Full wwPDB EM Validation Report (i)

Aug 1, 2026 – 07:43 am BST

PDB ID	:	28VY / pdb_000028vy
EMDB ID	:	EMD-56898
Title	:	sCMGE assembled on ARS1 DNA with Sld2 and RPA
Authors	:	Butryn, A.; Palm, G.; Costa, A.
Deposited on	:	2026-02-23
Resolution	:	2.70 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 (i) 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 (i)) were used in the production of this report:

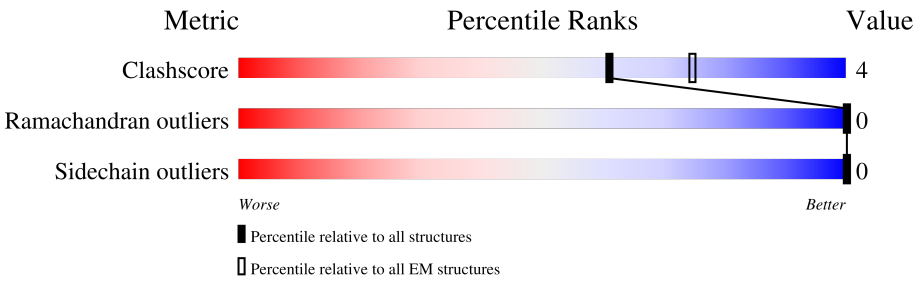
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

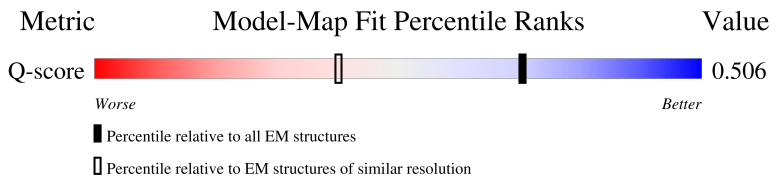
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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	10327 (2.20 - 3.20)

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	2	868	68% 8% 24%
2	3	1006	55% 5% 40%
3	4	933	59% 15% 26%
4	5	775	79% 9% 13%

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Mol	Chain	Length	Quality of chain
5	6	1017	54% 7% 39%
6	7	845	61% 14% 25%
7	A	27	7% 52% 33% 15%
7	B	27	30% 15% 56%
8	C	217	74% 9% 18%
9	D	294	72% 8% 20%
10	E	657	78% 8% 14%
11	F	689	72% 7% 21%
12	G	2222	35% 62%
13	H	208	87% 9%
14	I	213	84% 5% 11%

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 54130 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	2	661	5248	3296	939	994	19	1	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	3	607	4751	3000	844	895	12	0	0

There are 35 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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	4	692	5499	3450	958	1060	31	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	5	676	5364	3370	934	1036	24	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	6	618	4895	3091	851	928	25	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	7	633	5014	3168	870	949	27	0	0

- Molecule 7 is a DNA chain called DNA (5'-D(P*GP*AP*TP*CP*GP*AP*TP*CP*GP*AP*TP*CP*GP*AP*TP*CP*GP*AP*TP*CP*GP*AP*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	A	23	473	225	87	138	23	0	0
7	B	12	246	117	45	72	12	0	0

- Molecule 8 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	C	179	1436	932	232	264	8	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-22	MET	-	initiating methionine	UNP Q12146
C	-21	GLY	-	expression tag	UNP Q12146
C	-20	SER	-	expression tag	UNP Q12146
C	-19	SER	-	expression tag	UNP Q12146
C	-18	HIS	-	expression tag	UNP Q12146
C	-17	HIS	-	expression tag	UNP Q12146
C	-16	HIS	-	expression tag	UNP Q12146
C	-15	HIS	-	expression tag	UNP Q12146
C	-14	HIS	-	expression tag	UNP Q12146
C	-13	HIS	-	expression tag	UNP Q12146
C	-12	SER	-	expression tag	UNP Q12146
C	-11	SER	-	expression tag	UNP Q12146
C	-10	GLY	-	expression tag	UNP Q12146
C	-9	LEU	-	expression tag	UNP Q12146
C	-8	VAL	-	expression tag	UNP Q12146
C	-7	PRO	-	expression tag	UNP Q12146
C	-6	ARG	-	expression tag	UNP Q12146
C	-5	GLY	-	expression tag	UNP Q12146
C	-4	SER	-	expression tag	UNP Q12146
C	-3	HIS	-	expression tag	UNP Q12146
C	-2	MET	-	expression tag	UNP Q12146
C	-1	ALA	-	expression tag	UNP Q12146
C	0	SER	-	expression tag	UNP Q12146
C	45	ASN	SER	variant	UNP Q12146

- Molecule 9 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	D	236	1949	1243	320	372	14	0	0

- Molecule 10 is a protein called Cell division control protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	E	565	4590	2934	774	868	14	0	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	167F	ASP	-	linker	UNP Q08032
E	167G	TYR	-	linker	UNP Q08032
E	167H	LYS	-	linker	UNP Q08032
E	167I	ASP	-	linker	UNP Q08032
E	167J	ASP	-	linker	UNP Q08032
E	167K	ASP	-	linker	UNP Q08032
E	167L	GLY	-	linker	UNP Q08032
E	167M	ASP	-	linker	UNP Q08032
E	167N	TYR	-	linker	UNP Q08032
E	167O	LYS	-	linker	UNP Q08032
E	167P	ASP	-	linker	UNP Q08032
E	167Q	ASP	-	linker	UNP Q08032
E	167R	ASP	-	linker	UNP Q08032

- Molecule 11 is a protein called DNA polymerase epsilon subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	F	545	4366	2808	744	796	18	0	0

- Molecule 12 is a protein called DNA polymerase epsilon catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	G	849	6894	4466	1128	1263	37	0	0

- Molecule 13 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	H	199	1629	1022	281	317	9	0	0

- Molecule 14 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	I	189	1581	1016	278	283	4	0	0

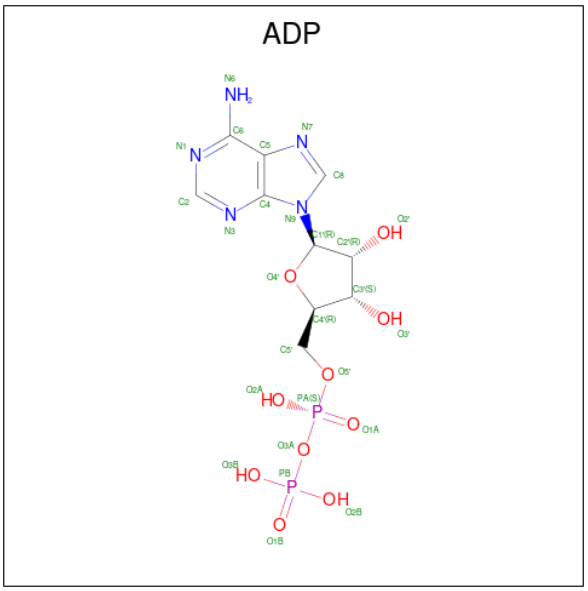
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
15	2	1	1	1	0
15	3	1	1	1	0
15	4	1	1	1	0
15	5	1	1	1	0
15	6	1	1	1	0
15	7	1	1	1	0

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

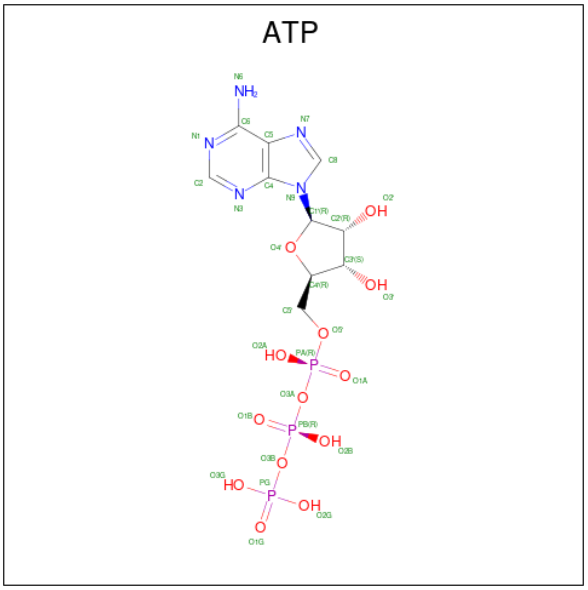
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
16	2	1	1	1	0
16	4	1	1	1	0
16	5	1	1	1	0
16	6	1	1	1	0
16	7	1	1	1	0
16	G	2	2	2	0

- Molecule 17 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
17	2	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 18 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
18	3	1	Total	C	N	O	P	0
			31	10	5	13	3	
18	4	1	Total	C	N	O	P	0
			31	10	5	13	3	
18	5	1	Total	C	N	O	P	0
			31	10	5	13	3	

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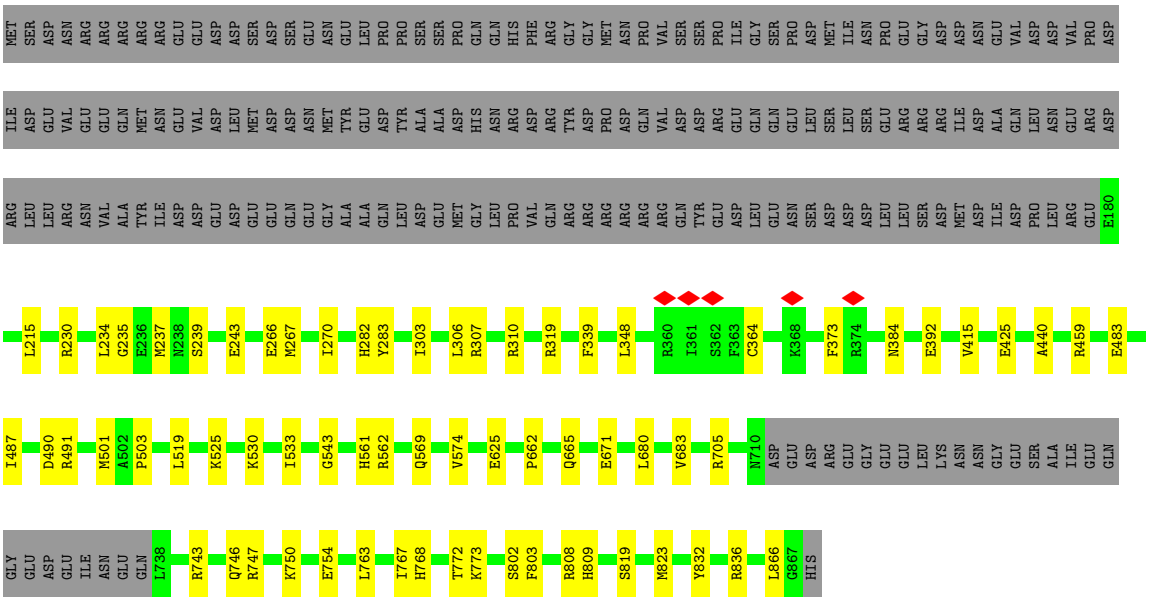
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
18	6	1	31	10	5	13	3	0
			Total	C	N	O	P	
18	7	1	31	10	5	13	3	0

3 Residue-property plots (i)

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

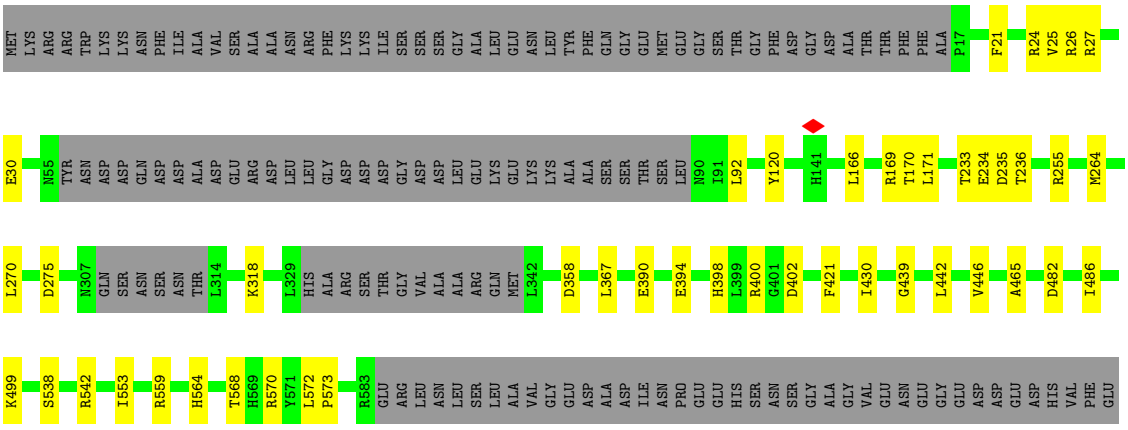
- Molecule 1: DNA replication licensing factor MCM2

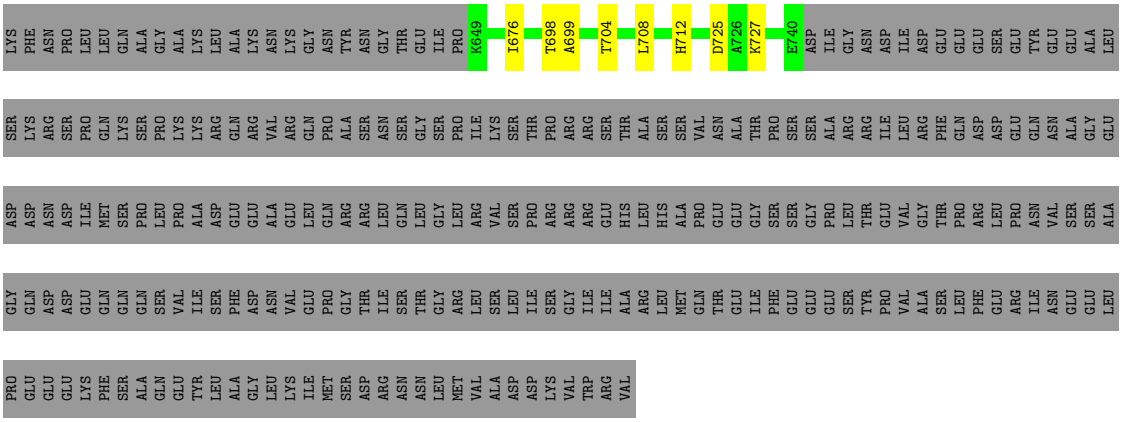
Chain 2:



- Molecule 2: DNA replication licensing factor MCM3

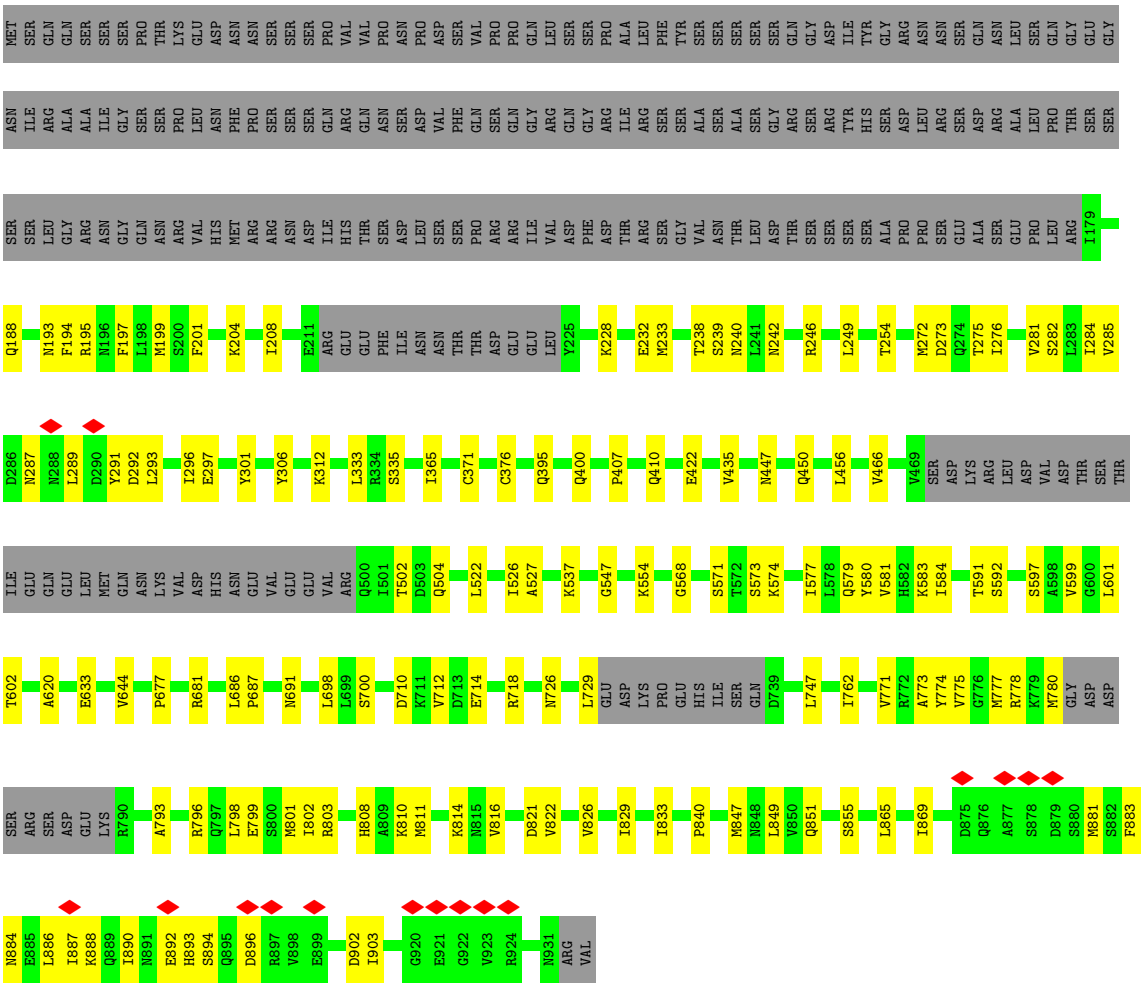
Chain 3:





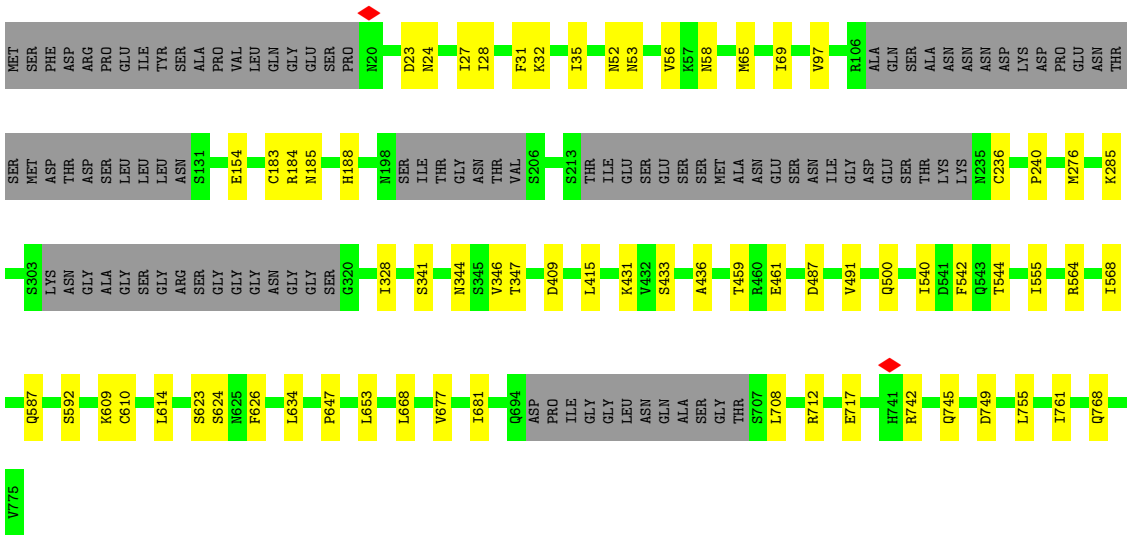
• Molecule 3: DNA replication licensing factor MCM4

Chain 4:



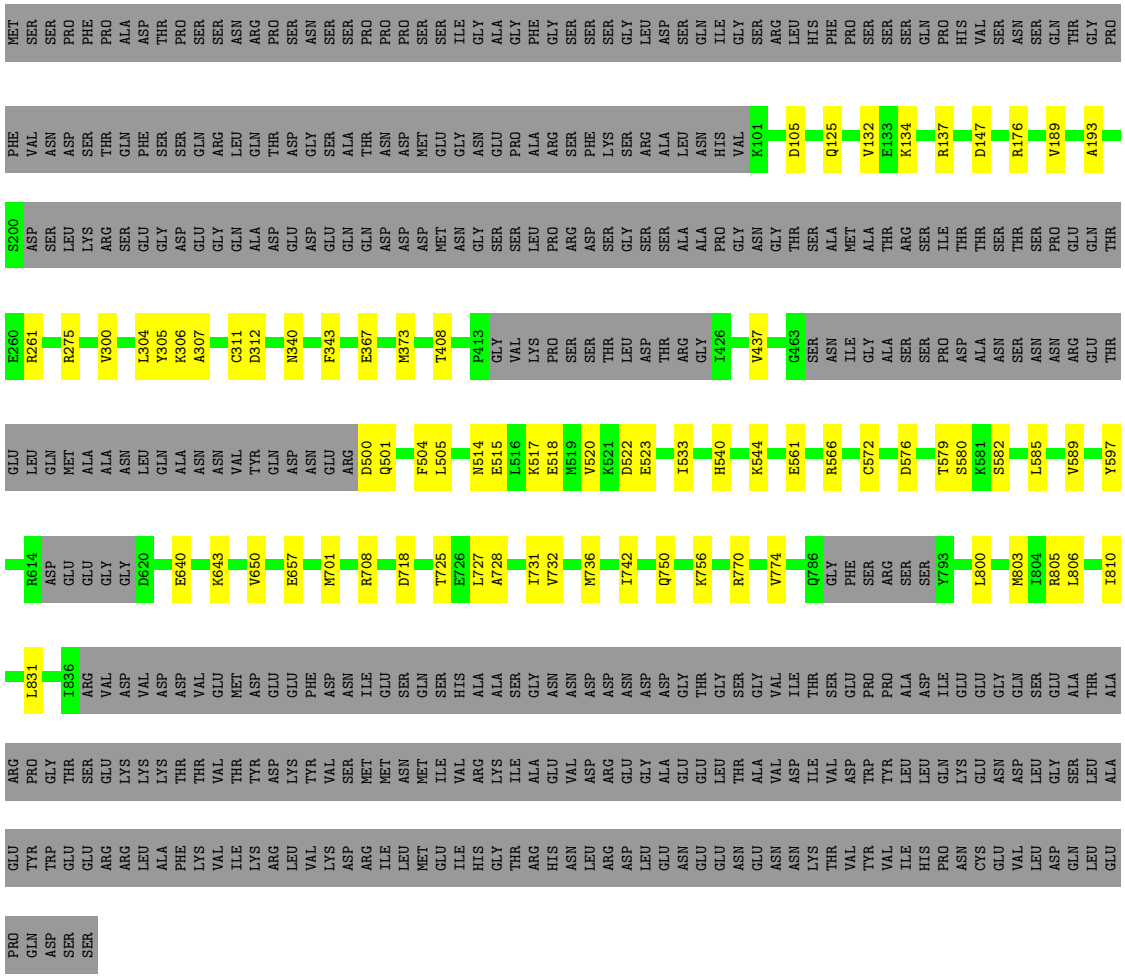
• Molecule 4: Minichromosome maintenance protein 5

Chain 5:



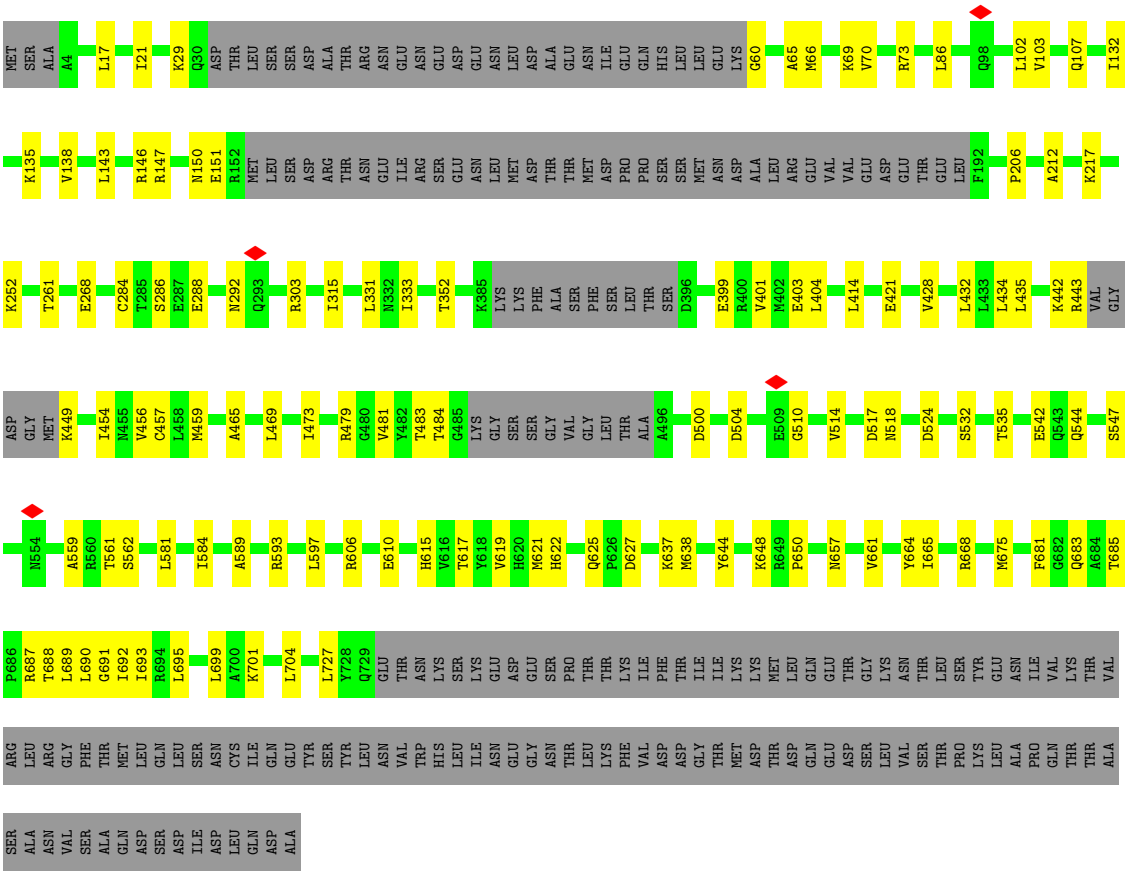
• Molecule 5: DNA replication licensing factor MCM6

Chain 6:



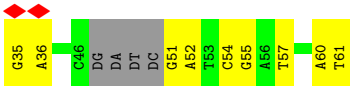
• Molecule 6: DNA replication licensing factor MCM7

Chain 7: 61% 14% 25%



• Molecule 7: DNA (5'-D(P*GP*AP*TP*CP*GP*AP*TP*CP*GP*AP*TP*CP*GP*AP*TP*CP*GP*AP*TP*CP*GP*AP*T)-3')

Chain A: 7% 52% 33% 15%

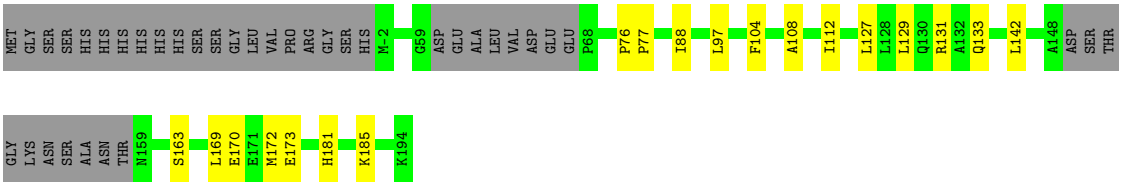


• Molecule 7: DNA (5'-D(P*GP*AP*TP*CP*GP*AP*TP*CP*GP*AP*TP*CP*GP*AP*TP*CP*GP*AP*TP*CP*GP*AP*T)-3')

Chain B: 30% 15% 56%

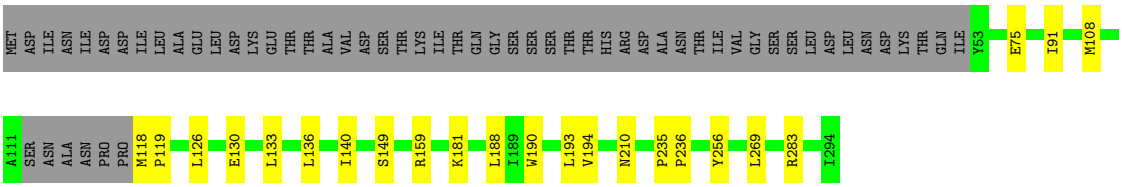
• Molecule 8: DNA replication complex GINS protein PSF3

Chain C: 74% 9% 18%



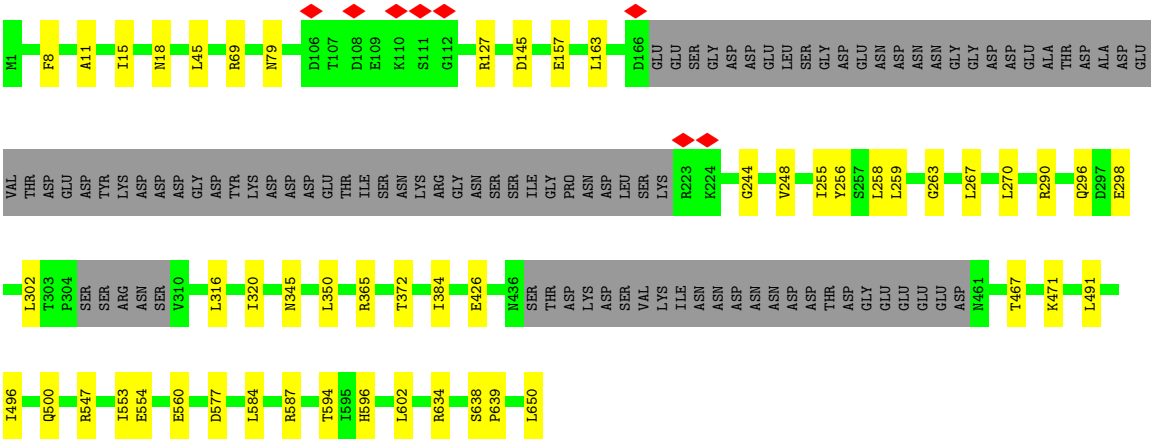
• Molecule 9: DNA replication complex GINS protein SLD5

Chain D:



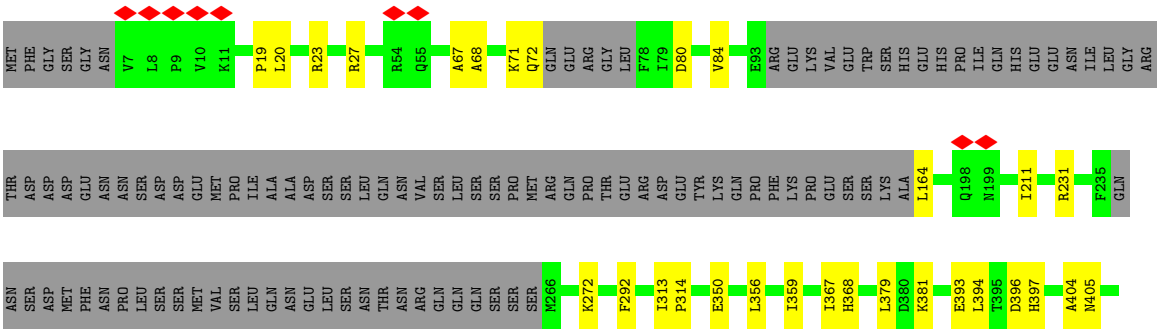
• Molecule 10: Cell division control protein 45

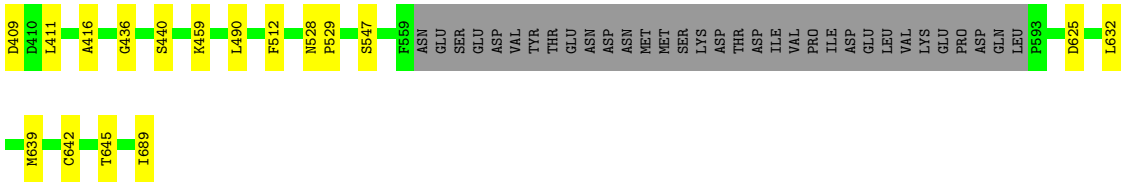
Chain E:



• Molecule 11: DNA polymerase epsilon subunit B

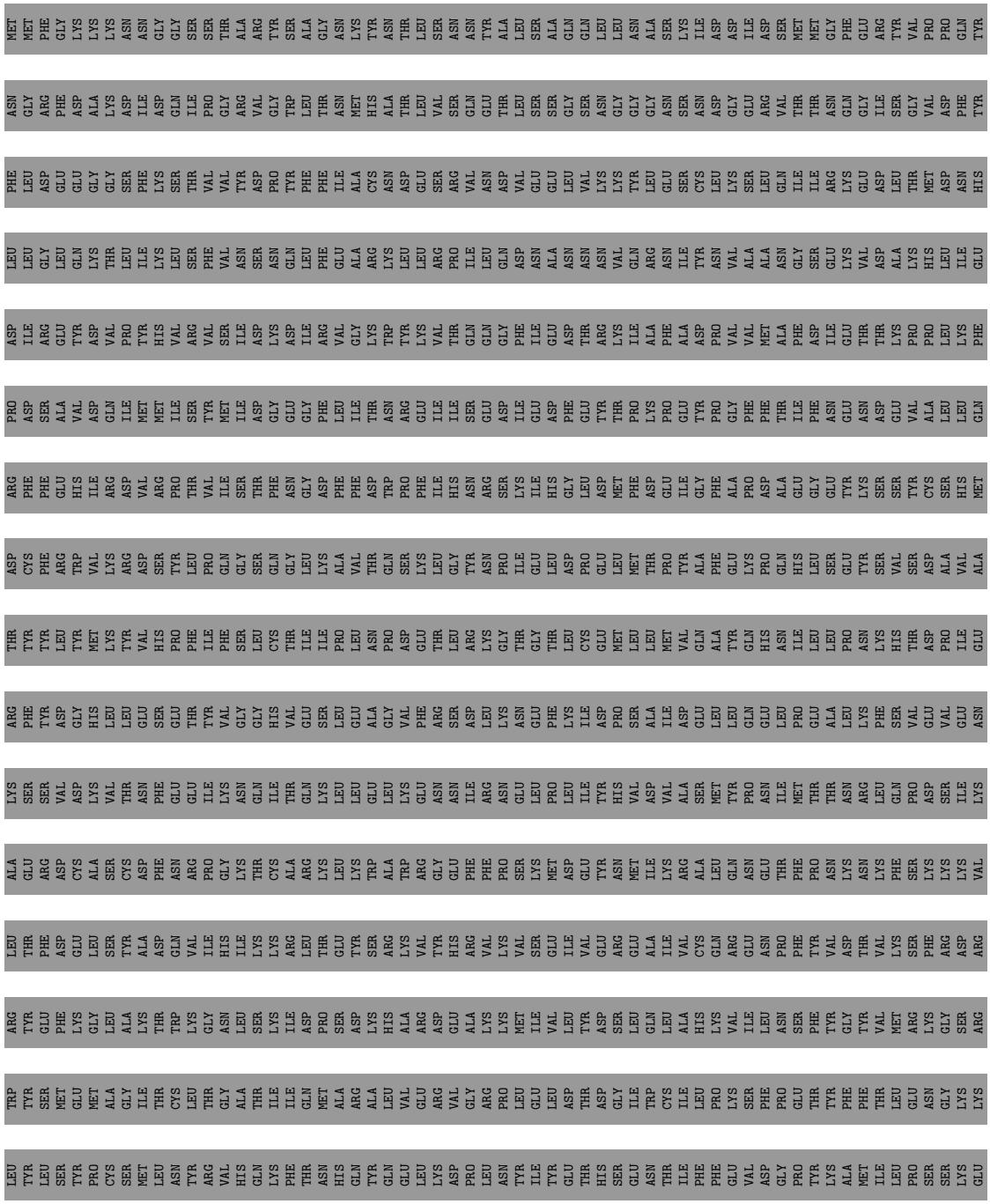
Chain F:

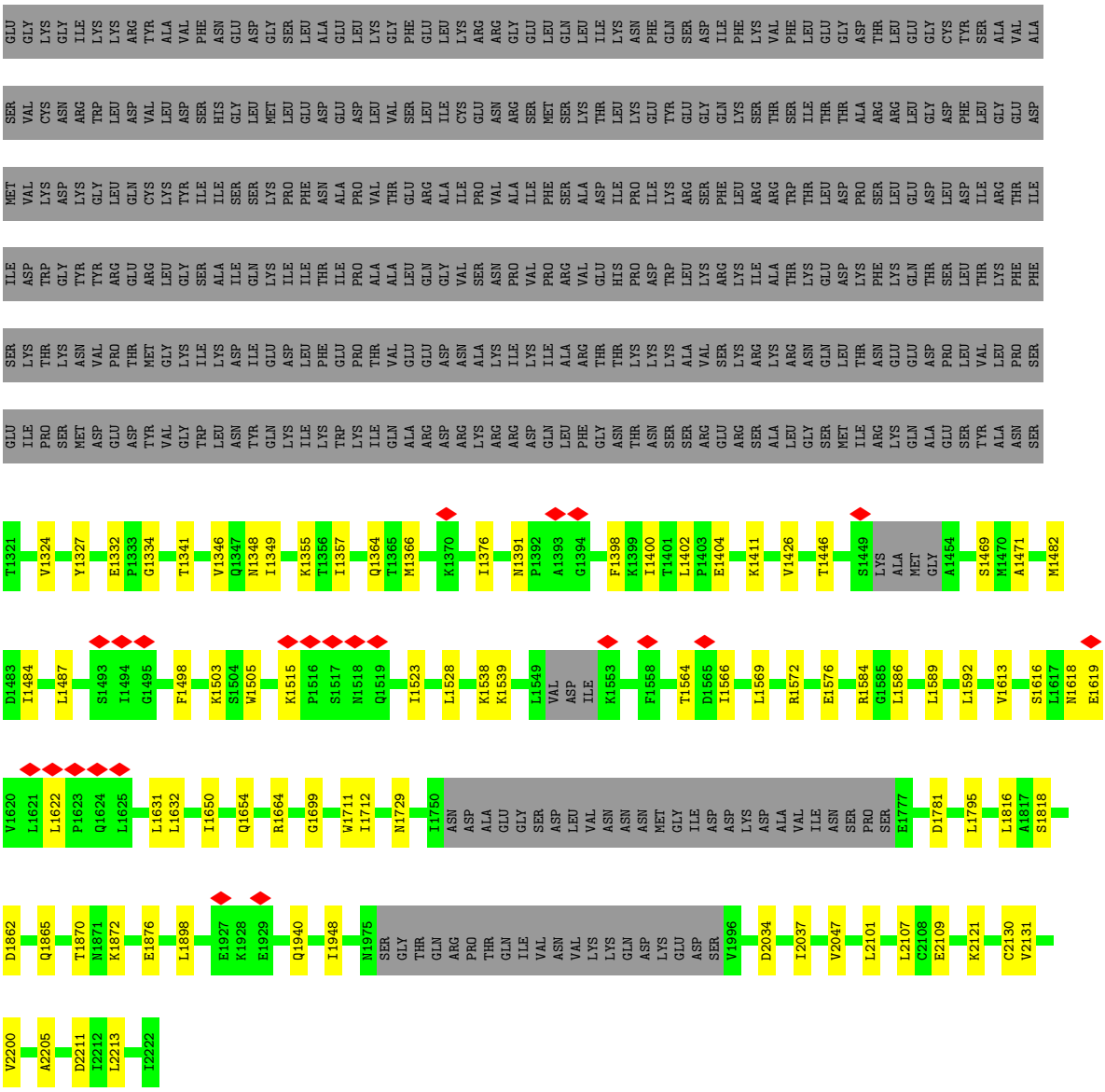




• Molecule 12: DNA polymerase epsilon catalytic subunit A

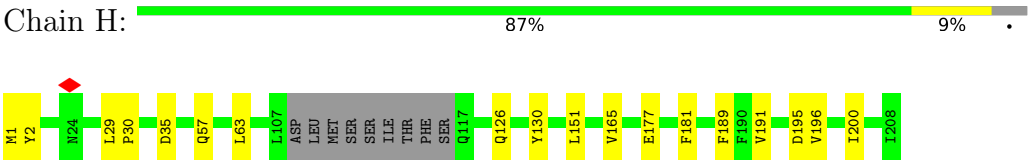
Chain G:





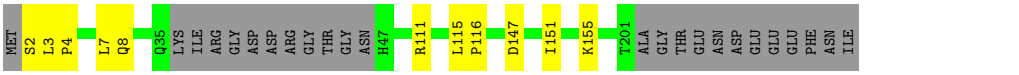
- Molecule 13: DNA replication complex GINS protein PSF1

Chain H:



- Molecule 14: DNA replication complex GINS protein PSF2

Chain I:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1125095	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	38.6	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	2900	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.530	Depositor
Minimum map value	-0.388	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	410.4, 410.4, 410.4	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.12	0/5340	0.27	0/7211
2	3	0.12	0/4835	0.27	0/6558
3	4	0.11	0/5572	0.29	0/7521
4	5	0.11	0/5442	0.26	0/7348
5	6	0.11	0/4972	0.28	0/6706
6	7	0.11	0/5092	0.30	0/6881
7	A	0.20	0/529	0.39	0/812
7	B	0.19	0/275	0.36	0/422
8	C	0.13	0/1469	0.27	0/1984
9	D	0.12	0/1988	0.25	0/2686
10	E	0.11	0/4676	0.26	0/6328
11	F	0.11	0/4464	0.27	0/6042
12	G	0.10	0/7046	0.26	0/9526
13	H	0.10	0/1649	0.24	0/2218
14	I	0.11	0/1614	0.25	0/2185
All	All	0.11	0/54963	0.27	0/74428

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	5248	0	5295	45	0
2	3	4751	0	4820	34	0
3	4	5499	0	5596	89	0
4	5	5364	0	5424	42	0
5	6	4895	0	4936	48	0
6	7	5014	0	5085	73	0
7	A	473	0	261	6	0
7	B	246	0	136	2	0
8	C	1436	0	1452	13	0
9	D	1949	0	1948	15	0
10	E	4590	0	4596	29	0
11	F	4366	0	4417	32	0
12	G	6894	0	6967	52	0
13	H	1629	0	1631	14	0
14	I	1581	0	1625	7	0
15	2	1	0	0	0	0
15	3	1	0	0	0	0
15	4	1	0	0	0	0
15	5	1	0	0	0	0
15	6	1	0	0	0	0
15	7	1	0	0	0	0
16	2	1	0	0	0	0
16	4	1	0	0	0	0
16	5	1	0	0	0	0
16	6	1	0	0	0	0
16	7	1	0	0	0	0
16	G	2	0	0	0	0
17	2	27	0	12	0	0
18	3	31	0	12	0	0
18	4	31	0	12	0	0
18	5	31	0	12	0	0
18	6	31	0	12	4	0
18	7	31	0	12	1	0
All	All	54130	0	54261	471	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 4.

All (471) 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)
3:4:197:PHE:HB2	3:4:254:THR:HG21	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:1366:MET:HE3	12:G:1366:MET:H	1.57	0.69
10:E:594:THR:HG22	10:E:596:HIS:H	1.58	0.68
8:C:97:LEU:HD11	8:C:127:LEU:HD21	1.75	0.68
5:6:657:GLU:HB2	5:6:708:ARG:HE	1.58	0.67
11:F:405:ASN:H	11:F:436:GLY:HA3	1.59	0.67
4:5:276:MET:HG2	4:5:328:ILE:HB	1.77	0.66
6:7:691:GLY:O	6:7:695:LEU:HD12	1.97	0.64
4:5:185:ASN:ND2	4:5:236:CYS:O	2.32	0.63
3:4:246:ARG:HD3	3:4:249:LEU:HD12	1.82	0.61
5:6:125:GLN:HG2	5:6:132:VAL:HG22	1.83	0.61
12:G:1940:GLN:HE22	12:G:2121:LYS:HA	1.67	0.60
3:4:591:THR:HG21	3:4:601:LEU:HD21	1.84	0.60
4:5:183:CYS:HB3	4:5:188:HIS:H	1.68	0.59
11:F:19:PRO:HA	13:H:177:GLU:HG2	1.84	0.59
1:2:543:GLY:HA3	1:2:683:VAL:HB	1.85	0.58
2:3:233:THR:HG23	2:3:234:GLU:HG3	1.85	0.58
3:4:778:ARG:HG2	3:4:793:ALA:HB3	1.85	0.58
4:5:344:ASN:HB2	4:5:346:VAL:HG12	1.85	0.57
4:5:52:ASN:ND2	8:C:142:LEU:O	2.37	0.57
3:4:700:SER:HB2	3:4:851:GLN:HG2	1.86	0.57
3:4:365:ILE:HD11	5:6:437:VAL:HB	1.86	0.57
7:B:18:DT:H2"	7:B:19:DC:H5"	1.86	0.57
8:C:88:ILE:HG23	8:C:127:LEU:HD13	1.87	0.57
12:G:1870:THR:HG22	12:G:1872:LYS:H	1.70	0.57
6:7:206:PRO:HG3	6:7:352:THR:HG21	1.87	0.56
6:7:517:ASP:HA	6:7:561:THR:HG22	1.87	0.56
12:G:1341:THR:HG22	12:G:1346:VAL:HG22	1.87	0.56
6:7:664:TYR:HB2	6:7:689:LEU:HD13	1.86	0.56
1:2:525:LYS:HB2	1:2:533:ILE:HD12	1.88	0.56
3:4:833:ILE:HD11	3:4:847:MET:HE1	1.88	0.56
10:E:372:THR:HG21	10:E:384:ILE:HD12	1.87	0.55
3:4:602:THR:HG22	3:4:644:VAL:HG11	1.87	0.55
1:2:561:HIS:CD2	1:2:562:ARG:HG3	2.41	0.55
3:4:883:PHE:O	3:4:887:ILE:HG13	2.06	0.55
5:6:540:HIS:O	5:6:544:LYS:HG3	2.06	0.55
12:G:1324:VAL:HG11	12:G:1327:TYR:CZ	2.40	0.55
12:G:2211:ASP:OD1	12:G:2211:ASP:N	2.39	0.55
3:4:814:LYS:HG2	3:4:816:VAL:H	1.71	0.55
2:3:358:ASP:OD1	2:3:358:ASP:N	2.40	0.55
2:3:400:ARG:NH1	2:3:402:ASP:O	2.40	0.55
4:5:184:ARG:N	4:5:240:PRO:O	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:585:LEU:O	5:6:589:VAL:HG23	2.07	0.55
6:7:465:ALA:N	18:7:1502:ATP:O1B	2.39	0.55
12:G:1729:ASN:ND2	12:G:1872:LYS:O	2.40	0.55
6:7:414:LEU:HD12	6:7:638:MET:HG3	1.88	0.54
3:4:796:ARG:NH1	18:6:1502:ATP:O3G	2.39	0.54
13:H:29:LEU:HD23	13:H:30:PRO:HD2	1.88	0.54
6:7:138:VAL:HG11	6:7:303:ARG:HD3	1.89	0.54
8:C:131:ARG:HH21	8:C:169:LEU:HD23	1.72	0.54
3:4:527:ALA:HB3	3:4:537:LYS:HE2	1.90	0.54
10:E:577:ASP:OD1	10:E:634:ARG:NH2	2.34	0.54
4:5:459:THR:HG22	4:5:461:GLU:HG3	1.89	0.54
5:6:105:ASP:OD2	5:6:176:ARG:NH1	2.42	0.53
12:G:1572:ARG:HH12	12:G:1576:GLU:HG2	1.74	0.53
1:2:490:ASP:OD1	1:2:491:ARG:N	2.42	0.53
6:7:315:ILE:HB	6:7:333:ILE:HD11	1.91	0.53
4:5:409:ASP:OD2	4:5:500:GLN:NE2	2.39	0.53
6:7:261:THR:HG22	6:7:268:GLU:HG3	1.91	0.53
6:7:457:CYS:HB3	6:7:597:LEU:HD13	1.90	0.53
12:G:1711:TRP:HD1	12:G:1712:ILE:HD12	1.73	0.53
12:G:1862:ASP:OD1	12:G:1865:GLN:N	2.40	0.53
13:H:35:ASP:OD1	13:H:35:ASP:N	2.42	0.53
13:H:57:GLN:HB2	13:H:63:LEU:HD11	1.91	0.53
11:F:528:ASN:HB3	11:F:529:PRO:HD3	1.89	0.53
3:4:894:SER:OG	3:4:896:ASP:O	2.25	0.53
2:3:255:ARG:NH1	2:3:275:ASP:OD2	2.42	0.53
6:7:288:GLU:O	6:7:292:ASN:ND2	2.42	0.53
10:E:553:ILE:HD11	10:E:584:LEU:HB3	1.91	0.53
6:7:627:ASP:OD1	6:7:627:ASP:N	2.41	0.53
11:F:367:ILE:HG23	11:F:368:HIS:CD2	2.43	0.53
2:3:676:ILE:HD13	6:7:617:THR:HB	1.91	0.52
4:5:32:LYS:HG2	4:5:97:VAL:HG23	1.91	0.52
5:6:803:MET:HG3	5:6:831:LEU:HD12	1.90	0.52
10:E:18:ASN:O	10:E:79:ASN:ND2	2.36	0.52
2:3:712:HIS:ND1	2:3:725:ASP:OD1	2.28	0.52
14:I:111:ARG:O	14:I:155:LYS:NZ	2.42	0.52
4:5:544:THR:HG22	4:5:647:PRO:HG3	1.92	0.52
12:G:1781:ASP:OD1	12:G:1781:ASP:N	2.42	0.52
5:6:728:ALA:O	5:6:732:VAL:HG23	2.10	0.52
9:D:193:LEU:HD13	13:H:130:TYR:HB2	1.91	0.52
12:G:1364:GLN:N	12:G:1364:GLN:OE1	2.41	0.52
3:4:687:PRO:O	3:4:691:ASN:ND2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:675:MET:HG3	6:7:683:GLN:NE2	2.24	0.52
1:2:303:ILE:HG13	1:2:319:ARG:HD3	1.92	0.52
2:3:559:ARG:NH1	4:5:623:SER:OG	2.43	0.52
2:3:482:ASP:O	2:3:486:ILE:HG12	2.10	0.52
2:3:390:GLU:OE2	2:3:398:HIS:NE2	2.43	0.52
3:4:801:MET:HG3	3:4:829:ILE:HD12	1.92	0.52
1:2:574:VAL:HG21	7:A:57:DT:H5"	1.93	0.51
10:E:267:LEU:HD13	10:E:316:LEU:HD23	1.91	0.51
12:G:1503:LYS:HB3	12:G:1505:TRP:HE3	1.75	0.51
12:G:1589:LEU:HD11	12:G:1613:VAL:HG23	1.91	0.51
6:7:661:VAL:O	6:7:665:ILE:HG13	2.10	0.51
1:2:662:PRO:HG2	1:2:665:GLN:HG3	1.92	0.51
12:G:1482:MET:HE1	12:G:1589:LEU:HB2	1.92	0.51
5:6:275:ARG:HD2	5:6:367:GLU:HG2	1.92	0.51
10:E:244:GLY:H	10:E:602:LEU:HD23	1.76	0.51
12:G:1622:LEU:HD11	12:G:1631:LEU:HD22	1.92	0.51
14:I:115:LEU:HD23	14:I:116:PRO:HD2	1.93	0.51
5:6:147:ASP:OD1	5:6:261:ARG:NH2	2.35	0.51
3:4:435:VAL:HG12	3:4:466:VAL:HG23	1.92	0.51
4:5:624:SER:HB3	11:F:272:LYS:HG2	1.93	0.51
12:G:1334:GLY:N	12:G:1404:GLU:OE1	2.44	0.51
1:2:440:ALA:HB1	5:6:408:THR:HG22	1.92	0.50
3:4:287:ASN:O	3:4:289:LEU:N	2.44	0.50
3:4:865:LEU:O	3:4:869:ILE:HG13	2.11	0.50
6:7:657:ASN:O	6:7:661:VAL:HG23	2.11	0.50
4:5:31:PHE:O	4:5:35:ILE:HG12	2.12	0.50
9:D:75:GLU:OE2	9:D:283:ARG:NH1	2.44	0.50
1:2:501:MET:HE1	1:2:519:LEU:HD12	1.93	0.50
10:E:157:GLU:OE1	10:E:157:GLU:N	2.45	0.50
3:4:502:THR:HG22	3:4:504:GLN:H	1.75	0.50
5:6:576:ASP:O	5:6:579:THR:OG1	2.21	0.50
10:E:270:LEU:HD22	10:E:302:LEU:HD12	1.93	0.50
6:7:146:ARG:O	6:7:150:ASN:ND2	2.44	0.50
11:F:416:ALA:HB2	11:F:689:ILE:HG12	1.94	0.50
12:G:1484:ILE:HD12	12:G:1589:LEU:HB3	1.94	0.50
12:G:1538:LYS:C	12:G:1539:LYS:HD3	2.37	0.50
13:H:1:MET:HG2	13:H:2:TYR:H	1.77	0.50
6:7:454:ILE:O	6:7:562:SER:OG	2.22	0.49
9:D:256:TYR:N	9:D:269:LEU:O	2.36	0.49
11:F:68:ALA:O	11:F:72:GLN:NE2	2.33	0.49
3:4:729:LEU:O	6:7:442:LYS:NZ	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:768:GLN:HG2	11:F:292:PHE:HA	1.94	0.49
1:2:306:LEU:HB2	1:2:392:GLU:HG3	1.93	0.49
6:7:589:ALA:O	6:7:593:ARG:HG2	2.12	0.49
10:E:467:THR:O	10:E:471:LYS:HG3	2.12	0.49
3:4:592:SER:OG	3:4:633:GLU:OE1	2.29	0.49
6:7:484:THR:HG22	6:7:524:ASP:HB3	1.94	0.49
11:F:632:LEU:HD13	11:F:639:MET:HE1	1.95	0.49
3:4:893:HIS:ND1	3:4:893:HIS:O	2.46	0.49
11:F:459:LYS:HB2	11:F:512:PHE:HD1	1.77	0.49
3:4:601:LEU:HD23	3:4:620:ALA:HB3	1.95	0.49
3:4:771:VAL:O	3:4:775:VAL:HG23	2.12	0.49
4:5:23:ASP:O	4:5:27:ILE:HG12	2.11	0.49
1:2:763:LEU:O	1:2:767:ILE:HG13	2.12	0.49
3:4:447:ASN:OD1	3:4:450:GLN:N	2.38	0.49
6:7:434:LEU:HD21	6:7:699:LEU:HG	1.95	0.49
1:2:768:HIS:O	1:2:772:THR:HG22	2.12	0.49
5:6:566:ARG:O	5:6:805:ARG:NH1	2.46	0.49
6:7:17:LEU:O	6:7:21:ILE:HG13	2.12	0.49
10:E:345:ASN:HA	10:E:350:LEU:HD13	1.94	0.49
1:2:282:HIS:O	10:E:365:ARG:NH1	2.44	0.49
1:2:319:ARG:NE	1:2:425:GLU:OE2	2.41	0.48
12:G:1446:THR:HG1	12:G:1469:SER:HG	1.60	0.48
4:5:154:GLU:OE1	4:5:154:GLU:N	2.46	0.48
11:F:547:SER:HB3	11:F:645:THR:HG23	1.94	0.48
3:4:849:LEU:HD13	3:4:855:SER:HB2	1.95	0.48
6:7:650:PRO:HD3	6:7:701:LYS:HZ3	1.78	0.48
12:G:1446:THR:HG23	12:G:1471:ALA:HB2	1.96	0.48
1:2:705:ARG:NH1	1:2:754:GLU:OE2	2.47	0.48
5:6:514:ASN:O	5:6:518:GLU:HG2	2.13	0.48
3:4:580:TYR:O	3:4:584:ILE:HG13	2.14	0.47
7:A:54:DC:H2"	7:A:55:DG:H5'	1.95	0.47
1:2:680:LEU:HD13	1:2:803:PHE:HE2	1.79	0.47
1:2:425:GLU:HB2	1:2:459:ARG:HD2	1.96	0.47
1:2:530:LYS:HA	4:5:431:LYS:HE3	1.95	0.47
2:3:166:LEU:HB3	2:3:170:THR:HG23	1.96	0.47
6:7:650:PRO:HD3	6:7:701:LYS:NZ	2.30	0.47
7:B:16:DG:H2"	7:B:17:DA:C8	2.49	0.47
12:G:2130:CYS:SG	12:G:2131:VAL:N	2.88	0.47
2:3:430:ILE:HG13	2:3:465:ALA:HB2	1.96	0.47
3:4:774:TYR:CZ	3:4:778:ARG:HD2	2.50	0.47
2:3:439:GLY:N	2:3:482:ASP:OD1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:1355:LYS:HB3	12:G:1357:ILE:HD11	1.97	0.47
1:2:746:GLN:O	1:2:750:LYS:HG2	2.15	0.47
2:3:21:PHE:O	2:3:25:VAL:HG23	2.15	0.47
3:4:240:ASN:ND2	3:4:422:GLU:OE1	2.43	0.47
3:4:554:LYS:HE3	5:6:742:ILE:HG13	1.96	0.47
3:4:571:SER:OG	6:7:687:ARG:NH1	2.48	0.47
4:5:346:VAL:HG21	8:C:163:SER:HB3	1.96	0.47
5:6:727:LEU:O	5:6:731:ILE:HG13	2.14	0.47
6:7:443:ARG:HA	6:7:449:LYS:HA	1.96	0.47
6:7:581:LEU:HD23	6:7:584:ILE:HD11	1.95	0.47
12:G:1482:MET:HE2	12:G:1482:MET:HB3	1.79	0.47
4:5:53:ASN:HB3	4:5:58:ASN:O	2.15	0.47
1:2:832[B]:TYR:HE2	1:2:836:ARG:HH21	1.63	0.47
3:4:798:LEU:O	3:4:802:ILE:HG13	2.14	0.47
4:5:24:ASN:O	4:5:28:ILE:HG13	2.14	0.47
4:5:587:GLN:HG3	4:5:592:SER:HB2	1.97	0.47
1:2:339:PHE:HB2	1:2:348:LEU:HD12	1.96	0.47
1:2:671:GLU:OE1	1:2:671:GLU:N	2.39	0.47
6:7:147:ARG:HA	6:7:147:ARG:CZ	2.45	0.47
12:G:1818:SER:HB2	12:G:2107:LEU:HD11	1.96	0.47
4:5:564:ARG:O	4:5:568:ILE:HG13	2.15	0.46
5:6:533:ILE:O	5:6:544:LYS:HD3	2.15	0.46
5:6:806:LEU:O	5:6:810:ILE:HG13	2.15	0.46
12:G:1498:PHE:HE2	12:G:1523:ILE:HD11	1.79	0.46
9:D:181:LYS:NZ	9:D:181:LYS:HB3	2.30	0.46
13:H:181:PHE:HZ	13:H:191:VAL:HG21	1.80	0.46
1:2:267:MET:HE3	1:2:267:MET:HB3	1.73	0.46
3:4:371:CYS:HB3	3:4:376:CYS:O	2.14	0.46
8:C:181:HIS:CE1	8:C:185:LYS:HE2	2.51	0.46
9:D:159:ARG:NH2	9:D:210:ASN:HD22	2.13	0.46
1:2:234:LEU:HD12	1:2:239:SER:HB3	1.97	0.46
1:2:772:THR:HG23	1:2:773:LYS:HG2	1.97	0.46
3:4:296:ILE:HG12	3:4:301:TYR:OH	2.16	0.46
5:6:580:SER:HB3	18:6:1502:ATP:C8	2.51	0.46
6:7:459:MET:HE3	6:7:584:ILE:HG22	1.98	0.46
6:7:615:HIS:O	6:7:619:VAL:HG23	2.15	0.46
8:C:129:LEU:O	8:C:133:GLN:HG2	2.15	0.46
1:2:235:GLY:HA3	1:2:283:TYR:CE2	2.51	0.46
5:6:340:ASN:OD1	5:6:343:PHE:HB2	2.16	0.46
9:D:91:ILE:HG23	9:D:133:LEU:HD11	1.98	0.46
11:F:394:LEU:HD23	11:F:397:HIS:NE2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:522:LEU:O	3:4:526:ILE:HG23	2.15	0.46
6:7:399:GLU:O	6:7:403:GLU:HG3	2.16	0.46
1:2:384:ASN:HB3	1:2:415:VAL:HG21	1.98	0.46
1:2:671:GLU:H	1:2:671:GLU:CD	2.24	0.46
2:3:570:ARG:NH1	4:5:614:LEU:O	2.48	0.46
3:4:747:LEU:HD23	3:4:747:LEU:HA	1.78	0.46
3:4:808:HIS:ND1	3:4:821:ASP:HA	2.31	0.46
4:5:52:ASN:O	4:5:56:VAL:HG22	2.15	0.46
4:5:433:SER:HB3	4:5:436:ALA:HB2	1.96	0.46
6:7:401:VAL:HG11	6:7:644:TYR:CD2	2.51	0.46
11:F:490:LEU:HD23	11:F:490:LEU:HA	1.79	0.46
12:G:1616:SER:HB3	12:G:1664:ARG:HH21	1.80	0.46
3:4:773:ALA:O	3:4:777:MET:HG3	2.15	0.46
6:7:514:VAL:HG22	6:7:559:ALA:HB2	1.97	0.46
8:C:169:LEU:HD22	8:C:173:GLU:HB3	1.98	0.46
11:F:27:ARG:NH2	13:H:177:GLU:OE1	2.49	0.46
3:4:547:GLY:O	3:4:810:LYS:NZ	2.35	0.46
6:7:479:ARG:HH11	6:7:518:ASN:HB2	1.81	0.46
12:G:1876:GLU:OE1	12:G:1876:GLU:N	2.33	0.46
13:H:165:VAL:HG23	13:H:189:PHE:HB2	1.97	0.46
3:4:333:LEU:HD23	3:4:333:LEU:HA	1.83	0.46
3:4:194:PHE:CE2	3:4:272:MET:HG2	2.51	0.45
3:4:808:HIS:HD2	3:4:811:MET:HE2	1.80	0.45
1:2:483:GLU:O	1:2:487:ILE:HG23	2.15	0.45
1:2:569:GLN:HG3	5:6:650:VAL:HG21	1.98	0.45
3:4:239:SER:HB3	3:4:301:TYR:HA	1.97	0.45
6:7:17:LEU:HD22	6:7:102:LEU:HD12	1.98	0.45
6:7:500:ASP:O	6:7:504:ASP:HA	2.16	0.45
3:4:714:GLU:O	3:4:718:ARG:HG3	2.16	0.45
3:4:822:VAL:O	3:4:826:VAL:HG23	2.15	0.45
4:5:487:ASP:O	4:5:491:VAL:HG23	2.16	0.45
4:5:540:ILE:HG22	4:5:542:PHE:H	1.81	0.45
3:4:281:VAL:O	3:4:285:VAL:HG22	2.17	0.45
10:E:259:LEU:O	10:E:263:GLY:N	2.48	0.45
3:4:573:SER:O	3:4:577:ILE:HG13	2.16	0.45
5:6:515:GLU:OE2	5:6:750:GLN:NE2	2.50	0.45
6:7:29:LYS:HZ2	6:7:60:GLY:HA2	1.82	0.45
6:7:532:SER:O	6:7:535:THR:OG1	2.33	0.45
10:E:8:PHE:HB3	10:E:258:LEU:HD13	1.97	0.45
1:2:237:MET:HA	1:2:237:MET:HE2	1.98	0.45
4:5:347:THR:HG21	4:5:609:LYS:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:500:ASP:OD1	5:6:501:GLN:N	2.49	0.45
10:E:45:LEU:HD21	10:E:255:ILE:HD12	1.98	0.45
9:D:149:SER:HB2	14:I:2:SER:HB2	1.99	0.45
9:D:193:LEU:HD12	13:H:126:GLN:HB3	1.99	0.45
11:F:409:ASP:OD2	11:F:440:SER:OG	2.28	0.45
12:G:1795:LEU:HD13	12:G:1816:LEU:HD22	1.99	0.45
3:4:204:LYS:O	3:4:208:ILE:HG12	2.17	0.45
3:4:291:TYR:CG	3:4:292:ASP:N	2.85	0.45
3:4:568:GLY:O	3:4:677:PRO:HD3	2.17	0.45
4:5:415:LEU:O	4:5:555:ILE:HA	2.17	0.45
2:3:704:THR:O	2:3:708:LEU:HD23	2.16	0.45
9:D:136:LEU:O	9:D:140:ILE:HG13	2.16	0.45
10:E:11:ALA:O	10:E:15:ILE:HG13	2.17	0.45
10:E:296:GLN:HG2	10:E:320:ILE:HD13	1.98	0.45
12:G:1618:ASN:OD1	12:G:1619:GLU:N	2.44	0.45
2:3:572:LEU:HD12	2:3:573:PRO:HD2	1.99	0.45
3:4:681:ARG:NH2	3:4:710:ASP:OD1	2.50	0.45
6:7:428:VAL:O	6:7:432:LEU:HG	2.17	0.44
2:3:264:MET:HE3	2:3:264:MET:HB3	1.84	0.44
6:7:435:LEU:HD13	6:7:456:VAL:HG12	1.99	0.44
9:D:188:LEU:HD23	9:D:188:LEU:HA	1.85	0.44
10:E:127:ARG:NH2	10:E:145:ASP:OD1	2.50	0.44
2:3:442:LEU:HD13	2:3:486:ILE:HD11	1.99	0.44
3:4:242:ASN:HB3	3:4:306:TYR:CE2	2.53	0.44
4:5:755:LEU:HB3	4:5:761:ILE:HG12	1.98	0.44
3:4:242:ASN:HB3	3:4:306:TYR:HE2	1.82	0.44
3:4:293:LEU:O	3:4:297:GLU:HG2	2.17	0.44
3:4:762:ILE:HB	5:6:736:MET:HG2	2.00	0.44
6:7:648:LYS:HE2	6:7:704:LEU:HD13	1.99	0.44
6:7:688:THR:O	6:7:692:ILE:HG12	2.18	0.44
11:F:20:LEU:HA	11:F:23:ARG:HH12	1.83	0.44
1:2:310:ARG:HH12	5:6:300:VAL:HG21	1.82	0.44
3:4:197:PHE:O	3:4:201:PHE:HB2	2.15	0.44
3:4:597:SER:OG	6:7:547:SER:O	2.24	0.44
3:4:881:MET:HE2	3:4:886:LEU:HA	2.00	0.44
3:4:902:ASP:OD1	3:4:903:ILE:N	2.50	0.44
1:2:230:ARG:NH1	1:2:243:GLU:O	2.48	0.44
3:4:890:ILE:O	3:4:894:SER:HB3	2.18	0.44
6:7:542:GLU:C	6:7:544:GLN:H	2.25	0.44
9:D:235:PRO:HA	9:D:236:PRO:HD3	1.87	0.44
1:2:266:GLU:O	1:2:270:ILE:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:446:VAL:HG23	2:3:499:LYS:HE3	1.98	0.44
6:7:147:ARG:HA	6:7:147:ARG:NH1	2.33	0.44
7:A:51:DG:H2"	7:A:52:DA:C8	2.53	0.44
9:D:126:LEU:O	9:D:130:GLU:HG3	2.18	0.44
2:3:727:LYS:HE3	2:3:727:LYS:HB2	1.63	0.44
5:6:580:SER:N	18:6:1502:ATP:O1B	2.50	0.44
11:F:625:ASP:N	11:F:625:ASP:OD1	2.50	0.44
2:3:553:ILE:HB	4:5:634:LEU:HD13	2.00	0.44
12:G:2107:LEU:HD23	12:G:2109:GLU:H	1.83	0.44
2:3:318:LYS:NZ	2:3:318:LYS:HB3	2.33	0.43
2:3:394:GLU:CD	2:3:394:GLU:H	2.26	0.43
5:6:189:VAL:O	5:6:193:ALA:N	2.49	0.43
5:6:311:CYS:SG	5:6:340:ASN:ND2	2.89	0.43
8:C:104:PHE:HB3	8:C:170:GLU:OE2	2.18	0.43
2:3:26:ARG:O	2:3:30:GLU:HG3	2.17	0.43
2:3:92:LEU:HD23	2:3:92:LEU:HA	1.84	0.43
5:6:589:VAL:HG21	5:6:597:TYR:HB2	2.00	0.43
14:I:4:PRO:O	14:I:8:GLN:HG3	2.18	0.43
8:C:76:PRO:HA	8:C:77:PRO:HD3	1.87	0.43
3:4:193:ASN:HB3	3:4:254:THR:HG22	2.00	0.43
3:4:195:ARG:HG2	3:4:199:MET:SD	2.58	0.43
6:7:143:LEU:O	6:7:147:ARG:HG2	2.19	0.43
11:F:164:LEU:HD23	11:F:164:LEU:HA	1.88	0.43
4:5:65:MET:O	4:5:69:ILE:HG13	2.18	0.43
6:7:479:ARG:NH1	6:7:518:ASN:HB2	2.33	0.43
12:G:2205:ALA:HB2	12:G:2213:LEU:HD23	2.00	0.43
2:3:24:ARG:HH12	2:3:120:TYR:HB3	1.84	0.43
2:3:169:ARG:NH2	2:3:270:LEU:O	2.50	0.43
5:6:305:TYR:CD2	5:6:306:LYS:HG3	2.53	0.43
2:3:698:THR:OG1	2:3:699:ALA:N	2.51	0.43
3:4:407:PRO:HB2	3:4:410:GLN:HB2	2.01	0.43
5:6:373:MET:HE2	5:6:373:MET:HB3	1.85	0.43
6:7:65:ALA:O	6:7:69:LYS:HG3	2.19	0.43
2:3:27:ARG:HD2	2:3:27:ARG:HA	1.87	0.43
3:4:799:GLU:HB3	3:4:803:ARG:NH1	2.34	0.43
7:A:60:DA:H2"	7:A:61:DT:C6	2.54	0.43
6:7:315:ILE:HG22	6:7:331:LEU:HB3	2.01	0.43
10:E:554:GLU:HG2	10:E:587:ARG:NH2	2.34	0.43
13:H:196:VAL:O	13:H:200:ILE:HG13	2.19	0.43
5:6:304:LEU:HD21	5:6:307:ALA:HB2	1.99	0.43
5:6:640:GLU:HB3	5:6:643:LYS:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:625:GLU:OE1	1:2:808:ARG:HD3	2.19	0.42
3:4:233:MET:HG3	3:4:238:THR:HG23	2.00	0.42
6:7:689:LEU:O	6:7:693:ILE:HG13	2.19	0.42
11:F:393:GLU:HG3	11:F:394:LEU:HD12	2.00	0.42
14:I:4:PRO:HD2	14:I:7:LEU:HD12	2.01	0.42
3:4:579:GLN:O	3:4:583:LYS:HG3	2.18	0.42
6:7:284:CYS:SG	6:7:286:SER:OG	2.65	0.42
1:2:819:SER:O	1:2:823:MET:HG3	2.18	0.42
6:7:681:PHE:HE2	6:7:727:LEU:HD11	1.84	0.42
11:F:368:HIS:CE1	11:F:379:LEU:HD12	2.55	0.42
11:F:404:ALA:HB2	11:F:642:CYS:SG	2.59	0.42
1:2:503:PRO:HD2	5:6:561:GLU:OE1	2.19	0.42
3:4:726:ASN:HA	3:4:729:LEU:HD13	2.01	0.42
3:4:888:LYS:O	3:4:892:GLU:HG2	2.20	0.42
5:6:522:ASP:OD1	5:6:523:GLU:N	2.52	0.42
6:7:66:MET:O	6:7:70:VAL:HG23	2.18	0.42
12:G:1376:ILE:HD11	12:G:1398:PHE:HB3	2.02	0.42
2:3:367:LEU:HD22	2:3:421:PHE:HE2	1.84	0.42
2:3:564:HIS:O	2:3:568:THR:HG23	2.19	0.42
3:4:847:MET:HE2	3:4:847:MET:HB2	1.90	0.42
6:7:135:LYS:H	6:7:135:LYS:HG3	1.70	0.42
6:7:469:LEU:O	6:7:473:ILE:HG12	2.20	0.42
10:E:491:LEU:HD23	10:E:491:LEU:HA	1.84	0.42
11:F:396:ASP:OD1	11:F:396:ASP:N	2.53	0.42
12:G:1332:GLU:OE1	12:G:1332:GLU:N	2.46	0.42
1:2:215:LEU:HD23	1:2:215:LEU:HA	1.90	0.42
3:4:456:LEU:HD11	6:7:252:LYS:HB2	2.01	0.42
3:4:775:VAL:HG21	5:6:725:THR:HG22	2.00	0.42
5:6:572:CYS:SG	5:6:701:MET:HE1	2.59	0.42
6:7:421:GLU:HG3	6:7:625:GLN:HE21	1.84	0.42
10:E:248:VAL:O	10:E:290:ARG:NH2	2.49	0.42
3:4:577:ILE:O	3:4:581:VAL:HG23	2.20	0.42
5:6:311:CYS:SG	5:6:312:ASP:N	2.93	0.42
3:4:599:VAL:HG12	3:4:601:LEU:H	1.85	0.42
3:4:884:ASN:O	3:4:888:LYS:HG3	2.19	0.42
5:6:831:LEU:HD23	5:6:831:LEU:HA	1.84	0.42
6:7:404:LEU:HD13	6:7:637:LYS:HE2	2.01	0.42
12:G:1505:TRP:HE1	12:G:1584:ARG:HD2	1.85	0.42
1:2:743:ARG:O	1:2:747:ARG:HG3	2.20	0.42
7:A:60:DA:H2"	7:A:61:DT:C5	2.55	0.42
9:D:190:TRP:O	9:D:194:VAL:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:E:163:LEU:HD12	10:E:163:LEU:HA	1.94	0.42
11:F:411:LEU:H	11:F:411:LEU:HD12	1.85	0.42
12:G:2037:ILE:HG12	12:G:2047:VAL:HB	2.01	0.42
14:I:3:LEU:HD23	14:I:8:GLN:HG2	2.01	0.42
2:3:235:ASP:OD1	2:3:236:THR:N	2.48	0.41
5:6:504:PHE:HE1	5:6:756:LYS:HE2	1.85	0.41
6:7:621:MET:HE3	6:7:622:HIS:NE2	2.35	0.41
12:G:1391:ASN:OD1	12:G:1391:ASN:N	2.51	0.41
1:2:364:CYS:HB2	1:2:373:PHE:HE1	1.85	0.41
10:E:496:ILE:O	10:E:500:GLN:HG3	2.21	0.41
12:G:1528:LEU:HB2	12:G:1632:LEU:HD13	2.03	0.41
2:3:538:SER:O	2:3:542:ARG:NH1	2.45	0.41
3:4:568:GLY:C	3:4:574:LYS:HZ1	2.28	0.41
3:4:780:MET:HE2	3:4:780:MET:HB3	1.90	0.41
4:5:610:CYS:HB2	4:5:668:LEU:HD23	2.02	0.41
6:7:147:ARG:O	6:7:151:GLU:HG3	2.20	0.41
12:G:1426:VAL:O	12:G:1699:GLY:HA2	2.20	0.41
3:4:188:GLN:H	3:4:188:GLN:CD	2.26	0.41
3:4:273:ASP:HA	3:4:276:ILE:HG22	2.02	0.41
3:4:712:VAL:HG22	6:7:668:ARG:HH21	1.85	0.41
5:6:134:LYS:HD2	5:6:137:ARG:NH1	2.36	0.41
5:6:582:SER:N	18:6:1502:ATP:O2B	2.40	0.41
11:F:80:ASP:O	11:F:84:VAL:HG23	2.20	0.41
11:F:381:LYS:HE3	11:F:381:LYS:HB2	1.76	0.41
3:4:194:PHE:HD2	3:4:275:THR:HB	1.86	0.41
3:4:312:LYS:HE2	3:4:312:LYS:HB3	1.85	0.41
10:E:426:GLU:OE1	10:E:547:ARG:NH2	2.52	0.41
12:G:2101:LEU:HD12	12:G:2200:VAL:HG23	2.02	0.41
1:2:866:LEU:HD23	1:2:866:LEU:HA	1.84	0.41
3:4:400:GLN:OE1	3:4:400:GLN:HA	2.21	0.41
5:6:806:LEU:HD23	5:6:806:LEU:HA	1.94	0.41
6:7:685:THR:O	6:7:688:THR:OG1	2.32	0.41
11:F:231:ARG:NH2	11:F:350:GLU:OE1	2.50	0.41
3:4:335:SER:OG	3:4:395:GLN:NE2	2.54	0.41
4:5:285:LYS:HE2	4:5:285:LYS:HB2	1.80	0.41
6:7:103:VAL:O	6:7:107:GLN:HG3	2.20	0.41
6:7:687:ARG:HA	6:7:690:LEU:HD12	2.03	0.41
7:A:35:DG:H2"	7:A:36:DA:C8	2.56	0.41
10:E:560:GLU:H	10:E:560:GLU:CD	2.29	0.41
12:G:1346:VAL:HB	12:G:1586:LEU:O	2.21	0.41
12:G:1566:ILE:HA	12:G:1569:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:341:SER:HA	4:5:346:VAL:O	2.20	0.41
4:5:626:PHE:CD1	4:5:653:LEU:HB2	2.56	0.41
4:5:745:GLN:NE2	4:5:749:ASP:OD2	2.54	0.41
11:F:72:GLN:N	11:F:72:GLN:CD	2.78	0.41
1:2:802:SER:OG	1:2:803:PHE:N	2.53	0.41
4:5:708:LEU:HD11	4:5:712:ARG:HE	1.85	0.41
4:5:717:GLU:OE2	4:5:742:ARG:NH2	2.54	0.41
5:6:770:ARG:O	5:6:774:VAL:HG23	2.20	0.41
6:7:212:ALA:HB1	6:7:217:LYS:O	2.20	0.41
6:7:401:VAL:HG11	6:7:644:TYR:HD2	1.85	0.41
6:7:510:GLY:HA3	6:7:514:VAL:HG21	2.03	0.41
8:C:97:LEU:HD23	8:C:97:LEU:HA	1.81	0.41
8:C:172:MET:HE2	8:C:172:MET:HB3	1.98	0.41
11:F:231:ARG:HH21	11:F:350:GLU:CD	2.29	0.41
12:G:1376:ILE:HD13	12:G:1400:ILE:HG12	2.03	0.41
13:H:181:PHE:CZ	13:H:191:VAL:HG21	2.56	0.41
13:H:195:ASP:N	13:H:195:ASP:OD1	2.53	0.41
14:I:147:ASP:O	14:I:151:ILE:HG13	2.21	0.41
3:4:228:LYS:O	3:4:232:GLU:HG3	2.21	0.41
3:4:686:LEU:C	3:4:840:PRO:HG3	2.46	0.41
4:5:677:VAL:O	4:5:681:ILE:HG13	2.21	0.41
4:5:742:ARG:HE	4:5:742:ARG:HB3	1.61	0.41
6:7:73:ARG:HD2	6:7:132:ILE:HG21	2.02	0.41
9:D:118:MET:HA	9:D:119:PRO:HD2	1.94	0.41
12:G:1357:ILE:HD13	12:G:1402:LEU:HD21	2.03	0.41
1:2:671:GLU:N	1:2:671:GLU:CD	2.79	0.40
5:6:505:LEU:HD23	5:6:505:LEU:HA	1.96	0.40
5:6:517:LYS:HA	5:6:520:VAL:HG22	2.03	0.40
10:E:69:ARG:HG2	10:E:69:ARG:NH1	2.36	0.40
10:E:638:SER:OG	10:E:639:PRO:HD3	2.21	0.40
11:F:211:ILE:HD13	11:F:211:ILE:HA	1.91	0.40
12:G:1650:ILE:O	12:G:1654:GLN:HG3	2.22	0.40
1:2:803:PHE:HE1	1:2:809:HIS:CE1	2.39	0.40
2:3:171:LEU:HD12	2:3:171:LEU:HA	1.86	0.40
4:5:276:MET:HE3	4:5:276:MET:HB2	1.84	0.40
5:6:718:ASP:OD1	5:6:718:ASP:C	2.65	0.40
6:7:481:VAL:HG22	6:7:483:THR:HG23	2.03	0.40
9:D:108:MET:HE2	9:D:108:MET:HB3	2.00	0.40
11:F:67:ALA:O	11:F:71:LYS:HG3	2.21	0.40
12:G:1348:ASN:C	12:G:1349:ILE:HD12	2.46	0.40
12:G:1948:ILE:HB	12:G:2034:ASP:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:284:ILE:HD12	3:4:296:ILE:HD12	2.02	0.40
6:7:86:LEU:HD12	6:7:86:LEU:HA	1.91	0.40
10:E:256:TYR:OH	10:E:298:GLU:OE1	2.30	0.40
10:E:650:LEU:HD23	10:E:650:LEU:HA	1.80	0.40
11:F:313:ILE:HA	11:F:314:PRO:HD3	1.95	0.40
12:G:1411:LYS:HB2	12:G:1411:LYS:HE3	1.83	0.40
3:4:712:VAL:HA	6:7:668:ARG:HH21	1.86	0.40
5:6:800:LEU:HA	5:6:803:MET:HE3	2.03	0.40
6:7:606:ARG:O	6:7:610:GLU:HG3	2.22	0.40
12:G:1487:LEU:HD23	12:G:1592:LEU:HD13	2.02	0.40
12:G:1515:LYS:HB2	12:G:1564:THR:HG22	2.02	0.40
1:2:307:ARG:HE	1:2:307:ARG:HB2	1.77	0.40
3:4:282:SER:HA	3:4:285:VAL:HG22	2.02	0.40
3:4:698:LEU:HD12	3:4:698:LEU:HA	1.91	0.40
8:C:108:ALA:O	8:C:112:ILE:HG13	2.22	0.40
11:F:356:LEU:HD23	11:F:359:ILE:HD11	2.03	0.40
12:G:1898:LEU:HD12	12:G:1898:LEU:HA	1.93	0.40
12:G:2034:ASP:OD1	12:G:2034:ASP:N	2.54	0.40
13:H:151:LEU:HD12	13:H:151:LEU:HA	1.93	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	2	658/868 (76%)	648 (98%)	10 (2%)	0	100	100
2	3	597/1006 (59%)	591 (99%)	6 (1%)	0	100	100
3	4	682/933 (73%)	667 (98%)	15 (2%)	0	100	100
4	5	664/775 (86%)	651 (98%)	13 (2%)	0	100	100
5	6	606/1017 (60%)	587 (97%)	19 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	7	621/845 (74%)	604 (97%)	17 (3%)	0	100	100
8	C	173/217 (80%)	171 (99%)	2 (1%)	0	100	100
9	D	232/294 (79%)	231 (100%)	1 (0%)	0	100	100
10	E	557/657 (85%)	551 (99%)	6 (1%)	0	100	100
11	F	535/689 (78%)	523 (98%)	12 (2%)	0	100	100
12	G	839/2222 (38%)	820 (98%)	19 (2%)	0	100	100
13	H	195/208 (94%)	191 (98%)	4 (2%)	0	100	100
14	I	185/213 (87%)	182 (98%)	3 (2%)	0	100	100
All	All	6544/9944 (66%)	6417 (98%)	127 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	580/770 (75%)	580 (100%)	0	100	100
2	3	525/864 (61%)	525 (100%)	0	100	100
3	4	627/848 (74%)	627 (100%)	0	100	100
4	5	609/688 (88%)	609 (100%)	0	100	100
5	6	541/886 (61%)	541 (100%)	0	100	100
6	7	561/753 (74%)	561 (100%)	0	100	100
8	C	160/192 (83%)	160 (100%)	0	100	100
9	D	227/279 (81%)	227 (100%)	0	100	100
10	E	510/592 (86%)	510 (100%)	0	100	100
11	F	492/629 (78%)	492 (100%)	0	100	100
12	G	781/2014 (39%)	781 (100%)	0	100	100
13	H	184/193 (95%)	184 (100%)	0	100	100
14	I	179/198 (90%)	179 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5976/8906 (67%)	5976 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	282	HIS
1	2	290	HIS
1	2	384	ASN
2	3	210	HIS
2	3	487	HIS
2	3	677	ASN
2	3	682	ASN
2	3	691	ASN
3	4	253	GLN
3	4	307	ASN
3	4	320	ASN
3	4	377	ASN
3	4	691	ASN
3	4	871	ASN
3	4	931	ASN
4	5	245	HIS
4	5	334	GLN
4	5	652	GLN
4	5	765	HIS
5	6	157	HIS
5	6	409	GLN
5	6	750	GLN
6	7	384	HIS
6	7	538	HIS
6	7	544	GLN
6	7	568	ASN
6	7	669	GLN
8	C	181	HIS
9	D	210	ASN
9	D	225	ASN
10	E	254	GLN
10	E	464	GLN
10	E	604	ASN
11	F	295	ASN
11	F	361	ASN

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Mol	Chain	Res	Type
11	F	648	GLN
12	G	1347	GLN
12	G	1698	HIS
12	G	1822	ASN
12	G	1824	ASN
12	G	1930	ASN
12	G	2001	ASN
12	G	2143	GLN
12	G	2148	GLN
13	H	7	ASN
14	I	17	GLN
14	I	62	ASN
14	I	139	HIS
14	I	153	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 19 ligands modelled in this entry, 13 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
18	ATP	7	1502	15	29,33,33	0.30	0	44,52,52	0.51	1 (2%)
18	ATP	6	1502	15	29,33,33	0.31	0	44,52,52	0.52	1 (2%)
18	ATP	4	1502	15	29,33,33	0.30	0	44,52,52	0.51	1 (2%)
18	ATP	5	1502	15	29,33,33	0.32	0	44,52,52	0.52	1 (2%)
17	ADP	2	1503	15	27,29,29	1.34	4 (14%)	42,45,45	1.97	11 (26%)
18	ATP	3	1502	15	29,33,33	0.31	0	44,52,52	0.49	1 (2%)

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
18	ATP	7	1502	15	-	2/22/38/38	0/3/3/3
18	ATP	6	1502	15	-	5/22/38/38	0/3/3/3
18	ATP	4	1502	15	-	2/22/38/38	0/3/3/3
18	ATP	5	1502	15	-	2/22/38/38	0/3/3/3
17	ADP	2	1503	15	-	3/16/32/32	0/3/3/3
18	ATP	3	1502	15	-	2/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	1503	ADP	C5-C4	4.38	1.47	1.39
17	2	1503	ADP	C5-C6	2.59	1.48	1.41
17	2	1503	ADP	C8-N7	2.37	1.36	1.31
17	2	1503	ADP	C5-N7	-2.25	1.34	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	2	1503	ADP	C5-C4-N3	-6.18	118.69	126.75
17	2	1503	ADP	N3-C4-N9	4.81	135.00	127.08
17	2	1503	ADP	C2-N3-C4	3.87	120.89	111.75
17	2	1503	ADP	PA-O3A-PB	-3.50	120.80	132.83
17	2	1503	ADP	C4-C5-N7	-3.25	106.66	110.62
17	2	1503	ADP	N3-C2-N1	-3.16	123.65	128.60
17	2	1503	ADP	C5-N7-C8	2.74	107.40	103.51
17	2	1503	ADP	C4-N9-C8	2.59	108.54	105.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	2	1503	ADP	C6-C5-N7	2.18	136.07	132.02
17	2	1503	ADP	C3'-C2'-C1'	2.15	105.51	101.43
17	2	1503	ADP	N9-C8-N7	-2.06	111.09	113.91
18	4	1502	ATP	PB-O3B-PG	2.05	139.85	132.83
18	7	1502	ATP	PB-O3B-PG	2.04	139.84	132.83
18	6	1502	ATP	PB-O3B-PG	2.04	139.84	132.83
18	5	1502	ATP	PB-O3B-PG	2.04	139.81	132.83
18	3	1502	ATP	PB-O3B-PG	2.03	139.79	132.83

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	2	1503	ADP	C5'-O5'-PA-O1A
17	2	1503	ADP	C5'-O5'-PA-O2A
18	3	1502	ATP	PB-O3B-PG-O2G
18	5	1502	ATP	C5'-O5'-PA-O2A
18	5	1502	ATP	C5'-O5'-PA-O3A
18	6	1502	ATP	C5'-O5'-PA-O1A
18	4	1502	ATP	O4'-C4'-C5'-O5'
18	7	1502	ATP	PG-O3B-PB-O1B
18	4	1502	ATP	C3'-C4'-C5'-O5'
18	6	1502	ATP	C5'-O5'-PA-O3A
18	6	1502	ATP	C5'-O5'-PA-O2A
18	6	1502	ATP	PG-O3B-PB-O3A
18	3	1502	ATP	PB-O3B-PG-O1G
18	7	1502	ATP	PB-O3B-PG-O3G
17	2	1503	ADP	C5'-O5'-PA-O3A
18	6	1502	ATP	PG-O3B-PB-O1B

There are no ring outliers.

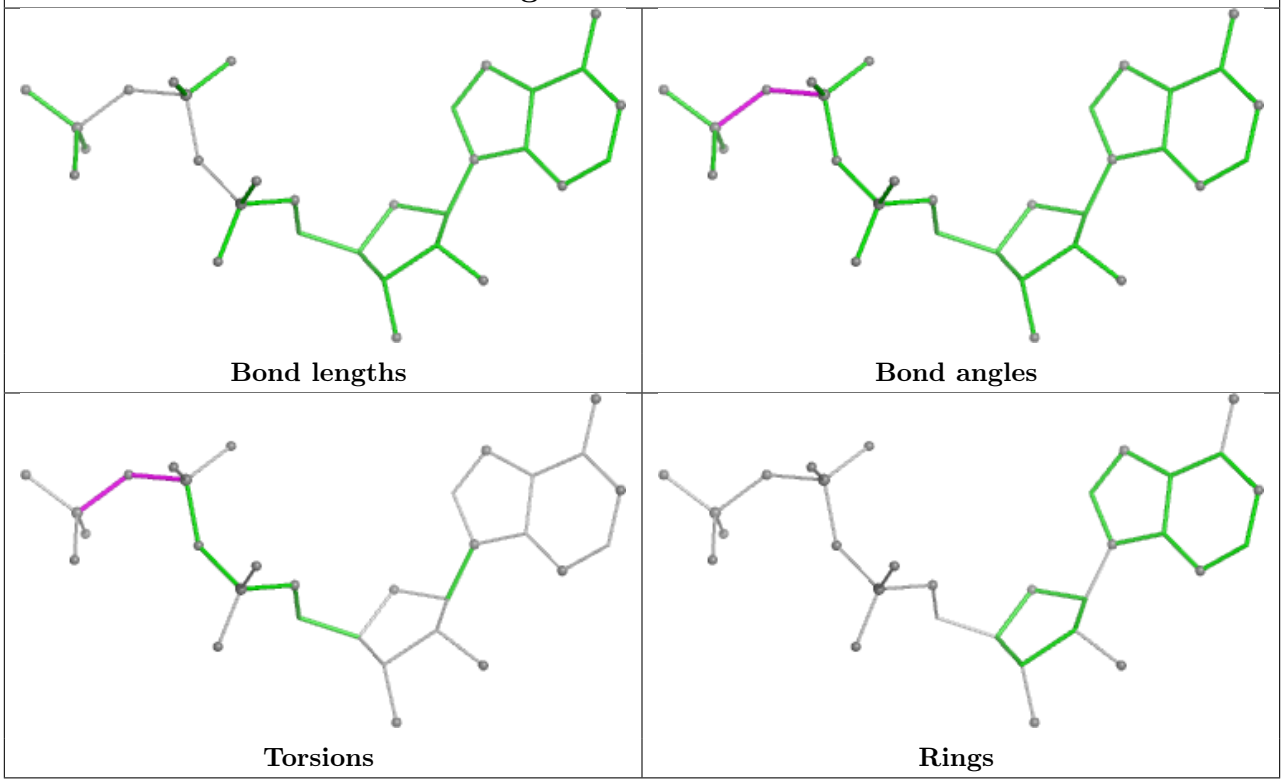
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	7	1502	ATP	1	0
18	6	1502	ATP	4	0

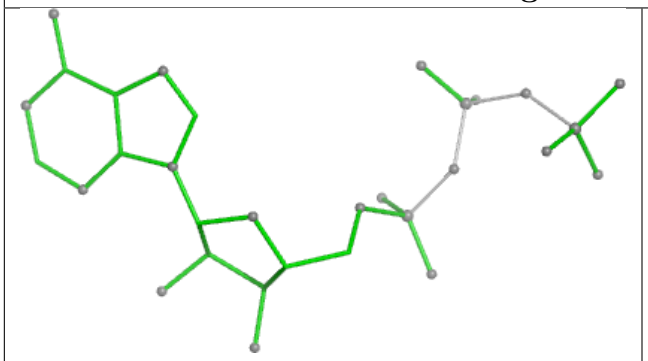
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

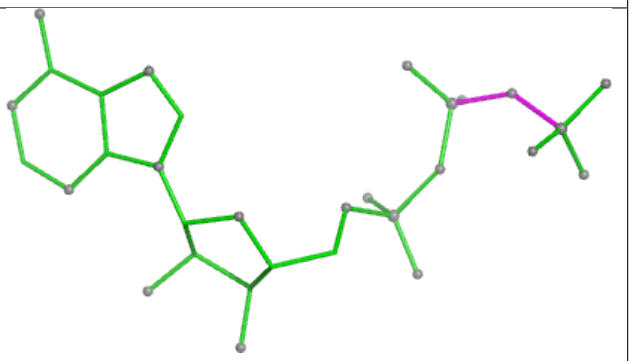
Ligand ATP 7 1502



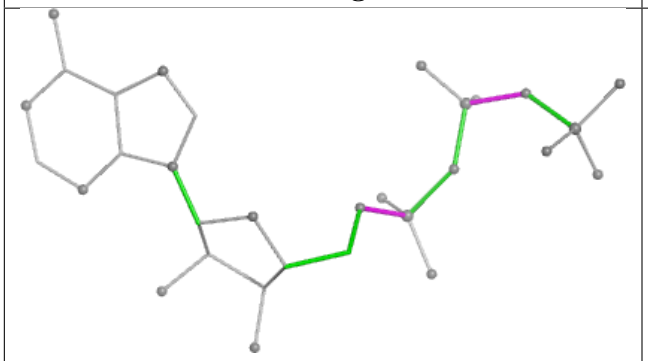
Ligand ATP 6 1502



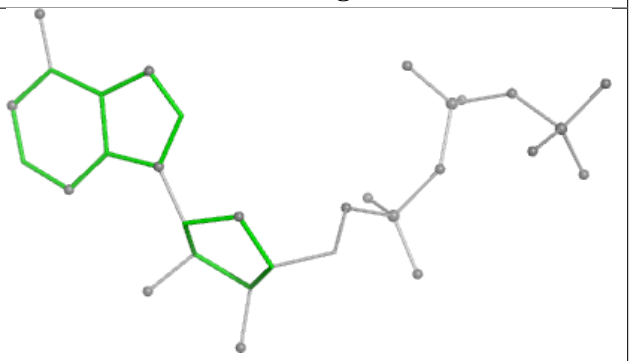
Bond lengths



Bond angles

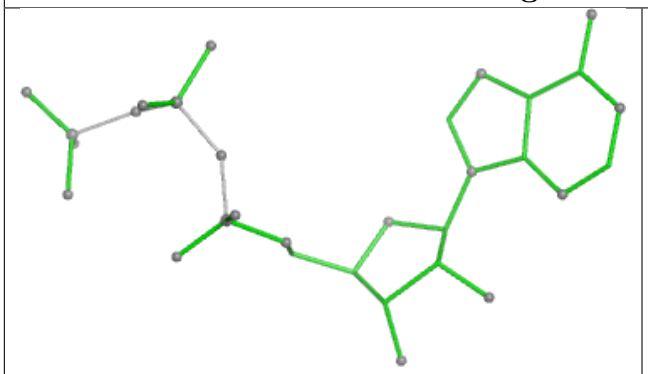


Torsions



Rings

Ligand ATP 4 1502



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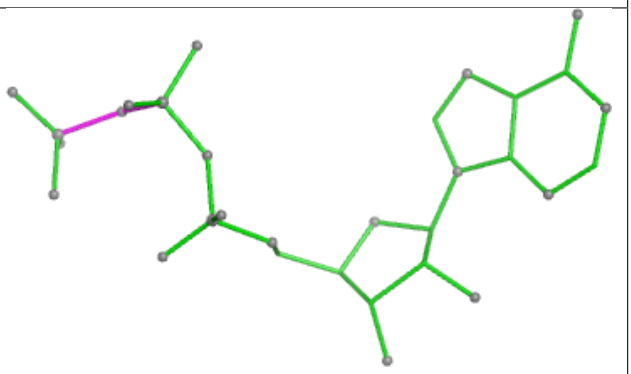
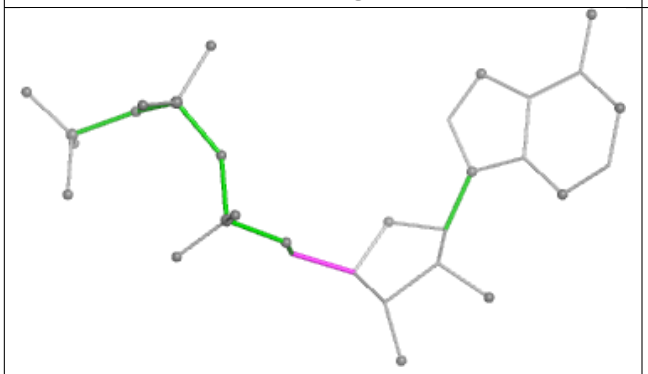
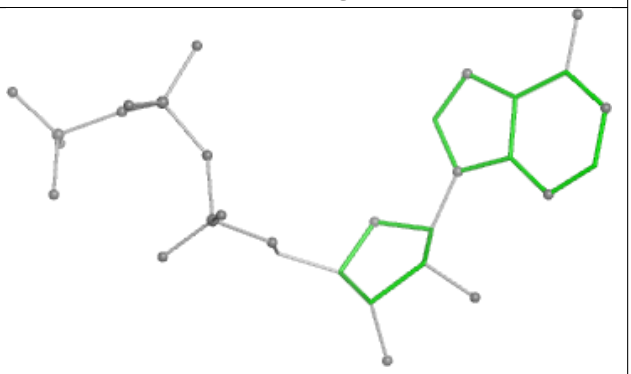


Bond angles

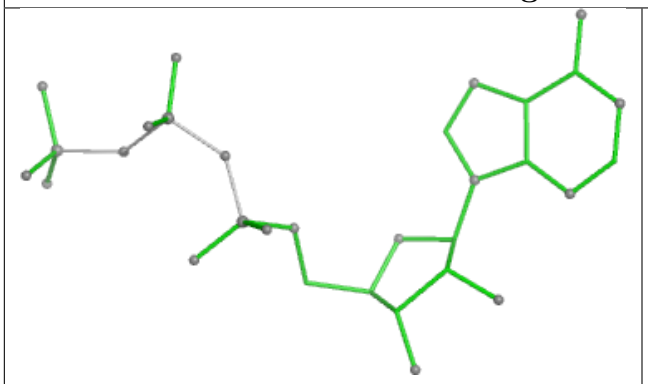


Torsions

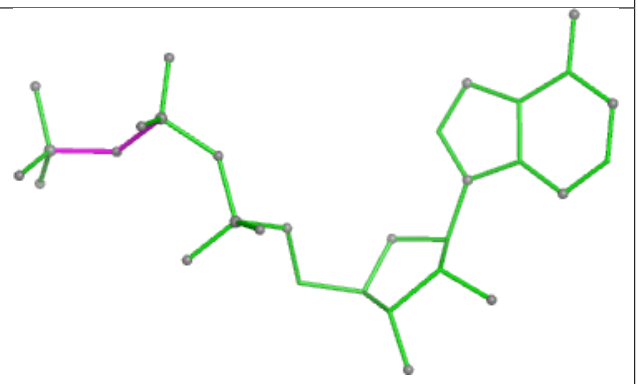


Rings

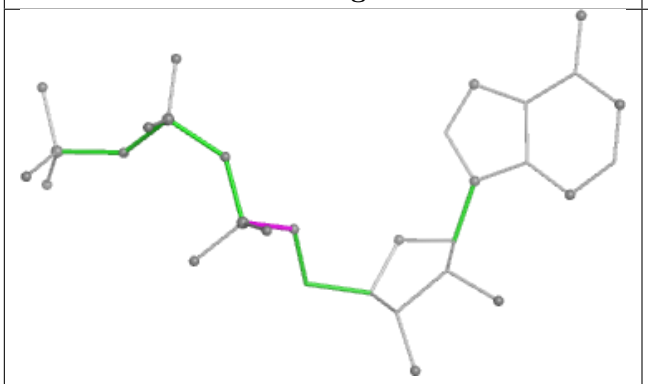
Ligand ATP 5 1502



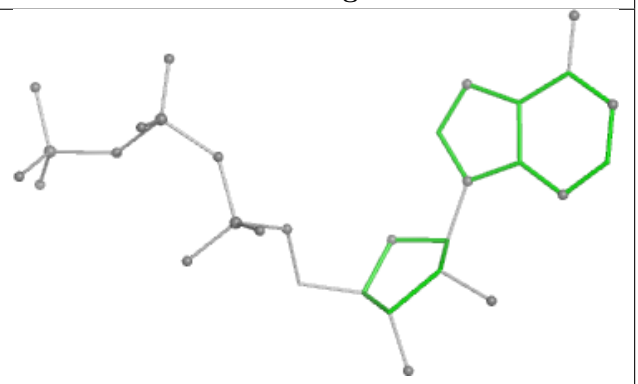
Bond lengths



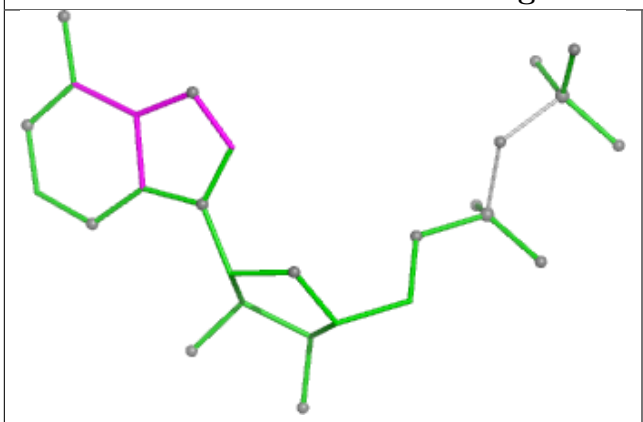
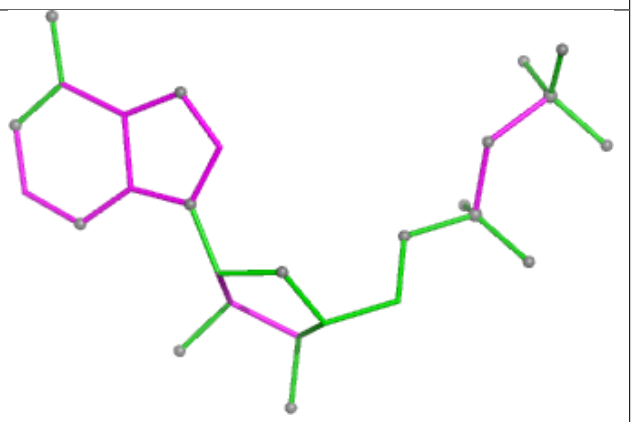
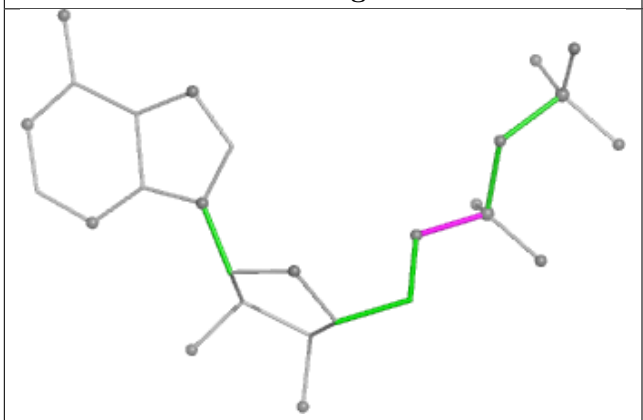
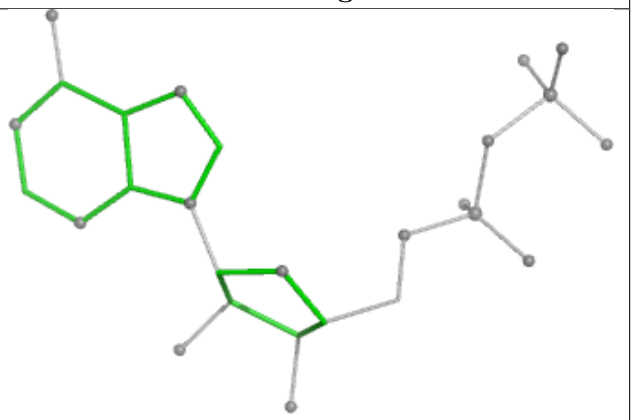
Bond angles

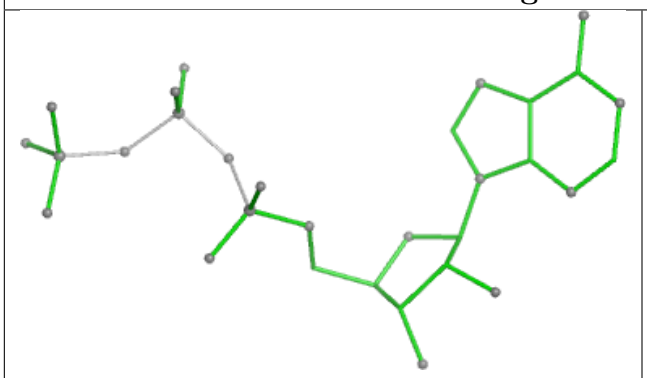
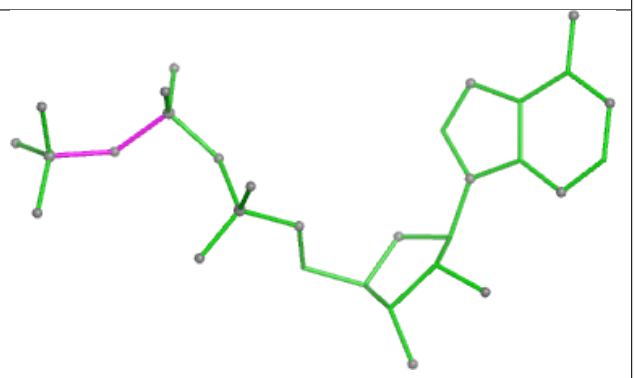
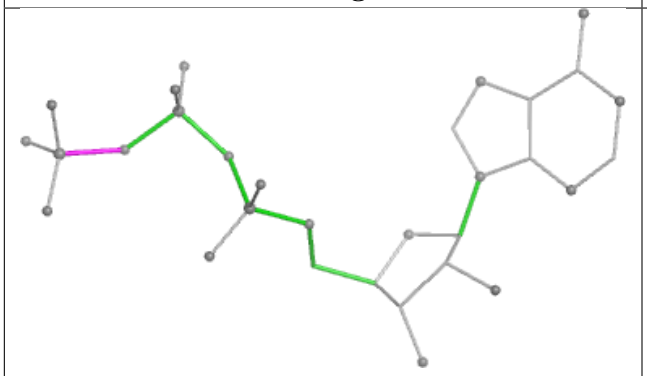
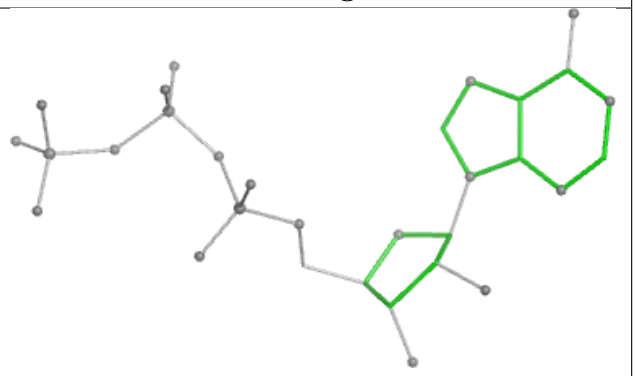


Torsions



Rings

Ligand ADP 2 1503	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ATP 3 1502	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

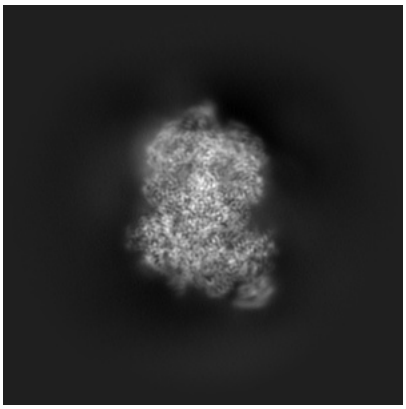
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-56898. These allow visual inspection of the internal detail of the map and identification of artifacts.

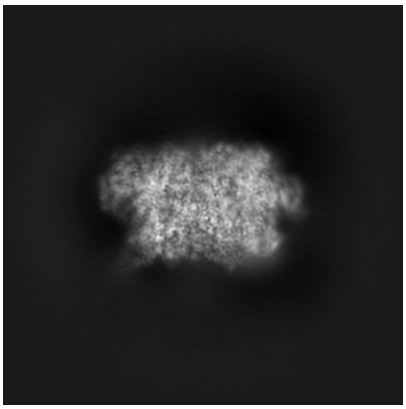
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

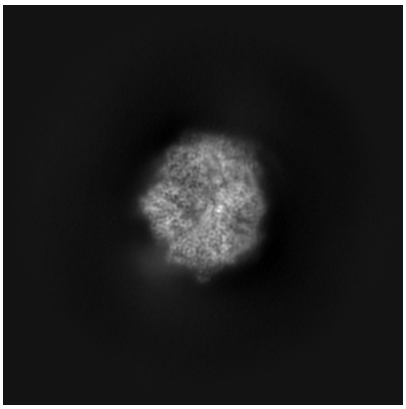
6.1.1 Primary map



X

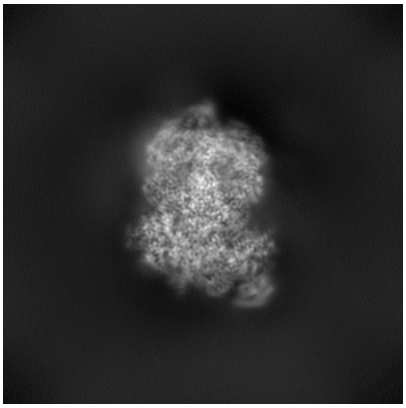


Y

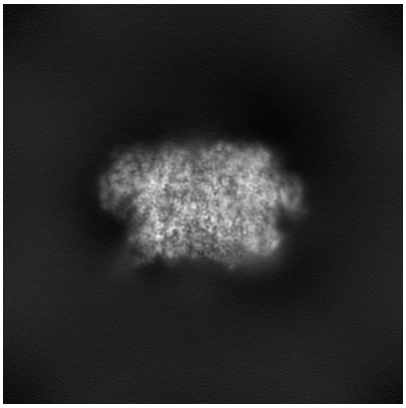


Z

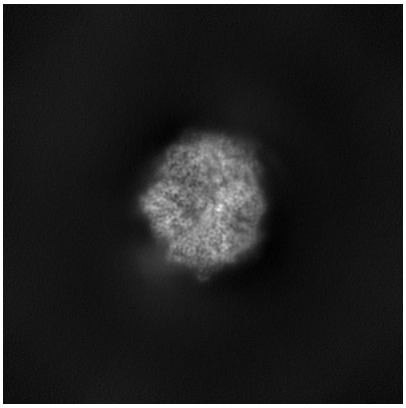
6.1.2 Raw map



X



Y

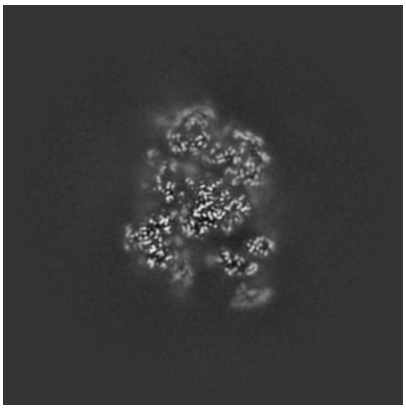


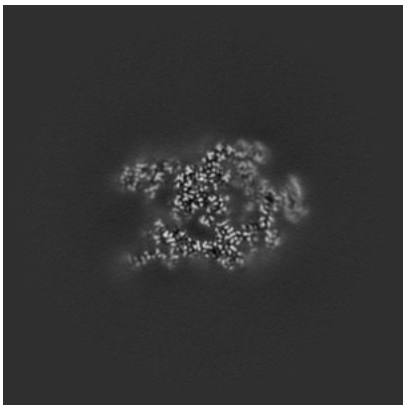
Z

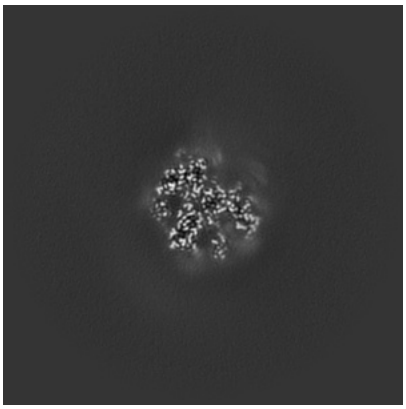
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

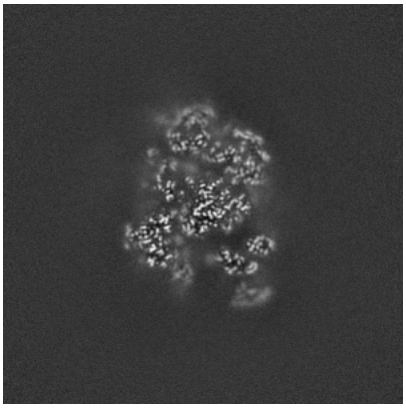
6.2.1 Primary map

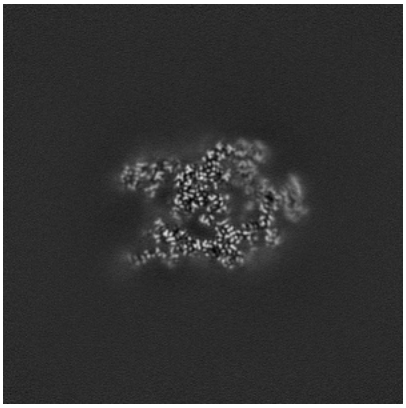

X Index: 216

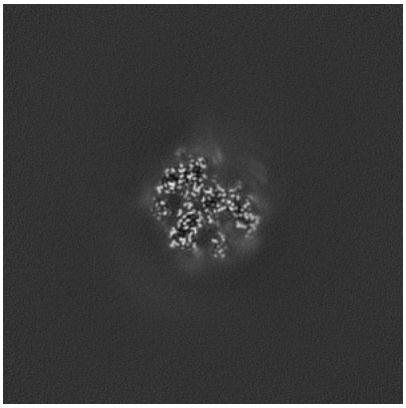

Y Index: 216


Z Index: 216

6.2.2 Raw map


X Index: 216

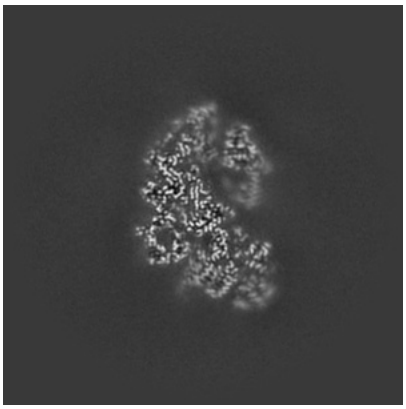

Y Index: 216


Z Index: 216

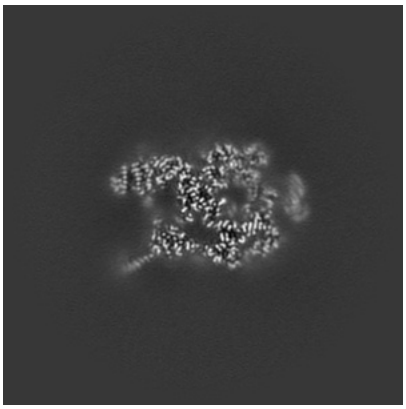
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

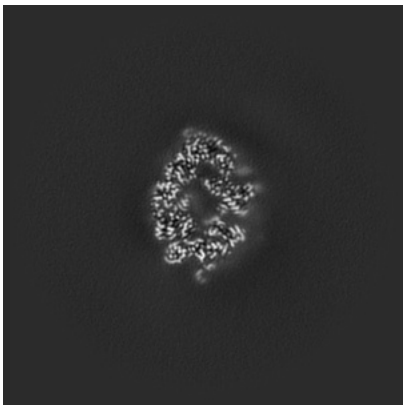
6.3.1 Primary map



X Index: 233

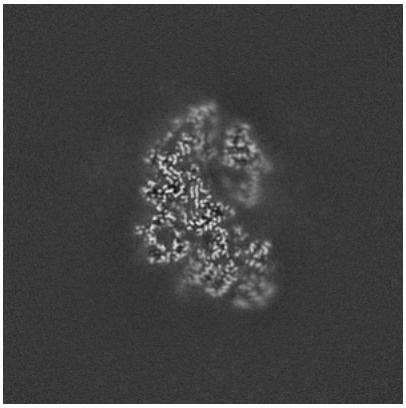


Y Index: 222

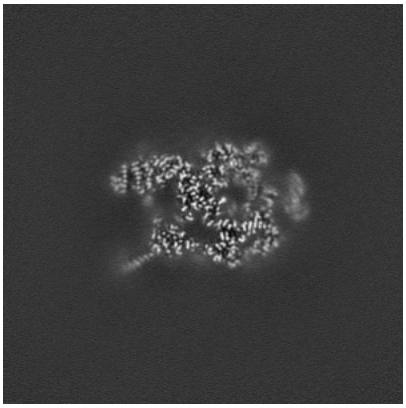


Z Index: 167

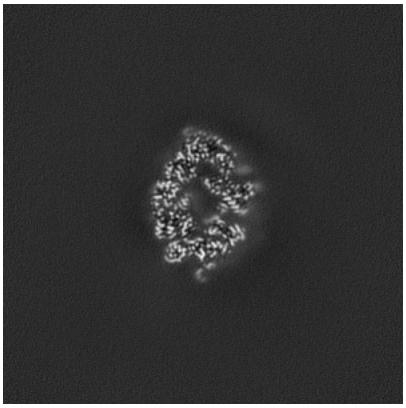
6.3.2 Raw map



X Index: 233



Y Index: 222

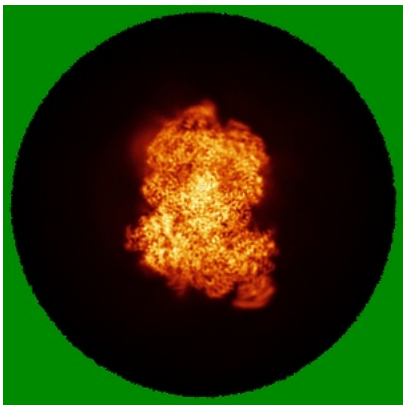


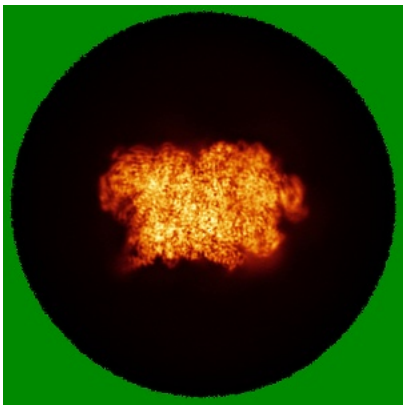
Z Index: 167

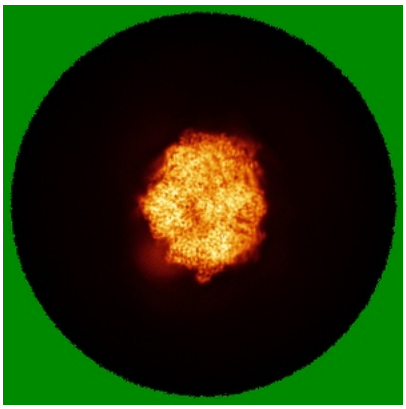
The images above show the largest variance slices of the map in three orthogonal directions.

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

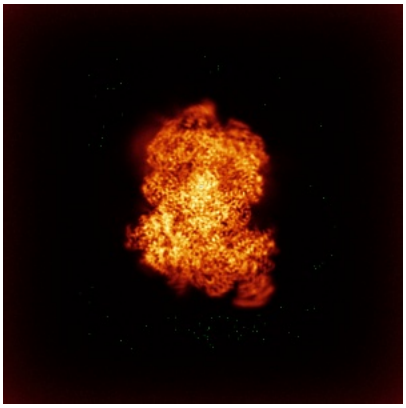
6.4.1 Primary map

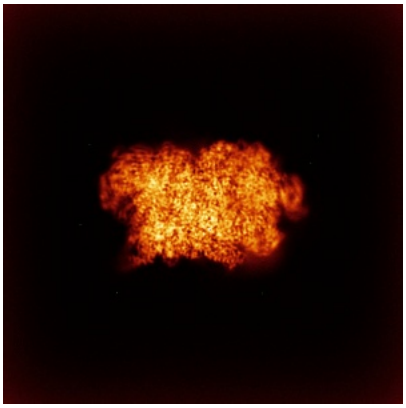

X

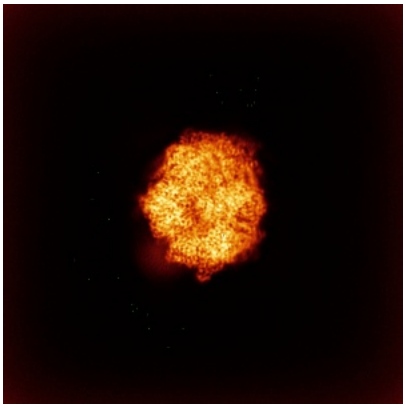

Y


Z

6.4.2 Raw map


X

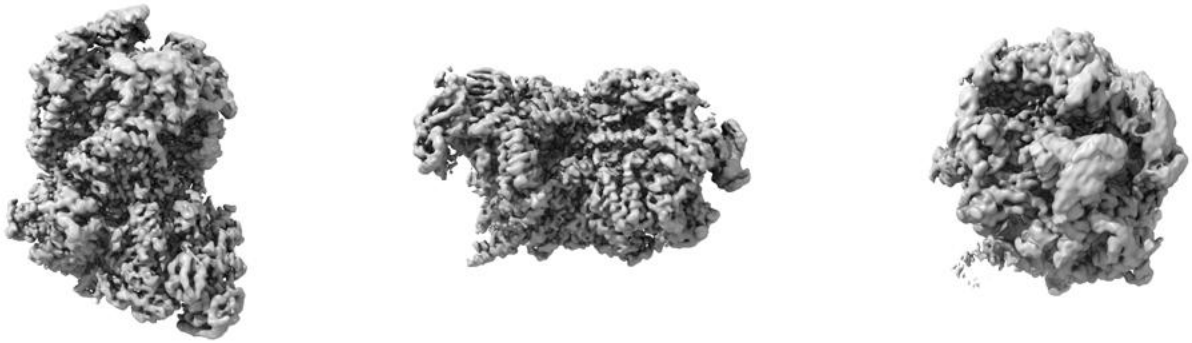

Y


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)

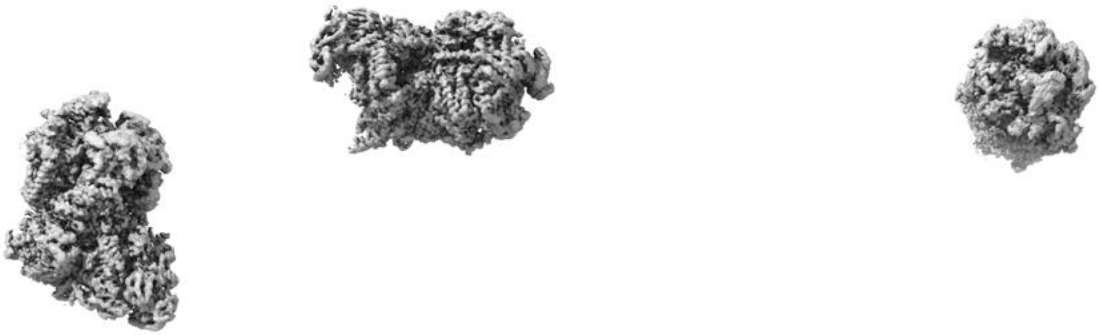
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. 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.

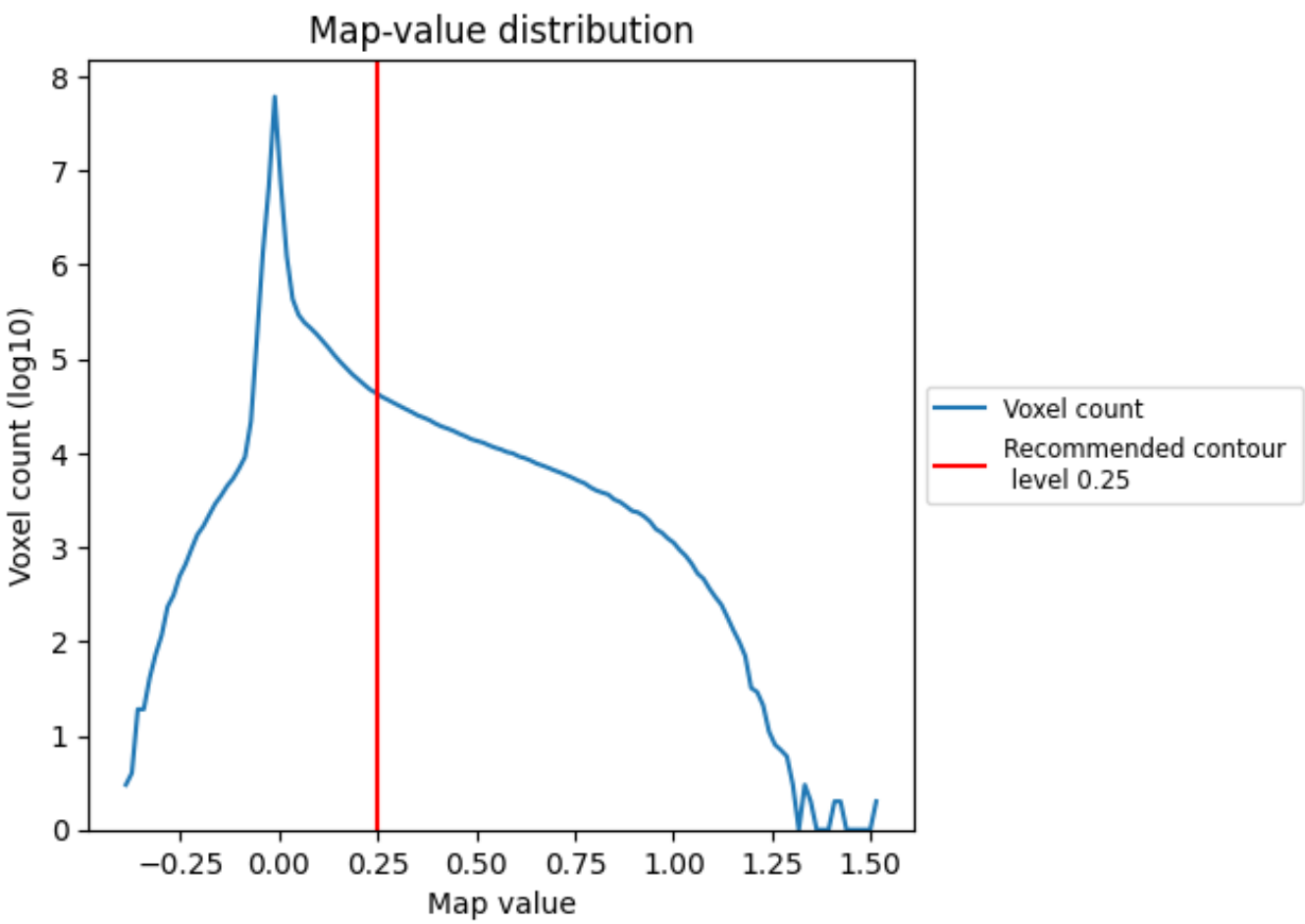
6.6 Mask visualisation (i)

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

7 Map analysis (i)

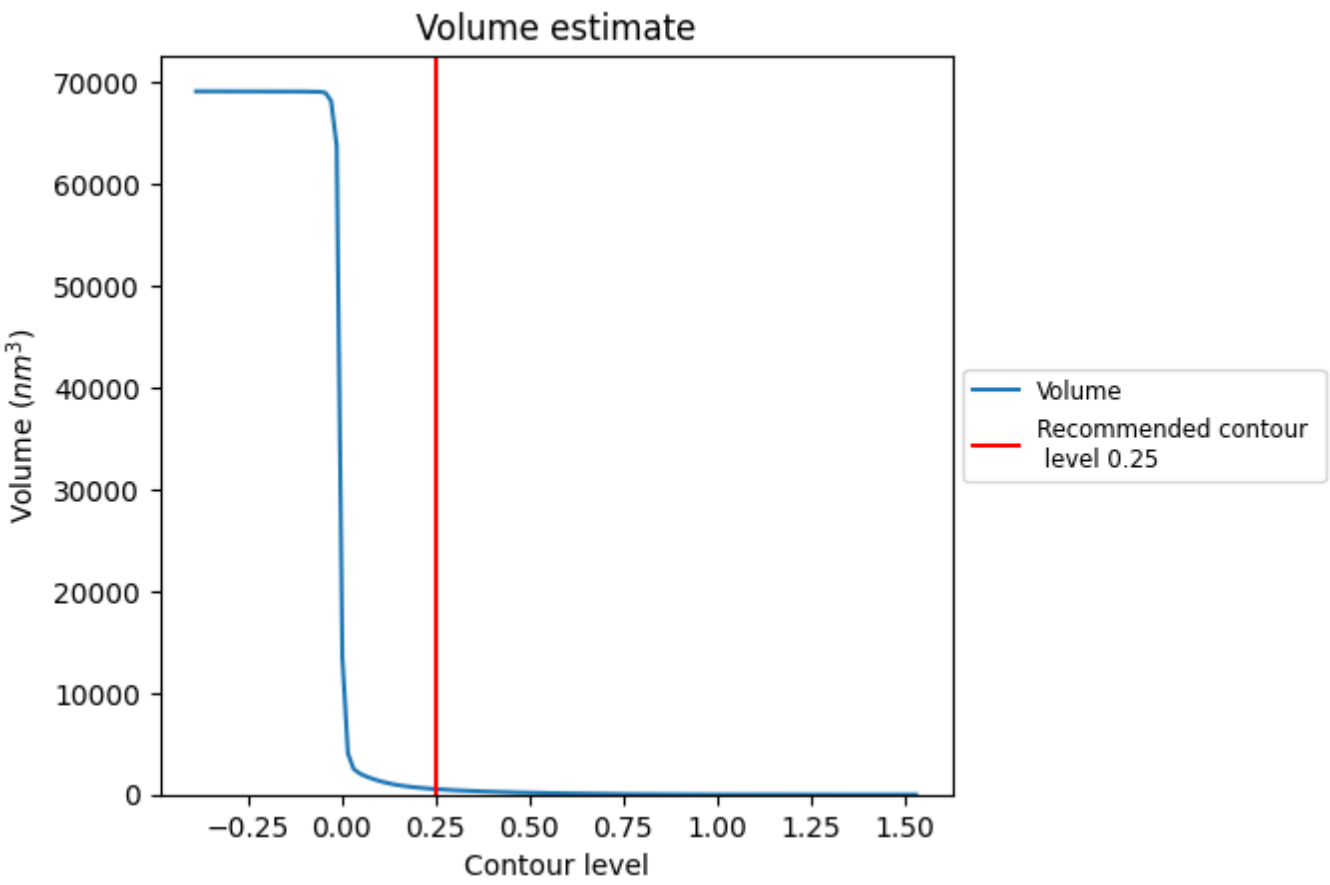
This section contains the results of statistical analysis of the map.

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.

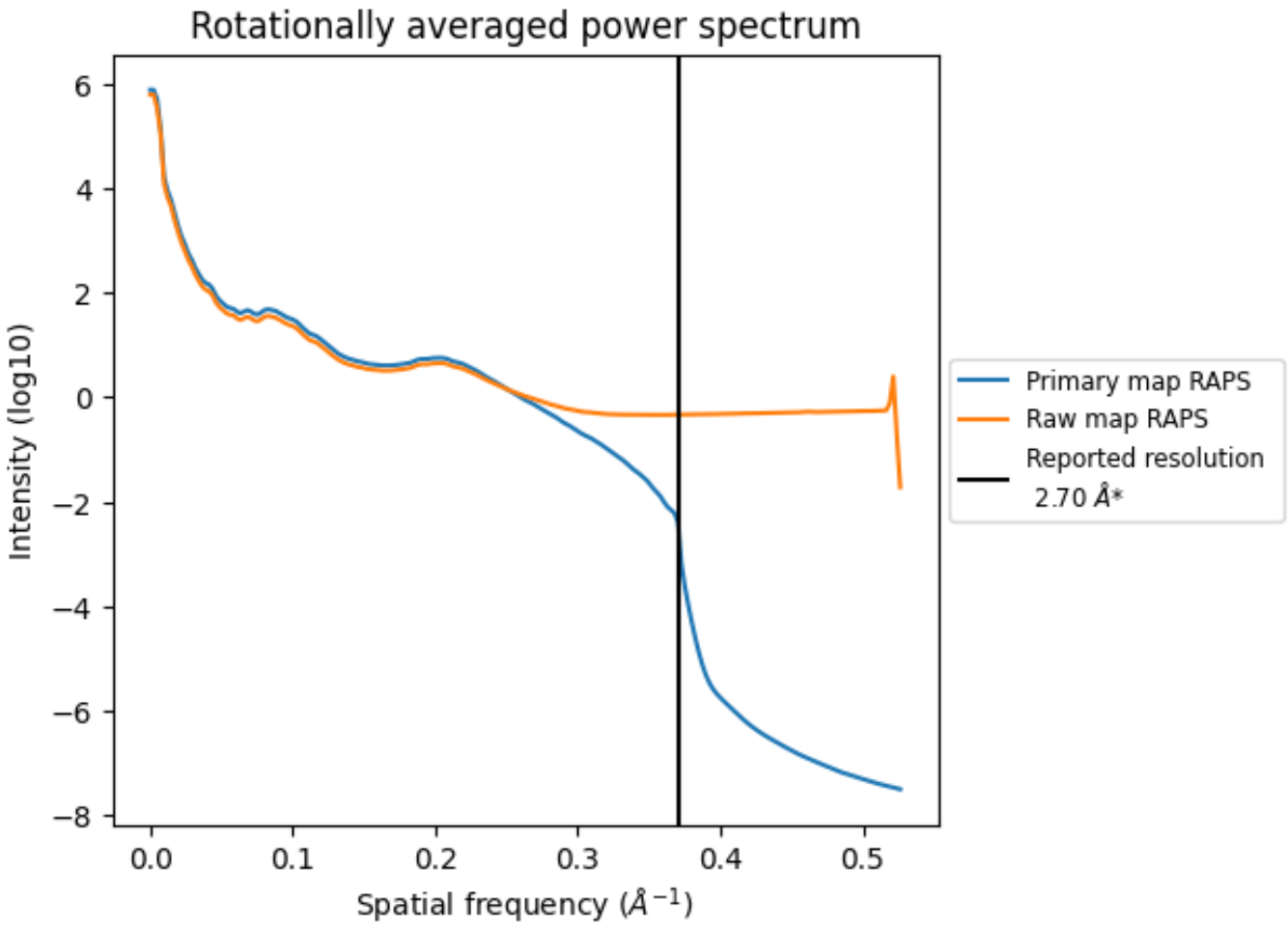
7.2 Volume estimate (i)



The volume at the recommended contour level is 539 nm^3; this corresponds to an approximate mass of 487 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)

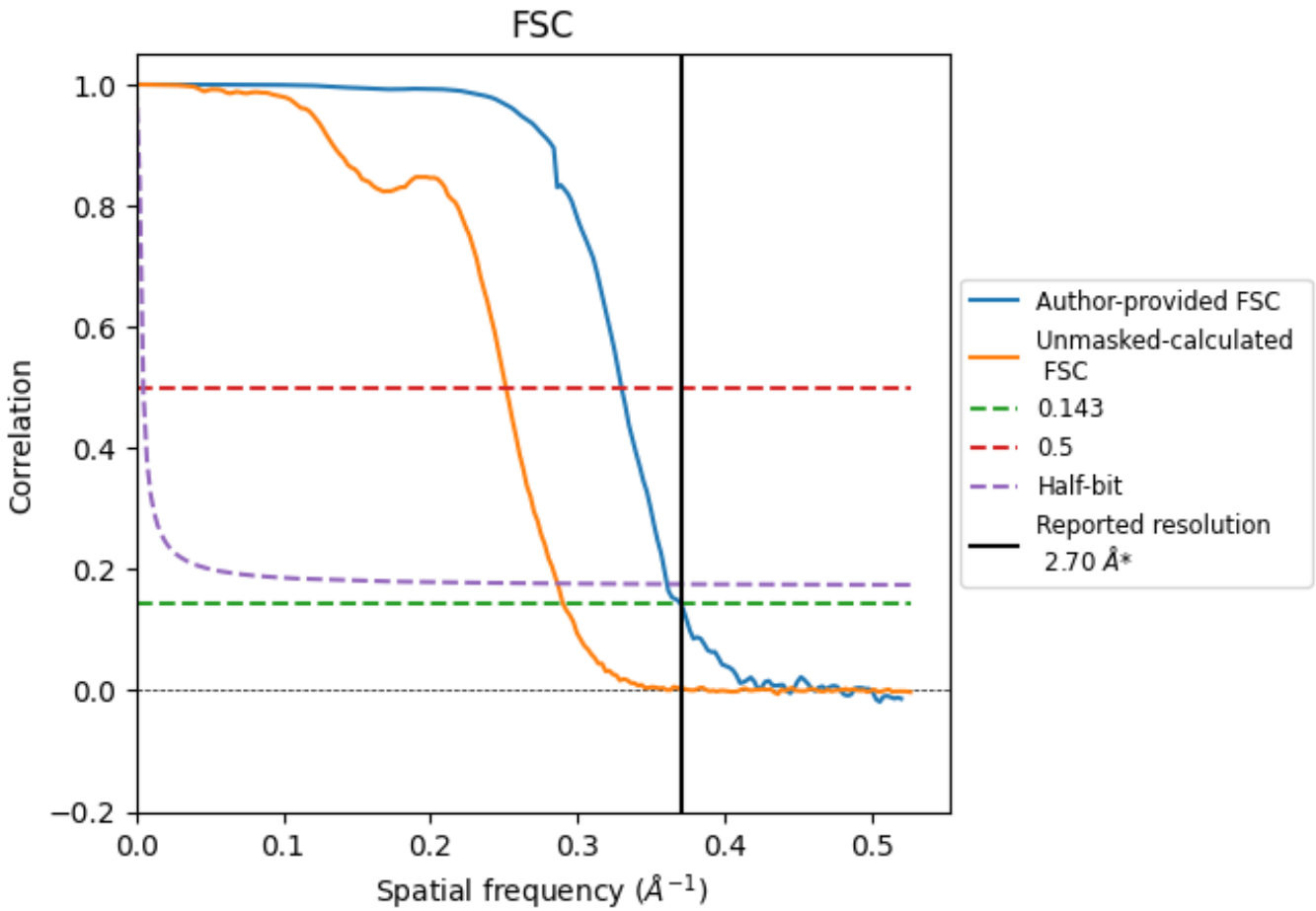


*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

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 0.370 Å^{-1}

8.2 Resolution estimates (i)

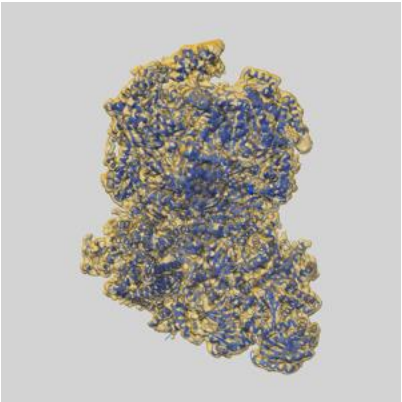
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.70	3.03	2.77
Unmasked-calculated*	3.45	3.98	3.49

*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 3.45 differs from the reported value 2.7 by more than 10 %

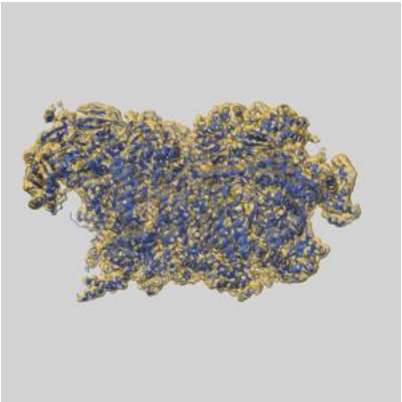
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-56898 and PDB model 28VY. Per-residue inclusion information can be found in section 3 on page 11.

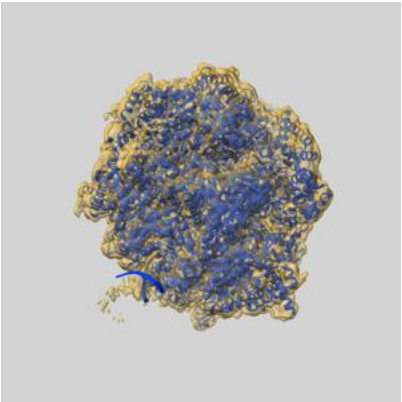
9.1 Map-model overlay (i)



X



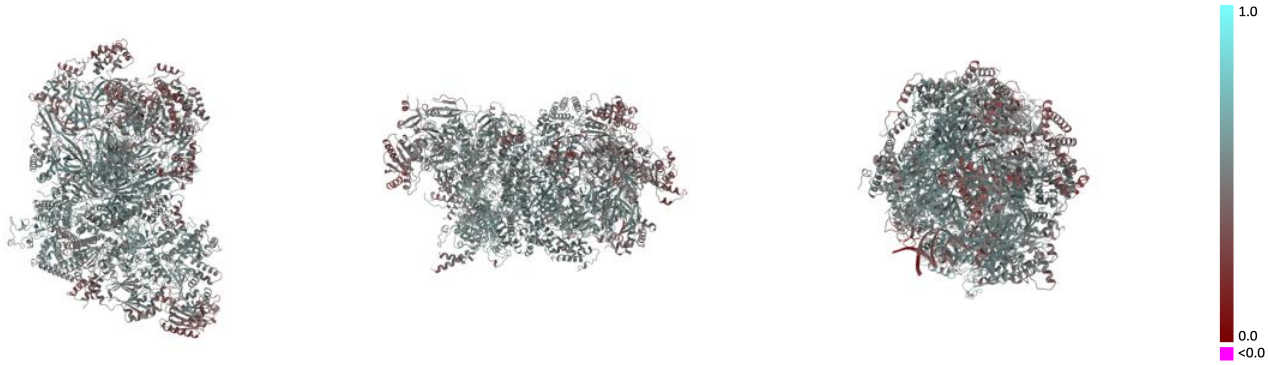
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25 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.

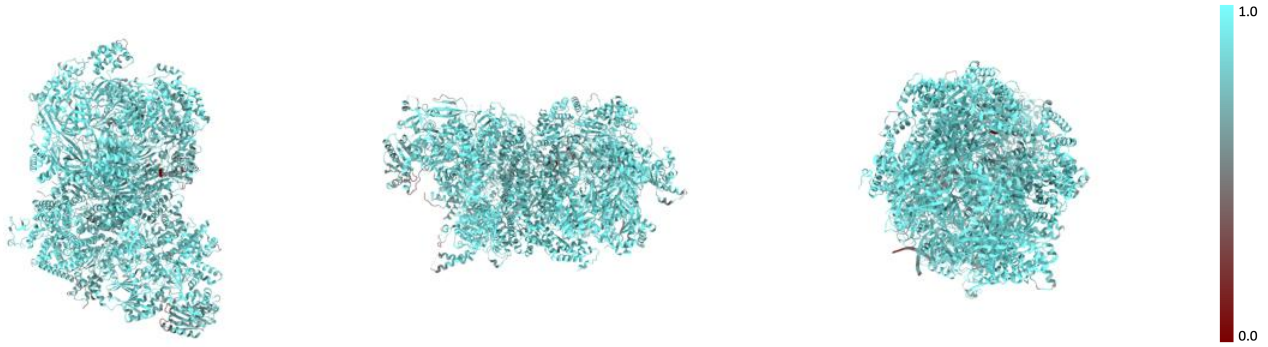
9.2 Q-score mapped to coordinate model (i)



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.

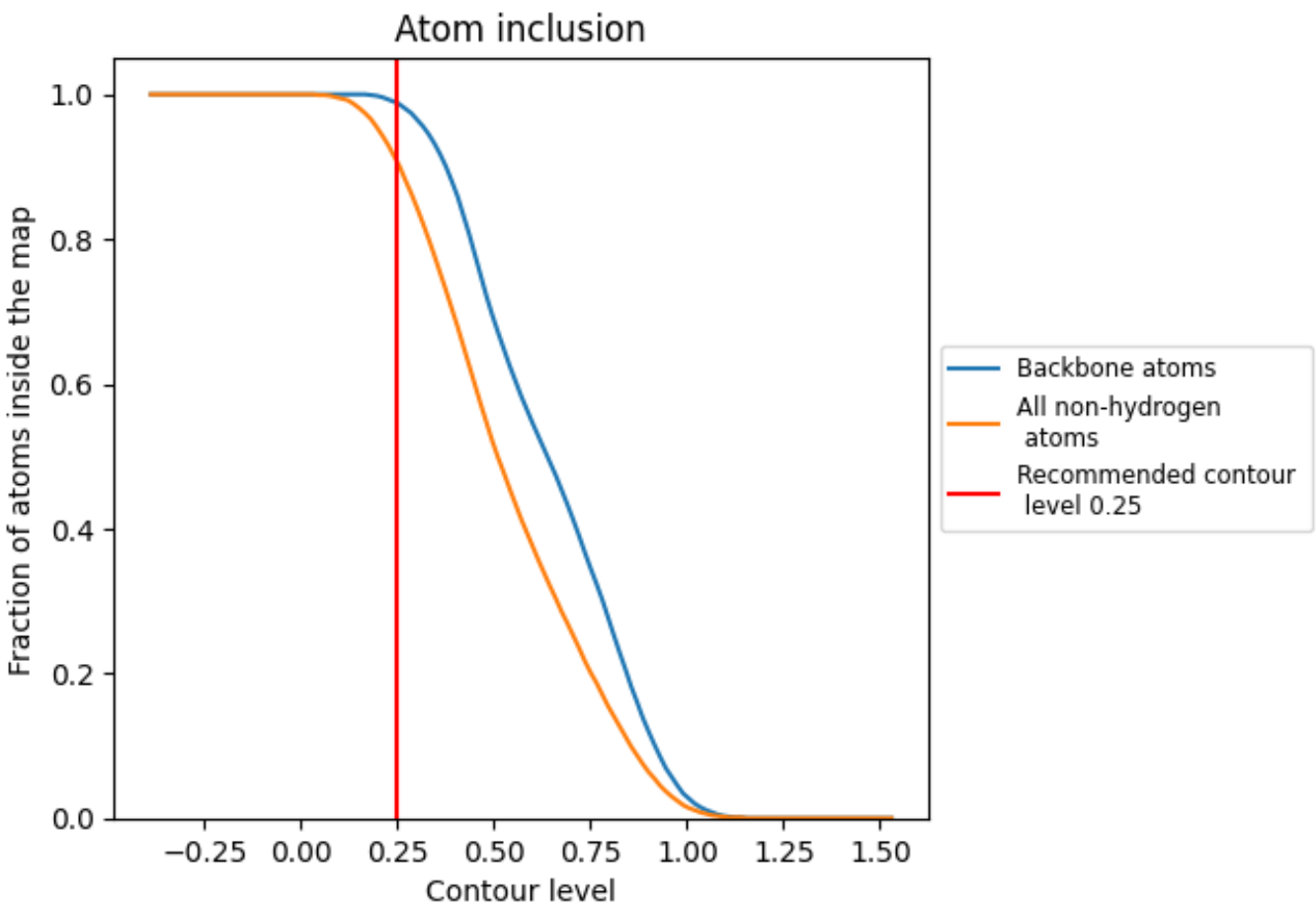
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.25).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9060	0.5060
2	0.9370	0.5450
3	0.9500	0.5430
4	0.8710	0.4390
5	0.9250	0.5440
6	0.9320	0.5070
7	0.8930	0.4510
A	0.8120	0.3970
B	0.7560	0.3070
C	0.9430	0.5390
D	0.9300	0.5210
E	0.9300	0.5380
F	0.8790	0.4950
G	0.8480	0.4890
H	0.9100	0.5050
I	0.9480	0.5570