:1:444:PRO:HD3	2.55	0.41
12:X:134:ASP:HB2	12:X:203:VAL:HG21	2.01	0.41
12:X:168:LYS:HG3	12:X:181:ILE:HG12	2.03	0.41
9:2:229:ARG:HD3	10:5:184:ARG:HA	2.00	0.41
10:5:165:ILE:HD13	10:5:165:ILE:HA	1.90	0.41
12:Z:83:ASN:C	12:Z:85:THR:H	2.24	0.41
4:E:564:GLY:HA2	4:E:1161:PRO:O	2.19	0.41
4:E:986:LEU:C	4:E:988:ARG:N	2.66	0.41
4:E:1036:MET:CB	5:D:131:PRO:HG3	2.50	0.41
10:5:49:LYS:HG2	16:5:401:ADP:O3B	2.20	0.41
10:5:275:SER:OG	10:5:276:VAL:N	2.54	0.41
11:1:214:ALA:O	11:1:215:GLY:C	2.59	0.41
12:Z:82:GLY:O	12:Z:86:ASP:CB	2.68	0.41
8:3:28:TYR:O	14:3:401:AGS:N6	2.50	0.41
9:2:75:ILE:HG21	9:2:169:ILE:HD11	2.03	0.41
9:2:228:LEU:HD23	14:2:401:AGS:C4	2.51	0.41
10:5:111:GLU:O	10:5:115:GLU:HG3	2.20	0.41
12:X:134:ASP:HB3	12:X:203:VAL:CG2	2.51	0.41
12:Z:151:LEU:HB3	12:Z:171:ALA:HB2	2.01	0.41
4:E:679:ARG:HB3	4:E:764:GLN:NE2	2.35	0.41
7:4:264:ILE:HD12	8:3:149:TYR:CE1	2.56	0.41
9:2:63:PHE:HD1	9:2:187:PHE:HB2	1.85	0.41
9:2:237:SER:HB3	10:5:186:LEU:HD11	2.03	0.41
5:D:98:ASP:N	5:D:98:ASP:OD1	2.54	0.41
8:3:244:LEU:HD21	8:3:280:GLY:HA3	2.02	0.41
9:2:79:THR:HB	9:2:92:ILE:HD11	2.03	0.41
9:2:124:HIS:CE1	9:2:128:ASN:HD21	2.39	0.41
4:E:824:LYS:HG2	4:E:828:ASN:HD21	1.85	0.41
4:E:842:TYR:CD2	4:E:843:SER:N	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1158:ILE:O	4:E:1161:PRO:HD2	2.21	0.41
10:5:264:HIS:O	10:5:268:ARG:HG2	2.20	0.41
8:3:215:CYS:SG	8:3:232:ILE:HD13	2.61	0.41
9:2:24:GLN:HB2	10:5:34:ARG:HD2	2.02	0.41
9:2:202:ARG:O	9:2:206:GLU:HG2	2.21	0.41
10:5:231:ARG:N	16:5:401:ADP:H4'	2.36	0.41
12:X:182:ILE:HD12	12:X:195:ILE:HD13	2.02	0.41
12:Y:112:ALA:HA	12:Z:179:SER:O	2.21	0.41
12:Z:134:ASP:HB3	12:Z:203:VAL:CG2	2.51	0.41
1:C:729:ALA:HA	4:E:452:ILE:CD1	2.50	0.41
12:Y:134:ASP:HB3	12:Y:203:VAL:CG2	2.51	0.41
12:Y:211:TYR:O	12:Y:215:ILE:HG13	2.20	0.41
12:Z:235:ALA:O	12:Z:249:PHE:HA	2.21	0.41
4:E:140:PHE:CE1	4:E:170:ILE:HD11	2.56	0.40
4:E:815:LEU:O	4:E:818:SER:OG	2.28	0.40
9:2:62:LEU:HD13	9:2:168:LEU:HB2	2.03	0.40
9:2:305:HIS:HB2	9:2:326:LEU:HD13	2.03	0.40
10:5:206:VAL:HB	10:5:211:ILE:HB	2.03	0.40
12:X:235:ALA:O	12:X:249:PHE:HA	2.22	0.40
4:E:119:PHE:CB	4:E:121:PHE:HE2	2.35	0.40
4:E:254:SER:O	4:E:260:ARG:NH1	2.52	0.40
4:E:653:ARG:NH2	4:E:768:PRO:HB3	2.37	0.40
9:2:63:PHE:HB3	9:2:71:LYS:HG2	2.03	0.40
12:Y:233:ALA:HB1	12:Y:234:PRO:HD2	2.04	0.40
4:E:346:PHE:HZ	6:B:111:ARG:NH1	2.19	0.40
4:E:570:LEU:CB	4:E:1011:THR:HA	2.51	0.40
4:E:780:ARG:O	4:E:784:PHE:CD2	2.74	0.40
12:X:83:ASN:C	12:X:85:THR:H	2.24	0.40
12:Z:233:ALA:HB1	12:Z:234:PRO:HD2	2.03	0.40
9:2:16:LEU:H	9:2:16:LEU:HD12	1.86	0.40
10:5:242:LEU:HD12	11:1:558:MET:HG2	2.04	0.40
11:1:348:LEU:HD21	11:1:359:CYS:HA	2.02	0.40
12:X:100:ILE:HA	12:X:114:TYR:O	2.22	0.40
12:X:211:TYR:O	12:X:215:ILE:HG13	2.20	0.40
12:Y:82:GLY:HA2	12:Y:103:PHE:HD2	1.86	0.40
12:Y:235:ALA:O	12:Y:249:PHE:HA	2.22	0.40
12:Z:137:LEU:HD12	12:Z:137:LEU:C	2.42	0.40
12:Z:211:TYR:O	12:Z:215:ILE:HG13	2.20	0.40
7:4:175:LEU:O	7:4:179:ILE:HG12	2.21	0.40
9:2:291:MET:HG3	9:2:340:HIS:CG	2.56	0.40
14:2:401:AGS:O2G	10:5:184:ARG:NH1	2.51	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	C	24/26 (92%)	22 (92%)	2 (8%)	0	100	100
4	E	1115/2222 (50%)	1046 (94%)	54 (5%)	15 (1%)	10	42
5	D	130/132 (98%)	127 (98%)	3 (2%)	0	100	100
6	B	167/380 (44%)	150 (90%)	12 (7%)	5 (3%)	3	26
7	4	317/319 (99%)	304 (96%)	12 (4%)	1 (0%)	37	71
8	3	325/327 (99%)	316 (97%)	9 (3%)	0	100	100
9	2	338/340 (99%)	334 (99%)	4 (1%)	0	100	100
10	5	331/354 (94%)	327 (99%)	4 (1%)	0	100	100
11	1	447/741 (60%)	422 (94%)	21 (5%)	4 (1%)	14	50
12	X	256/258 (99%)	239 (93%)	12 (5%)	5 (2%)	6	34
12	Y	256/258 (99%)	239 (93%)	12 (5%)	5 (2%)	6	34
12	Z	252/258 (98%)	237 (94%)	11 (4%)	4 (2%)	8	39
All	All	3958/5615 (70%)	3763 (95%)	156 (4%)	39 (1%)	16	48

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	833	TYR
4	E	845	GLU
4	E	846	MET
4	E	987	LYS
4	E	1053	SER
4	E	1055	THR
6	B	334	ARG
6	B	335	LEU
11	1	249	SER

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Mol	Chain	Res	Type
12	X	190	HIS
12	Y	190	HIS
12	Z	190	HIS
4	E	659	ILE
4	E	1061	GLY
6	B	342	GLU
12	X	109	ASP
12	X	255	ASN
12	Y	109	ASP
12	Y	255	ASN
12	Z	109	ASP
4	E	128	SER
4	E	986	LEU
6	B	340	ASP
6	B	353	SER
7	4	231	PRO
11	1	219	LYS
12	X	150	ASP
12	Y	150	ASP
12	Z	150	ASP
4	E	712	LYS
4	E	718	LYS
12	X	83	ASN
12	Y	83	ASN
12	Z	83	ASN
4	E	834	VAL
4	E	798	ILE
4	E	1043	VAL
11	1	455	LYS
11	1	478	GLY

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	C	20/24 (83%)	20 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	E	942/2014 (47%)	940 (100%)	2 (0%)	92 94
5	D	110/119 (92%)	110 (100%)	0	100 100
6	B	153/352 (44%)	153 (100%)	0	100 100
7	4	267/280 (95%)	264 (99%)	3 (1%)	70 80
8	3	279/284 (98%)	279 (100%)	0	100 100
9	2	298/301 (99%)	298 (100%)	0	100 100
10	5	299/324 (92%)	298 (100%)	1 (0%)	91 92
11	1	385/671 (57%)	385 (100%)	0	100 100
12	X	226/233 (97%)	226 (100%)	0	100 100
12	Y	224/233 (96%)	224 (100%)	0	100 100
12	Z	220/233 (94%)	219 (100%)	1 (0%)	86 90
All	All	3423/5068 (68%)	3416 (100%)	7 (0%)	91 94

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	256	ASP
4	E	795	LEU
7	4	229	ASP
7	4	231	PRO
7	4	294	LEU
10	5	287	TYR
12	Z	198	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	728	ASN
4	E	638	HIS
4	E	713	ASN
4	E	794	ASN
4	E	828	ASN
4	E	993	GLN
4	E	997	ASN
6	B	29	GLN
7	4	18	GLN
7	4	60	HIS

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Mol	Chain	Res	Type
7	4	92	GLN
7	4	177	GLN
7	4	220	ASN
7	4	244	ASN
7	4	320	ASN
8	3	180	ASN
8	3	317	GLN
9	2	96	ASN
9	2	128	ASN
9	2	236	GLN
9	2	288	ASN
9	2	303	GLN
9	2	345	ASN
9	2	352	GLN
10	5	18	HIS
10	5	19	ASN
10	5	80	ASN
10	5	86	ASN
10	5	144	ASN
10	5	244	ASN
11	1	477	ASN
11	1	534	GLN
12	X	64	HIS
12	X	159	ASN
12	Y	64	HIS
12	Y	83	ASN
12	Y	159	ASN
12	Z	64	HIS
12	Z	83	ASN
12	Z	159	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	SF4	E	2301	4	0,12,12	-	-	-		
14	AGS	2	401	15	28,33,33	0.76	1 (3%)	31,52,52	0.93	2 (6%)
14	AGS	3	401	15	28,33,33	0.74	1 (3%)	31,52,52	0.94	2 (6%)
16	ADP	5	401	-	24,29,29	0.73	0	29,45,45	0.76	1 (3%)
14	AGS	4	401	15	28,33,33	0.74	1 (3%)	31,52,52	0.94	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	SF4	E	2301	4	-	-	0/6/5/5
14	AGS	2	401	15	-	2/17/38/38	0/3/3/3
14	AGS	3	401	15	-	2/17/38/38	0/3/3/3
16	ADP	5	401	-	-	1/12/32/32	0/3/3/3
14	AGS	4	401	15	-	5/17/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	2	401	AGS	PG-S1G	2.15	1.95	1.90
14	4	401	AGS	PG-S1G	2.13	1.95	1.90
14	3	401	AGS	PG-S1G	2.09	1.95	1.90

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	3	401	AGS	PB-O3B-PG	-3.55	120.16	133.17
14	4	401	AGS	PB-O3B-PG	-3.52	120.29	133.17
14	2	401	AGS	PB-O3B-PG	-3.51	120.32	133.17
14	3	401	AGS	C5-C6-N6	2.31	123.83	120.31
14	2	401	AGS	C5-C6-N6	2.31	123.83	120.31
16	5	401	ADP	C5-C6-N6	2.28	123.78	120.31
14	4	401	AGS	C5-C6-N6	2.25	123.74	120.31

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	4	401	AGS	PB-O3B-PG-O2G
14	4	401	AGS	PB-O3B-PG-O3G
14	4	401	AGS	C5'-O5'-PA-O1A
14	3	401	AGS	PB-O3B-PG-O2G
14	3	401	AGS	PB-O3B-PG-O3G
14	4	401	AGS	C5'-O5'-PA-O2A
14	4	401	AGS	C5'-O5'-PA-O3A
16	5	401	ADP	C4'-C5'-O5'-PA
14	2	401	AGS	PA-O3A-PB-O1B
14	2	401	AGS	PA-O3A-PB-O2B

There are no ring outliers.

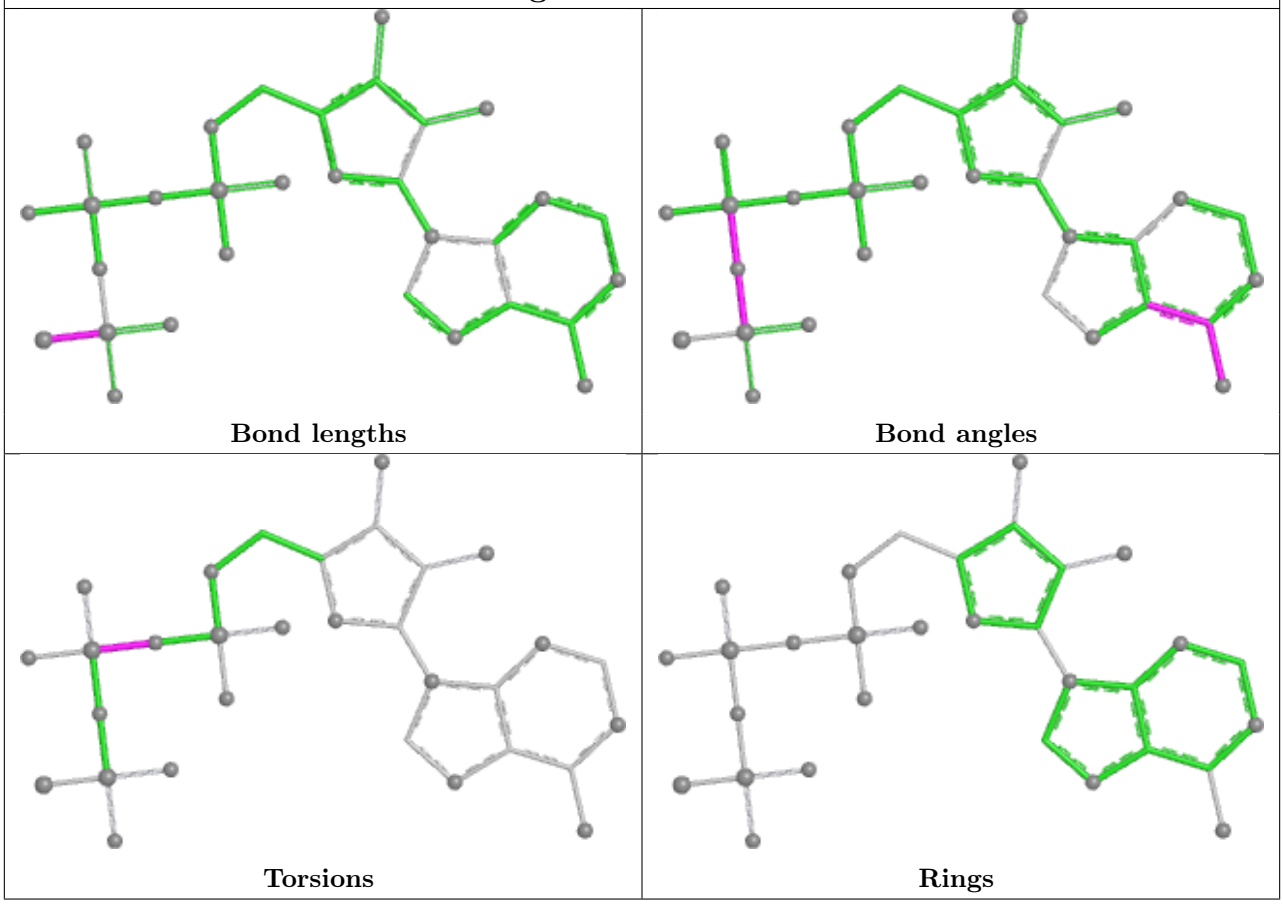
5 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	E	2301	SF4	6	0
14	2	401	AGS	3	0
14	3	401	AGS	2	0
16	5	401	ADP	9	0
14	4	401	AGS	3	0

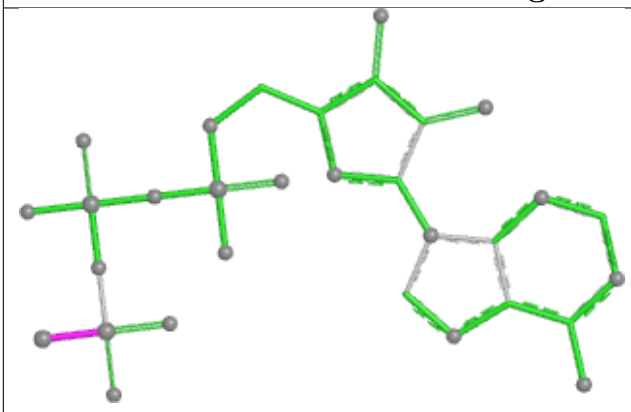
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

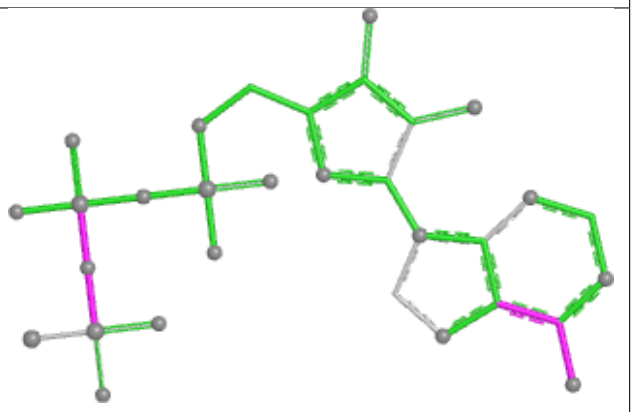
Ligand AGS 2 401



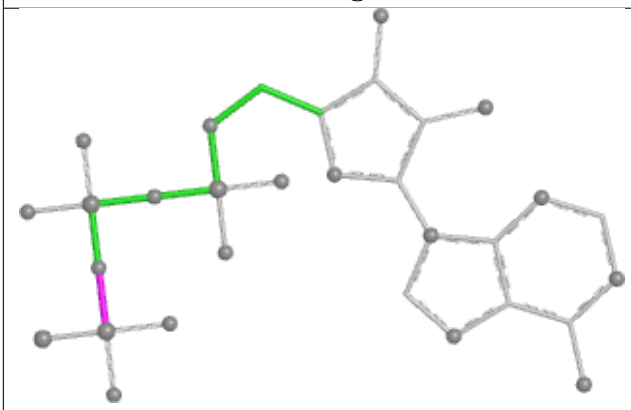
Ligand AGS 3 401



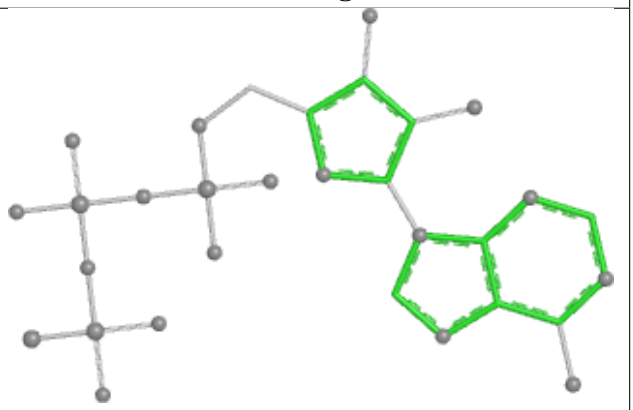
Bond lengths



Bond angles

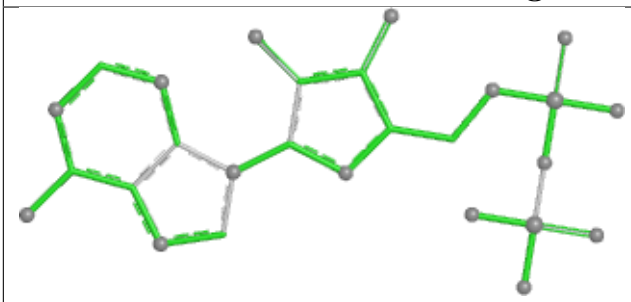


Torsions

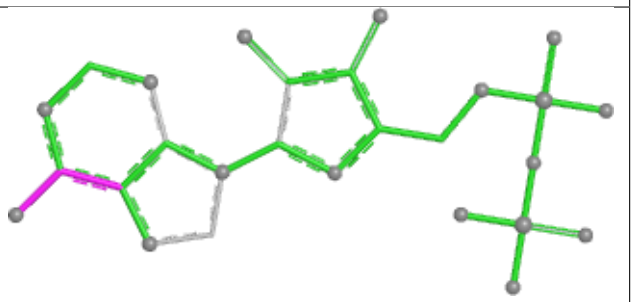


Rings

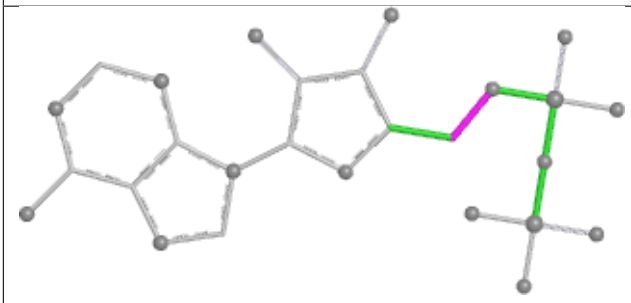
Ligand ADP 5 401



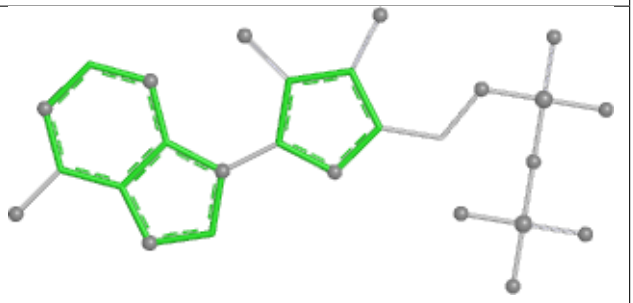
Bond lengths



Bond angles

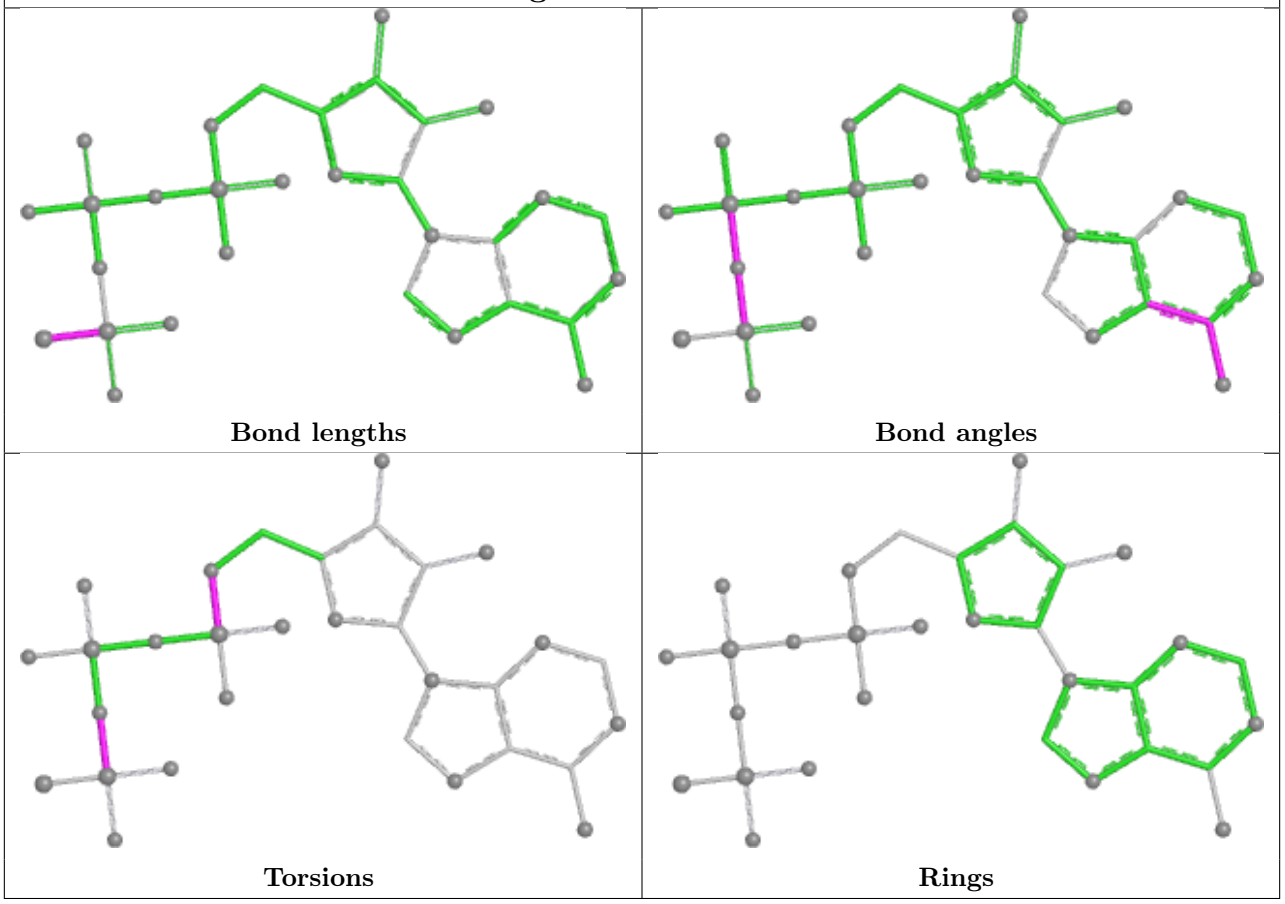


Torsions



Rings

Ligand AGS 4 401



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.

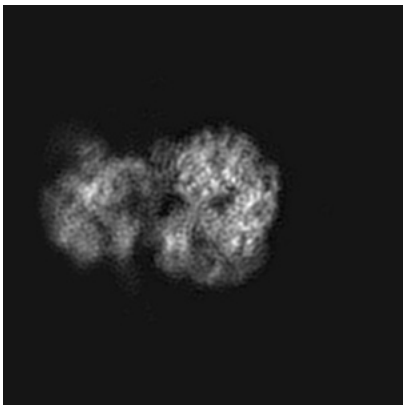
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-41664. These allow visual inspection of the internal detail of the map and identification of artifacts.

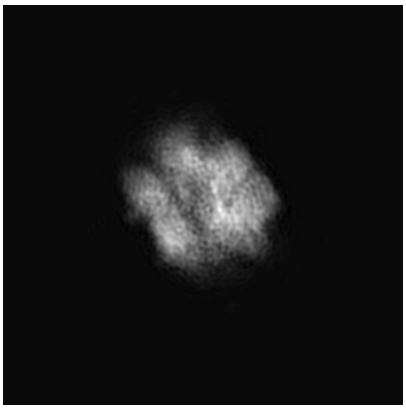
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

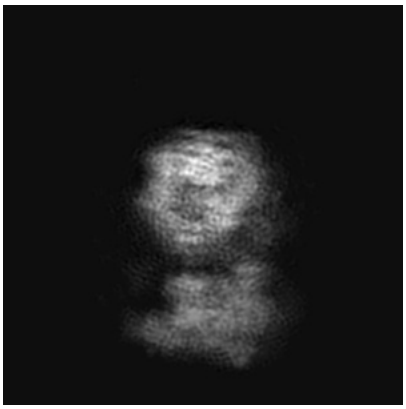
6.1.1 Primary map



X

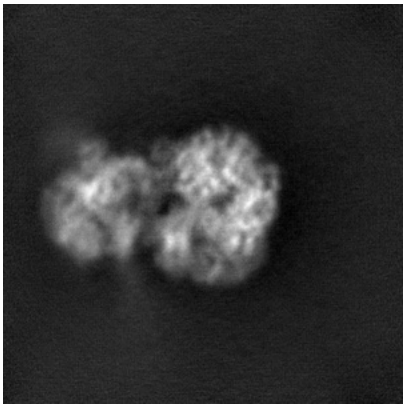


Y

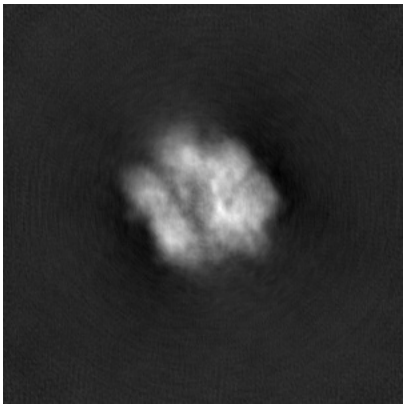


Z

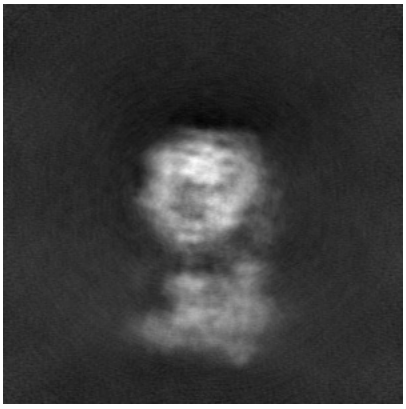
6.1.2 Raw map



X



Y

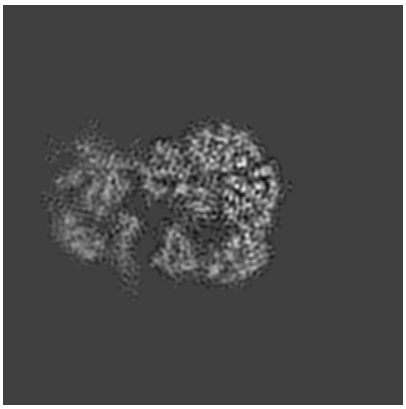


Z

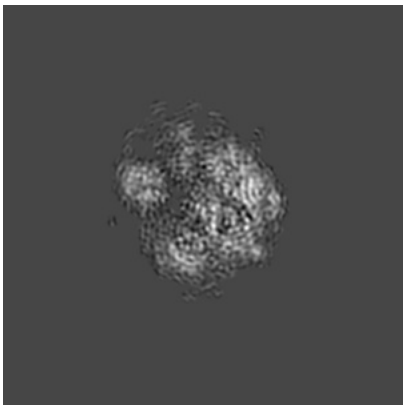
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

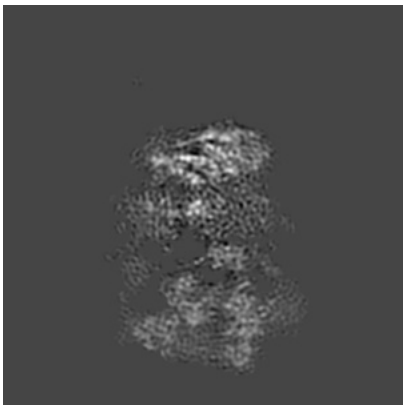
6.2.1 Primary map



X Index: 180

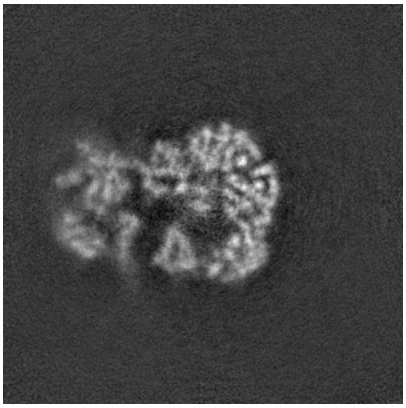


Y Index: 180

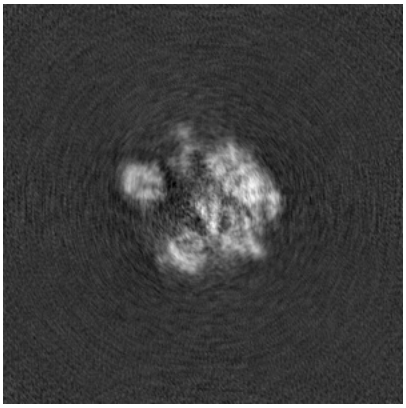


Z Index: 180

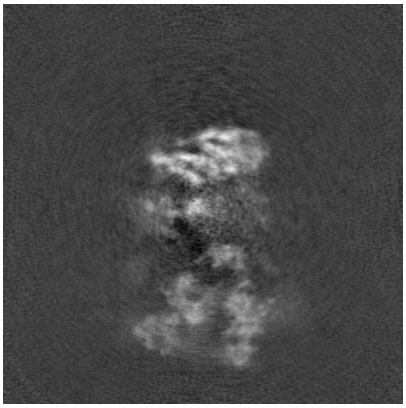
6.2.2 Raw map



X Index: 180



Y Index: 180



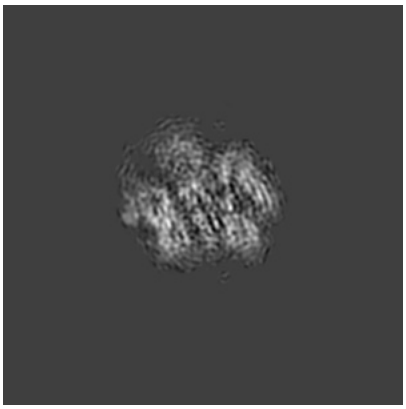
Z Index: 180

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

6.3 Largest variance slices (i)

6.3.1 Primary map

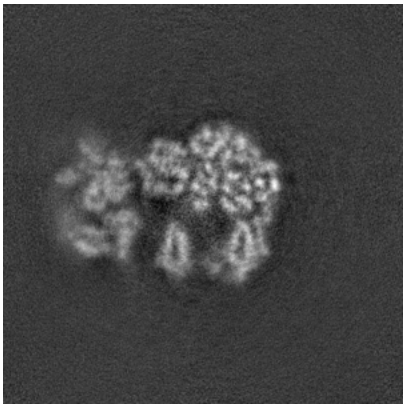
X Index: 175



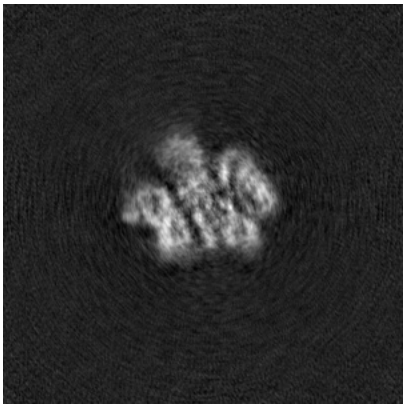
Y Index: 208

Z Index: 197

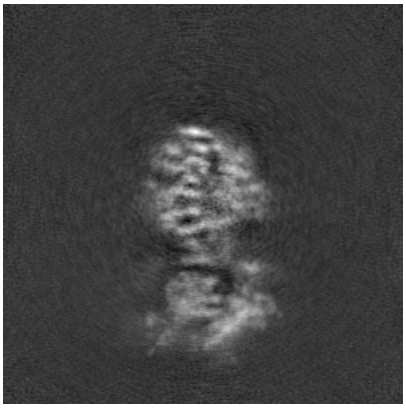
6.3.2 Raw map



X Index: 175



Y Index: 209

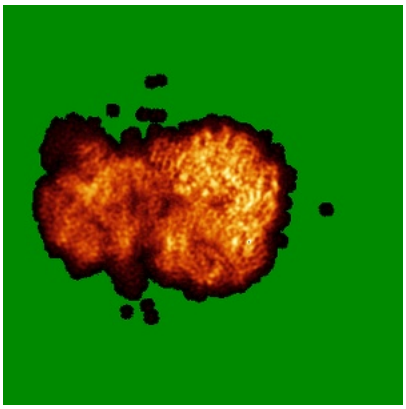


Z Index: 197

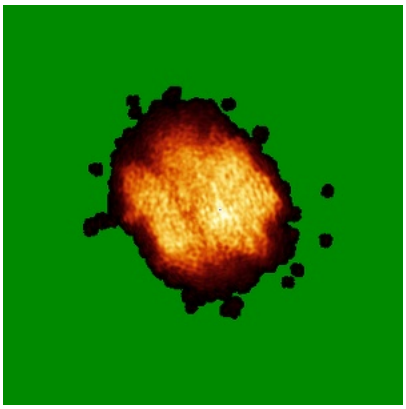
The images above show the largest variance slices of the map in three orthogonal directions.

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

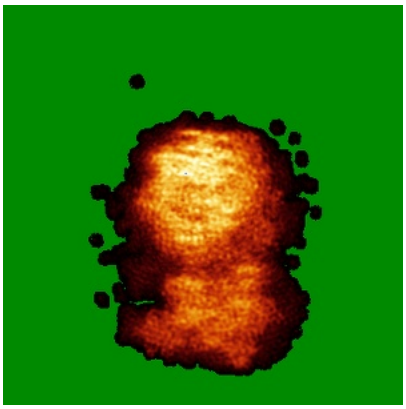
6.4.1 Primary map



X

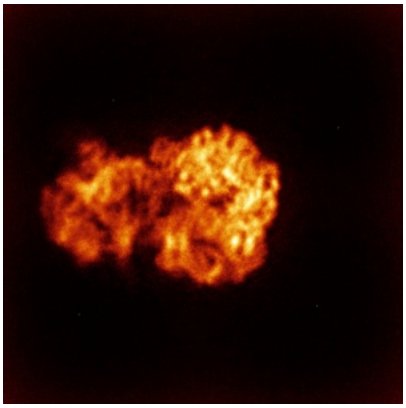


Y

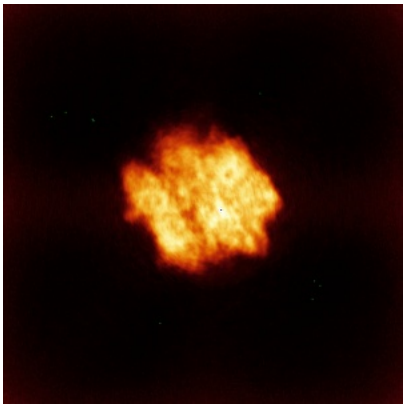


Z

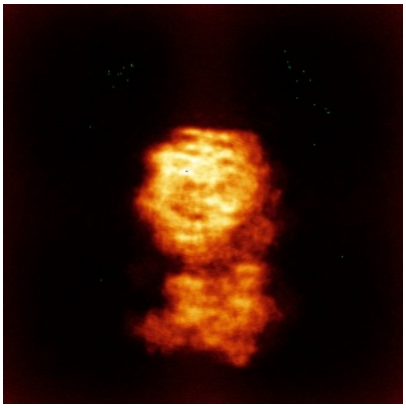
6.4.2 Raw map



X



Y

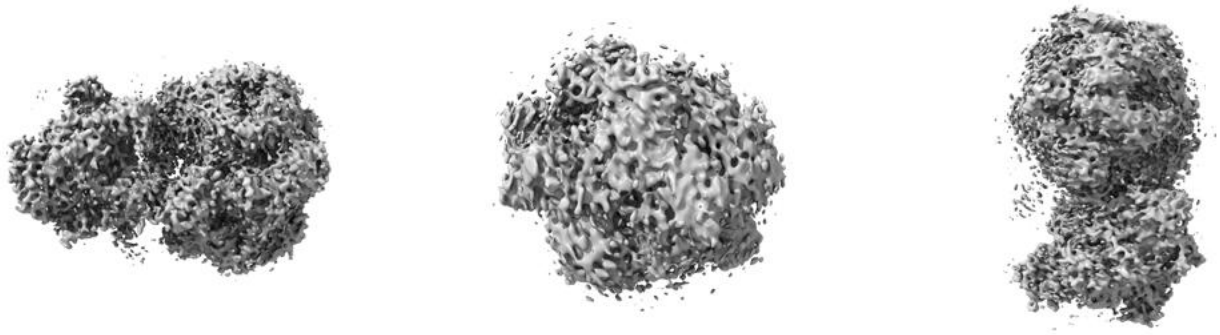


Z

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)

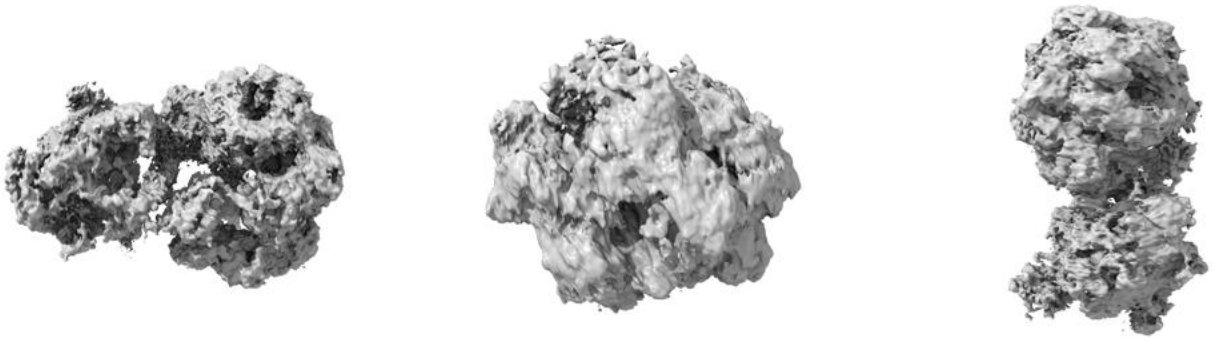
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.144. 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.

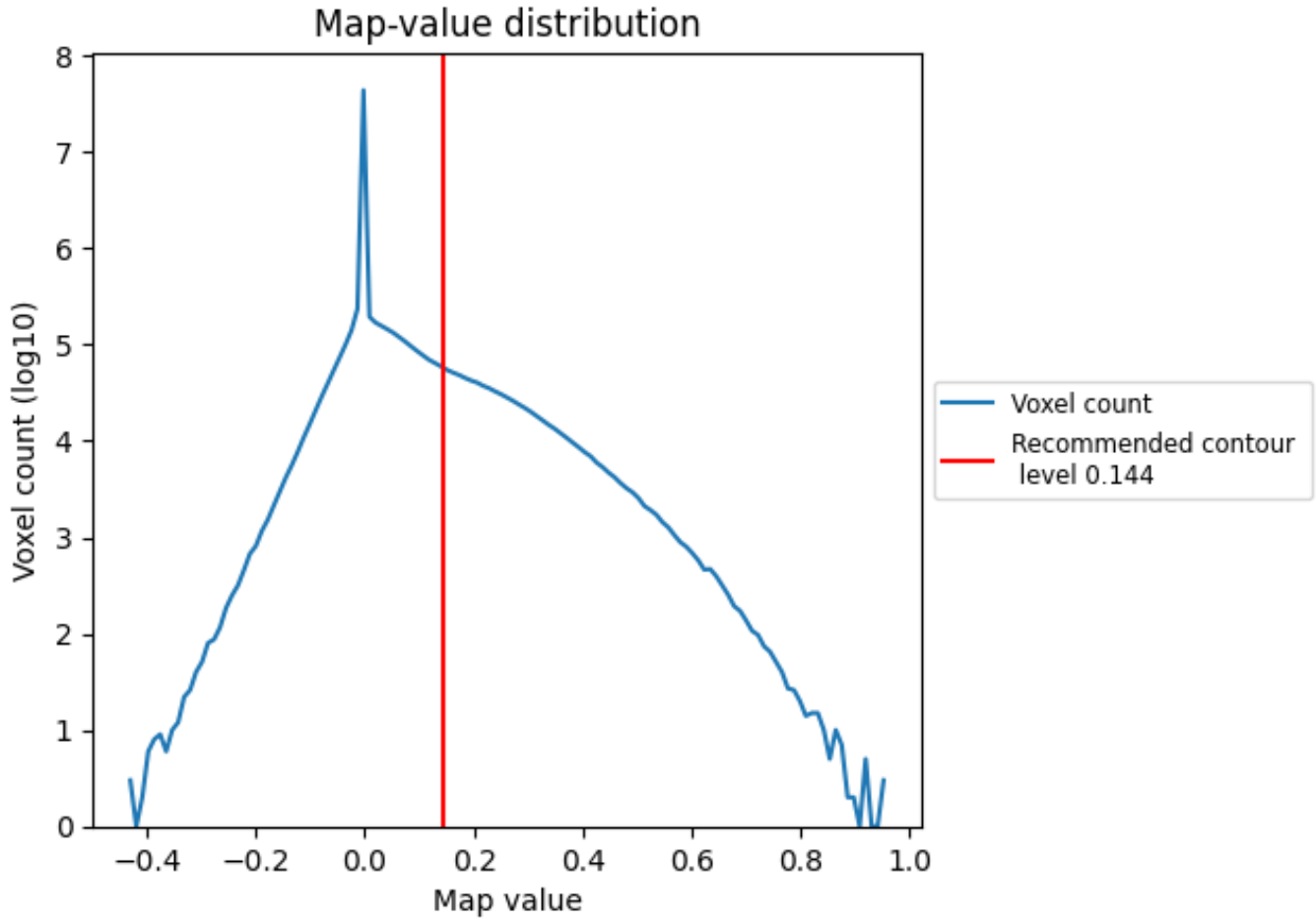
6.6 Mask visualisation (i)

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

7 Map analysis

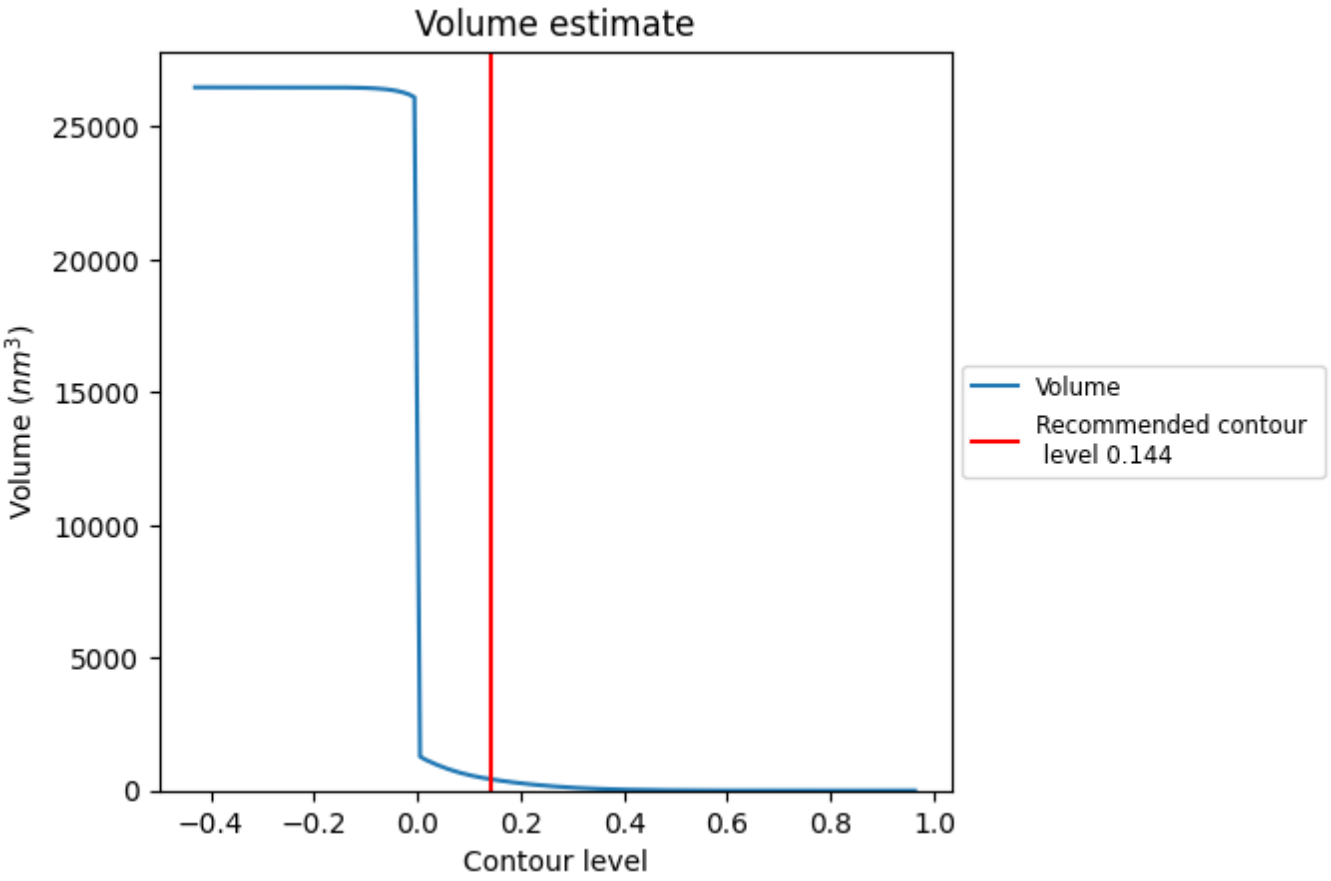
This section contains the results of statistical analysis of the map.

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.

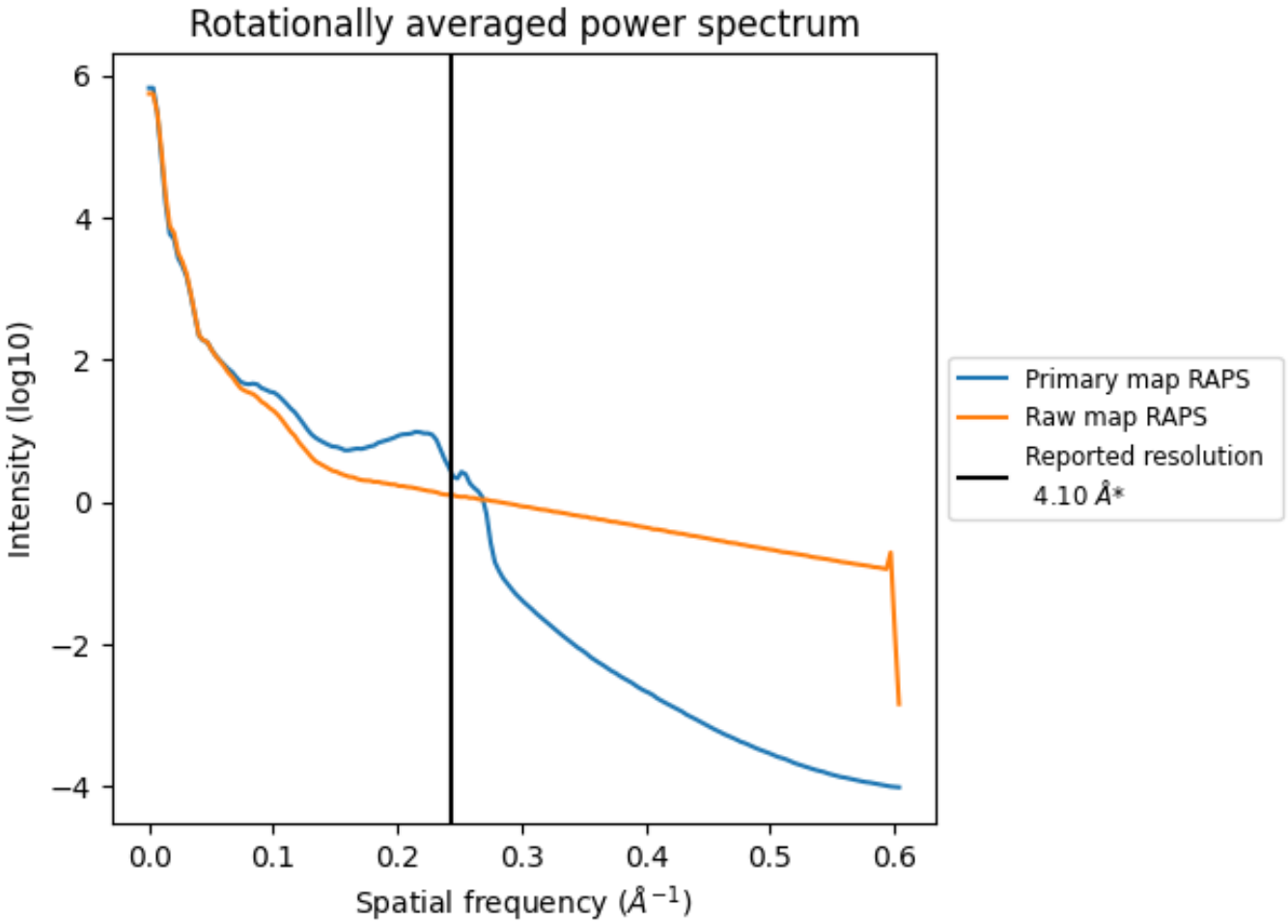
7.2 Volume estimate



The volume at the recommended contour level is 422 nm^3; this corresponds to an approximate mass of 381 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)

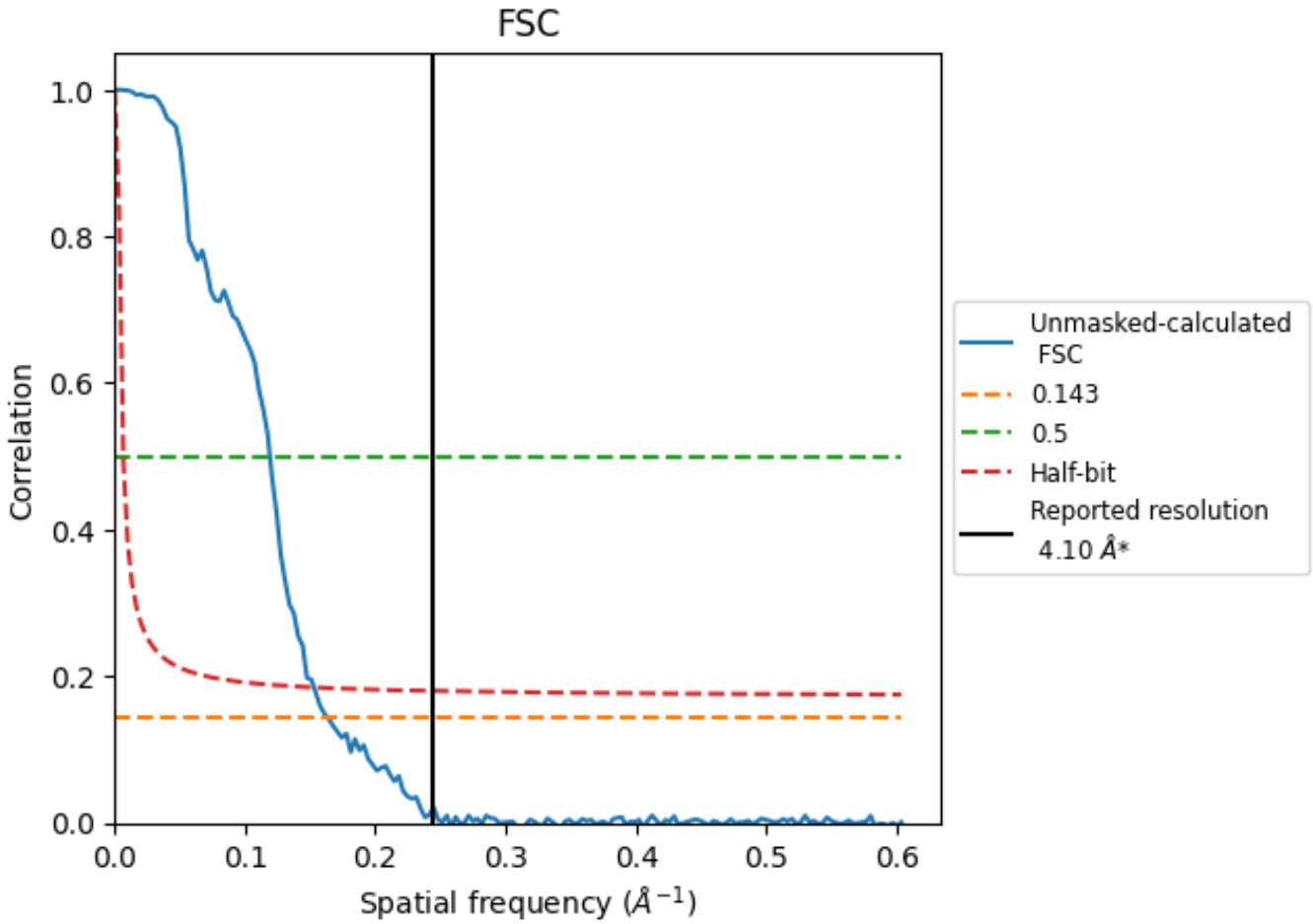


*Reported resolution corresponds to spatial frequency of 0.244 Å^{-1}

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 0.244 Å^{-1}

8.2 Resolution estimates (i)

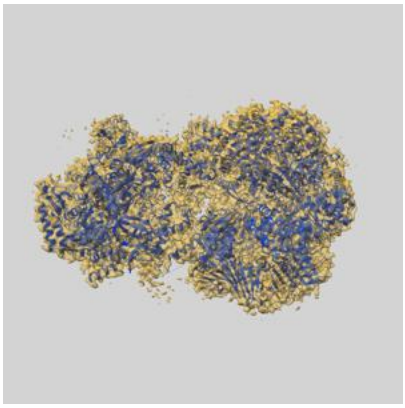
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.11	8.40	6.54

*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 6.11 differs from the reported value 4.1 by more than 10 %

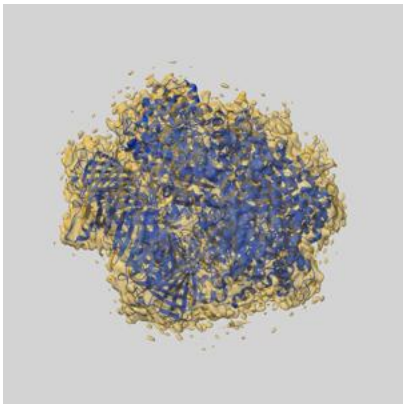
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-41664 and PDB model 8TWA. Per-residue inclusion information can be found in section 3 on page 9.

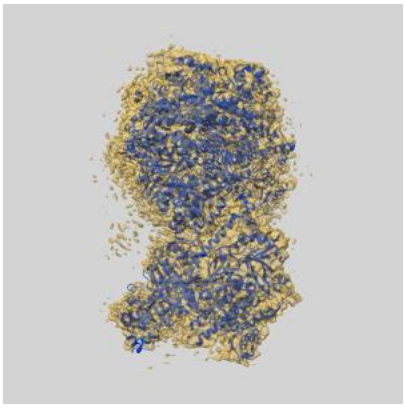
9.1 Map-model overlay



X



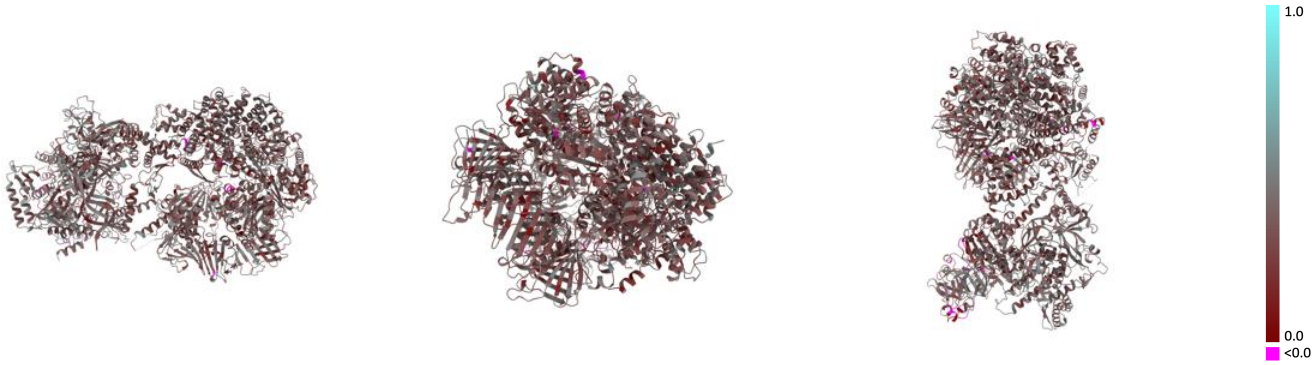
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.144 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.

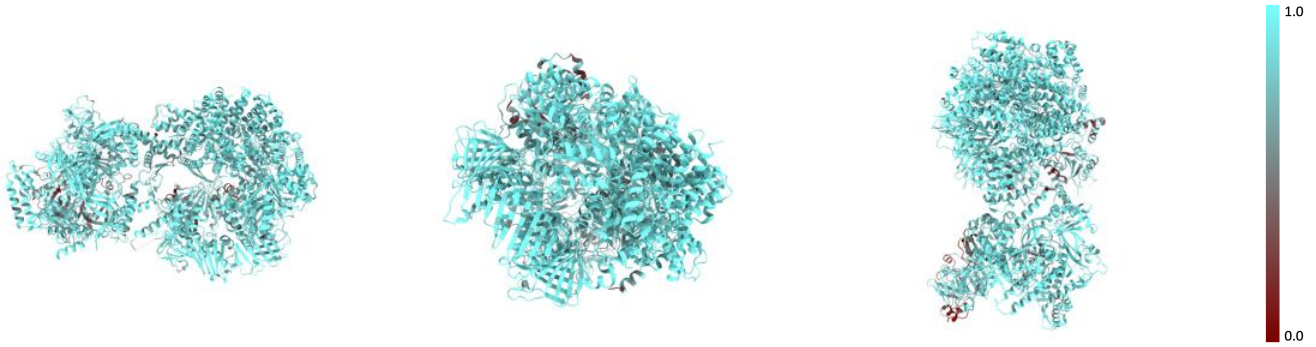
9.2 Q-score mapped to coordinate model (i)



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.

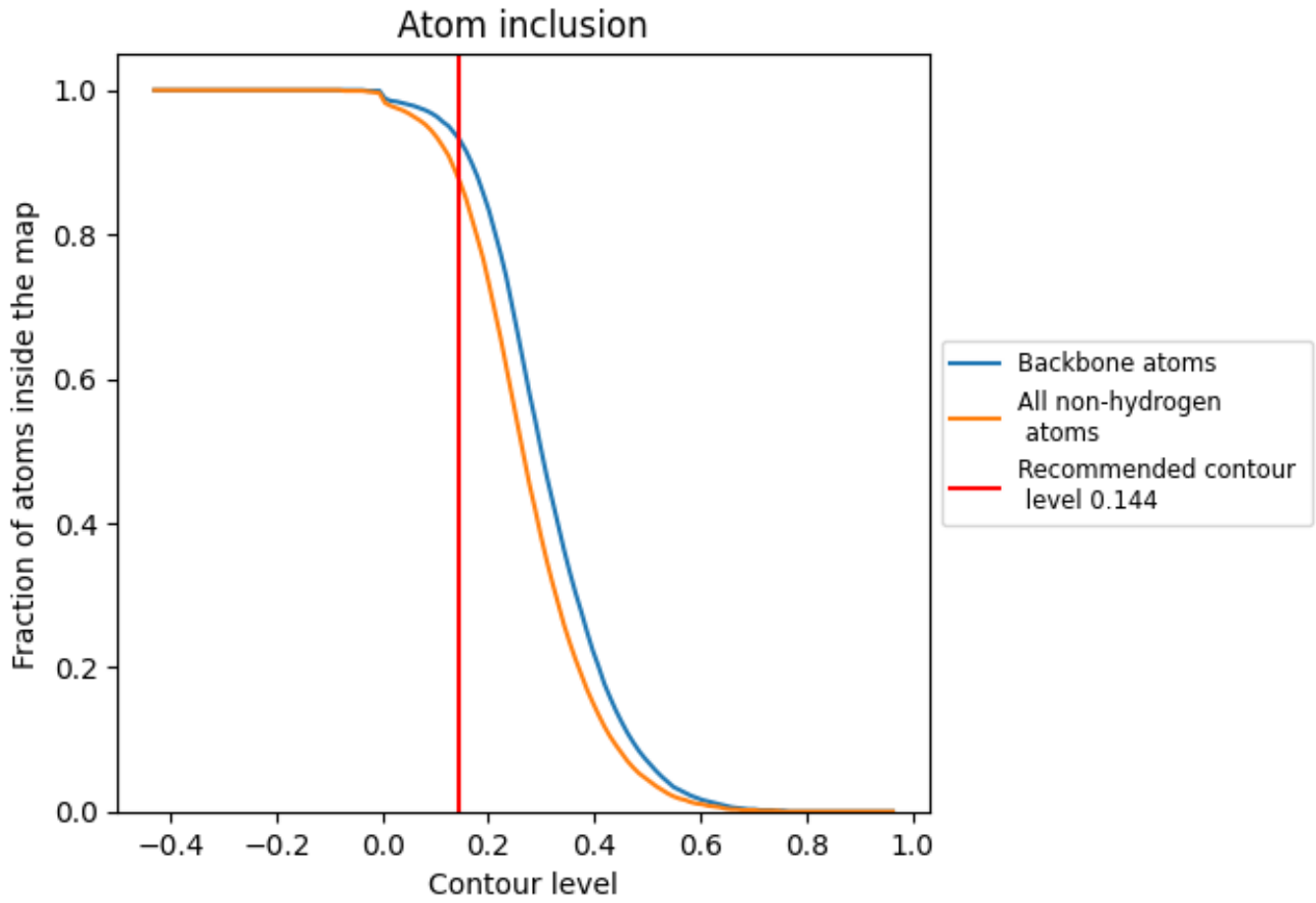
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.144).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 88% 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 (0.144) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8770	0.3490
1	0.8110	0.3280
2	0.9340	0.3480
3	0.9370	0.3480
4	0.8950	0.3300
5	0.9260	0.3410
B	0.6950	0.3290
C	0.8710	0.4140
D	0.6380	0.3060
E	0.8770	0.3690
P	0.8690	0.3290
T	0.7720	0.3360
X	0.9110	0.3440
Y	0.9270	0.3630
Z	0.9380	0.3590