



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 06:22 PM UTC

PDB ID : 7P30 / pdb_00007p30
EMDB ID : EMD-13176
Title : 3.0 Å resolution structure of a DNA-loaded MCM double hexamer
Authors : Greiwe, J.F.; Miller, T.C.R.; Martino, F.; Costa, A.
Deposited on : 2021-07-06
Resolution : 3.00 Å (reported)
Based on initial models : 6F0L, 6EYC, 5BK4

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

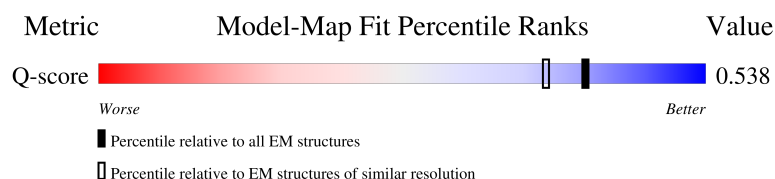
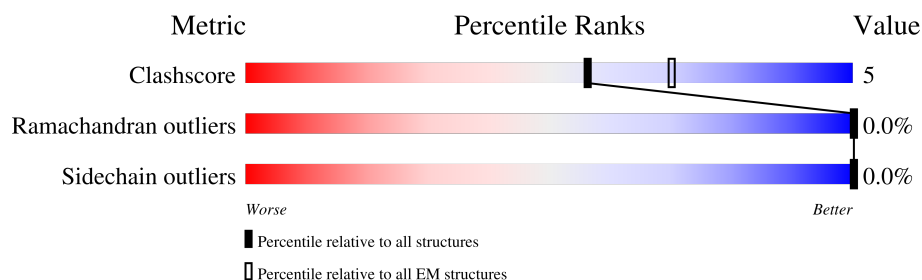
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	868	11% 62% 9% 28%
1	A	868	11% 63% 9% 28%
2	3	1006	53% 6% 41%
2	B	1006	54% 5% 41%

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Mol	Chain	Length	Quality of chain
3	4	933	
3	C	933	
4	5	775	
4	D	775	
5	6	1017	
5	E	1017	
6	7	845	
6	F	845	
7	X	53	
8	Y	53	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 123819 atoms, of which 61072 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 replication licensing factor MCM2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	2	623	Total	C	H	N	O	S	0	0
			9918	3109	4986	877	927	19		
1	A	623	Total	C	H	N	O	S	0	0
			9918	3109	4986	877	927	19		

- Molecule 2 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	3	595	Total	C	H	N	O	S	0	0
			9381	2930	4726	833	879	13		
2	B	595	Total	C	H	N	O	S	0	0
			9381	2930	4726	833	879	13		

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	-34	MET	-	initiating methionine	UNP P24279
3	-33	LYS	-	expression tag	UNP P24279
3	-32	ARG	-	expression tag	UNP P24279
3	-31	ARG	-	expression tag	UNP P24279
3	-30	TRP	-	expression tag	UNP P24279
3	-29	LYS	-	expression tag	UNP P24279
3	-28	LYS	-	expression tag	UNP P24279
3	-27	ASN	-	expression tag	UNP P24279
3	-26	PHE	-	expression tag	UNP P24279
3	-25	ILE	-	expression tag	UNP P24279
3	-24	ALA	-	expression tag	UNP P24279
3	-23	VAL	-	expression tag	UNP P24279
3	-22	SER	-	expression tag	UNP P24279
3	-21	ALA	-	expression tag	UNP P24279
3	-20	ALA	-	expression tag	UNP P24279
3	-19	ASN	-	expression tag	UNP P24279
3	-18	ARG	-	expression tag	UNP P24279

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Chain	Residue	Modelled	Actual	Comment	Reference
3	-17	PHE	-	expression tag	UNP P24279
3	-16	LYS	-	expression tag	UNP P24279
3	-15	LYS	-	expression tag	UNP P24279
3	-14	ILE	-	expression tag	UNP P24279
3	-13	SER	-	expression tag	UNP P24279
3	-12	SER	-	expression tag	UNP P24279
3	-11	SER	-	expression tag	UNP P24279
3	-10	GLY	-	expression tag	UNP P24279
3	-9	ALA	-	expression tag	UNP P24279
3	-8	LEU	-	expression tag	UNP P24279
3	-7	GLU	-	expression tag	UNP P24279
3	-6	ASN	-	expression tag	UNP P24279
3	-5	LEU	-	expression tag	UNP P24279
3	-4	TYR	-	expression tag	UNP P24279
3	-3	PHE	-	expression tag	UNP P24279
3	-2	GLN	-	expression tag	UNP P24279
3	-1	GLY	-	expression tag	UNP P24279
3	0	GLU	-	expression tag	UNP P24279
B	-34	MET	-	initiating methionine	UNP P24279
B	-33	LYS	-	expression tag	UNP P24279
B	-32	ARG	-	expression tag	UNP P24279
B	-31	ARG	-	expression tag	UNP P24279
B	-30	TRP	-	expression tag	UNP P24279
B	-29	LYS	-	expression tag	UNP P24279
B	-28	LYS	-	expression tag	UNP P24279
B	-27	ASN	-	expression tag	UNP P24279
B	-26	PHE	-	expression tag	UNP P24279
B	-25	ILE	-	expression tag	UNP P24279
B	-24	ALA	-	expression tag	UNP P24279
B	-23	VAL	-	expression tag	UNP P24279
B	-22	SER	-	expression tag	UNP P24279
B	-21	ALA	-	expression tag	UNP P24279
B	-20	ALA	-	expression tag	UNP P24279
B	-19	ASN	-	expression tag	UNP P24279
B	-18	ARG	-	expression tag	UNP P24279
B	-17	PHE	-	expression tag	UNP P24279
B	-16	LYS	-	expression tag	UNP P24279
B	-15	LYS	-	expression tag	UNP P24279
B	-14	ILE	-	expression tag	UNP P24279
B	-13	SER	-	expression tag	UNP P24279
B	-12	SER	-	expression tag	UNP P24279
B	-11	SER	-	expression tag	UNP P24279

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	GLY	-	expression tag	UNP P24279
B	-9	ALA	-	expression tag	UNP P24279
B	-8	LEU	-	expression tag	UNP P24279
B	-7	GLU	-	expression tag	UNP P24279
B	-6	ASN	-	expression tag	UNP P24279
B	-5	LEU	-	expression tag	UNP P24279
B	-4	TYR	-	expression tag	UNP P24279
B	-3	PHE	-	expression tag	UNP P24279
B	-2	GLN	-	expression tag	UNP P24279
B	-1	GLY	-	expression tag	UNP P24279
B	0	GLU	-	expression tag	UNP P24279

- Molecule 3 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	4	654	Total	C	H	N	O	S	0	0
			10452	3259	5256	896	1011	30		
3	C	654	Total	C	H	N	O	S	0	0
			10452	3259	5256	896	1011	30		

- Molecule 4 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	5	652	Total	C	H	N	O	S	0	0
			10253	3198	5150	873	1007	25		
4	D	652	Total	C	H	N	O	S	0	0
			10251	3198	5148	873	1007	25		

- Molecule 5 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	6	609	Total	C	H	N	O	S	0	0
			9681	3041	4862	840	913	25		
5	E	609	Total	C	H	N	O	S	0	0
			9681	3041	4862	840	913	25		

- Molecule 6 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	7	689	Total	C	H	N	O	S	0	0
			10935	3421	5502	942	1041	29		

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Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	689	Total	C	H	N	O	S	0	0
			10935	3421	5502	942	1041	29		

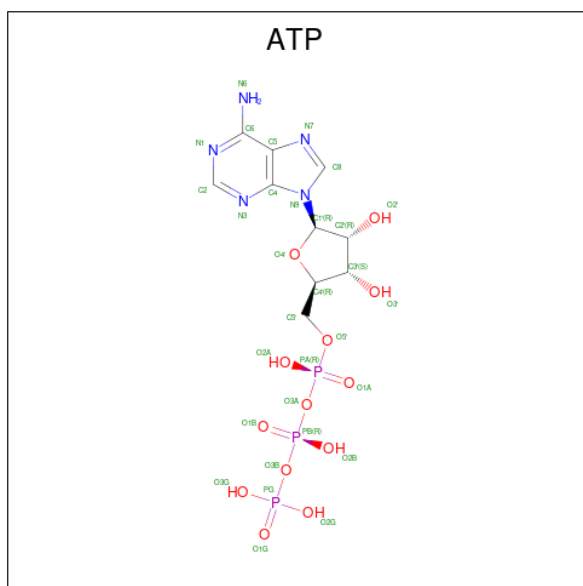
- Molecule 7 is a DNA chain called DNA (53-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	X	53	Total	C	N	O	P	0	0
			1086	515	199	319	53		

- Molecule 8 is a DNA chain called DNA (53-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Y	53	Total	C	N	O	P	0	0
			1087	515	202	317	53		

- Molecule 9 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

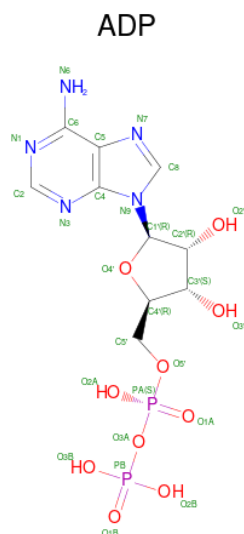


Mol	Chain	Residues	Atoms		AltConf
10	2	1	Total 1	Mg 1	0
10	3	1	Total 1	Mg 1	0
10	5	1	Total 1	Mg 1	0
10	7	2	Total 2	Mg 2	0
10	A	1	Total 1	Mg 1	0
10	B	1	Total 1	Mg 1	0
10	D	1	Total 1	Mg 1	0
10	F	2	Total 2	Mg 2	0

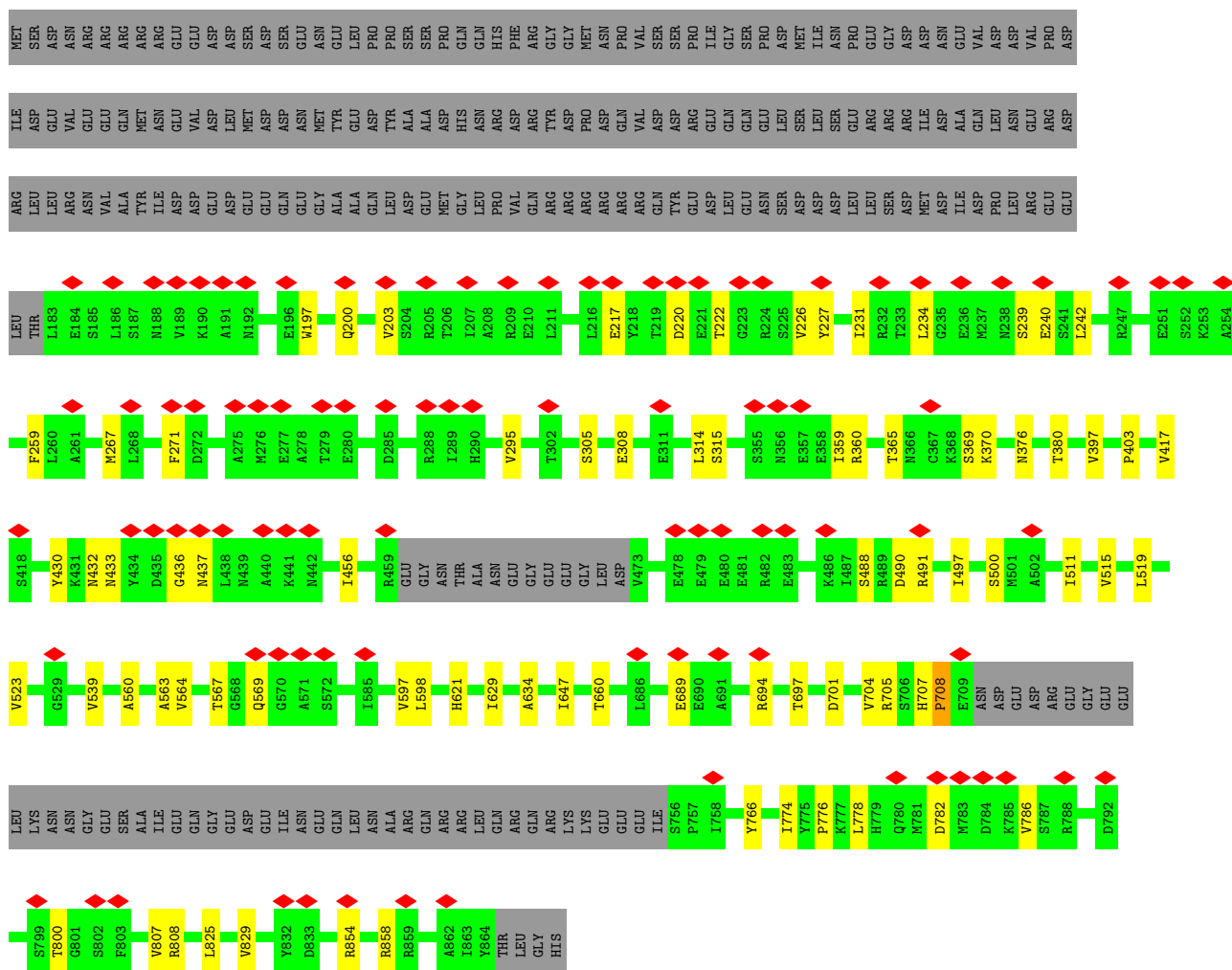
- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
11	2	1	Total 1	Zn 1	0
11	4	1	Total 1	Zn 1	0
11	5	1	Total 1	Zn 1	0
11	6	1	Total 1	Zn 1	0
11	7	1	Total 1	Zn 1	0
11	A	1	Total 1	Zn 1	0
11	C	1	Total 1	Zn 1	0
11	D	1	Total 1	Zn 1	0
11	E	1	Total 1	Zn 1	0
11	F	1	Total 1	Zn 1	0

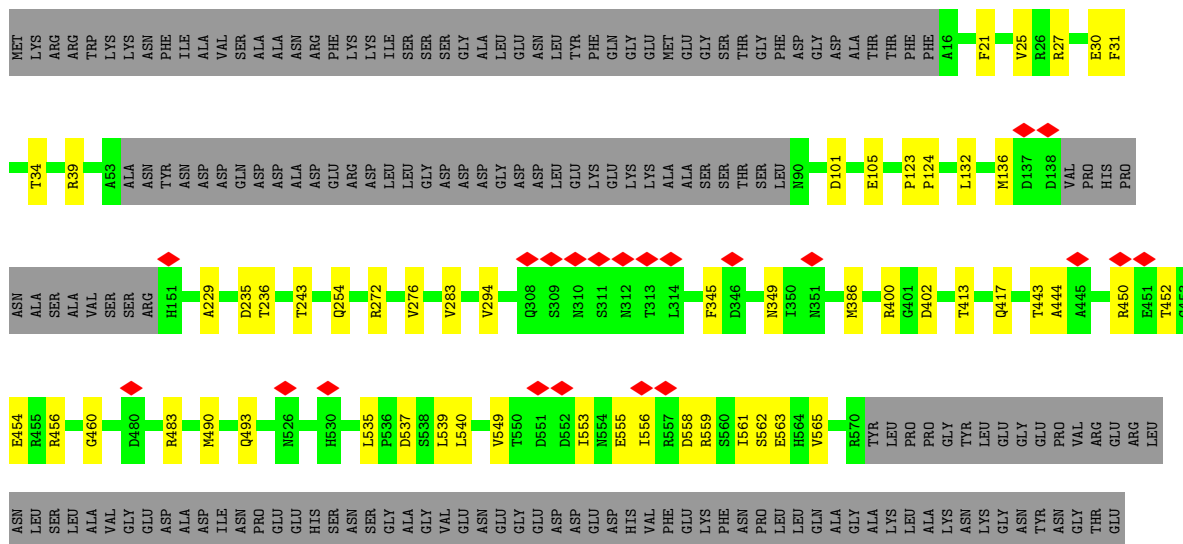
- Molecule 12 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

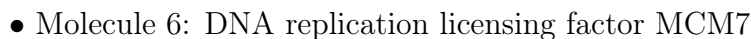


Mol	Chain	Residues	Atoms						AltConf
12	3	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
12	4	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
12	5	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
12	7	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
12	B	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
12	C	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
12	D	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
12	F	1	Total 38	C 10	H 11	N 5	O 10	P 2	0

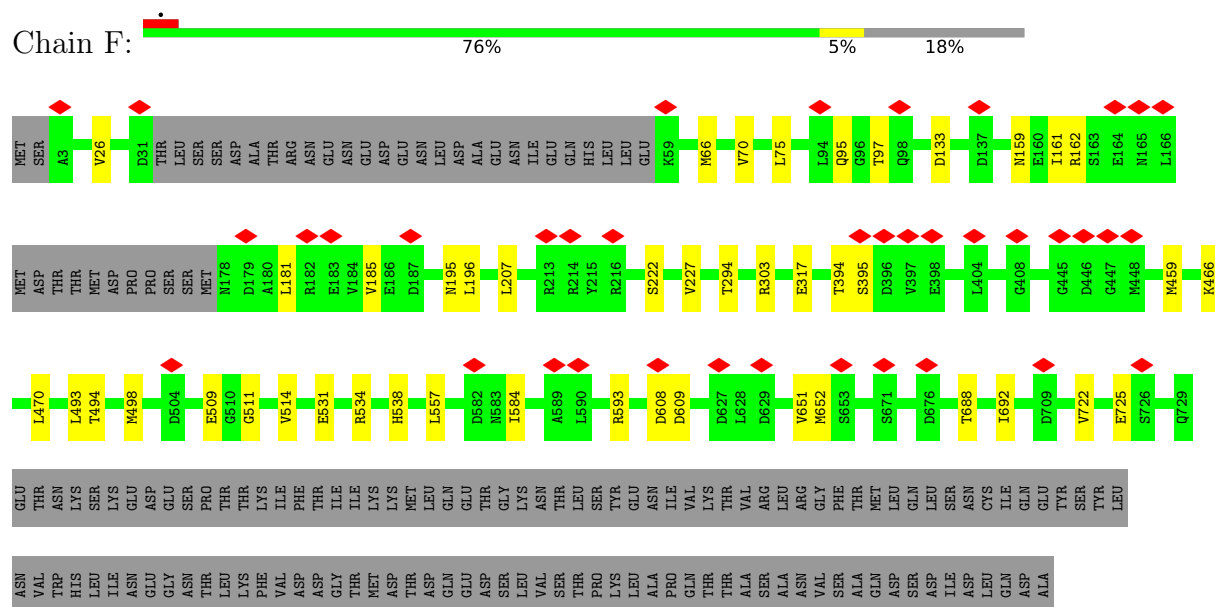


- Molecule 2: DNA replication licensing factor MCM3

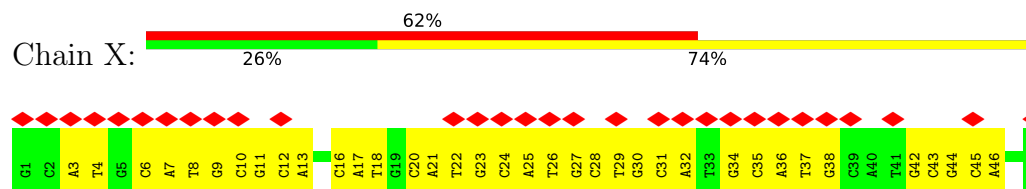




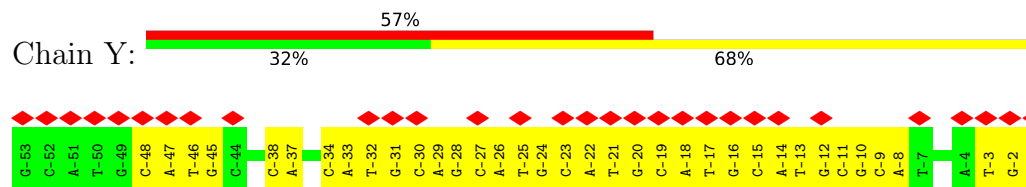
- Molecule 6: DNA replication licensing factor MCM7



- Molecule 7: DNA (53-MER)



- Molecule 8: DNA (53-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	238620	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.3	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4100	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.081	Depositor
Minimum map value	-1.358	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.074	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	276.48, 276.48, 276.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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, ATP, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	2	0.10	0/5019	0.26	0/6781
1	A	0.14	1/5019 (0.0%)	0.30	2/6781 (0.0%)
2	3	0.11	0/4733	0.27	0/6417
2	B	0.11	0/4733	0.27	0/6417
3	4	0.10	0/5270	0.25	0/7123
3	C	0.09	0/5270	0.25	0/7123
4	5	0.23	2/5176 (0.0%)	0.37	3/7000 (0.0%)
4	D	0.19	1/5176 (0.0%)	0.36	4/7000 (0.1%)
5	6	0.10	0/4896	0.28	0/6601
5	E	0.10	0/4896	0.26	0/6601
6	7	0.11	0/5516	0.27	0/7454
6	F	0.10	0/5516	0.27	0/7454
7	X	0.15	0/1217	0.32	0/1876
8	Y	0.17	0/1219	0.33	0/1879
All	All	0.13	4/63656 (0.0%)	0.29	9/86507 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	525	PRO	CG-CD	-13.40	1.05	1.50
4	D	525	PRO	CG-CD	-10.65	1.14	1.50
1	A	708	PRO	CG-CD	-6.01	1.30	1.50
4	5	525	PRO	N-CD	5.21	1.55	1.47

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	525	PRO	N-CD-CG	-14.59	81.31	103.20
4	D	525	PRO	N-CD-CG	-13.23	83.36	103.20
4	5	525	PRO	CA-N-CD	-10.16	97.78	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	525	PRO	CA-N-CD	-8.28	100.42	112.00
1	A	708	PRO	N-CD-CG	-8.14	90.98	103.20
4	5	525	PRO	CA-CB-CG	-7.86	89.58	104.50
4	D	525	PRO	CA-CB-CG	-6.62	91.92	104.50
1	A	708	PRO	CA-N-CD	-6.52	102.87	112.00
4	D	525	PRO	N-CA-CB	-5.08	98.22	103.15

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2	4932	4986	4984	63	0
1	A	4932	4986	4984	53	0
2	3	4655	4726	4723	39	0
2	B	4655	4726	4723	36	0
3	4	5196	5256	5254	42	0
3	C	5196	5256	5254	44	0
4	5	5103	5150	5147	61	0
4	D	5103	5148	5147	65	0
5	6	4819	4862	4856	52	0
5	E	4819	4862	4856	47	0
6	7	5433	5502	5500	37	0
6	F	5433	5502	5500	28	0
7	X	1086	0	596	41	0
8	Y	1087	0	595	43	0
9	2	31	11	12	0	0
9	A	31	11	12	0	0
10	2	1	0	0	0	0
10	3	1	0	0	0	0
10	5	1	0	0	0	0
10	7	2	0	0	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
10	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	F	2	0	0	0	0
11	2	1	0	0	0	0
11	4	1	0	0	0	0
11	5	1	0	0	0	0
11	6	1	0	0	0	0
11	7	1	0	0	0	0
11	A	1	0	0	0	0
11	C	1	0	0	0	0
11	D	1	0	0	0	0
11	E	1	0	0	0	0
11	F	1	0	0	0	0
12	3	27	11	12	1	0
12	4	27	11	12	1	0
12	5	27	11	12	2	0
12	7	27	11	12	0	0
12	B	27	11	12	1	0
12	C	27	11	12	1	0
12	D	27	11	12	2	0
12	F	27	11	12	0	0
All	All	62747	61072	62239	617	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 5.

All (617) 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)
4:5:621:LYS:NZ	4:5:678:ASP:OD1	2.05	0.89
8:Y:-12:DG:H4'	8:Y:-11:DC:OP1	1.72	0.87
6:7:401:VAL:O	6:7:405:ILE:HD12	1.74	0.87
7:X:7:DA:H2''	7:X:8:DT:H71	1.59	0.84
3:4:350:ASN:OD1	3:4:381:SER:OG	1.94	0.84
6:7:95:GLN:NE2	6:7:97:THR:OG1	2.11	0.82
6:F:95:GLN:NE2	6:F:97:THR:OG1	2.13	0.82
5:6:616:GLU:OE1	5:6:619:GLY:N	2.13	0.81
2:3:402:ASP:OD2	2:3:493:GLN:NE2	2.15	0.80
2:B:402:ASP:OD2	2:B:493:GLN:NE2	2.15	0.80
5:E:657:GLU:OE2	5:E:708:ARG:NH2	2.15	0.80
2:B:417:GLN:NE2	4:D:499:GLN:OE1	2.14	0.80
5:E:616:GLU:OE1	5:E:619:GLY:N	2.14	0.80
8:Y:-47:DA:H2''	8:Y:-46:DT:H5'	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:417:GLN:NE2	4:5:499:GLN:OE1	2.14	0.79
7:X:7:DA:C2'	7:X:8:DT:H71	2.15	0.77
1:2:438:LEU:HD21	7:X:34:DG:H5''	1.67	0.76
5:E:168:MET:HE2	5:E:168:MET:N	1.99	0.76
3:C:815:ASN:O	3:C:815:ASN:ND2	2.19	0.75
2:B:559:ARG:O	2:B:562:SER:OG	2.02	0.75
5:6:553:GLY:O	5:6:812:ARG:NH1	2.19	0.75
3:4:815:ASN:O	3:4:815:ASN:ND2	2.18	0.74
8:Y:-30:DC:H2''	8:Y:-29:DA:C8	2.22	0.74
3:C:732:LYS:NZ	3:C:734:GLU:OE1	2.21	0.74
4:D:90:PHE:CE2	4:D:137:LEU:HD13	2.23	0.74
7:X:6:DC:H2''	7:X:7:DA:C8	2.23	0.74
1:2:597:VAL:HG23	1:2:629:ILE:HD12	1.70	0.73
7:X:37:DT:H2''	7:X:38:DG:C8	2.23	0.73
8:Y:-21:DT:H4'	8:Y:-20:DG:OP1	1.87	0.73
3:C:350:ASN:OD1	3:C:381:SER:OG	2.06	0.72
4:D:407:ARG:NH1	4:D:497:MET:O	2.22	0.72
4:5:90:PHE:CE2	4:5:137:LEU:HD13	2.24	0.72
7:X:24:DC:H2''	7:X:25:DA:C8	2.24	0.72
1:2:774:ILE:HG22	1:2:776:PRO:HD3	1.72	0.71
7:X:45:DC:H2''	7:X:46:DA:C8	2.25	0.71
3:4:732:LYS:NZ	3:4:734:GLU:OE1	2.24	0.71
2:3:559:ARG:O	2:3:562:SER:OG	2.06	0.71
1:A:621:HIS:NE2	4:D:481:GLU:OE1	2.24	0.70
1:A:315:SER:N	1:A:430:TYR:O	2.25	0.70
1:2:621:HIS:NE2	4:5:481:GLU:OE1	2.25	0.69
1:2:807:VAL:HG21	12:5:801:ADP:C8	2.28	0.69
1:A:778:LEU:HD23	1:A:829:VAL:HG11	1.75	0.69
1:A:807:VAL:HG21	12:D:801:ADP:C8	2.28	0.69
4:D:144:ASN:O	4:D:144:ASN:ND2	2.26	0.69
6:7:66:MET:O	6:7:70:VAL:HG23	1.94	0.68
1:A:488:SER:OG	1:A:766:TYR:OH	1.94	0.68
6:F:493:LEU:O	6:F:494:THR:OG1	2.11	0.68
3:4:775:VAL:HG21	5:6:725:THR:HG22	1.77	0.67
5:E:340:ASN:OD1	5:E:341:ARG:N	2.27	0.67
6:7:493:LEU:O	6:7:494:THR:OG1	2.11	0.67
4:D:39:ARG:NH2	4:D:42:SER:OG	2.28	0.67
6:7:407:SER:OG	6:7:413:ARG:NH1	2.27	0.67
1:A:707:HIS:ND1	1:A:708:PRO:O	2.26	0.66
1:2:359:ILE:O	1:2:360:ARG:NE	2.28	0.66
1:2:315:SER:N	1:2:430:TYR:O	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:227:TYR:O	1:2:231:ILE:HD12	1.96	0.66
1:2:707:HIS:ND1	1:2:708:PRO:O	2.29	0.66
5:6:340:ASN:OD1	5:6:341:ARG:N	2.28	0.66
3:4:621:LEU:HD23	3:4:648:VAL:HG21	1.78	0.66
1:A:227:TYR:O	1:A:231:ILE:HD12	1.96	0.65
5:E:510:SER:O	5:E:513:ILE:HD12	1.97	0.65
4:D:74:ASP:OD1	4:D:75:ILE:N	2.30	0.65
5:E:584:PHE:O	5:E:588:VAL:HG23	1.96	0.65
1:2:689:GLU:OE2	5:6:782:LYS:NZ	2.30	0.65
8:Y:-12:DG:H1'	8:Y:-11:DC:C5'	2.27	0.65
3:C:758:ILE:HD11	3:C:810:LYS:O	1.96	0.65
4:D:473:ASP:OD1	4:D:516:ARG:N	2.30	0.65
7:X:31:DC:H2''	7:X:32:DA:N7	2.12	0.65
3:C:621:LEU:HD23	3:C:648:VAL:HG21	1.79	0.64
7:X:22:DT:H2''	7:X:23:DG:C8	2.33	0.64
8:Y:-12:DG:H1'	8:Y:-11:DC:H5'	1.79	0.64
4:5:74:ASP:OD1	4:5:75:ILE:N	2.30	0.64
4:5:149:ARG:NH1	4:5:260:GLU:OE2	2.30	0.64
1:A:359:ILE:O	1:A:360:ARG:NE	2.31	0.64
4:5:473:ASP:OD1	4:5:516:ARG:N	2.31	0.64
3:C:230:LEU:HD12	3:C:280:MET:HG2	1.80	0.64
2:3:558:ASP:OD1	4:5:630:ARG:NE	2.30	0.63
8:Y:-23:DC:H2''	8:Y:-22:DA:C8	2.33	0.63
3:C:575:SER:N	12:C:1001:ADP:O2B	2.32	0.63
5:6:510:SER:O	5:6:513:ILE:HD12	1.98	0.63
1:A:314:LEU:HD22	1:A:432:ASN:OD1	1.99	0.63
2:B:400:ARG:NH1	2:B:490:MET:O	2.31	0.63
2:B:101:ASP:O	2:B:105:GLU:OE1	2.17	0.62
5:E:566:ARG:NH1	5:E:568:ASP:O	2.32	0.62
7:X:35:DC:H2''	7:X:36:DA:H8	1.64	0.62
1:A:490:ASP:OD1	1:A:491:ARG:N	2.33	0.62
4:5:569:ALA:O	4:5:573:ILE:HD12	2.00	0.61
2:3:101:ASP:O	2:3:105:GLU:OE1	2.17	0.61
1:2:490:ASP:OD1	1:2:491:ARG:N	2.33	0.61
2:3:400:ARG:NH1	2:3:490:MET:O	2.32	0.61
1:A:220:ASP:OD2	1:A:222:THR:OG1	2.10	0.61
2:B:558:ASP:OD1	4:D:630:ARG:NE	2.33	0.61
4:D:90:PHE:HE2	4:D:137:LEU:HD13	1.63	0.61
8:Y:-17:DT:H2''	8:Y:-16:DG:C8	2.36	0.61
4:5:90:PHE:HE2	4:5:137:LEU:HD13	1.64	0.61
6:7:659:TYR:OH	6:7:714:GLU:OE2	2.17	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:35:DC:H2''	7:X:36:DA:C8	2.36	0.61
6:7:207:LEU:O	6:7:222:SER:OG	2.10	0.60
2:B:559:ARG:O	2:B:563:GLU:OE1	2.18	0.60
3:C:431:ASP:OD1	3:C:587:ARG:NH1	2.34	0.60
5:6:566:ARG:NH1	5:6:568:ASP:O	2.33	0.60
1:A:519:LEU:O	1:A:519:LEU:HD23	2.01	0.60
8:Y:-13:DT:H2''	8:Y:-12:DG:C8	2.36	0.60
1:2:564:VAL:HG21	1:2:598:LEU:HD22	1.83	0.60
4:5:39:ARG:NH2	4:5:42:SER:OG	2.34	0.60
4:D:569:ALA:O	4:D:573:ILE:HD12	2.00	0.60
3:C:640:SER:OG	5:E:601:LYS:NZ	2.35	0.60
7:X:44:DG:H2''	7:X:45:DC:C6	2.37	0.60
8:Y:-18:DA:H2''	8:Y:-17:DT:H5'	1.83	0.60
2:B:413:THR:HG21	2:B:549:VAL:CG2	2.32	0.60
5:6:691:ARG:HH21	5:6:716:LEU:HD13	1.66	0.59
1:2:220:ASP:OD2	1:2:222:THR:OG1	2.12	0.59
2:3:235:ASP:OD1	2:3:236:THR:N	2.35	0.59
4:D:20:ASN:OD1	4:D:21:ASP:N	2.34	0.59
3:4:189:GLU:N	3:4:189:GLU:OE1	2.35	0.59
5:6:770:ARG:O	5:6:774:VAL:HG23	2.03	0.59
1:A:774:ILE:HG22	1:A:776:PRO:HD3	1.84	0.59
3:4:550:LYS:NZ	3:4:806:GLU:OE1	2.35	0.59
3:C:189:GLU:N	3:C:189:GLU:OE1	2.35	0.59
2:3:413:THR:HG21	2:3:549:VAL:CG2	2.32	0.59
3:C:329:LYS:NZ	3:C:404:ASP:OD1	2.36	0.59
5:E:522:ASP:OD1	5:E:523:GLU:N	2.36	0.59
3:C:758:ILE:HD13	3:C:813:LEU:HA	1.85	0.58
8:Y:-10:DG:H2''	8:Y:-9:DC:C6	2.38	0.58
2:3:559:ARG:O	2:3:563:GLU:OE1	2.20	0.58
4:5:153:SER:O	4:5:156:VAL:HG23	2.03	0.58
6:F:466:LYS:O	6:F:470:LEU:HD23	2.03	0.58
5:6:549:LEU:HD21	5:6:810:ILE:CG1	2.32	0.58
5:E:770:ARG:O	5:E:774:VAL:HG23	2.04	0.58
7:X:31:DC:H2''	7:X:32:DA:C8	2.38	0.58
2:B:562:SER:O	2:B:566:LEU:HD23	2.04	0.58
3:4:366:GLN:NE2	6:7:297:GLN:OE1	2.34	0.58
5:E:549:LEU:HD21	5:E:810:ILE:CG1	2.34	0.58
3:4:519:TYR:CD1	3:4:811:MET:HE1	2.39	0.57
3:4:575:SER:N	12:4:1001:ADP:O2B	2.37	0.57
1:A:808:ARG:NH2	12:D:801:ADP:O3B	2.37	0.57
6:F:161:ILE:HD12	6:F:185:VAL:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:466:LYS:O	6:7:470:LEU:HD23	2.03	0.57
8:Y:-38:DC:H2''	8:Y:-37:DA:C8	2.38	0.57
5:6:629:MET:HE1	5:6:673:ASN:O	2.04	0.57
3:4:370:ARG:NH2	3:4:377:ASN:O	2.36	0.57
4:5:524:ASN:OD1	4:5:525:PRO:HD3	2.05	0.57
1:A:437:ASN:ND2	8:Y:-20:DG:OP2	2.37	0.57
1:2:544:ASP:OD2	1:2:656:ARG:NH1	2.37	0.57
6:7:494:THR:O	6:7:511:GLY:N	2.36	0.57
6:7:597:LEU:O	6:7:723:SER:OG	2.23	0.57
6:F:181:LEU:O	6:F:185:VAL:HG23	2.04	0.57
6:F:494:THR:O	6:F:511:GLY:N	2.36	0.57
1:A:597:VAL:HG23	1:A:629:ILE:HD12	1.86	0.57
4:5:493:ILE:HG22	4:5:497:MET:HE3	1.87	0.57
4:D:153:SER:O	4:D:156:VAL:HG23	2.05	0.57
5:E:549:LEU:HD21	5:E:810:ILE:HG12	1.86	0.57
5:E:555:VAL:HG22	5:E:808:GLU:OE2	2.05	0.56
2:3:345:PHE:O	2:3:349:ASN:ND2	2.39	0.56
4:5:20:ASN:OD1	4:5:21:ASP:N	2.38	0.56
6:F:159:ASN:OD1	6:F:162:ARG:NH2	2.37	0.56
8:Y:-48:DC:H2''	8:Y:-47:DA:C8	2.40	0.56
8:Y:-18:DA:H2''	8:Y:-17:DT:C5'	2.35	0.56
1:2:566:ALA:O	1:2:567:THR:OG1	2.24	0.56
4:5:450:THR:HG22	4:5:451:ALA:H	1.71	0.56
8:Y:-34:DC:H2'	8:Y:-33:DA:H8	1.70	0.56
8:Y:-34:DC:H2'	8:Y:-33:DA:C8	2.40	0.56
4:5:374:ILE:O	4:5:385:LYS:NZ	2.39	0.56
3:C:226:TYR:O	3:C:230:LEU:HD23	2.04	0.56
6:F:207:LEU:O	6:F:222:SER:OG	2.10	0.56
1:2:239:SER:OG	1:2:240:GLU:N	2.39	0.56
1:2:598:LEU:O	1:2:598:LEU:HD23	2.05	0.56
1:2:808:ARG:NH2	12:5:801:ADP:O3B	2.38	0.55
3:4:640:SER:OG	5:6:601:LYS:NZ	2.35	0.55
3:C:572:THR:HG21	3:C:708:VAL:HG11	1.89	0.55
1:2:376:ASN:O	1:2:380:THR:OG1	2.22	0.55
4:D:69:ILE:HD12	4:D:76:TYR:CE2	2.42	0.55
3:4:572:THR:HG21	3:4:708:VAL:HG11	1.89	0.55
7:X:29:DT:H2''	7:X:30:DG:N7	2.21	0.55
7:X:22:DT:H2''	7:X:23:DG:N7	2.22	0.55
5:6:549:LEU:HD21	5:6:810:ILE:HG12	1.88	0.55
5:6:629:MET:HA	5:6:629:MET:HE3	1.89	0.55
1:A:239:SER:OG	1:A:240:GLU:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:567:THR:HG22	1:2:569:GLN:H	1.71	0.54
4:5:432:VAL:HG23	4:5:596:ILE:HG13	1.90	0.54
2:3:21:PHE:O	2:3:25:VAL:HG23	2.07	0.54
5:6:522:ASP:OD1	5:6:523:GLU:N	2.39	0.54
4:D:432:VAL:HG23	4:D:596:ILE:HG13	1.89	0.54
1:2:314:LEU:HD22	1:2:432:ASN:OD1	2.07	0.54
8:Y:-32:DT:H2''	8:Y:-31:DG:C8	2.43	0.54
4:D:493:ILE:HG22	4:D:497:MET:HE3	1.89	0.54
8:Y:-15:DC:H2''	8:Y:-14:DA:O5'	2.08	0.54
2:B:21:PHE:O	2:B:25:VAL:HG23	2.08	0.54
7:X:24:DC:H2''	7:X:25:DA:N7	2.23	0.54
1:2:774:ILE:HG13	1:2:825:LEU:HD13	1.89	0.54
2:B:450:ARG:HE	2:B:456:ARG:NH1	2.05	0.54
1:2:259:PHE:HB3	1:2:267:MET:HE1	1.90	0.54
1:2:548:ALA:O	1:2:552:ILE:HD12	2.08	0.53
7:X:36:DA:H2''	7:X:37:DT:C5'	2.38	0.53
7:X:51:DT:H2''	7:X:52:DG:H8	1.71	0.53
3:4:639:ASP:OD1	3:4:642:ARG:NH2	2.42	0.53
1:A:634:ALA:N	4:D:465:GLU:OE2	2.38	0.53
4:D:456:ASP:N	4:D:461:GLU:O	2.38	0.53
2:B:272:ARG:NE	4:D:171:VAL:HG12	2.24	0.53
4:D:460:ARG:HD3	4:D:460:ARG:O	2.08	0.53
7:X:36:DA:H2''	7:X:37:DT:H5'	1.90	0.53
3:C:370:ARG:NH2	3:C:377:ASN:O	2.38	0.53
4:D:74:ASP:OD1	4:D:75:ILE:HG23	2.09	0.53
7:X:12:DC:H2''	7:X:13:DA:C8	2.44	0.53
7:X:51:DT:H2''	7:X:52:DG:C8	2.43	0.53
2:3:39:ARG:CG	2:3:136:MET:HE1	2.39	0.53
2:3:272:ARG:NE	4:5:171:VAL:HG12	2.24	0.53
4:5:74:ASP:OD1	4:5:75:ILE:HG23	2.09	0.53
3:4:684:PRO:HB3	3:4:847:MET:HE3	1.91	0.52
8:Y:-21:DT:H2''	8:Y:-20:DG:H8	1.74	0.52
6:7:227:VAL:HG22	6:7:317:GLU:CG	2.39	0.52
1:A:259:PHE:CB	1:A:267:MET:HE1	2.39	0.52
2:B:345:PHE:O	2:B:349:ASN:ND2	2.39	0.52
1:2:271:PHE:CD2	1:2:295:VAL:HG21	2.45	0.52
1:2:488:SER:OG	1:2:766:TYR:OH	1.98	0.52
6:7:180:ALA:CB	4:D:107:ALA:HB2	2.39	0.52
2:B:27:ARG:NH1	2:B:30:GLU:OE1	2.42	0.52
2:B:413:THR:O	2:B:413:THR:HG22	2.08	0.52
3:C:322:ILE:O	6:F:303:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:26:DT:H2''	7:X:27:DG:C8	2.44	0.52
2:3:676:ILE:O	2:3:680:VAL:HG23	2.09	0.52
1:2:695:LEU:HD21	5:6:797:VAL:HG11	1.91	0.52
4:5:583:MET:O	4:5:585:ASN:N	2.43	0.52
4:D:450:THR:HG22	4:D:451:ALA:H	1.75	0.52
7:X:29:DT:H2''	7:X:30:DG:C8	2.44	0.52
1:2:271:PHE:HD2	1:2:295:VAL:HG21	1.74	0.52
4:5:552:MET:HE2	4:5:659:ILE:HD11	1.92	0.52
5:6:797:VAL:O	5:6:800:LEU:N	2.43	0.52
4:5:89:LEU:O	4:5:92:THR:HG22	2.11	0.51
4:5:469:MET:HE2	4:5:496:ALA:HB1	1.91	0.51
1:A:397:VAL:HG21	1:A:403:PRO:HG3	1.91	0.51
4:D:432:VAL:HG21	4:D:599:MET:CE	2.40	0.51
2:B:676:ILE:O	2:B:680:VAL:HG23	2.11	0.51
6:7:718:ARG:NH1	6:7:722:VAL:CG2	2.73	0.51
4:D:469:MET:HE2	4:D:496:ALA:HB1	1.90	0.51
7:X:34:DG:H1'	7:X:35:DC:H5'	1.91	0.51
1:2:689:GLU:O	1:2:692:ASP:N	2.44	0.51
1:2:704:VAL:HG21	5:6:770:ARG:HH21	1.74	0.51
3:4:239:SER:OG	3:4:300:PHE:O	2.28	0.51
2:3:413:THR:O	2:3:413:THR:HG22	2.10	0.51
5:6:550:GLN:OE1	5:6:571:ILE:HD12	2.11	0.51
6:7:181:LEU:O	6:7:185:VAL:HG23	2.10	0.51
3:C:639:ASP:OD1	3:C:642:ARG:NH2	2.43	0.51
5:E:613:VAL:HG13	5:E:613:VAL:O	2.11	0.51
1:2:634:ALA:N	4:5:465:GLU:OE2	2.39	0.51
7:X:12:DC:H4'	7:X:12:DC:OP1	2.10	0.51
8:Y:-27:DC:H2''	8:Y:-26:DA:C8	2.46	0.51
1:2:519:LEU:O	1:2:519:LEU:HD23	2.12	0.50
1:A:689:GLU:N	1:A:689:GLU:OE1	2.44	0.50
2:B:395:ASN:OD1	2:B:396:GLY:N	2.44	0.50
4:D:144:ASN:HD22	4:D:144:ASN:C	2.07	0.50
5:E:639:ASP:OD1	5:E:640:GLU:N	2.45	0.50
8:Y:-29:DA:H2''	8:Y:-28:DG:C8	2.45	0.50
3:C:519:TYR:CD1	3:C:811:MET:HE1	2.46	0.50
5:6:154:ASP:OD1	5:6:155:TYR:N	2.45	0.50
5:6:648:ASP:OD1	5:6:649:GLN:N	2.45	0.50
1:A:259:PHE:HB3	1:A:267:MET:HE1	1.93	0.50
1:A:689:GLU:OE2	5:E:782:LYS:NZ	2.44	0.50
1:2:689:GLU:O	1:2:693:GLU:OE1	2.29	0.50
4:5:141:SER:OG	4:5:161:ARG:NE	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:413:THR:HG21	2:B:549:VAL:HG21	1.94	0.50
3:C:239:SER:OG	3:C:300:PHE:O	2.29	0.50
3:C:684:PRO:HB3	3:C:847:MET:HE3	1.94	0.50
6:F:593:ARG:O	6:F:593:ARG:HG2	2.11	0.50
5:E:168:MET:O	5:E:172:GLU:OE1	2.29	0.50
6:F:459:MET:SD	6:F:584:ILE:HD13	2.52	0.50
3:4:650:GLU:OE1	3:4:651:GLN:HG2	2.12	0.50
1:2:198:ILE:HG22	1:2:198:ILE:O	2.10	0.50
5:6:576:ASP:OD1	5:6:579:THR:HG23	2.11	0.50
12:B:1001:ADP:O3B	4:D:651:ARG:NH2	2.45	0.50
5:E:648:ASP:OD1	5:E:649:GLN:N	2.45	0.50
6:F:26:VAL:HG12	6:F:26:VAL:O	2.12	0.50
4:D:374:ILE:O	4:D:385:LYS:NZ	2.45	0.50
7:X:28:DC:H2''	7:X:29:DT:C6	2.47	0.50
4:5:148:LEU:O	4:5:148:LEU:HD23	2.13	0.49
5:6:780:LEU:CD2	5:6:795:ILE:HG21	2.42	0.49
6:7:405:ILE:HD12	6:7:405:ILE:H	1.78	0.49
6:7:608:ASP:OD1	6:7:609:ASP:N	2.45	0.49
7:X:9:DG:H2''	7:X:10:DC:C6	2.46	0.49
7:X:42:DG:H1'	7:X:43:DC:H5'	1.95	0.49
2:3:229:ALA:HB2	4:D:187:ARG:HH21	1.78	0.49
12:3:1001:ADP:O3B	4:5:651:ARG:NH2	2.45	0.49
4:D:89:LEU:O	4:D:92:THR:HG22	2.11	0.49
7:X:27:DG:H2''	7:X:28:DC:C6	2.46	0.49
8:Y:-12:DG:H1'	8:Y:-11:DC:H5''	1.94	0.49
4:5:351:GLU:OE1	4:5:351:GLU:HA	2.12	0.49
3:C:503:ASP:OD1	3:C:504:GLN:N	2.45	0.49
4:D:156:VAL:O	4:D:157:SER:OG	2.26	0.49
2:3:27:ARG:NH1	2:3:30:GLU:OE1	2.42	0.49
6:7:26:VAL:HG12	6:7:26:VAL:O	2.12	0.49
5:6:639:ASP:OD1	5:6:640:GLU:N	2.45	0.49
4:D:149:ARG:NH1	4:D:260:GLU:OE2	2.46	0.49
4:D:404:MET:HA	4:D:404:MET:HE2	1.95	0.49
8:Y:-46:DT:H2''	8:Y:-45:DG:C8	2.47	0.49
3:4:503:ASP:OD1	3:4:504:GLN:N	2.45	0.49
3:4:507:ALA:O	3:4:511:GLU:HG2	2.13	0.49
5:6:157:HIS:HA	5:6:160:MET:HE2	1.95	0.49
2:B:276:VAL:HG11	2:B:294:VAL:HG21	1.95	0.49
6:7:133:ASP:OD1	6:7:133:ASP:N	2.46	0.48
2:3:452:THR:OG1	2:3:454:GLU:OE1	2.21	0.48
4:5:385:LYS:O	4:5:389:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:107:THR:O	5:6:111:VAL:HG23	2.13	0.48
5:E:550:GLN:OE1	5:E:571:ILE:HD12	2.14	0.48
5:6:739:ASP:OD1	5:6:740:GLU:N	2.46	0.48
4:D:141:SER:OG	4:D:161:ARG:NE	2.43	0.48
4:D:599:MET:O	4:D:603:ILE:HG13	2.14	0.48
5:E:136:TYR:O	5:E:140:ILE:HG13	2.12	0.48
7:X:43:DC:H2''	7:X:44:DG:C8	2.48	0.48
2:B:452:THR:OG1	2:B:454:GLU:OE1	2.20	0.48
6:F:227:VAL:HG22	6:F:317:GLU:CG	2.44	0.48
1:2:198:ILE:HD12	1:2:267:MET:CE	2.44	0.48
4:5:456:ASP:N	4:5:461:GLU:O	2.46	0.48
4:D:385:LYS:O	4:D:389:VAL:HG23	2.13	0.48
4:D:650:ILE:O	4:D:654:GLU:OE1	2.31	0.48
5:E:109:GLU:OE1	5:E:112:ARG:NH2	2.42	0.48
5:E:168:MET:O	5:E:171:SER:N	2.46	0.48
1:2:689:GLU:N	1:2:689:GLU:OE1	2.46	0.48
4:5:57:LYS:O	4:5:57:LYS:HG2	2.14	0.48
1:A:497:ILE:O	1:A:500:SER:OG	2.30	0.48
6:F:608:ASP:OD1	6:F:609:ASP:N	2.46	0.48
4:5:679:GLU:OE1	4:5:682:ARG:NH2	2.46	0.48
4:5:695:ASP:HB2	4:5:696:PRO:HD3	1.95	0.48
6:F:514:VAL:HG21	6:F:557:LEU:HD23	1.96	0.48
3:4:681:ARG:NH2	6:7:683:GLN:HB3	2.29	0.48
5:6:555:VAL:HG22	5:6:808:GLU:OE2	2.14	0.48
2:B:36:THR:HG22	2:B:36:THR:O	2.14	0.48
8:Y:-19:DC:H2''	8:Y:-18:DA:C8	2.48	0.48
1:2:438:LEU:CD2	7:X:34:DG:H5''	2.42	0.47
1:2:497:ILE:O	1:2:500:SER:OG	2.31	0.47
4:5:489:ASP:O	4:5:493:ILE:HG13	2.14	0.47
4:5:650:ILE:O	4:5:654:GLU:OE1	2.31	0.47
7:X:36:DA:H2''	7:X:37:DT:O5'	2.14	0.47
4:5:354:GLU:O	4:5:358:LEU:HD13	2.14	0.47
4:D:497:MET:HE2	4:D:519:VAL:HG11	1.96	0.47
8:Y:-2:DG:H2''	8:Y:-1:DC:C6	2.49	0.47
2:3:413:THR:HG21	2:3:549:VAL:HG21	1.95	0.47
1:2:560:ALA:HB3	1:2:563:ALA:HB2	1.95	0.47
3:4:234:ARG:HB2	3:4:280:MET:HE1	1.95	0.47
1:A:564:VAL:HG21	1:A:598:LEU:HD22	1.96	0.47
1:A:774:ILE:HG13	1:A:825:LEU:HD13	1.96	0.47
8:Y:-25:DT:H2''	8:Y:-24:DG:C8	2.49	0.47
5:6:174:TYR:CZ	5:6:178:LEU:HD13	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:797:VAL:O	5:6:801:GLU:OE1	2.33	0.47
4:D:583:MET:O	4:D:585:ASN:N	2.46	0.47
8:Y:-19:DC:H2"	8:Y:-18:DA:H8	1.80	0.47
1:2:397:VAL:HG21	1:2:403:PRO:HG3	1.95	0.47
3:4:839:ASP:OD2	3:4:842:THR:HG22	2.15	0.47
4:5:458:MET:HG2	4:5:459:THR:HG23	1.95	0.47
5:6:523:GLU:OE1	5:6:524:HIS:CE1	2.68	0.47
5:6:739:ASP:OD1	5:6:739:ASP:C	2.58	0.47
5:6:742:ILE:HG23	5:6:743:GLU:N	2.30	0.47
1:A:567:THR:HG22	1:A:569:GLN:H	1.80	0.47
5:E:174:TYR:CZ	5:E:178:LEU:HD13	2.50	0.47
4:5:599:MET:O	4:5:603:ILE:HG13	2.15	0.47
1:A:226:VAL:HG23	1:A:227:TYR:N	2.30	0.47
4:D:695:ASP:HB2	4:D:696:PRO:HD3	1.96	0.47
5:E:409:GLN:NE2	5:E:450:TYR:O	2.46	0.47
5:E:553:GLY:O	5:E:812:ARG:NH2	2.48	0.47
1:2:226:VAL:HG23	1:2:227:TYR:N	2.30	0.47
6:7:227:VAL:HG22	6:7:317:GLU:HG2	1.96	0.47
1:A:854:ARG:O	1:A:858:ARG:HG2	2.15	0.47
7:X:44:DG:H2"	7:X:45:DC:H6	1.78	0.47
6:7:514:VAL:HG21	6:7:557:LEU:HD23	1.96	0.46
2:B:444:ALA:HB2	2:B:460:GLY:H	1.80	0.46
6:F:394:THR:HG22	6:F:395:SER:N	2.30	0.46
3:C:230:LEU:HD13	3:C:280:MET:HE2	1.97	0.46
8:Y:-21:DT:H2"	8:Y:-20:DG:C8	2.50	0.46
8:Y:-3:DT:H2"	8:Y:-2:DG:C8	2.49	0.46
1:2:854:ARG:O	1:2:858:ARG:HG2	2.14	0.46
3:C:605:ILE:HG12	3:C:616:LEU:HD23	1.98	0.46
6:F:531:GLU:OE1	6:F:534:ARG:NH2	2.48	0.46
8:Y:-3:DT:H2"	8:Y:-2:DG:H8	1.80	0.46
1:2:800:THR:HG22	1:2:800:THR:O	2.15	0.46
6:7:498:MET:HE3	6:7:509:GLU:HG3	1.97	0.46
1:A:271:PHE:HD2	1:A:295:VAL:HG21	1.79	0.46
3:C:293:LEU:HD12	3:C:293:LEU:C	2.40	0.46
4:D:354:GLU:O	4:D:358:LEU:HD13	2.15	0.46
7:X:20:DC:H2"	7:X:21:DA:H8	1.81	0.46
3:C:203:TYR:HH	3:C:225:TYR:HE2	1.61	0.46
5:E:548:LEU:O	5:E:549:LEU:HB2	2.16	0.46
3:4:569:ASP:O	3:4:572:THR:HG22	2.16	0.46
4:D:432:VAL:O	4:D:432:VAL:HG22	2.15	0.46
4:D:489:ASP:O	4:D:493:ILE:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:447:ASN:OD1	3:4:449:ARG:N	2.48	0.46
6:7:394:THR:HG22	6:7:395:SER:N	2.30	0.46
5:E:742:ILE:HG23	5:E:743:GLU:N	2.31	0.46
6:F:498:MET:HE3	6:F:509:GLU:HG3	1.97	0.46
5:6:409:GLN:NE2	5:6:450:TYR:O	2.46	0.46
5:E:642:ASP:OD1	5:E:642:ASP:N	2.46	0.46
4:5:695:ASP:HB2	4:5:696:PRO:CD	2.46	0.46
6:7:718:ARG:O	6:7:722:VAL:HG23	2.16	0.46
1:A:511:ILE:O	1:A:515:VAL:HG23	2.16	0.46
3:C:569:ASP:O	3:C:572:THR:HG22	2.16	0.45
7:X:36:DA:C8	7:X:37:DT:H72	2.52	0.45
5:6:721:GLU:O	5:6:725:THR:HG23	2.16	0.45
1:A:800:THR:HG22	1:A:800:THR:O	2.17	0.45
4:D:695:ASP:HB2	4:D:696:PRO:CD	2.46	0.45
5:E:160:MET:O	5:E:160:MET:HG2	2.16	0.45
1:2:782:ASP:O	1:2:786:VAL:HG23	2.17	0.45
3:C:447:ASN:OD1	3:C:449:ARG:N	2.48	0.45
8:Y:-10:DG:H2''	8:Y:-9:DC:H6	1.82	0.45
4:5:407:ARG:NH1	4:5:498:GLU:OE1	2.50	0.45
5:6:803:MET:HE3	5:6:828:TYR:HB2	1.98	0.45
4:D:100:ARG:O	4:D:104:LEU:HD13	2.16	0.45
8:Y:-12:DG:C1'	8:Y:-11:DC:H5'	2.46	0.45
2:3:555:GLU:HG2	2:3:556:ILE:N	2.32	0.45
4:5:553:ILE:O	4:5:687:SER:OG	2.34	0.45
8:Y:-47:DA:C2'	8:Y:-46:DT:H5'	2.39	0.45
2:3:444:ALA:HB2	2:3:460:GLY:H	1.81	0.45
5:6:523:GLU:OE1	5:6:524:HIS:ND1	2.50	0.45
6:7:404:LEU:HD23	6:7:641:TYR:CD2	2.51	0.45
7:X:17:DA:H2''	7:X:18:DT:H5''	1.97	0.45
8:Y:-34:DC:H2''	8:Y:-33:DA:O4'	2.16	0.45
5:6:548:LEU:O	5:6:549:LEU:HB2	2.16	0.45
4:D:632:GLN:HA	4:D:632:GLN:OE1	2.17	0.45
4:D:407:ARG:NH1	4:D:411:ASN:OD1	2.48	0.45
8:Y:-9:DC:H2''	8:Y:-8:DA:C8	2.52	0.45
2:3:561:ILE:O	2:3:565:VAL:HG23	2.17	0.44
1:A:660:THR:HG22	1:A:660:THR:O	2.16	0.44
3:C:625:ASP:OD2	3:C:668:ARG:N	2.49	0.44
5:E:629:MET:HE1	5:E:672:LEU:HB3	1.99	0.44
1:2:271:PHE:CD2	1:2:295:VAL:HG11	2.53	0.44
2:3:656:LEU:O	2:3:660:VAL:HG23	2.18	0.44
4:D:450:THR:HG22	4:D:451:ALA:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:3:DA:C8	7:X:4:DT:H72	2.51	0.44
1:A:197:TRP:O	1:A:203:VAL:HG11	2.17	0.44
5:E:622:THR:HG22	5:E:623:ILE:N	2.32	0.44
5:E:780:LEU:CD2	5:E:795:ILE:HG21	2.47	0.44
4:5:449:LEU:HD21	4:5:493:ILE:HD11	1.99	0.44
4:5:450:THR:HG22	4:5:451:ALA:N	2.32	0.44
1:A:694:ARG:O	1:A:697:THR:HG22	2.18	0.44
1:2:660:THR:HG22	1:2:660:THR:O	2.18	0.44
1:A:305:SER:OG	1:A:308:GLU:OE2	2.27	0.44
1:A:782:ASP:O	1:A:786:VAL:HG23	2.17	0.44
4:D:148:LEU:HD23	4:D:148:LEU:O	2.18	0.44
4:D:569:ALA:O	4:D:573:ILE:CD1	2.66	0.44
5:E:509:SER:HB2	5:E:513:ILE:HD11	1.99	0.44
5:E:559:THR:HG22	5:E:560:VAL:N	2.32	0.44
5:E:766:THR:HG22	5:E:767:LYS:N	2.32	0.44
1:A:539:VAL:HG22	1:A:647:ILE:HG12	1.98	0.44
2:B:555:GLU:HG2	2:B:556:ILE:N	2.32	0.44
4:5:69:ILE:HD13	4:5:76:TYR:CD1	2.53	0.44
4:5:425:LEU:O	4:5:429:VAL:HG23	2.17	0.44
1:A:376:ASN:O	1:A:380:THR:OG1	2.30	0.44
4:D:650:ILE:HG22	4:D:654:GLU:OE1	2.18	0.44
1:2:231:ILE:HG13	1:2:242:LEU:HD11	1.99	0.44
2:B:483:ARG:HA	2:B:486:ILE:HG22	2.00	0.44
4:D:425:LEU:O	4:D:429:VAL:HG23	2.18	0.44
6:F:195:ASN:OD1	6:F:196:LEU:N	2.50	0.44
3:4:754:ALA:HA	3:4:758:ILE:HD13	2.00	0.44
5:6:622:THR:HG22	5:6:623:ILE:N	2.33	0.44
1:A:200:GLN:HB2	1:A:203:VAL:HG12	1.99	0.44
4:D:90:PHE:O	4:D:94:ILE:HG13	2.18	0.44
1:2:598:LEU:HD23	1:2:598:LEU:C	2.43	0.43
2:3:243:THR:OG1	4:D:4:ASP:OD1	2.30	0.43
5:6:613:VAL:HG13	5:6:613:VAL:O	2.17	0.43
1:A:417:VAL:HG21	1:A:456:ILE:HG21	2.00	0.43
3:C:451:ARG:NE	5:E:445:VAL:HG11	2.33	0.43
3:C:507:ALA:O	3:C:511:GLU:HG2	2.18	0.43
4:D:618:ALA:HB1	4:D:677:VAL:HG21	1.99	0.43
5:E:576:ASP:OD1	5:E:579:THR:HG23	2.17	0.43
3:4:711:LYS:NZ	3:4:850:VAL:O	2.48	0.43
4:5:618:ALA:HB1	4:5:677:VAL:HG21	1.99	0.43
1:A:234:LEU:C	1:A:234:LEU:HD23	2.44	0.43
6:F:538:HIS:O	6:F:593:ARG:NH1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:650:ILE:HG22	4:5:654:GLU:OE1	2.18	0.43
2:B:443:THR:O	2:B:444:ALA:HB3	2.18	0.43
4:5:517:THR:HG22	4:5:518:SER:N	2.34	0.43
1:A:369:SER:OG	1:A:370:LYS:N	2.52	0.43
8:Y:-12:DG:C4'	8:Y:-11:DC:OP1	2.57	0.43
4:5:579:ASN:O	4:5:583:MET:N	2.48	0.43
5:6:777:TYR:OH	5:6:781:ARG:NH1	2.50	0.43
1:A:523:VAL:O	1:A:523:VAL:HG13	2.18	0.43
3:C:815:ASN:HD22	3:C:815:ASN:C	2.23	0.43
5:E:816:VAL:HG12	5:E:818:GLU:H	1.83	0.43
4:5:66:GLU:O	4:5:69:ILE:HG22	2.18	0.43
4:5:569:ALA:O	4:5:573:ILE:CD1	2.66	0.43
2:B:386:MET:HE2	2:B:660:VAL:HG22	1.99	0.43
6:F:66:MET:O	6:F:70:VAL:HG23	2.19	0.43
8:Y:-20:DG:OP2	8:Y:-20:DG:H3'	2.18	0.43
2:3:276:VAL:HG11	2:3:294:VAL:HG21	2.00	0.43
2:3:537:ASP:OD2	6:7:573:ARG:NH1	2.52	0.43
2:B:692:THR:HG23	2:B:692:THR:O	2.19	0.43
3:C:581:VAL:HA	3:C:584:ILE:HG22	2.00	0.43
3:C:773:ALA:HB3	3:C:801:MET:HE1	2.01	0.43
4:5:90:PHE:O	4:5:94:ILE:HG13	2.19	0.43
4:5:432:VAL:HG22	4:5:432:VAL:O	2.19	0.43
3:C:392:ALA:O	5:E:281:SER:OG	2.30	0.43
3:C:602:THR:HG23	3:C:654:ILE:HG21	2.00	0.43
1:2:690:GLU:O	1:2:694:ARG:NE	2.48	0.43
5:6:347:ASN:OD1	5:6:349:THR:OG1	2.23	0.43
6:7:658:ASP:O	6:7:661:VAL:HG22	2.19	0.43
1:A:560:ALA:HB3	1:A:563:ALA:HB2	2.01	0.43
1:A:701:ASP:HA	1:A:704:VAL:HG22	2.00	0.43
1:A:829:VAL:HG13	1:A:829:VAL:O	2.19	0.43
8:Y:-20:DG:H2''	8:Y:-19:DC:OP2	2.18	0.43
1:2:197:TRP:CZ2	1:2:203:VAL:HG21	2.53	0.43
1:2:523:VAL:O	1:2:523:VAL:HG13	2.19	0.43
5:E:158:LEU:HD23	5:E:158:LEU:O	2.18	0.43
5:E:777:TYR:OH	5:E:781:ARG:NH1	2.51	0.43
2:B:656:LEU:O	2:B:660:VAL:HG23	2.18	0.42
3:C:451:ARG:CZ	5:E:445:VAL:HG11	2.49	0.42
4:D:449:LEU:HD21	4:D:493:ILE:HD11	2.00	0.42
2:3:123:PRO:HB2	2:3:124:PRO:HD3	2.02	0.42
2:3:444:ALA:HB2	2:3:460:GLY:N	2.34	0.42
5:6:584:PHE:O	5:6:588:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:561:ILE:O	2:B:565:VAL:HG23	2.19	0.42
6:F:651:VAL:HG22	6:F:652:MET:N	2.34	0.42
1:2:701:ASP:HA	1:2:704:VAL:HG12	2.01	0.42
3:4:266:GLN:CD	3:4:266:GLN:H	2.26	0.42
3:4:696:PRO:N	3:4:697:PRO:CD	2.83	0.42
5:6:648:ASP:O	5:6:652:ILE:HG13	2.19	0.42
2:B:444:ALA:HB2	2:B:460:GLY:N	2.34	0.42
8:Y:-23:DC:H2''	8:Y:-22:DA:N7	2.34	0.42
6:7:537:ILE:O	6:7:541:MET:HG3	2.19	0.42
4:D:517:THR:HG22	4:D:518:SER:N	2.34	0.42
8:Y:-33:DA:H2'	8:Y:-32:DT:H72	2.00	0.42
1:2:197:TRP:O	1:2:203:VAL:HG11	2.20	0.42
1:2:369:SER:OG	1:2:370:LYS:N	2.53	0.42
2:3:386:MET:HE2	2:3:660:VAL:HG22	2.01	0.42
2:3:537:ASP:OD1	2:3:696:PRO:HG3	2.19	0.42
1:A:701:ASP:O	1:A:705:ARG:HG3	2.20	0.42
4:D:56:VAL:O	4:D:57:LYS:HB2	2.19	0.42
5:E:808:GLU:HB2	5:E:819:ILE:HD11	2.00	0.42
7:X:11:DG:H2''	7:X:12:DC:O5'	2.19	0.42
2:3:31:PHE:O	2:3:34:THR:HG22	2.20	0.42
3:4:234:ARG:HB2	3:4:280:MET:CE	2.50	0.42
6:7:294:THR:O	6:7:294:THR:HG23	2.19	0.42
1:2:694:ARG:O	1:2:697:THR:HG22	2.19	0.42
6:7:138:VAL:HG21	6:7:303:ARG:HH21	1.84	0.42
1:A:433:ASN:O	1:A:436:GLY:N	2.53	0.42
2:B:254:GLN:OE1	2:B:283:VAL:O	2.38	0.42
3:4:431:ASP:OD1	3:4:587:ARG:NH1	2.53	0.42
3:C:204:LYS:NZ	3:C:222:GLU:OE1	2.44	0.42
4:5:395:GLY:N	4:5:408:GLY:O	2.51	0.42
3:C:615:VAL:HG22	3:C:616:LEU:N	2.35	0.42
3:C:696:PRO:N	3:C:697:PRO:CD	2.83	0.42
3:4:481:ILE:HA	3:4:484:GLU:OE1	2.20	0.42
2:B:535:LEU:HB2	2:B:540:LEU:HD21	2.02	0.42
2:3:535:LEU:HB2	2:3:540:LEU:HD21	2.01	0.41
2:3:553:ILE:H	2:3:553:ILE:HD12	1.85	0.41
3:4:293:LEU:HD12	3:4:293:LEU:C	2.45	0.41
5:6:816:VAL:HG12	5:6:818:GLU:H	1.84	0.41
1:2:701:ASP:O	1:2:705:ARG:HG3	2.21	0.41
2:3:443:THR:O	2:3:444:ALA:HB3	2.18	0.41
6:7:195:ASN:OD1	6:7:196:LEU:N	2.53	0.41
6:7:718:ARG:NH1	6:7:722:VAL:HG21	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:GLU:N	1:A:217:GLU:OE2	2.53	0.41
3:C:769:GLU:OE1	3:C:772:ARG:NH2	2.54	0.41
3:4:581:VAL:HA	3:4:584:ILE:HG22	2.02	0.41
5:6:767:LYS:HA	5:6:770:ARG:HH11	1.86	0.41
2:B:553:ILE:HD12	2:B:553:ILE:H	1.85	0.41
2:3:254:GLN:OE1	2:3:283:VAL:O	2.38	0.41
4:5:13:VAL:HG12	4:5:14:LEU:HD12	2.02	0.41
4:5:338:GLU:C	4:5:339:THR:HG22	2.45	0.41
6:7:161:ILE:HD12	6:7:185:VAL:HG22	2.01	0.41
3:4:224:LEU:HD13	3:4:227:ILE:HG13	2.01	0.41
4:D:579:ASN:O	4:D:583:MET:N	2.48	0.41
6:F:70:VAL:HG22	6:F:75:LEU:HB3	2.02	0.41
2:3:450:ARG:HE	2:3:456:ARG:HD3	1.85	0.41
2:3:692:THR:O	2:3:692:THR:HG23	2.20	0.41
5:6:519:MET:HE1	5:6:754:TYR:HB2	2.02	0.41
6:F:722:VAL:HG23	6:F:725:GLU:CD	2.45	0.41
7:X:16:DC:H2''	7:X:17:DA:C8	2.55	0.41
7:X:43:DC:H2''	7:X:44:DG:H8	1.84	0.41
1:2:539:VAL:HG22	1:2:647:ILE:HG12	2.02	0.41
6:7:444:VAL:HG12	6:7:444:VAL:O	2.20	0.41
2:B:123:PRO:HB2	2:B:124:PRO:HD3	2.01	0.41
4:D:338:GLU:C	4:D:339:THR:HG22	2.45	0.41
3:4:234:ARG:HG3	3:4:280:MET:CE	2.50	0.41
3:4:684:PRO:CB	3:4:847:MET:HE3	2.50	0.41
3:C:481:ILE:HA	3:C:484:GLU:OE1	2.20	0.41
6:F:651:VAL:HG22	6:F:652:MET:H	1.85	0.41
8:Y:-11:DC:H2''	8:Y:-10:DG:OP2	2.20	0.41
1:2:687:VAL:O	1:2:687:VAL:HG13	2.21	0.41
1:2:693:GLU:HG3	5:6:778:LYS:HD2	2.02	0.41
2:3:132:LEU:HD23	2:3:132:LEU:O	2.21	0.41
2:3:483:ARG:HD2	2:3:539:LEU:HD22	2.02	0.41
3:4:481:ILE:HD12	3:4:485:LEU:HD21	2.03	0.41
6:7:133:ASP:OD1	6:7:136:ASP:OD2	2.39	0.41
1:A:227:TYR:O	1:A:231:ILE:CD1	2.67	0.41
1:A:234:LEU:HD13	1:A:242:LEU:CD2	2.51	0.41
2:B:129:LEU:HD22	2:B:155:LEU:HD11	2.03	0.41
2:B:474:GLU:HG3	4:D:491:VAL:HG13	2.02	0.41
3:C:194:PHE:O	3:C:198:LEU:HD23	2.21	0.41
7:X:52:DG:H2''	7:X:53:DC:O5'	2.21	0.41
4:5:456:ASP:OD1	4:5:457:PRO:HD2	2.21	0.41
5:6:608:LEU:HD23	5:6:627:ALA:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:395:GLY:N	4:D:408:GLY:O	2.49	0.41
3:4:233:MET:O	3:4:237:GLY:N	2.47	0.40
3:4:602:THR:HG23	3:4:654:ILE:HG21	2.02	0.40
4:5:56:VAL:O	4:5:57:LYS:HB3	2.21	0.40
5:6:559:THR:HG22	5:6:560:VAL:N	2.35	0.40
5:6:610:ALA:HB3	5:6:663:ILE:HD11	2.03	0.40
5:E:154:ASP:OD1	5:E:155:TYR:N	2.53	0.40
5:E:691:ARG:HH21	5:E:716:LEU:HD13	1.86	0.40
1:2:197:TRP:CE2	1:2:203:VAL:HG21	2.56	0.40
4:D:258:LEU:HB2	4:D:276:MET:HE2	2.02	0.40
6:F:688:THR:O	6:F:692:ILE:HG12	2.20	0.40
1:2:200:GLN:HB2	1:2:203:VAL:HG12	2.02	0.40
1:2:567:THR:HG23	1:2:607:ASP:O	2.21	0.40
3:4:625:ASP:OD1	3:4:668:ARG:N	2.50	0.40
4:5:626:PHE:CZ	4:5:630:ARG:HD2	2.57	0.40
5:6:545:LYS:O	5:6:548:LEU:O	2.40	0.40
4:D:31:PHE:CG	4:D:90:PHE:HD1	2.39	0.40
6:F:294:THR:O	6:F:294:THR:HG23	2.21	0.40
8:Y:-33:DA:H2'	8:Y:-32:DT:C7	2.50	0.40
3:4:380:ASN:OD1	1:A:365:THR:HG22	2.21	0.40
3:C:445:ARG:NH1	5:E:447:ASP:OD2	2.50	0.40
3:C:602:THR:HG22	3:C:656:ILE:HD11	2.03	0.40
4:D:346:VAL:HG13	4:D:346:VAL:O	2.22	0.40
6:F:133:ASP:OD1	6:F:133:ASP:N	2.54	0.40
1:2:255:ILE:HG23	1:2:256:LEU:N	2.37	0.40
3:4:602:THR:HG22	3:4:656:ILE:HD11	2.02	0.40
4:5:56:VAL:O	4:5:56:VAL:CG1	2.69	0.40
6:7:75:LEU:O	6:7:199:ARG:NH1	2.55	0.40
5:E:134:LYS:CD	5:E:137:ARG:NH1	2.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	617/868 (71%)	602 (98%)	15 (2%)	0	100	100
1	A	617/868 (71%)	606 (98%)	11 (2%)	0	100	100
2	3	587/1006 (58%)	571 (97%)	16 (3%)	0	100	100
2	B	587/1006 (58%)	571 (97%)	16 (3%)	0	100	100
3	4	646/933 (69%)	626 (97%)	20 (3%)	0	100	100
3	C	646/933 (69%)	625 (97%)	21 (3%)	0	100	100
4	5	644/775 (83%)	621 (96%)	22 (3%)	1 (0%)	43	76
4	D	644/775 (83%)	619 (96%)	24 (4%)	1 (0%)	43	76
5	6	597/1017 (59%)	574 (96%)	23 (4%)	0	100	100
5	E	597/1017 (59%)	574 (96%)	23 (4%)	0	100	100
6	7	683/845 (81%)	660 (97%)	23 (3%)	0	100	100
6	F	683/845 (81%)	663 (97%)	20 (3%)	0	100	100
All	All	7548/10888 (69%)	7312 (97%)	234 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	5	337	VAL
4	D	337	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	547/770 (71%)	547 (100%)	0	100	100
1	A	547/770 (71%)	547 (100%)	0	100	100
2	3	514/864 (60%)	514 (100%)	0	100	100
2	B	514/864 (60%)	514 (100%)	0	100	100
3	4	593/848 (70%)	592 (100%)	1 (0%)	87	92
3	C	593/848 (70%)	592 (100%)	1 (0%)	87	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	5	584/688 (85%)	584 (100%)	0	100	100
4	D	584/688 (85%)	583 (100%)	1 (0%)	87	92
5	6	531/886 (60%)	531 (100%)	0	100	100
5	E	531/886 (60%)	531 (100%)	0	100	100
6	7	608/753 (81%)	608 (100%)	0	100	100
6	F	608/753 (81%)	608 (100%)	0	100	100
All	All	6754/9618 (70%)	6751 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	4	815	ASN
3	C	815	ASN
4	D	144	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	353	GLN
1	2	437	ASN
1	2	526	ASN
1	2	569	GLN
1	2	613	ASN
1	2	760	GLN
1	2	779	HIS
1	2	809	HIS
2	3	177	ASN
2	3	417	GLN
2	3	507	ASN
3	4	196	ASN
3	4	253	GLN
3	4	274	GLN
3	4	318	ASN
3	4	386	HIS
3	4	387	ASN
3	4	413	HIS
3	4	504	GLN
3	4	579	GLN
3	4	685	ASN

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Mol	Chain	Res	Type
3	4	716	ASN
4	5	96	GLN
4	5	185	ASN
4	5	223	ASN
4	5	284	ASN
4	5	579	ASN
4	5	673	GLN
5	6	570	ASN
6	7	68	GLN
6	7	95	GLN
6	7	209	GLN
6	7	425	ASN
6	7	468	GLN
6	7	683	GLN
1	A	294	HIS
1	A	613	ASN
1	A	703	HIS
1	A	760	GLN
1	A	779	HIS
1	A	809	HIS
2	B	177	ASN
2	B	310	ASN
2	B	312	ASN
2	B	417	GLN
2	B	507	ASN
2	B	517	ASN
2	B	673	GLN
3	C	196	ASN
3	C	253	GLN
3	C	318	ASN
3	C	386	HIS
3	C	683	ASN
3	C	685	ASN
4	D	253	GLN
4	D	574	ASN
4	D	579	ASN
4	D	673	GLN
5	E	157	HIS
5	E	264	GLN
5	E	570	ASN
5	E	653	HIS
5	E	669	HIS

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Mol	Chain	Res	Type
6	F	68	GLN
6	F	95	GLN
6	F	112	HIS
6	F	209	GLN
6	F	455	ASN
6	F	468	GLN
6	F	625	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 20 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	ADP	D	801	10	28,29,29	1.39	4 (14%)	43,45,45	1.89	10 (23%)
9	ATP	2	901	10	32,33,33	0.36	0	48,52,52	0.68	0
12	ADP	5	801	10	28,29,29	1.38	4 (14%)	43,45,45	1.87	10 (23%)
12	ADP	F	902	10	28,29,29	1.39	4 (14%)	43,45,45	1.92	11 (25%)
9	ATP	A	901	10	32,33,33	0.36	0	48,52,52	0.68	0
12	ADP	3	1001	10	28,29,29	1.38	4 (14%)	43,45,45	1.90	11 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	ADP	4	1001	10	28,29,29	1.40	4 (14%)	43,45,45	1.88	10 (23%)
12	ADP	C	1001	10	28,29,29	1.41	4 (14%)	43,45,45	1.86	10 (23%)
12	ADP	7	902	10	28,29,29	1.39	4 (14%)	43,45,45	1.91	11 (25%)
12	ADP	B	1001	10	28,29,29	1.38	4 (14%)	43,45,45	1.90	11 (25%)

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
12	ADP	D	801	10	-	3/16/32/32	0/3/3/3
9	ATP	2	901	10	-	7/22/38/38	0/3/3/3
12	ADP	5	801	10	-	3/16/32/32	0/3/3/3
12	ADP	F	902	10	-	1/16/32/32	0/3/3/3
9	ATP	A	901	10	-	7/22/38/38	0/3/3/3
12	ADP	3	1001	10	-	3/16/32/32	0/3/3/3
12	ADP	4	1001	10	-	8/16/32/32	0/3/3/3
12	ADP	C	1001	10	-	8/16/32/32	0/3/3/3
12	ADP	7	902	10	-	1/16/32/32	0/3/3/3
12	ADP	B	1001	10	-	3/16/32/32	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	4	1001	ADP	C5-C4	4.59	1.47	1.39
12	F	902	ADP	C5-C4	4.57	1.47	1.39
12	C	1001	ADP	C5-C4	4.56	1.47	1.39
12	7	902	ADP	C5-C4	4.55	1.47	1.39
12	D	801	ADP	C5-C4	4.52	1.47	1.39
12	5	801	ADP	C5-C4	4.50	1.47	1.39
12	3	1001	ADP	C5-C4	4.48	1.47	1.39
12	B	1001	ADP	C5-C4	4.48	1.47	1.39
12	4	1001	ADP	C5-C6	2.66	1.48	1.41
12	F	902	ADP	C5-C6	2.65	1.48	1.41
12	C	1001	ADP	C5-C6	2.64	1.48	1.41
12	7	902	ADP	C5-C6	2.63	1.48	1.41
12	D	801	ADP	C5-C6	2.60	1.48	1.41
12	3	1001	ADP	C5-C6	2.60	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	1001	ADP	C5-C6	2.58	1.48	1.41
12	5	801	ADP	C5-C6	2.57	1.48	1.41
12	D	801	ADP	C5-N7	-2.47	1.34	1.39
12	5	801	ADP	C5-N7	-2.43	1.34	1.39
12	C	1001	ADP	C5-N7	-2.39	1.34	1.39
12	B	1001	ADP	C5-N7	-2.39	1.34	1.39
12	4	1001	ADP	C5-N7	-2.38	1.34	1.39
12	3	1001	ADP	C5-N7	-2.36	1.34	1.39
12	F	902	ADP	C5-N7	-2.35	1.34	1.39
12	7	902	ADP	C5-N7	-2.33	1.34	1.39
12	C	1001	ADP	C8-N7	2.31	1.36	1.31
12	B	1001	ADP	C8-N7	2.30	1.36	1.31
12	4	1001	ADP	C8-N7	2.29	1.36	1.31
12	F	902	ADP	C8-N7	2.29	1.36	1.31
12	7	902	ADP	C8-N7	2.27	1.36	1.31
12	3	1001	ADP	C8-N7	2.27	1.36	1.31
12	D	801	ADP	C8-N7	2.24	1.36	1.31
12	5	801	ADP	C8-N7	2.23	1.36	1.31

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	4	1001	ADP	C5-C4-N3	-5.95	118.53	126.72
12	C	1001	ADP	C5-C4-N3	-5.91	118.58	126.72
12	D	801	ADP	C5-C4-N3	-5.90	118.59	126.72
12	5	801	ADP	C5-C4-N3	-5.88	118.62	126.72
12	7	902	ADP	C5-C4-N3	-5.88	118.62	126.72
12	F	902	ADP	C5-C4-N3	-5.83	118.69	126.72
12	3	1001	ADP	C5-C4-N3	-5.76	118.79	126.72
12	B	1001	ADP	C5-C4-N3	-5.73	118.82	126.72
12	7	902	ADP	N3-C4-N9	4.77	135.28	127.17
12	D	801	ADP	N3-C4-N9	4.75	135.24	127.17
12	5	801	ADP	N3-C4-N9	4.74	135.23	127.17
12	F	902	ADP	N3-C4-N9	4.73	135.21	127.17
12	4	1001	ADP	N3-C4-N9	4.72	135.19	127.17
12	C	1001	ADP	N3-C4-N9	4.71	135.18	127.17
12	3	1001	ADP	N3-C4-N9	4.64	135.06	127.17
12	B	1001	ADP	N3-C4-N9	4.64	135.05	127.17
12	C	1001	ADP	C2-N3-C4	3.88	121.30	111.83
12	4	1001	ADP	C2-N3-C4	3.87	121.27	111.83
12	7	902	ADP	C2-N3-C4	3.86	121.26	111.83
12	D	801	ADP	C2-N3-C4	3.85	121.24	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	3	1001	ADP	C2-N3-C4	3.85	121.23	111.83
12	F	902	ADP	C2-N3-C4	3.84	121.21	111.83
12	B	1001	ADP	C2-N3-C4	3.83	121.19	111.83
12	5	801	ADP	C2-N3-C4	3.83	121.19	111.83
12	B	1001	ADP	N3-C2-N1	-3.70	122.98	128.58
12	3	1001	ADP	N3-C2-N1	-3.70	122.98	128.58
12	D	801	ADP	N3-C2-N1	-3.68	123.02	128.58
12	7	902	ADP	N3-C2-N1	-3.67	123.03	128.58
12	5	801	ADP	N3-C2-N1	-3.65	123.06	128.58
12	F	902	ADP	N3-C2-N1	-3.65	123.06	128.58
12	C	1001	ADP	N3-C2-N1	-3.57	123.18	128.58
12	4	1001	ADP	N3-C2-N1	-3.57	123.18	128.58
12	F	902	ADP	C4-C5-N7	-3.51	106.57	110.58
12	4	1001	ADP	C4-C5-N7	-3.47	106.62	110.58
12	7	902	ADP	C4-C5-N7	-3.45	106.64	110.58
12	3	1001	ADP	C4-C5-N7	-3.40	106.69	110.58
12	C	1001	ADP	C4-C5-N7	-3.40	106.69	110.58
12	B	1001	ADP	C4-C5-N7	-3.38	106.71	110.58
12	D	801	ADP	C4-C5-N7	-3.34	106.76	110.58
12	5	801	ADP	C4-C5-N7	-3.29	106.82	110.58
12	F	902	ADP	C4-N9-C8	3.00	108.88	105.74
12	B	1001	ADP	C4-N9-C8	2.96	108.84	105.74
12	7	902	ADP	C4-N9-C8	2.94	108.83	105.74
12	3	1001	ADP	C4-N9-C8	2.92	108.81	105.74
12	F	902	ADP	C5-N7-C8	2.81	107.87	103.45
12	7	902	ADP	C5-N7-C8	2.76	107.79	103.45
12	D	801	ADP	C4-N9-C8	2.71	108.59	105.74
12	5	801	ADP	C4-N9-C8	2.69	108.56	105.74
12	4	1001	ADP	C4-N9-C8	2.68	108.55	105.74
12	4	1001	ADP	C5-N7-C8	2.68	107.66	103.45
12	C	1001	ADP	C3'-C2'-C1'	2.67	106.51	101.46
12	3	1001	ADP	C5-N7-C8	2.66	107.63	103.45
12	B	1001	ADP	C5-N7-C8	2.66	107.63	103.45
12	C	1001	ADP	C4-N9-C8	2.65	108.52	105.74
12	C	1001	ADP	C5-N7-C8	2.64	107.60	103.45
12	D	801	ADP	C5-N7-C8	2.63	107.58	103.45
12	4	1001	ADP	C3'-C2'-C1'	2.62	106.42	101.46
12	5	801	ADP	C5-N7-C8	2.58	107.50	103.45
12	D	801	ADP	C3'-C2'-C1'	2.56	106.31	101.46
12	5	801	ADP	C3'-C2'-C1'	2.56	106.30	101.46
12	3	1001	ADP	C3'-C2'-C1'	2.52	106.23	101.46
12	B	1001	ADP	C3'-C2'-C1'	2.51	106.22	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	902	ADP	N9-C8-N7	-2.37	110.58	113.94
12	F	902	ADP	C3'-C2'-C1'	2.36	105.92	101.46
12	7	902	ADP	C3'-C2'-C1'	2.33	105.88	101.46
12	7	902	ADP	N9-C8-N7	-2.32	110.64	113.94
12	B	1001	ADP	N9-C8-N7	-2.29	110.69	113.94
12	3	1001	ADP	N9-C8-N7	-2.27	110.71	113.94
12	4	1001	ADP	N9-C8-N7	-2.14	110.90	113.94
12	F	902	ADP	C6-C5-N7	2.13	136.20	132.09
12	D	801	ADP	N9-C8-N7	-2.13	110.91	113.94
12	B	1001	ADP	C6-C5-N7	2.13	136.19	132.09
12	3	1001	ADP	C6-C5-N7	2.12	136.19	132.09
12	C	1001	ADP	N9-C8-N7	-2.11	110.94	113.94
12	5	801	ADP	N9-C8-N7	-2.08	110.98	113.94
12	7	902	ADP	C6-C5-N7	2.08	136.10	132.09
12	F	902	ADP	C2-N1-C6	2.08	122.14	118.73
12	7	902	ADP	C2-N1-C6	2.07	122.14	118.73
12	4	1001	ADP	C6-C5-N7	2.07	136.08	132.09
12	D	801	ADP	C2-N1-C6	2.06	122.11	118.73
12	3	1001	ADP	C2-N1-C6	2.05	122.10	118.73
12	C	1001	ADP	C6-C5-N7	2.05	136.05	132.09
12	B	1001	ADP	C2-N1-C6	2.02	122.05	118.73
12	5	801	ADP	C2-N1-C6	2.02	122.04	118.73

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	3	1001	ADP	C5'-O5'-PA-O1A
12	4	1001	ADP	PA-O3A-PB-O2B
12	4	1001	ADP	C5'-O5'-PA-O2A
12	4	1001	ADP	C5'-O5'-PA-O3A
12	5	801	ADP	C5'-O5'-PA-O1A
12	5	801	ADP	C5'-O5'-PA-O3A
12	B	1001	ADP	C5'-O5'-PA-O1A
12	C	1001	ADP	PA-O3A-PB-O2B
12	C	1001	ADP	C5'-O5'-PA-O1A
12	C	1001	ADP	C5'-O5'-PA-O2A
12	C	1001	ADP	C5'-O5'-PA-O3A
12	D	801	ADP	C5'-O5'-PA-O1A
12	D	801	ADP	C5'-O5'-PA-O3A
12	C	1001	ADP	O4'-C4'-C5'-O5'
12	4	1001	ADP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
12	C	1001	ADP	C3'-C4'-C5'-O5'
12	4	1001	ADP	C3'-C4'-C5'-O5'
9	2	901	ATP	PB-O3B-PG-O1G
9	A	901	ATP	PB-O3B-PG-O1G
9	A	901	ATP	O4'-C4'-C5'-O5'
12	3	1001	ADP	C5'-O5'-PA-O2A
12	3	1001	ADP	C5'-O5'-PA-O3A
12	4	1001	ADP	C5'-O5'-PA-O1A
12	5	801	ADP	C5'-O5'-PA-O2A
12	7	902	ADP	C5'-O5'-PA-O1A
12	B	1001	ADP	C5'-O5'-PA-O2A
12	B	1001	ADP	C5'-O5'-PA-O3A
12	D	801	ADP	C5'-O5'-PA-O2A
12	F	902	ADP	C5'-O5'-PA-O1A
12	C	1001	ADP	PA-O3A-PB-O1B
9	2	901	ATP	O4'-C4'-C5'-O5'
9	2	901	ATP	PG-O3B-PB-O1B
9	2	901	ATP	PB-O3B-PG-O2G
9	2	901	ATP	PB-O3B-PG-O3G
9	A	901	ATP	PB-O3B-PG-O2G
9	A	901	ATP	PB-O3B-PG-O3G
12	4	1001	ADP	PA-O3A-PB-O3B
12	C	1001	ADP	PA-O3A-PB-O3B
9	2	901	ATP	PG-O3B-PB-O2B
9	A	901	ATP	PG-O3B-PB-O1B
9	A	901	ATP	PG-O3B-PB-O2B
12	4	1001	ADP	PA-O3A-PB-O1B
9	2	901	ATP	PA-O3A-PB-O2B
9	A	901	ATP	PA-O3A-PB-O2B

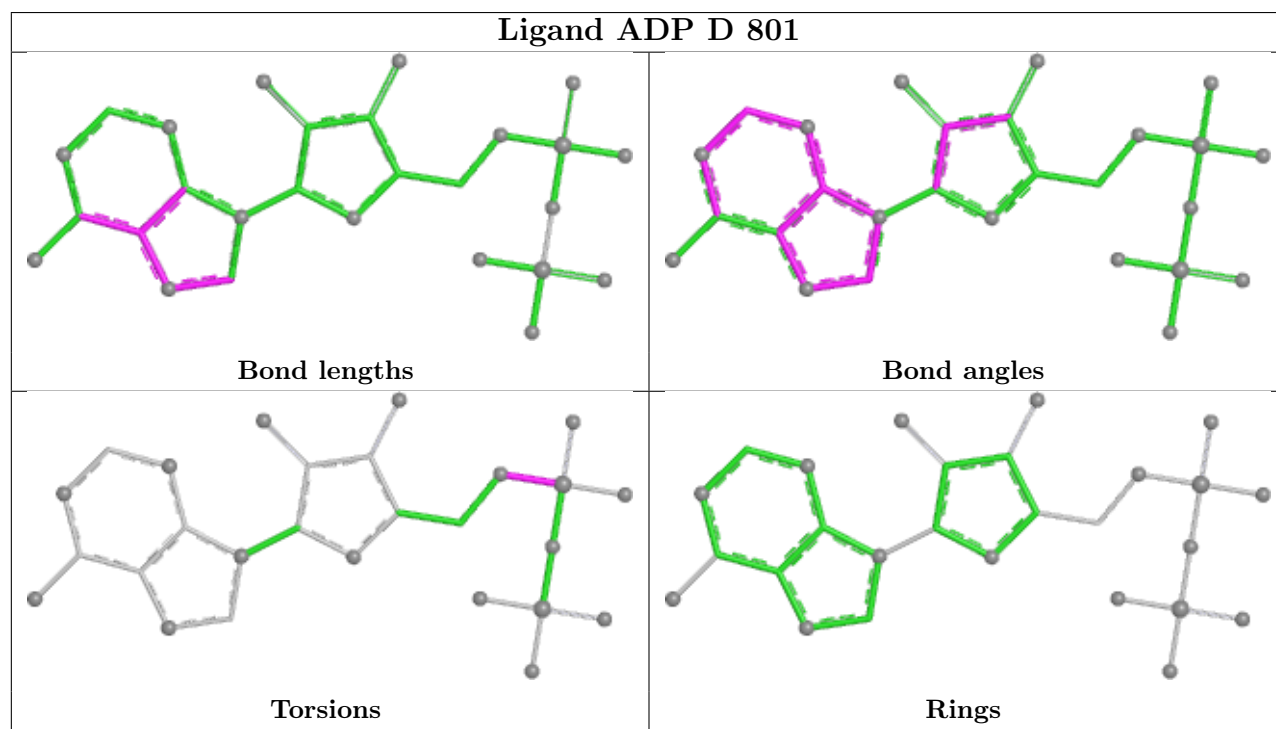
There are no ring outliers.

6 monomers are involved in 8 short contacts:

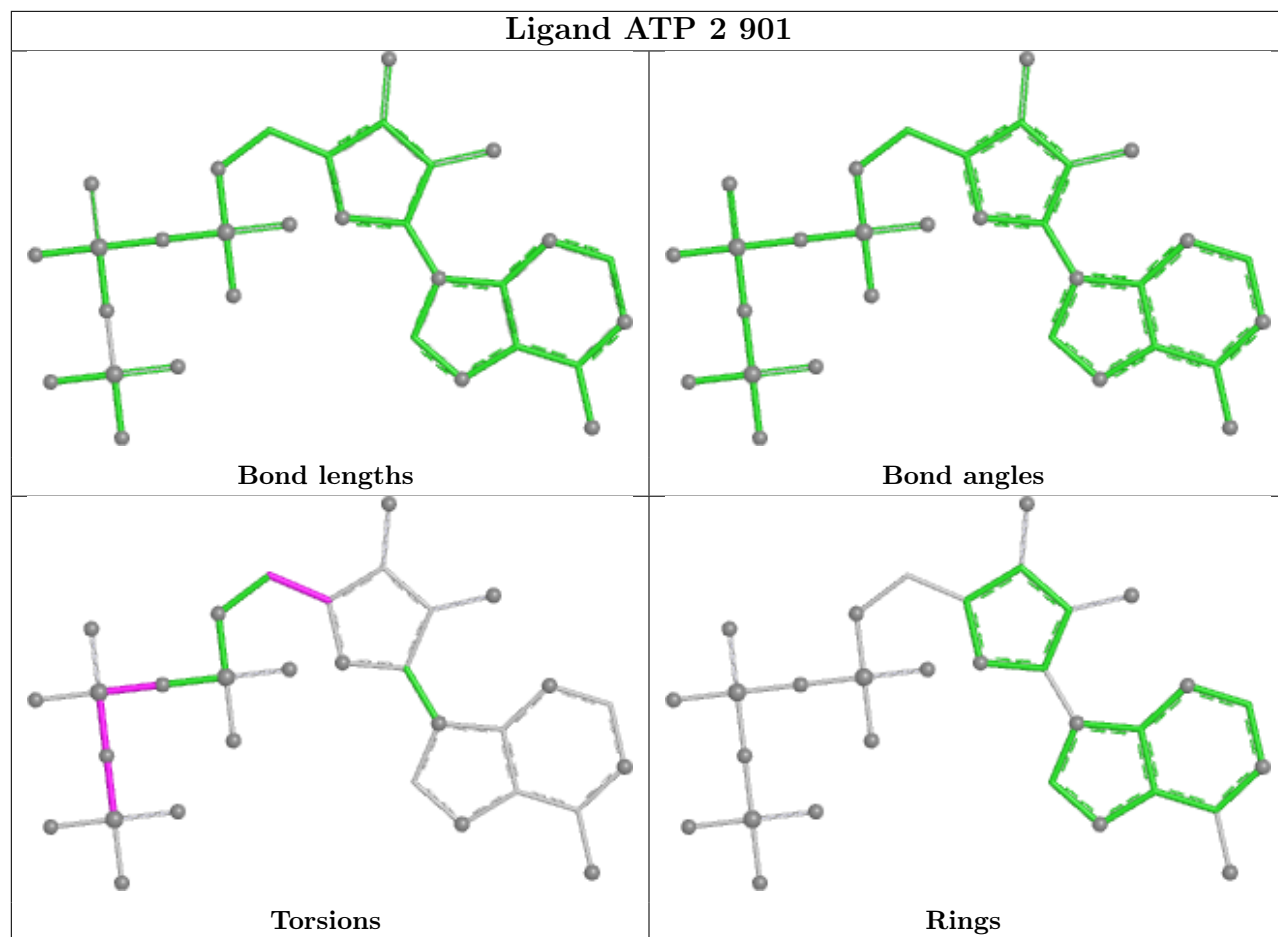
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	D	801	ADP	2	0
12	5	801	ADP	2	0
12	3	1001	ADP	1	0
12	4	1001	ADP	1	0
12	C	1001	ADP	1	0
12	B	1001	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

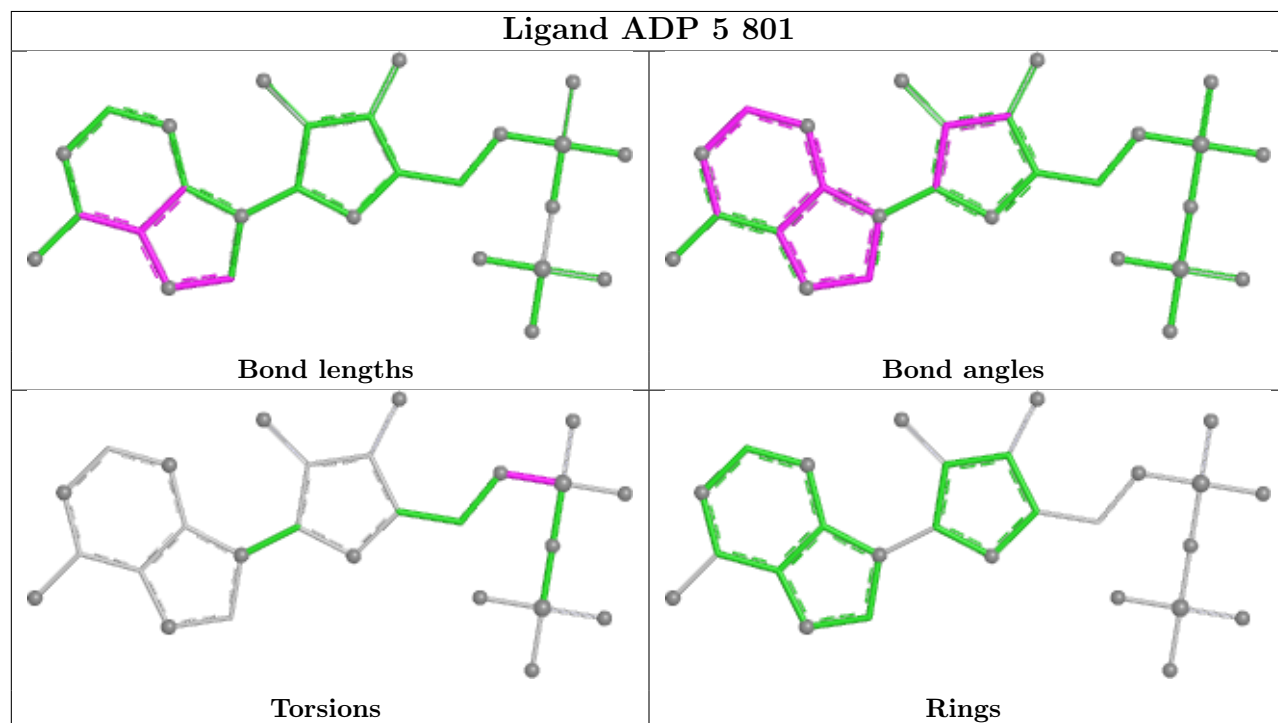
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within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

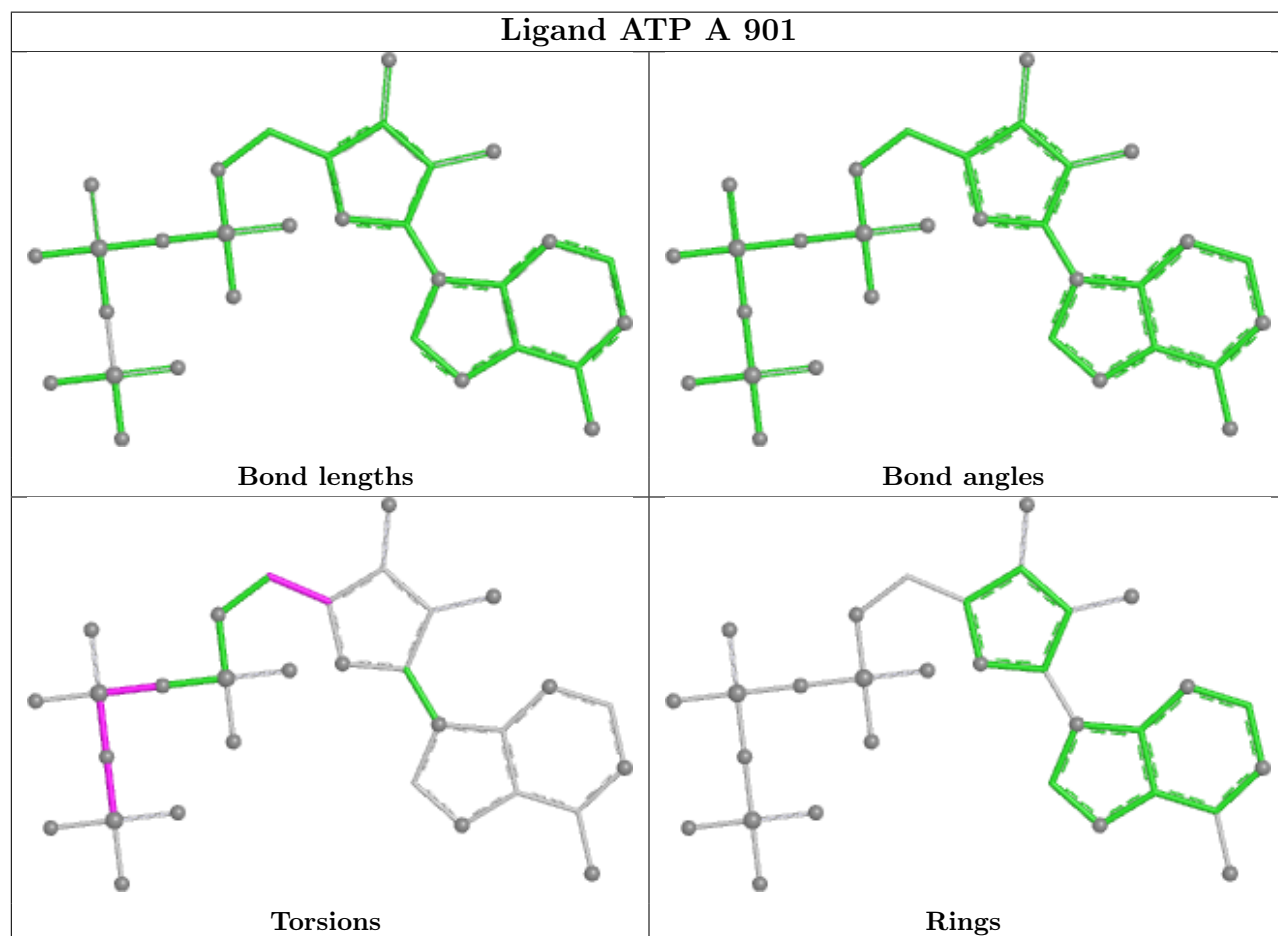
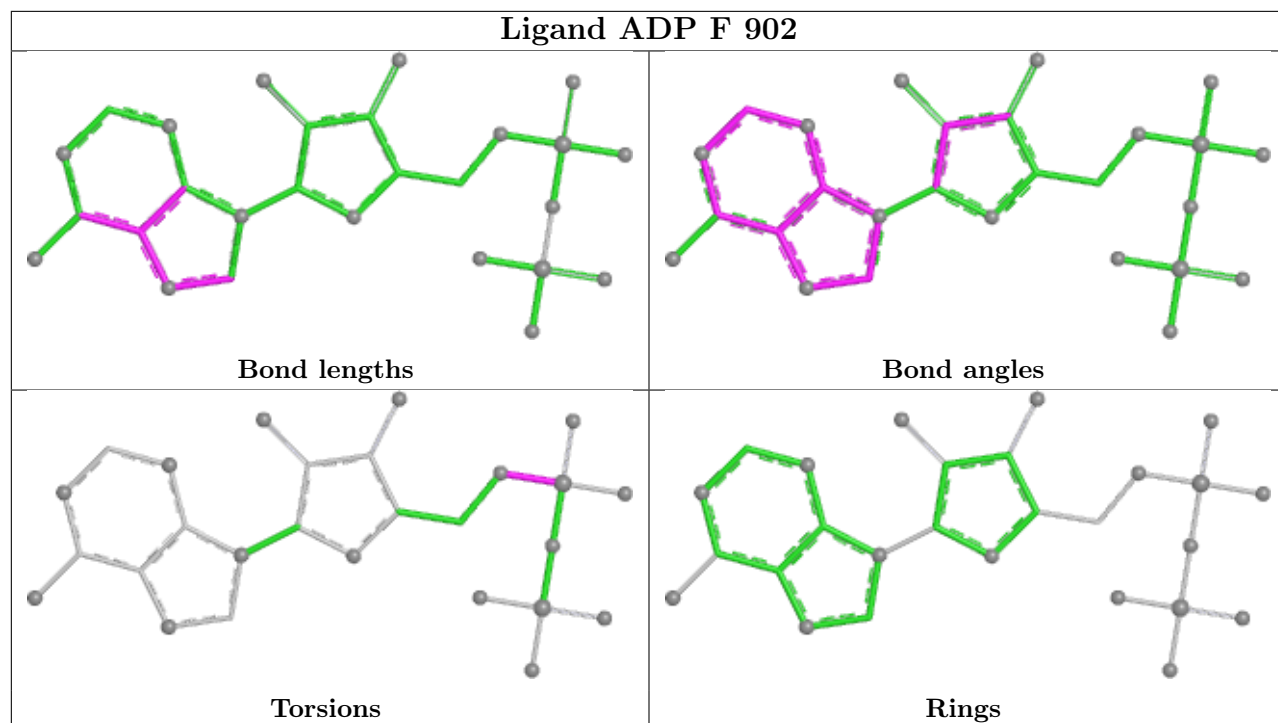


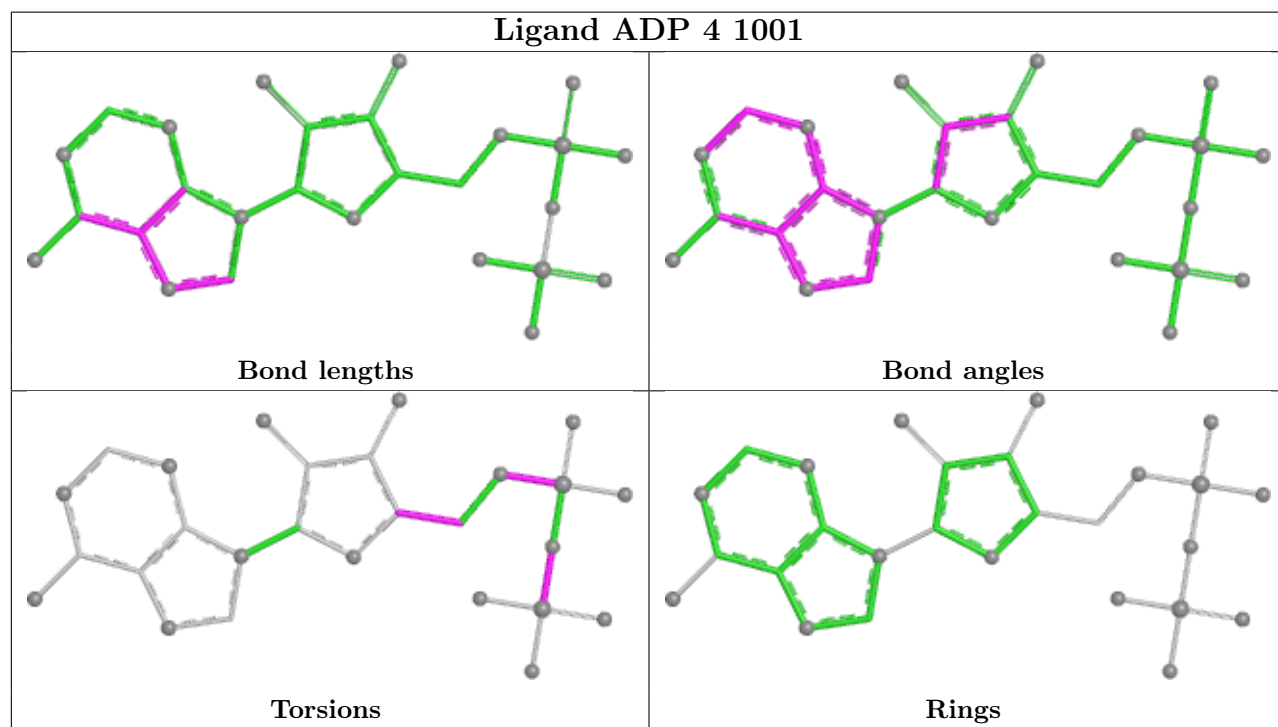
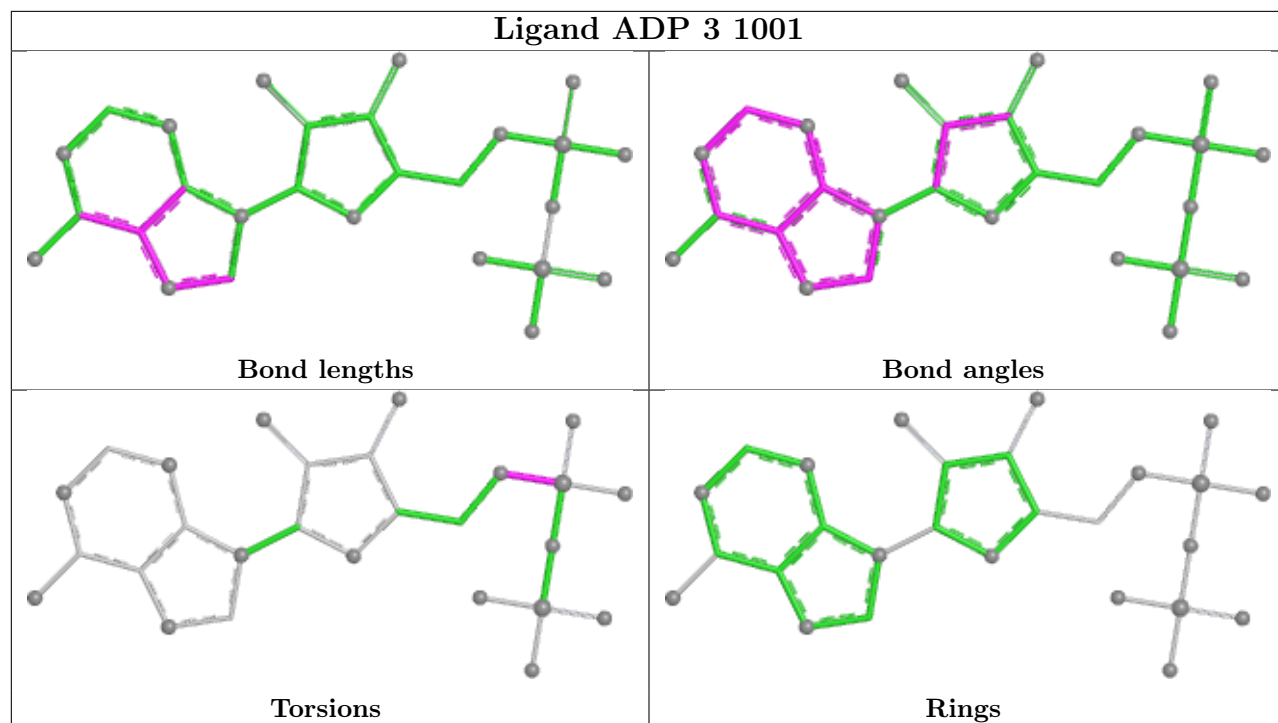
Ligand ATP 2 901

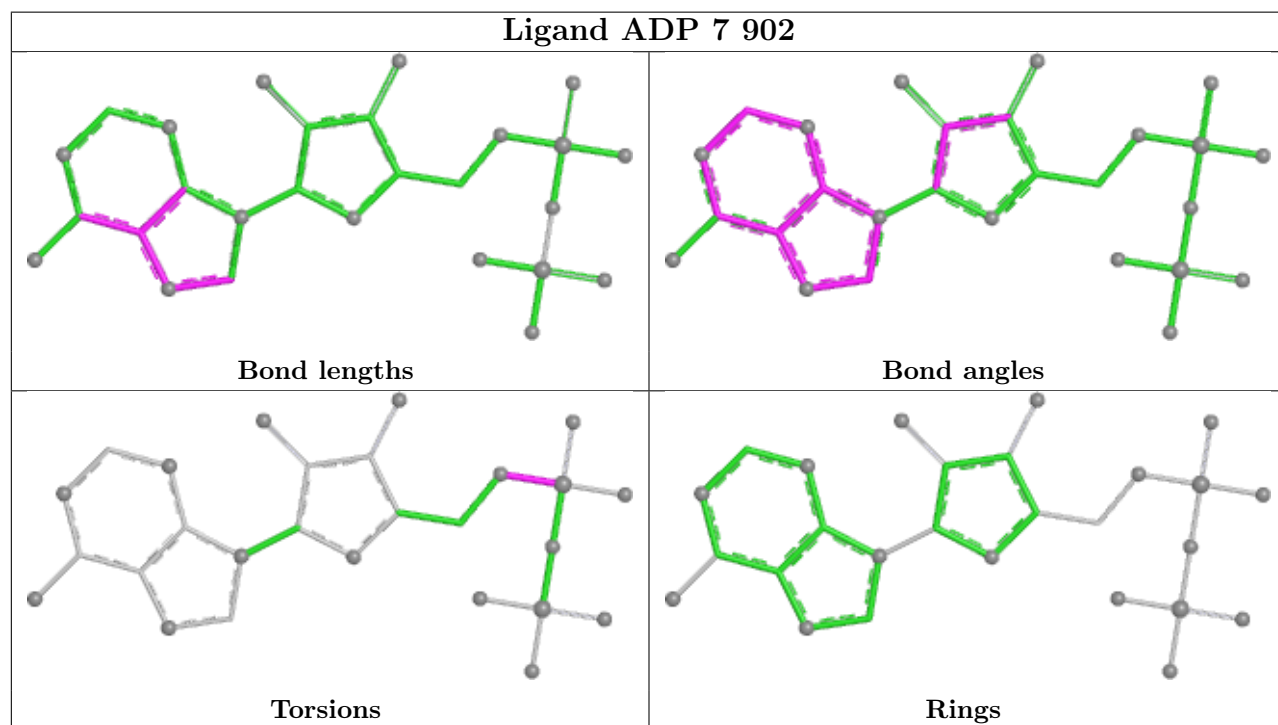
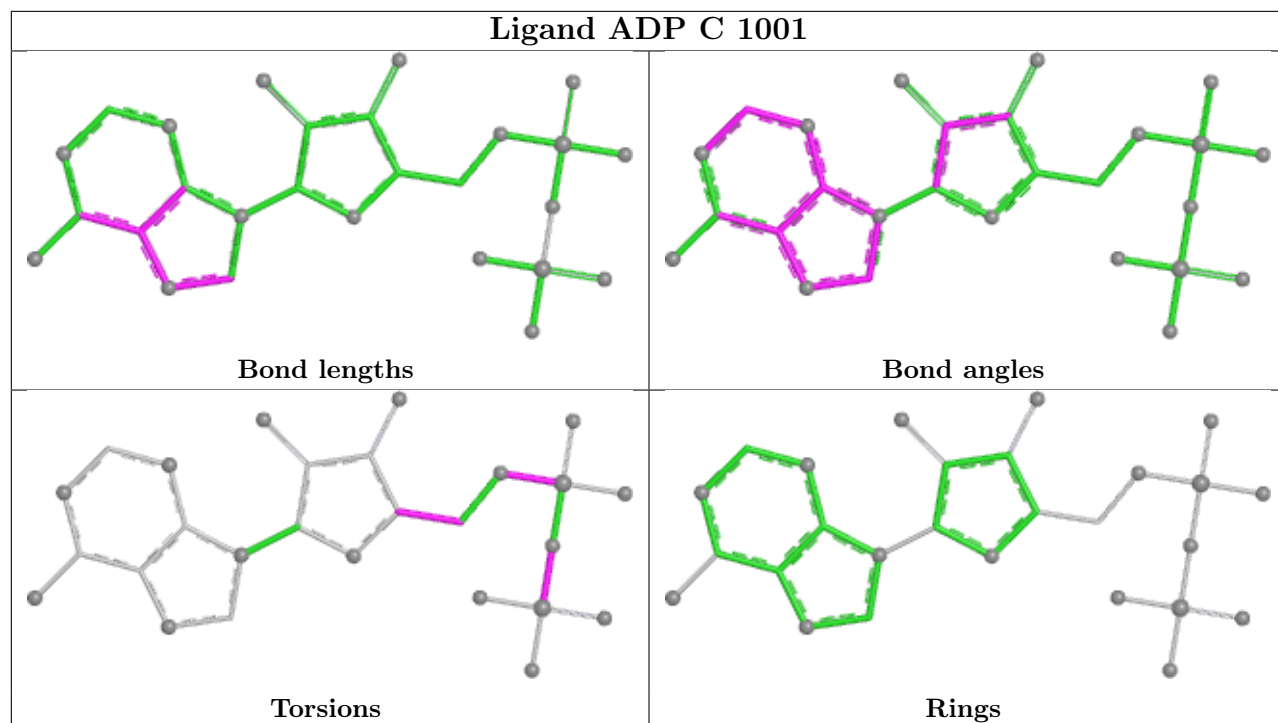


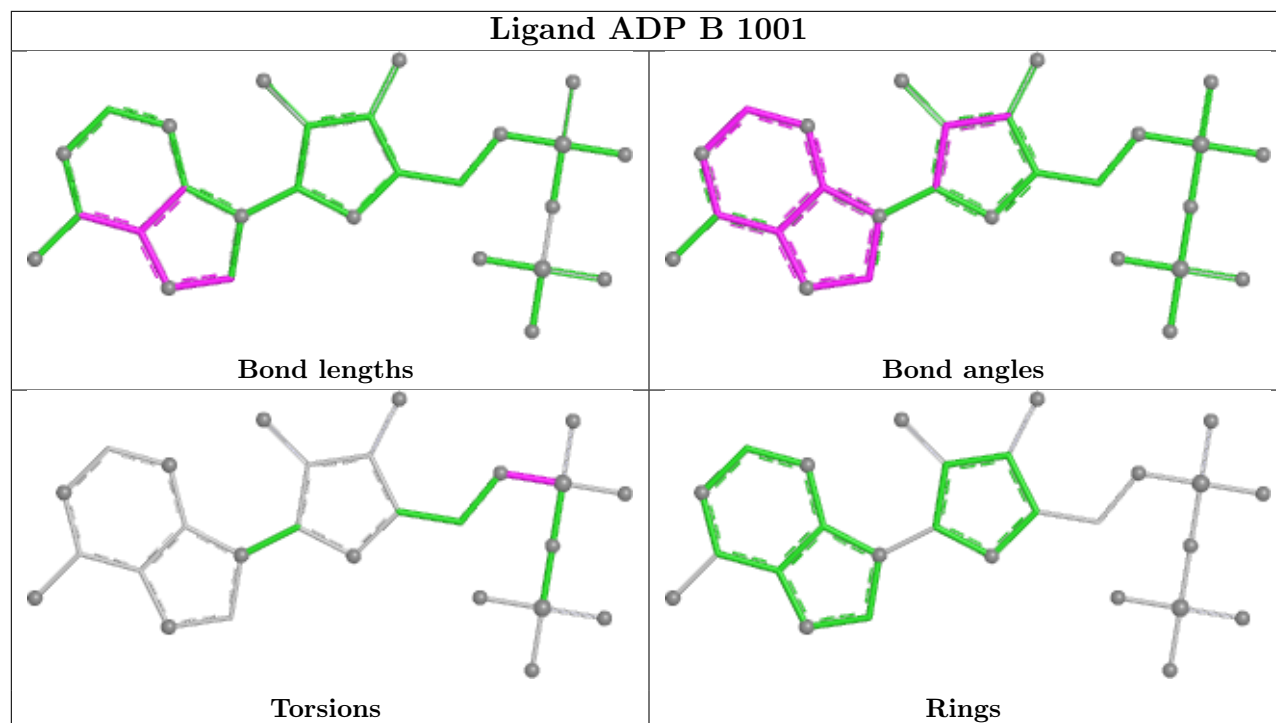
Ligand ADP 5 801











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

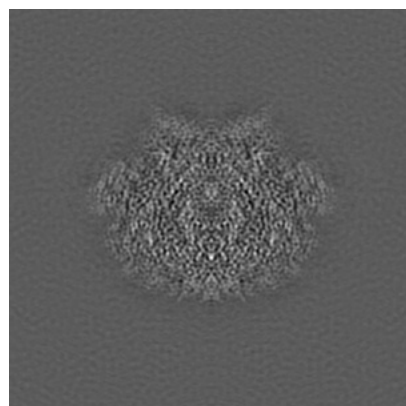
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13176. These allow visual inspection of the internal detail of the map and identification of artifacts.

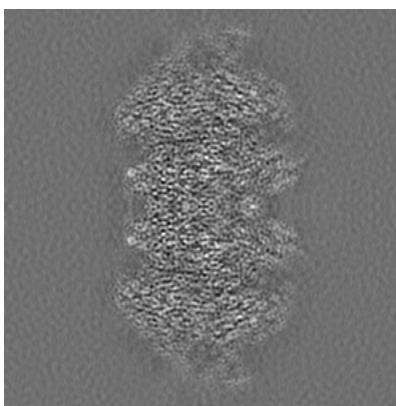
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

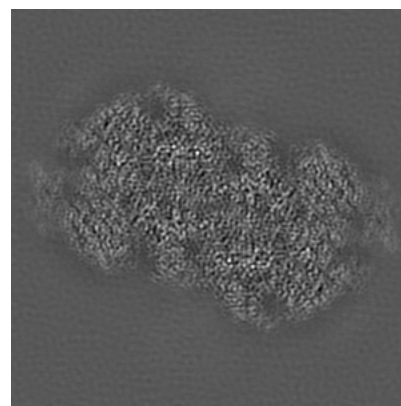
6.1.1 Primary map



X

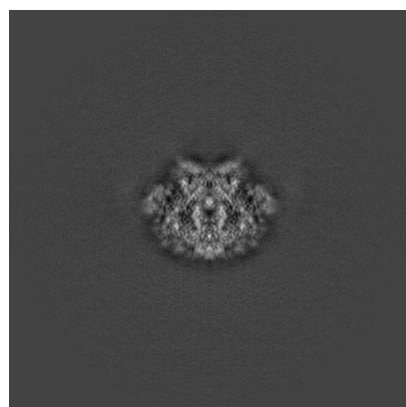


Y

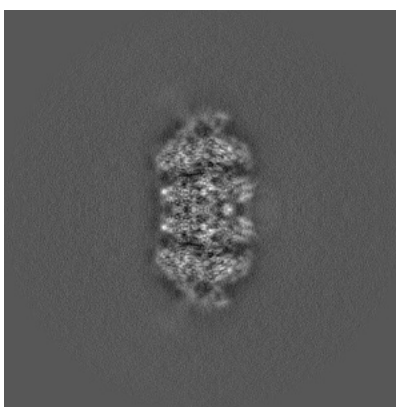


Z

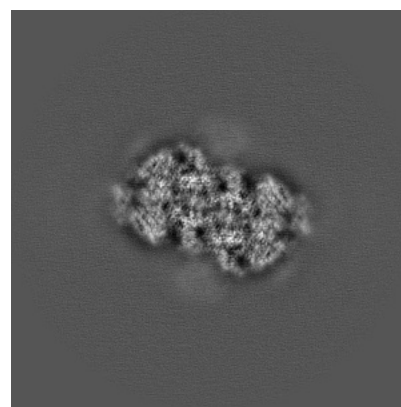
6.1.2 Raw map



X



Y

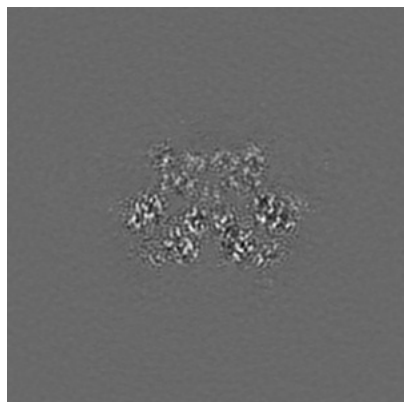


Z

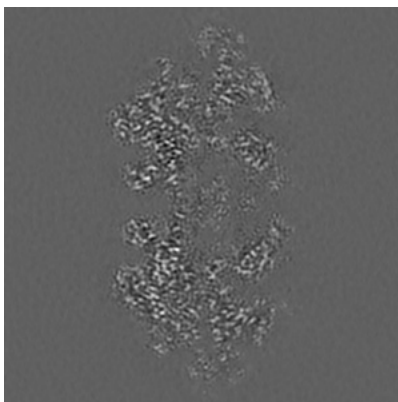
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

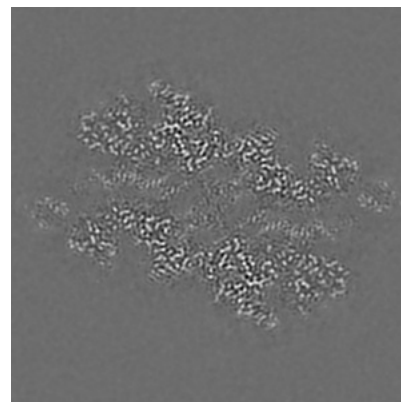
6.2.1 Primary map



X Index: 128

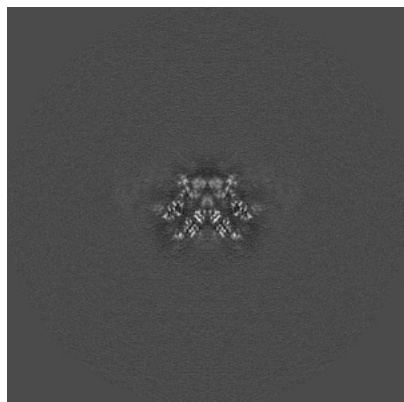


Y Index: 128

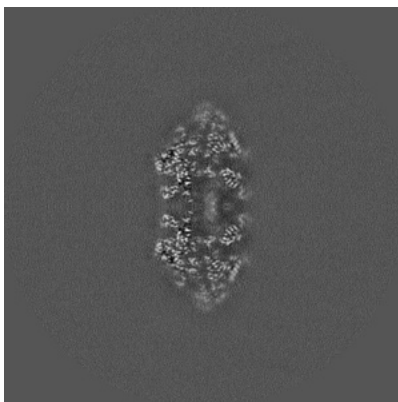


Z Index: 128

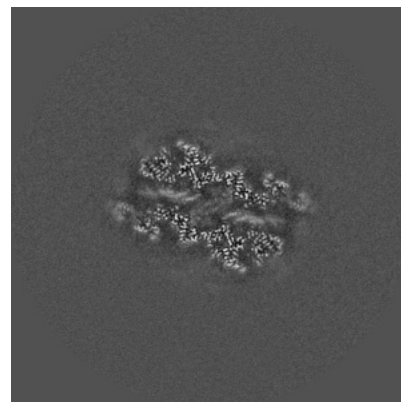
6.2.2 Raw map



X Index: 240



Y Index: 240

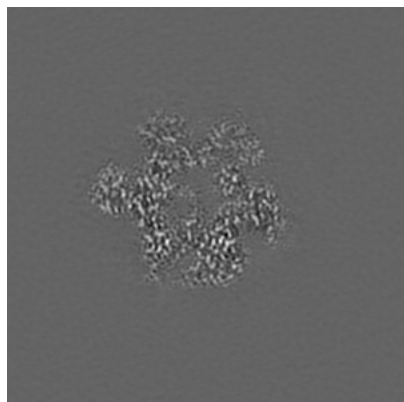


Z Index: 240

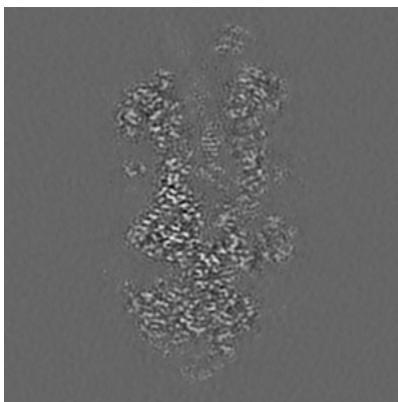
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

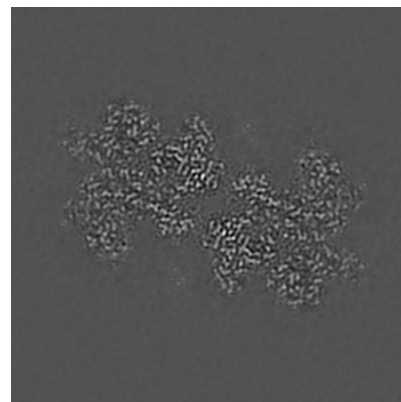
6.3.1 Primary map



X Index: 153

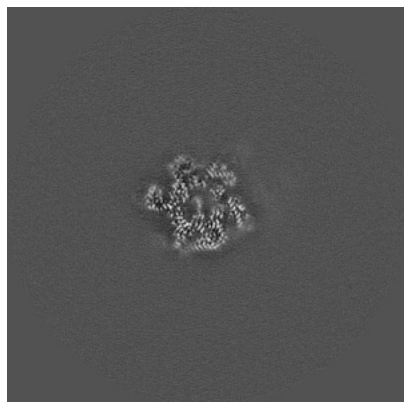


Y Index: 117

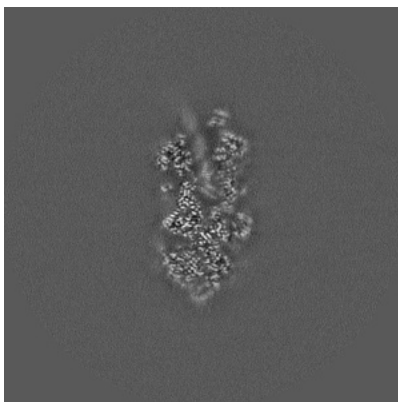


Z Index: 102

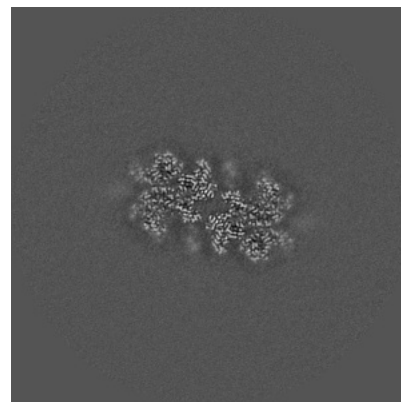
6.3.2 Raw map



X Index: 263



Y Index: 228

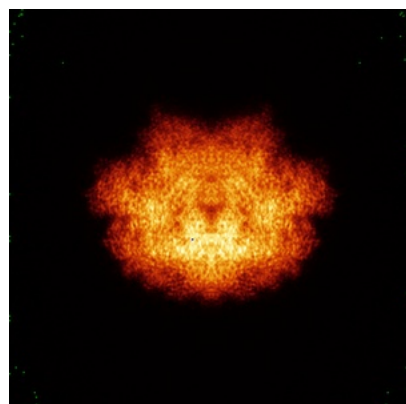


Z Index: 213

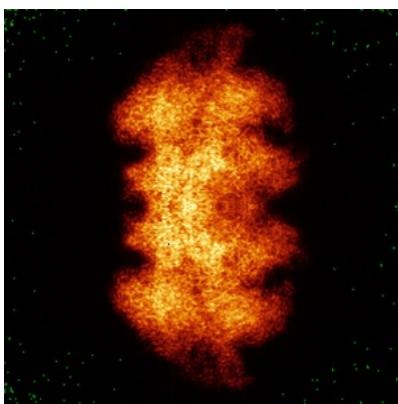
The images above show the largest variance slices of the map in three orthogonal directions.

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

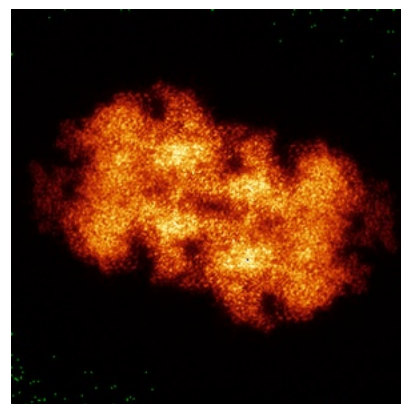
6.4.1 Primary map



X

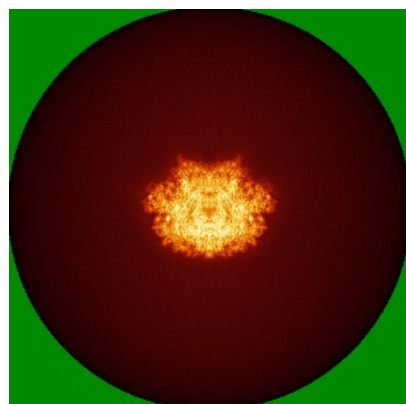


Y

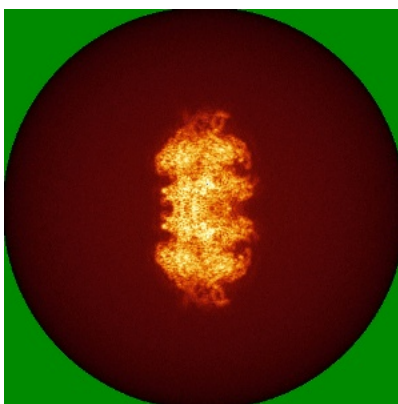


Z

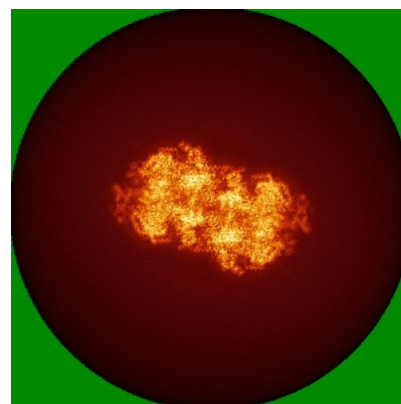
6.4.2 Raw map



X



Y

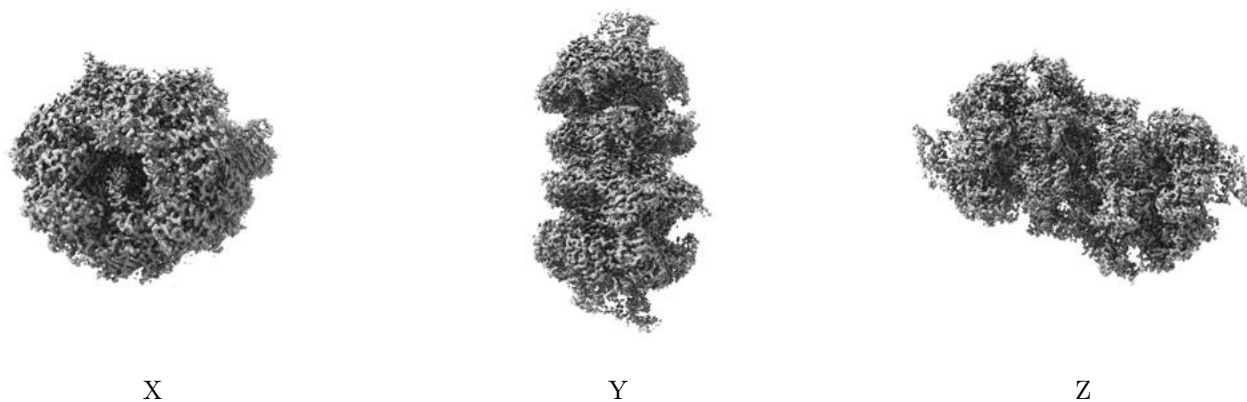


Z

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

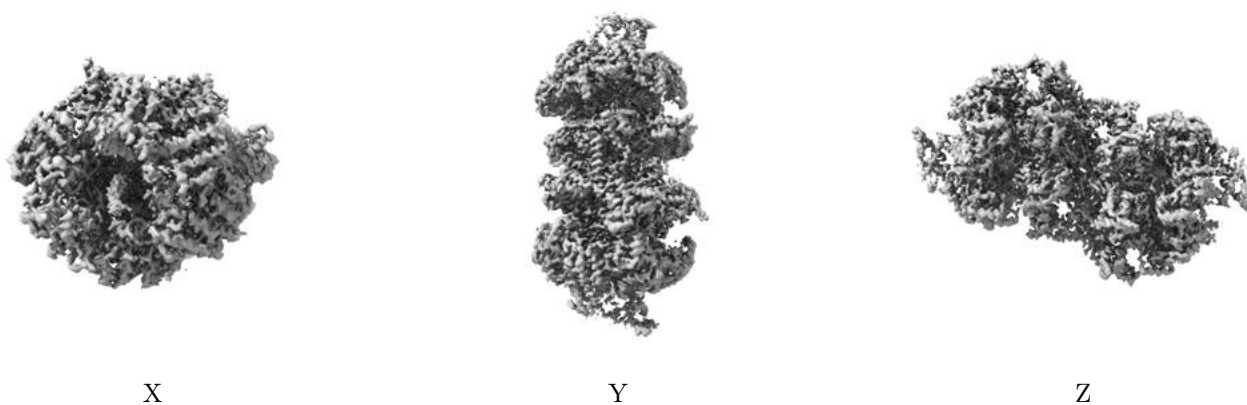
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

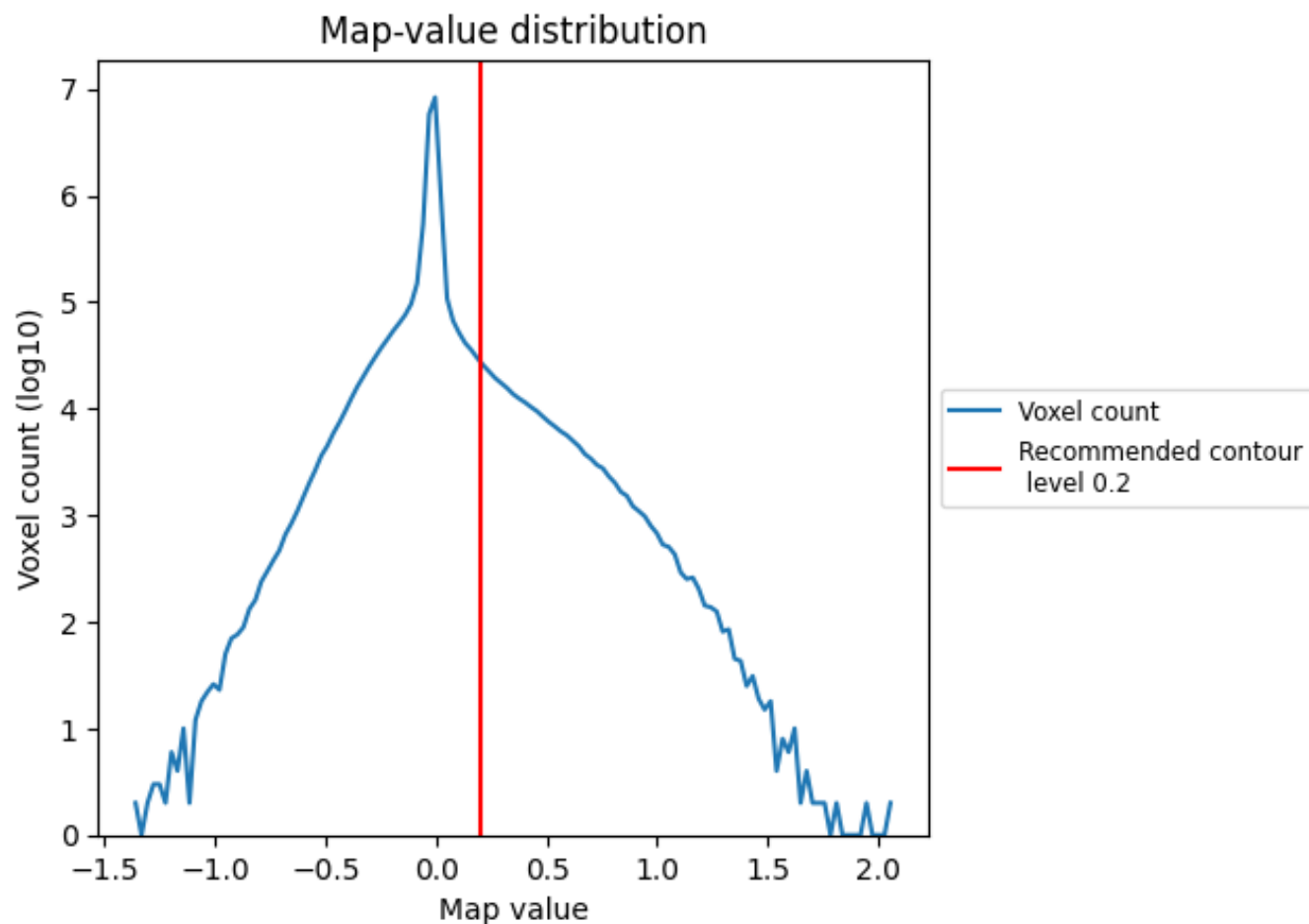
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

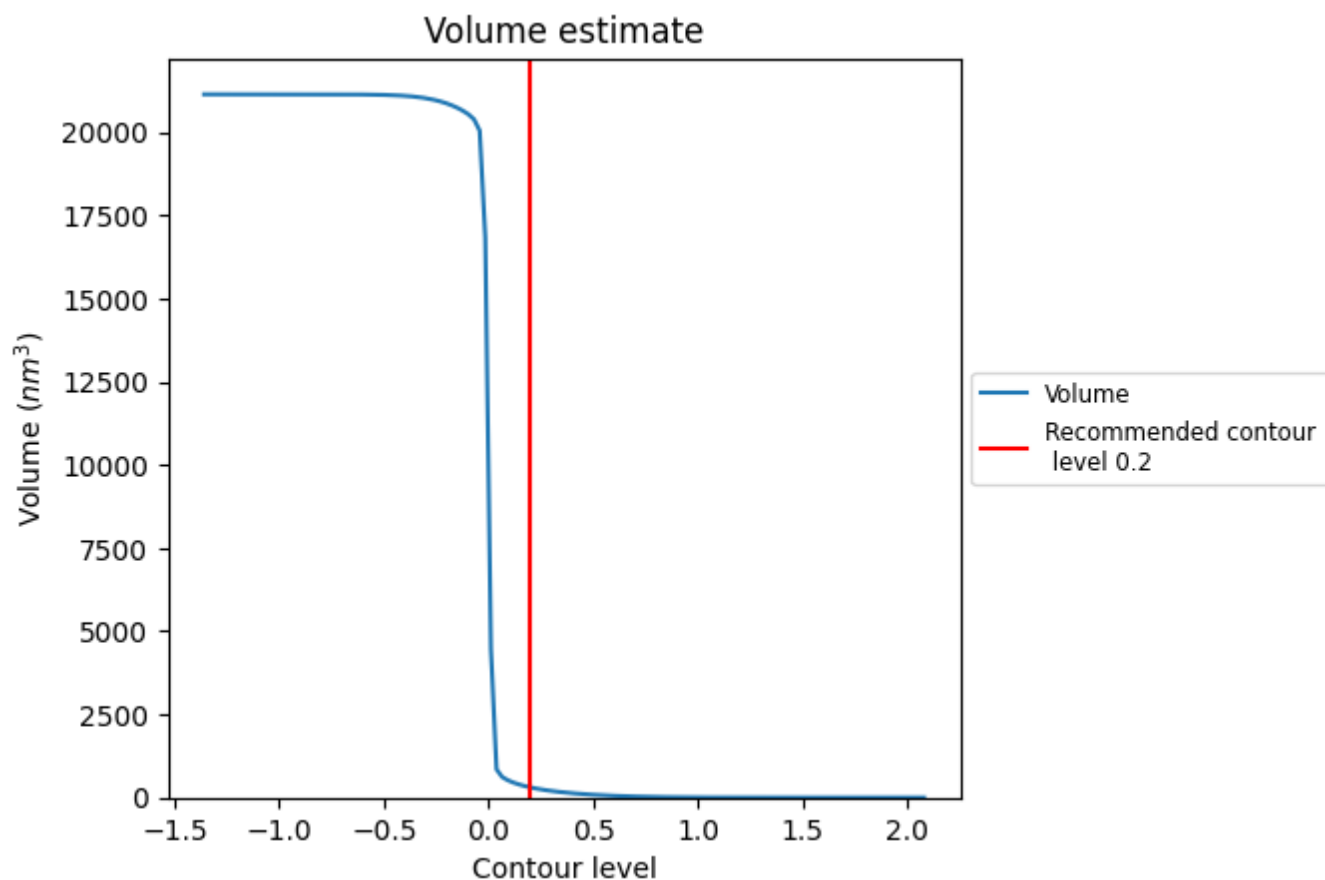
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

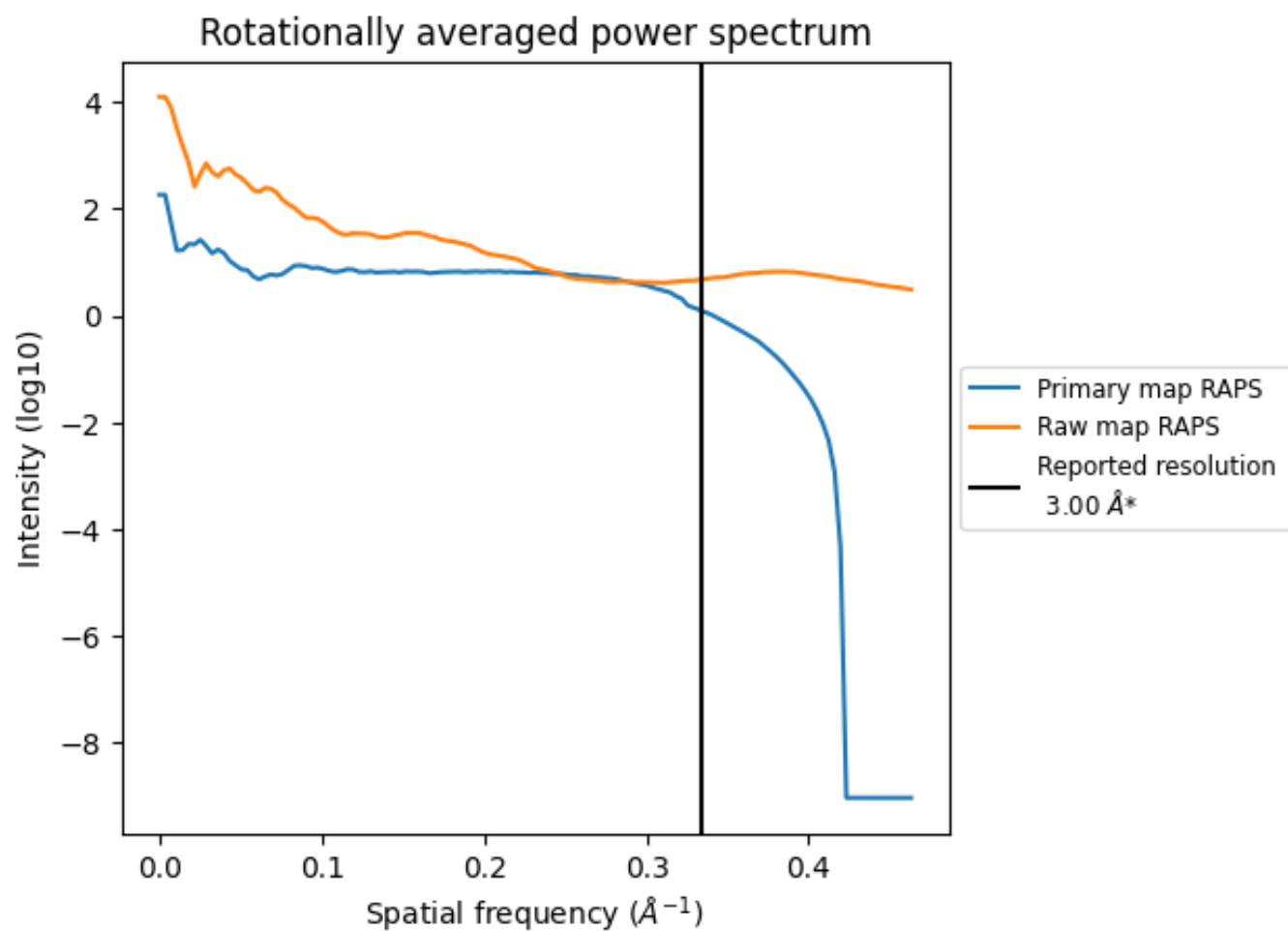
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 306 nm^3 ; this corresponds to an approximate mass of 277 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

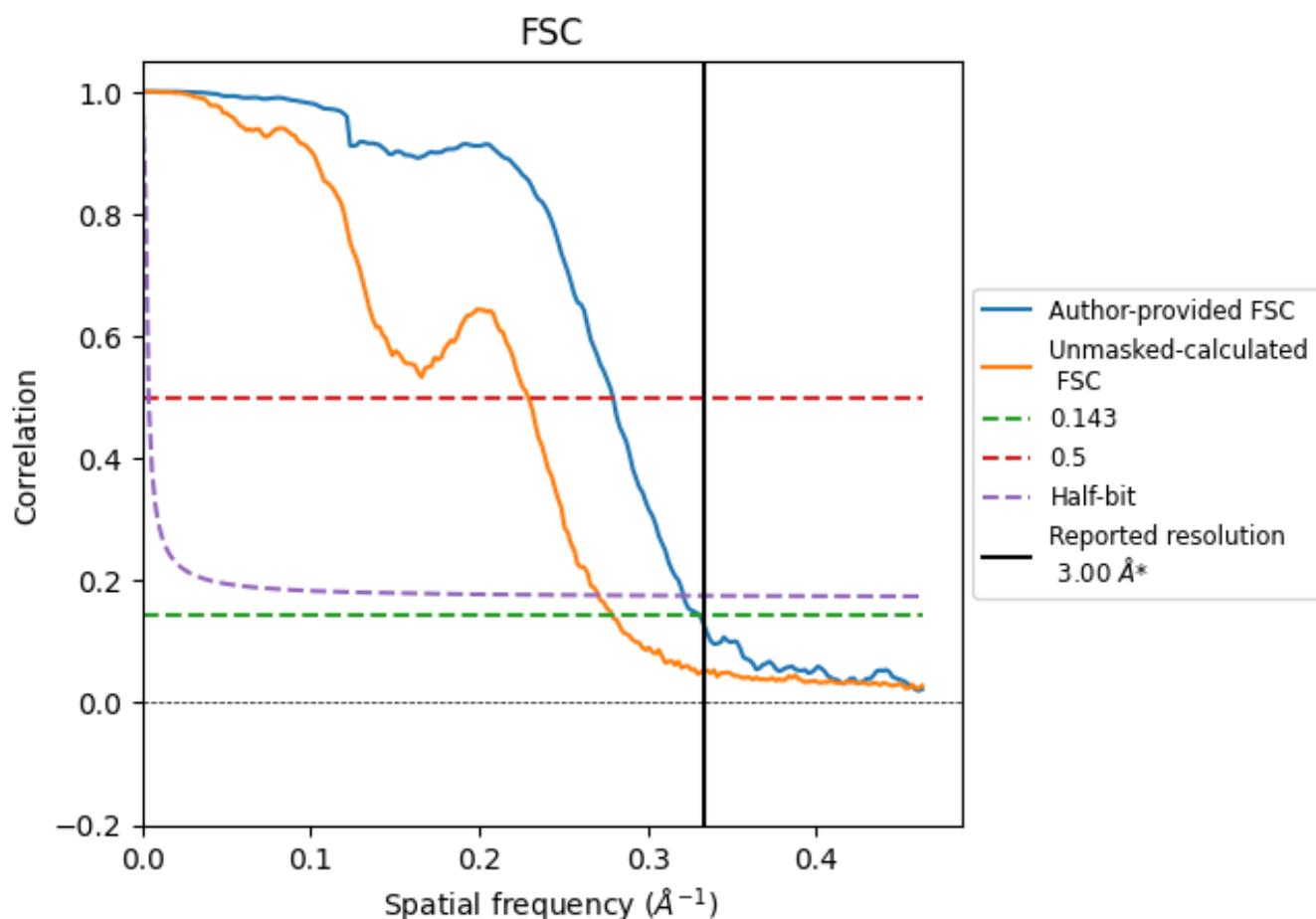


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

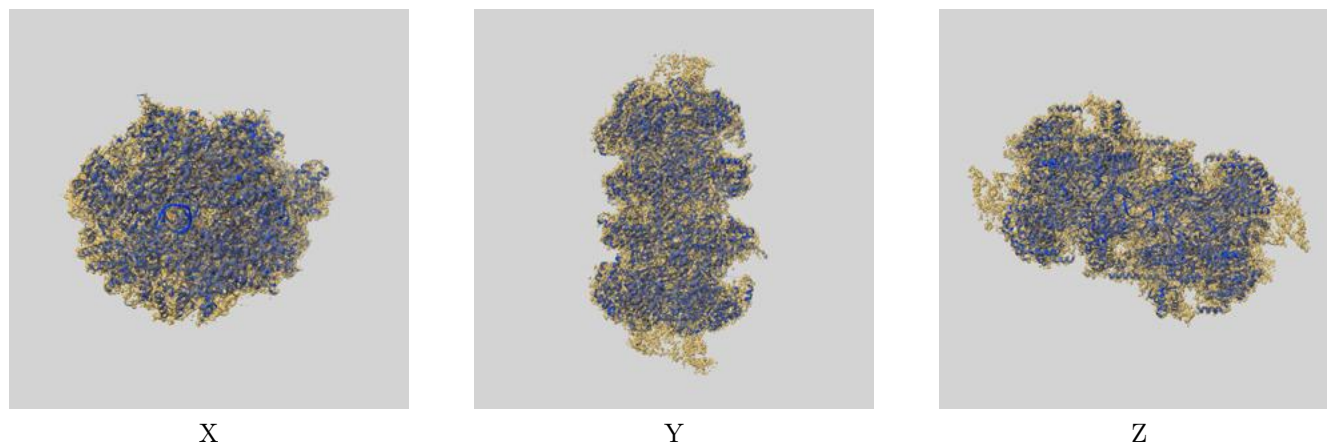
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.02	3.58	3.11
Unmasked-calculated*	3.59	4.36	3.69

*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 3.59 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

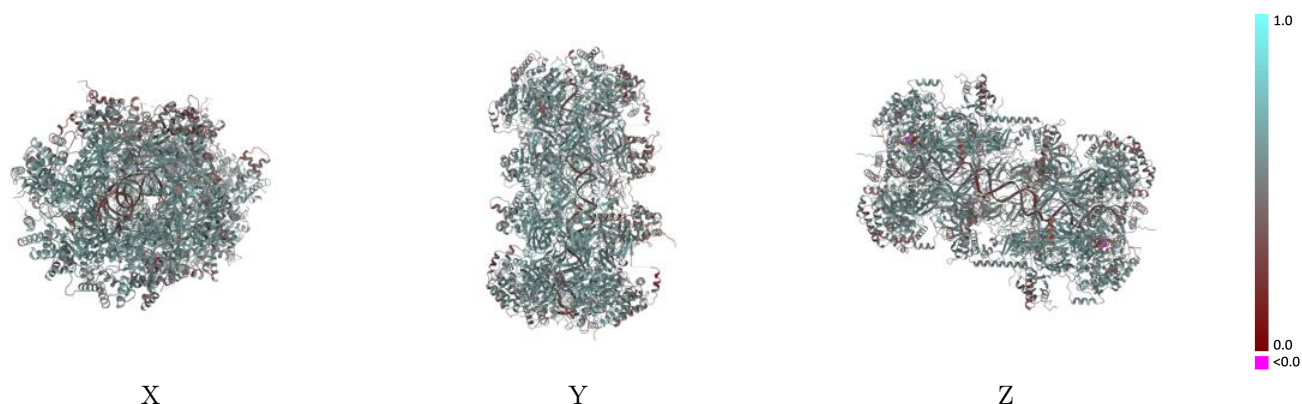
This section contains information regarding the fit between EMDB map EMD-13176 and PDB model 7P30. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



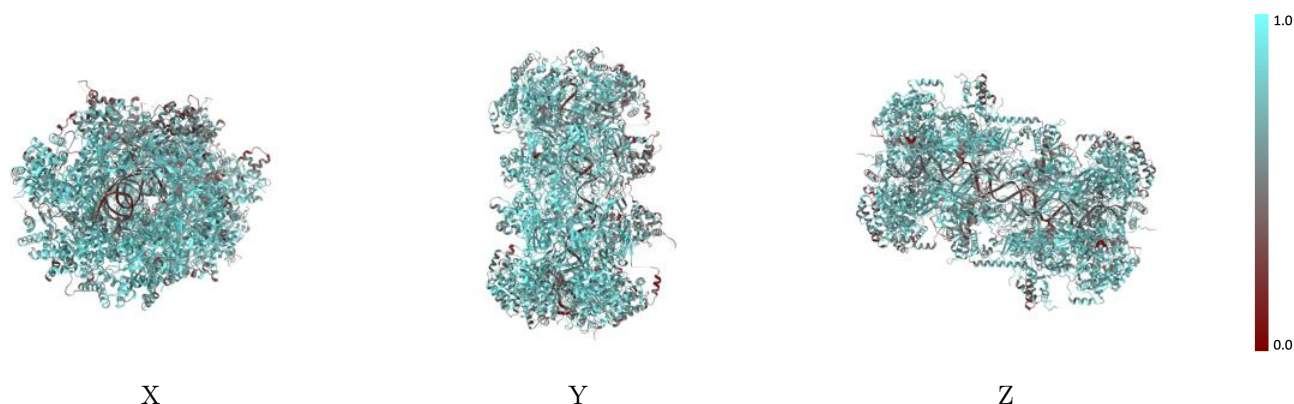
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



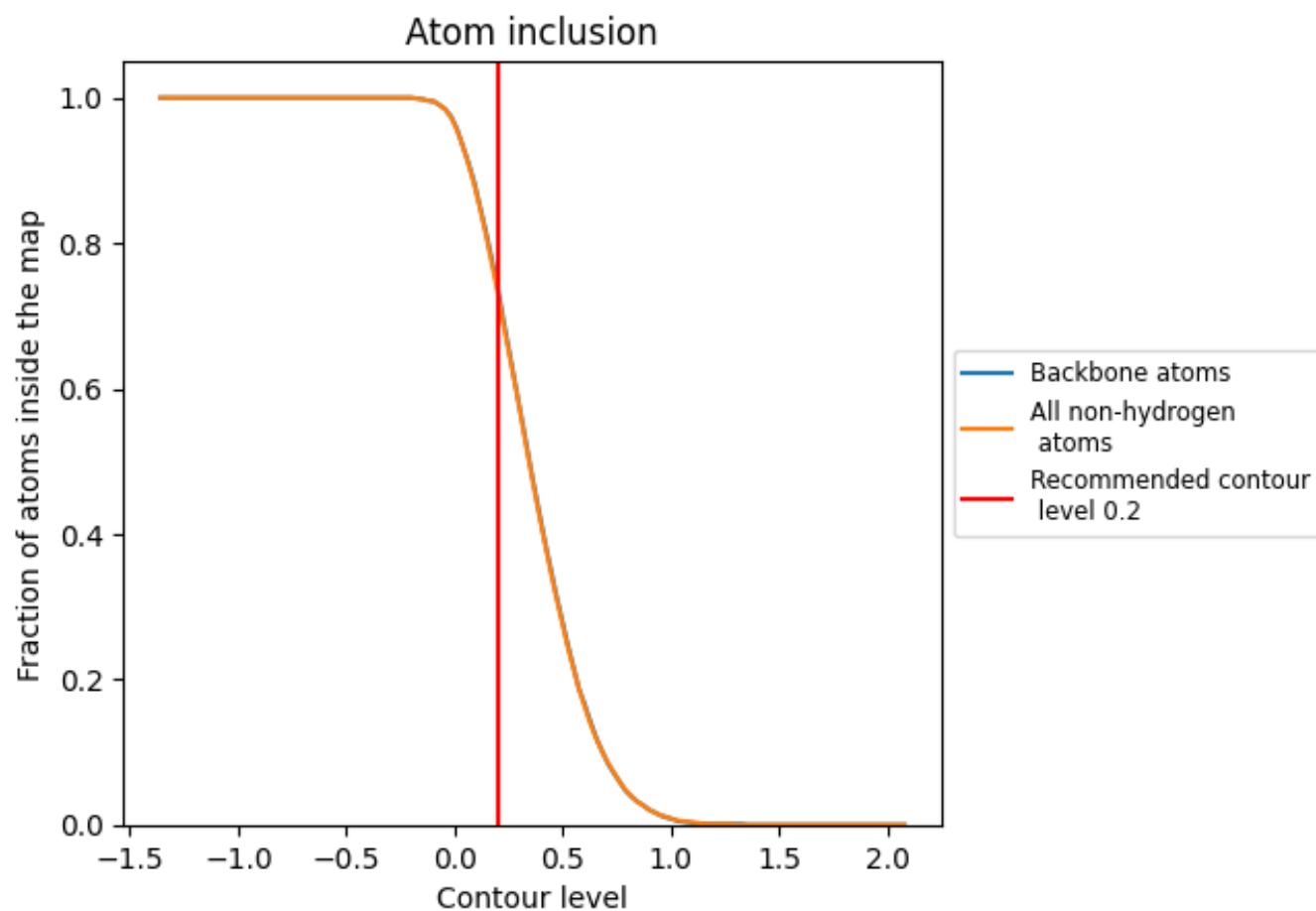
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 73% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7330	0.5380
2	0.6840	0.5130
3	0.8070	0.5630
4	0.7620	0.5560
5	0.7670	0.5510
6	0.6660	0.5120
7	0.7980	0.5660
A	0.6840	0.5140
B	0.8070	0.5610
C	0.7620	0.5560
D	0.7670	0.5500
E	0.6690	0.5120
F	0.7940	0.5660
X	0.3670	0.3760
Y	0.3800	0.3790

