Full wwPDB EM Validation Report ⓘ

May 20, 2024 – 02:05 pm BST

PDB ID	:	8P62
EMDB ID	:	EMD-17458
Title	:	S. cerevisiae ssDNA-sCMGE after DNA replication initiation
Authors	:	Henrikus, S.S.; Willhoft, O.
Deposited on	:	2023-05-25
Resolution	:	3.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

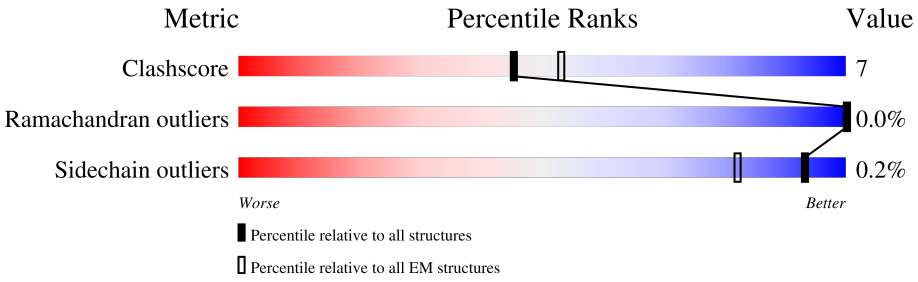
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	65% 11% 24%
2	3	1006	55% 9% 35%
3	4	933	52% 12% 37%
4	5	775	77% 12% 11%
5	6	1017	52% 11% 37%
6	7	845	5% 62% 16% 22%
7	A	9	33% 67%
8	C	229	67% 9% 24%

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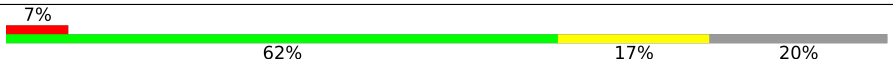
Mol	Chain	Length	Quality of chain
9	D	294	
10	E	657	
11	F	689	
12	G	2222	
13	H	208	
14	I	213	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 53042 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
1	2	662	Total	C	N	O	S	0	0
			5235	3283	940	993	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	649	Total	C	N	O	S	0	0
			5067	3191	904	959	13		

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
3	4	592	Total	C	N	O	S	0	0
			4702	2963	816	896	27		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	693	Total	C	N	O	S	0	0
			5447	3418	948	1057	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	636	Total	C	N	O	S	0	0
			5032	3173	879	955	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	663	Total	C	N	O	S	0	0
			5223	3301	903	990	29		

- Molecule 7 is a DNA chain called DNA (9-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	9	Total	C	N	O	P	0	0
			189	90	45	45	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	175	Total	C	N	O	S	0	0
			1408	914	226	261	7		

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-34	TRP	-	expression tag	UNP Q12146
C	-33	SER	-	expression tag	UNP Q12146
C	-32	HIS	-	expression tag	UNP Q12146
C	-31	PRO	-	expression tag	UNP Q12146
C	-30	GLN	-	expression tag	UNP Q12146
C	-29	PHE	-	expression tag	UNP Q12146
C	-28	GLU	-	expression tag	UNP Q12146
C	-27	LYS	-	expression tag	UNP Q12146
C	-26	GLY	-	expression tag	UNP Q12146
C	-25	GLY	-	expression tag	UNP Q12146
C	-24	GLY	-	expression tag	UNP Q12146
C	-23	SER	-	expression tag	UNP Q12146
C	-22	GLY	-	expression tag	UNP Q12146
C	-21	GLY	-	expression tag	UNP Q12146
C	-20	GLY	-	expression tag	UNP Q12146
C	-19	SER	-	expression tag	UNP Q12146
C	-18	GLY	-	expression tag	UNP Q12146
C	-17	GLY	-	expression tag	UNP Q12146
C	-16	GLY	-	expression tag	UNP Q12146
C	-15	SER	-	expression tag	UNP Q12146
C	-14	TRP	-	expression tag	UNP Q12146
C	-13	SER	-	expression tag	UNP Q12146
C	-12	HIS	-	expression tag	UNP Q12146
C	-11	PRO	-	expression tag	UNP Q12146
C	-10	GLN	-	expression tag	UNP Q12146
C	-9	PHE	-	expression tag	UNP Q12146
C	-8	GLU	-	expression tag	UNP Q12146
C	-7	LYS	-	expression tag	UNP Q12146
C	-6	GLU	-	expression tag	UNP Q12146
C	-5	ASN	-	expression tag	UNP Q12146
C	-4	LEU	-	expression tag	UNP Q12146

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	TYR	-	expression tag	UNP Q12146
C	-2	PHE	-	expression tag	UNP Q12146
C	-1	GLN	-	expression tag	UNP Q12146
C	0	SER	-	expression tag	UNP Q12146

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	245	Total	C	N	O	S	0	0
			2014	1282	332	386	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	549	Total	C	N	O	S	0	0
			4276	2747	708	808	13		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	164J	TYR	GLU	conflict	UNP Q08032
E	164K	LYS	GLU	conflict	UNP Q08032
E	164M	ASP	GLU	conflict	UNP Q08032
E	164O	GLY	-	insertion	UNP Q08032
E	164P	ASP	-	insertion	UNP Q08032
E	164Q	TYR	-	insertion	UNP Q08032
E	164R	LYS	-	insertion	UNP Q08032
E	164S	ASP	-	insertion	UNP Q08032
E	164T	ASP	-	insertion	UNP Q08032
E	164U	ASP	-	insertion	UNP Q08032

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	548	Total	C	N	O	S	0	0
			4379	2806	755	800	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	825	Total	C	N	O	S	0	0
			6628	4289	1089	1213	37		

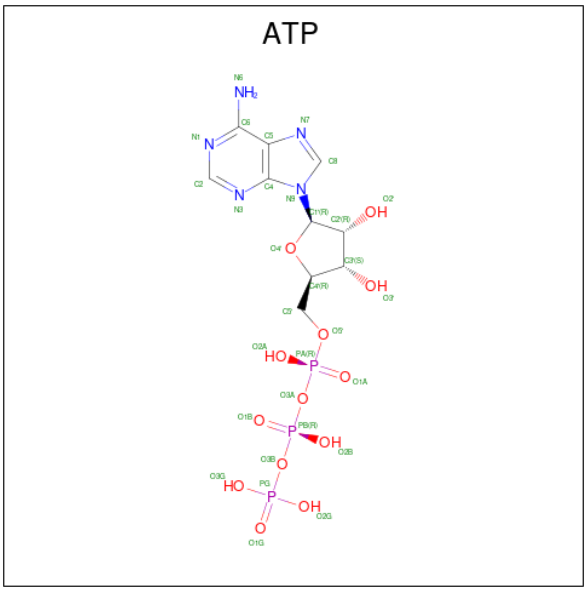
- Molecule 13 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	204	Total	C	N	O	S	0	0
			1663	1041	286	327	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	190	Total	C	N	O	S	0	0
			1591	1024	280	283	4		

- Molecule 15 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
15	2	1	Total	C	N	O	P	0
			31	10	5	13	3	
15	3	1	Total	C	N	O	P	0
			31	10	5	13	3	
15	5	1	Total	C	N	O	P	0
			31	10	5	13	3	
15	7	1	Total	C	N	O	P	0
			31	10	5	13	3	

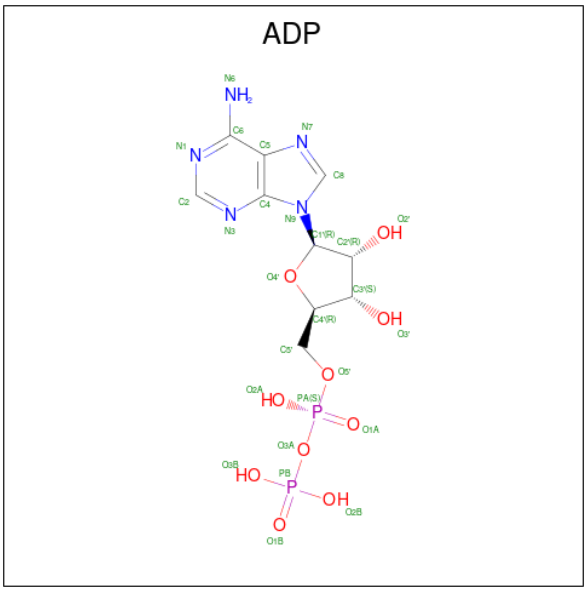
- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
17	3	1	Total Mg 1 1	0
17	5	1	Total Mg 1 1	0
17	7	1	Total Mg 1 1	0

- Molecule 18 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



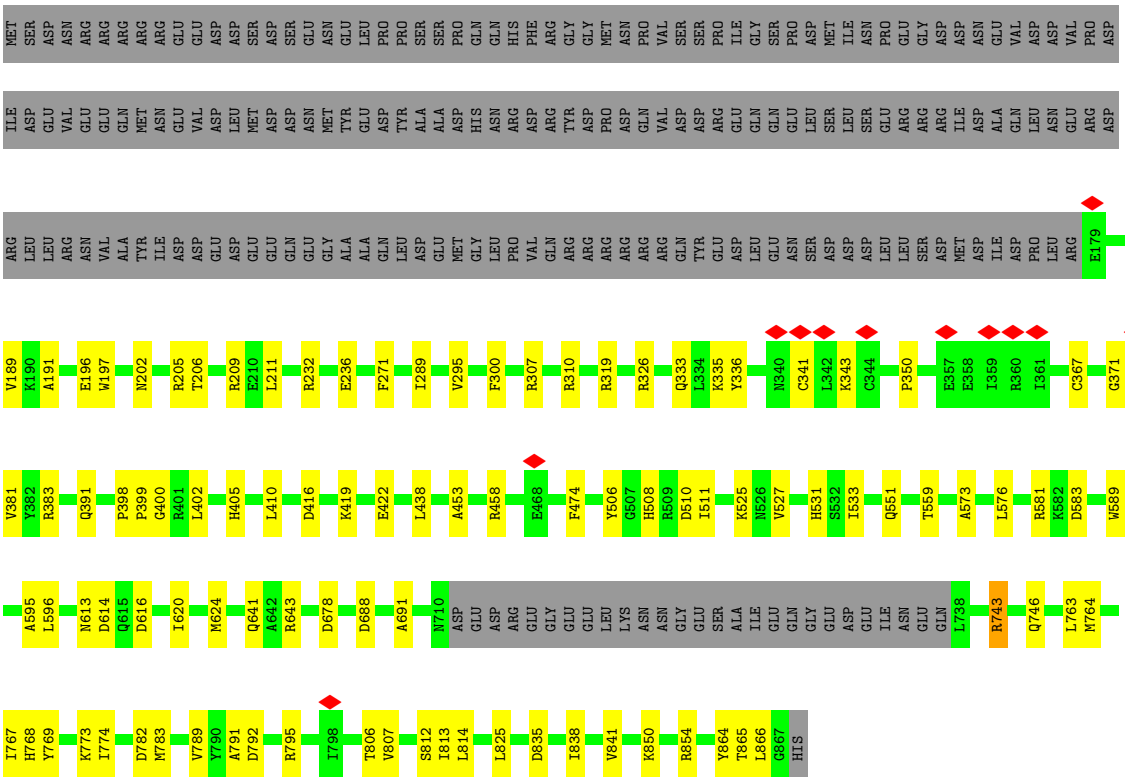
Mol	Chain	Residues	Atoms					AltConf
18	4	1	Total	C	N	O	P	0
			27	10	5	10	2	
18	6	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots (i)

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

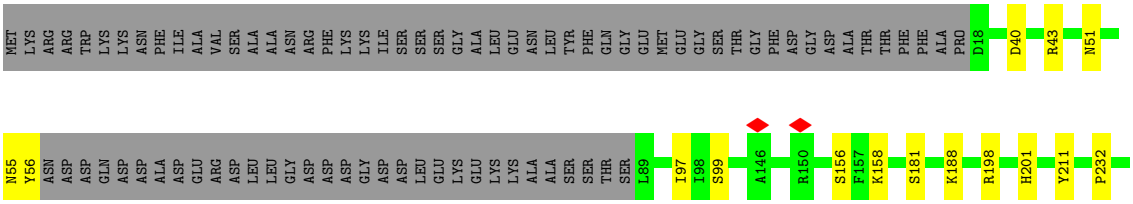
• Molecule 1: DNA replication licensing factor MCM2

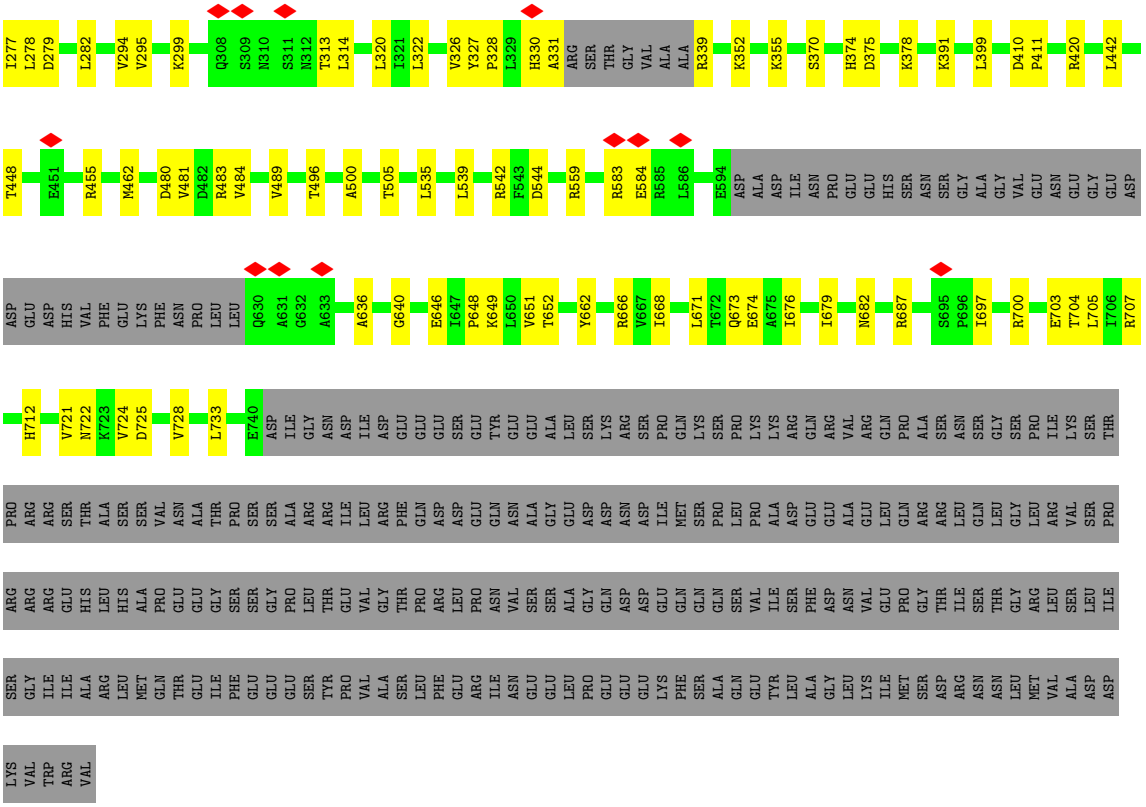
Chain 2:



• Molecule 2: DNA replication licensing factor MCM3

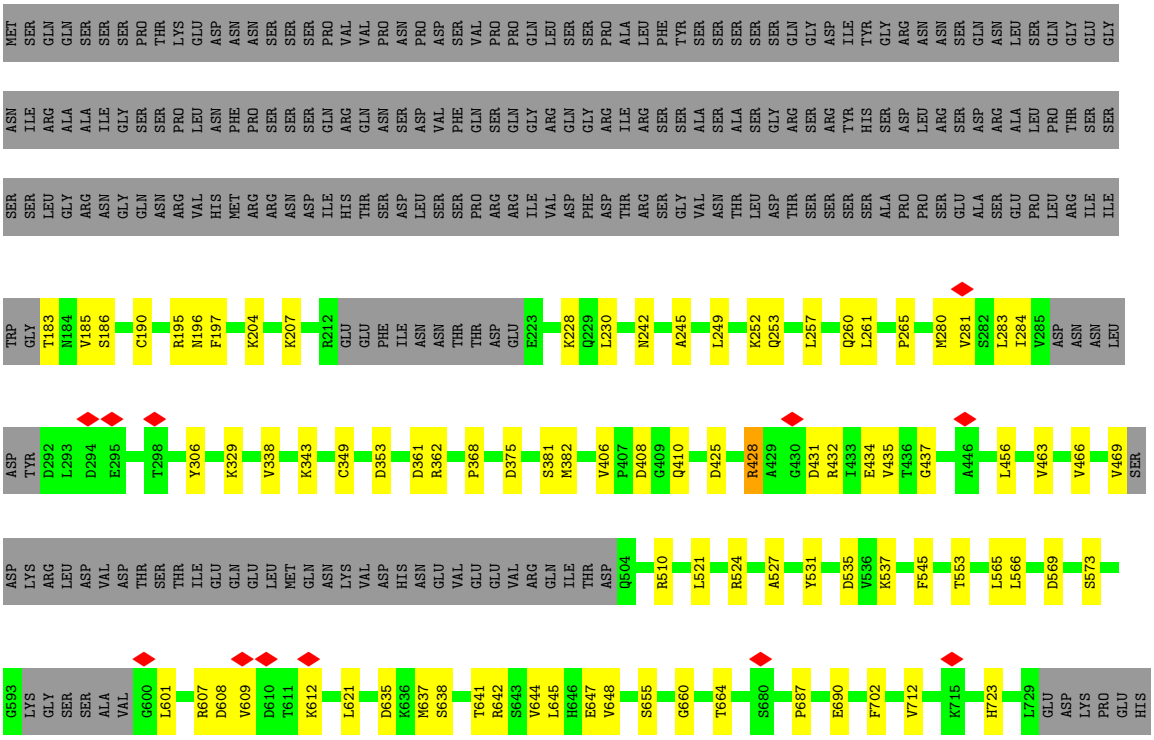
Chain 3:

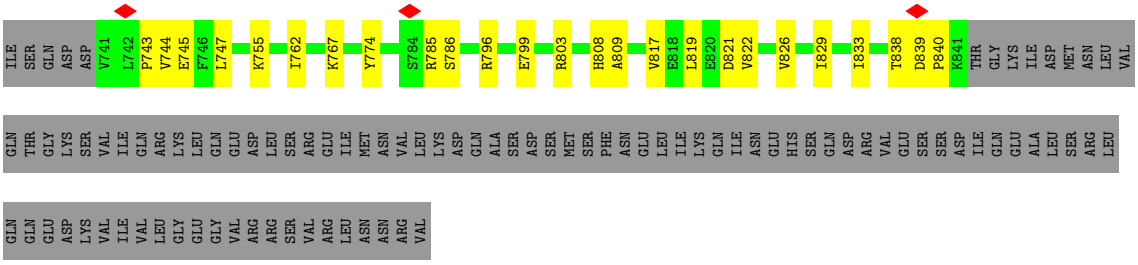




• Molecule 3: DNA replication licensing factor MCM4

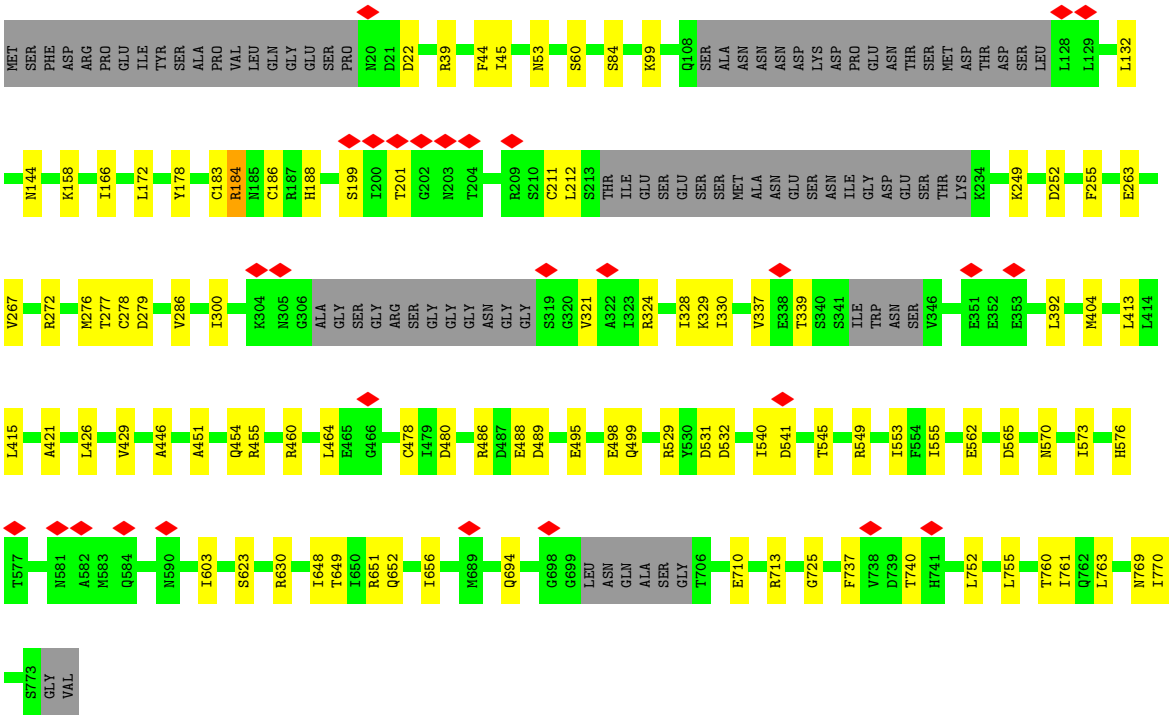
Chain 4:





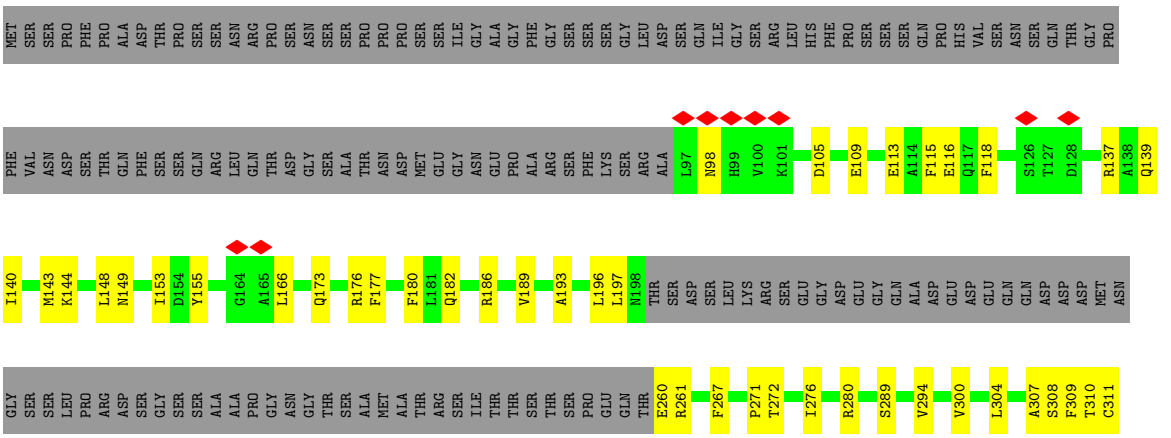
• Molecule 4: Minichromosome maintenance protein 5

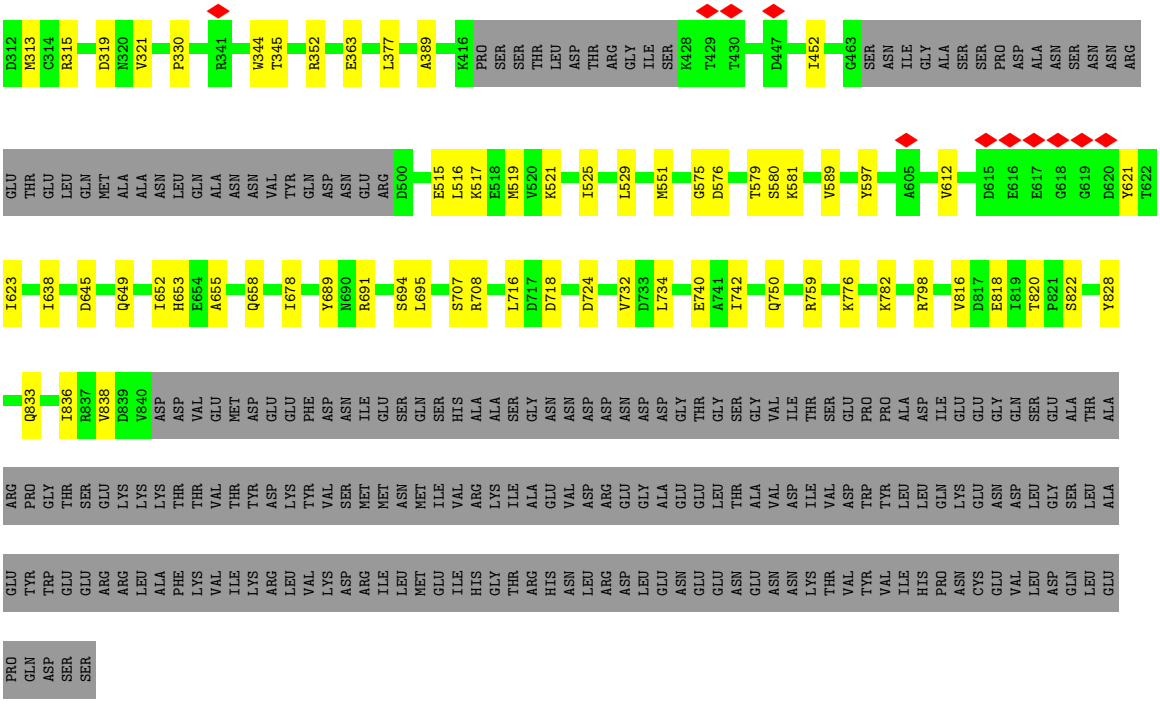
Chain 5:



• Molecule 5: DNA replication licensing factor MCM6

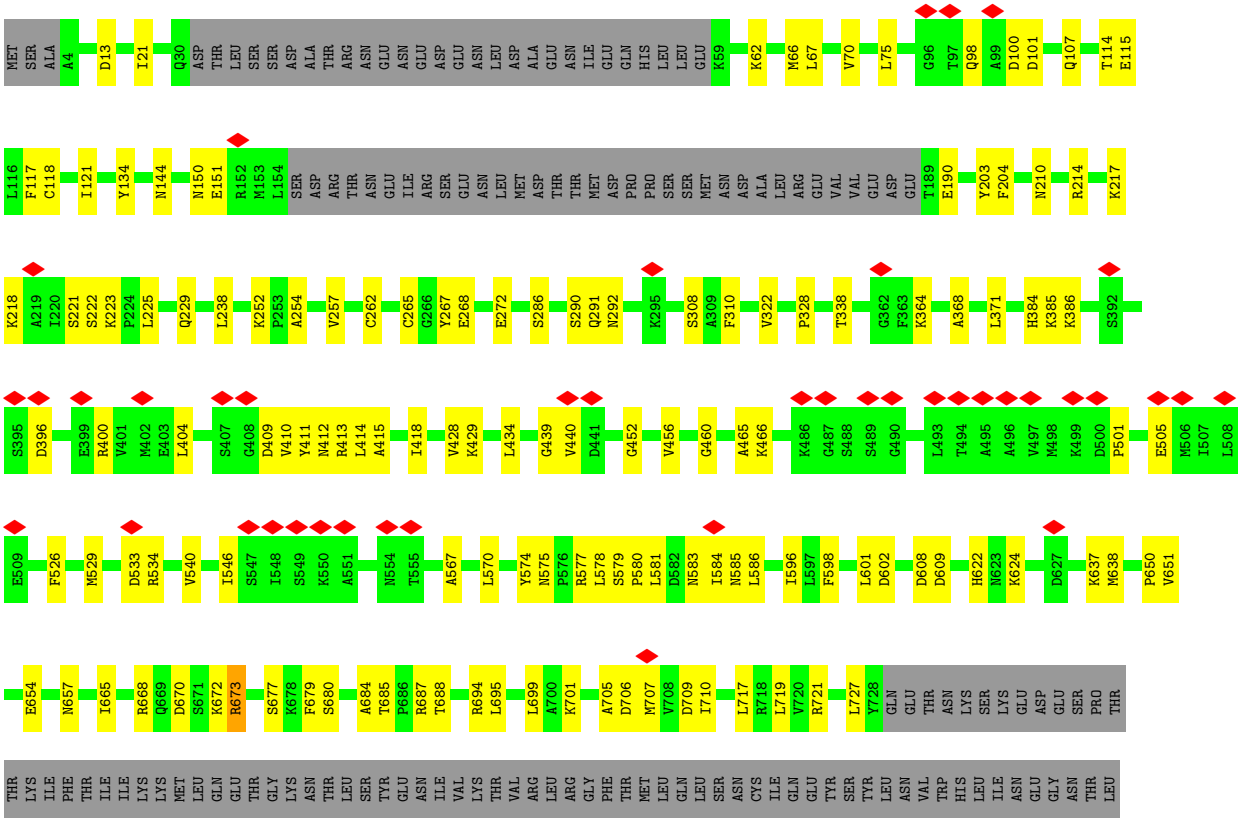
Chain 6:

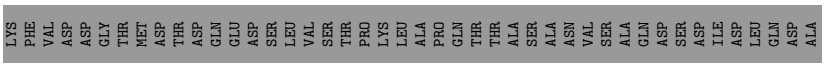




• Molecule 6: DNA replication licensing factor MCM7

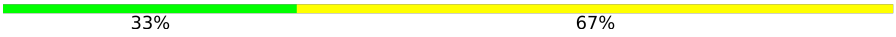
Chain 7:

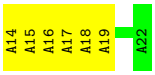




• Molecule 7: DNA (9-MER)

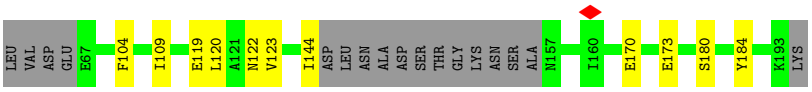
Chain A:





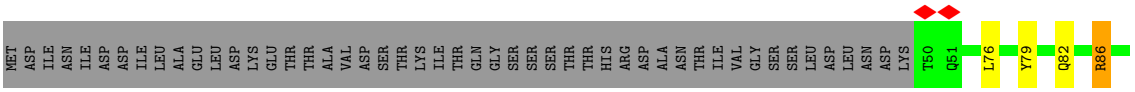
• Molecule 8: DNA replication complex GINS protein PSF3

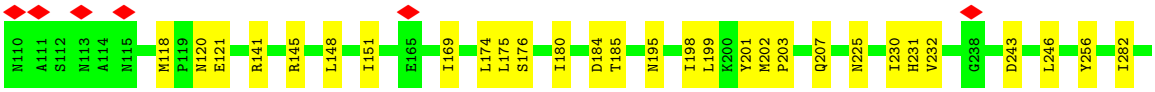
Chain C:

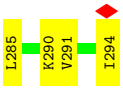


• Molecule 9: DNA replication complex GINS protein SLD5

Chain D:

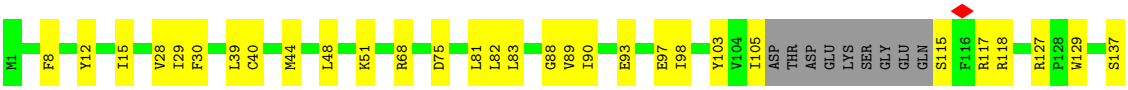


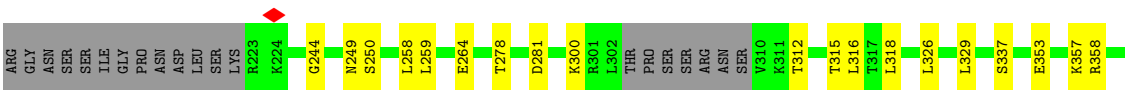


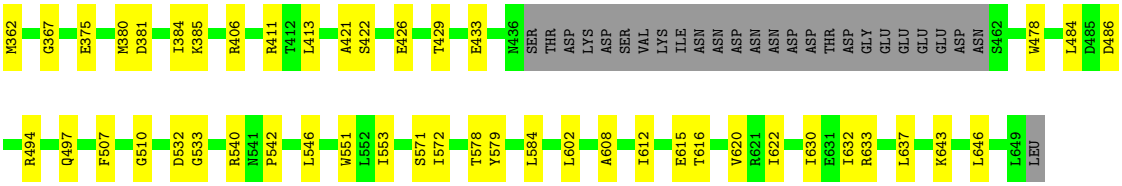


• Molecule 10: Cell division control protein 45

Chain E:

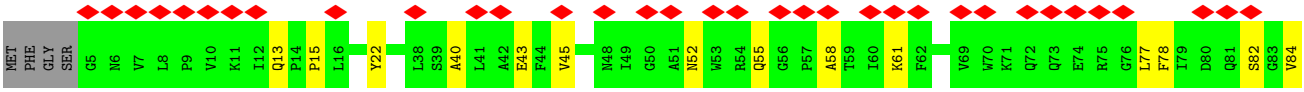


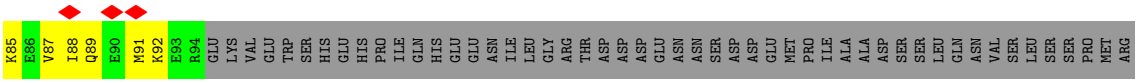


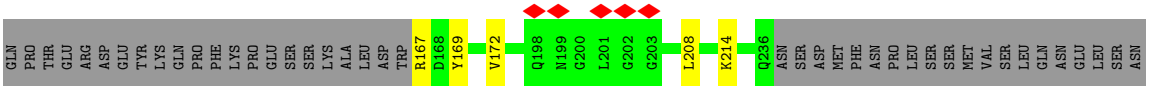


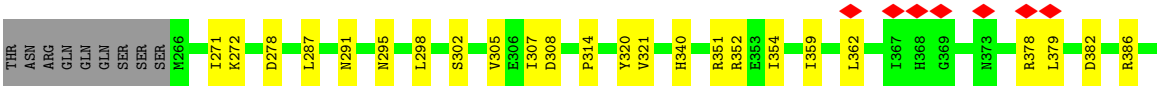
• Molecule 11: DNA polymerase epsilon subunit B

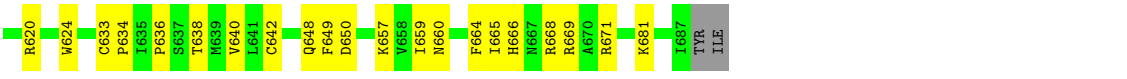
Chain F:

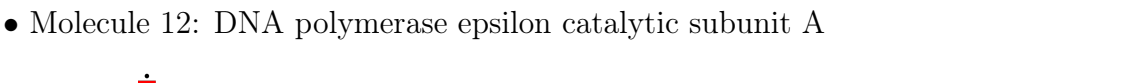


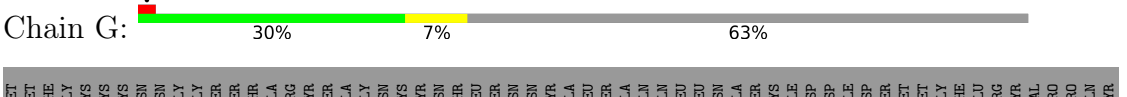


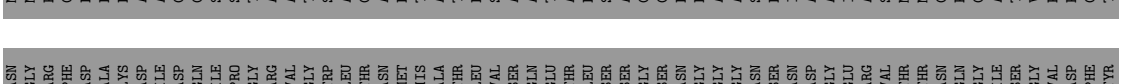


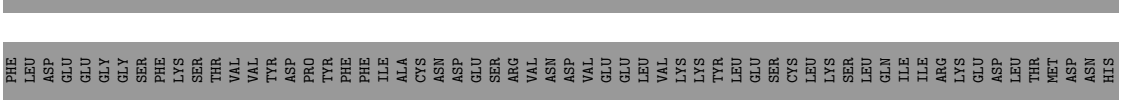


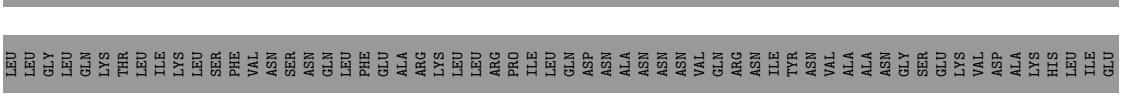


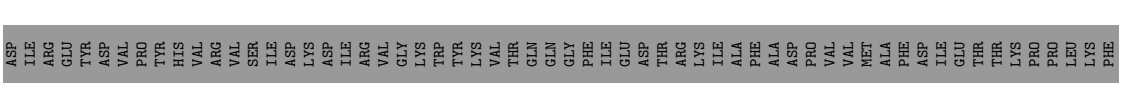






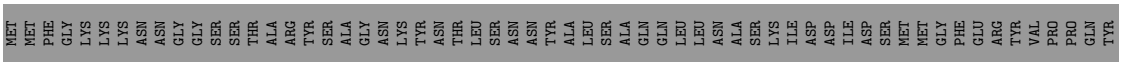


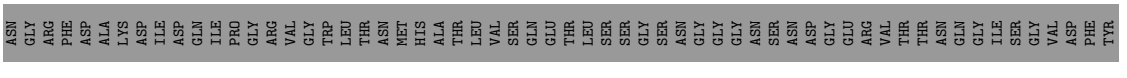




• Molecule 12: DNA polymerase epsilon catalytic subunit A

Chain G:





PRO ASP SER ALA VAL ASP GLN ILE MET MET ILE SER TYR MET ILE ASP GLY GLU GLY PHE LEU ILE THR ASN ARG GLU ILE ILE SER GLU ASP ILE GLU ASP PHE GLU TYR THR PRO LYS PRO GLU TYR PRO GLY PHE PHE THR ILE PHE ASN GLU ASN ASP GLU VAL ALA LEU LEU GLN

ARG PHE PHE GLU HIS ILE ARG ASP VAL ARG PRO THR VAL ILE SER THR PHE ASN GLY ASP PHE PHE ASP TRP PRO PHE ILE HIS ASN ARG SER LYS ILE HIS GLY LEU ASP MET PHE ASP GLU ILE GLY PHE ALA PRO ASP ALA GLU GLY GLU TYR LYS SER SER TYR CYS SER HIS MET

ASP CYS PHE ARG TRP VAL LYS ARG ASP SER TYR LEU PRO GLN GLY SER GLN GLY LEU LYS ALA VAL THR GLN SER LYS LEU GLY TYR ASN PRO ILE GLU LEU ASP PRO GLU LEU MET THR PRO TYR ALA PHE GLU LYS PRO GLN HIS LEU SER GLU TYR SER VAL SER ASP ALA VAL ALA

THR TYR TYR LEU TYR MET LYS TYR VAL HIS PRO PHE ILE PHE SER LEU CYS THR ILE ILE PRO LEU ASN PRO ASP GLU THR LEU ARG LYS GLY THR GLY THR LEU CYS GLU MET LEU LEU MET VAL GLN ALA TYR GLN HIS ASN ILE LEU LEU PRO ASN LYS HIS THR ASP PRO ILE GLU

ARG PHE TYR ASP GLY HIS LEU LEU GLU SER GLU THR TYR VAL GLY GLY HIS VAL GLU SER LEU GLU ALA GLY VAL PHE ARG SER ASP LEU LYS ASN GLU PHE LYS ILE ASP PRO SER ALA ILE ASP GLU LEU LEU GLN GLU LEU PRO GLU ALA LEU LYS PHE SER VAL GLU VAL GLU ASN

LYS SER SER VAL ASP LYS VAL THR ASN PHE GLU GLU ILE LYS ASN GLN ILE THR GLN LYS LEU LEU GLU LEU LYS GLU ASN ASN ILE ARG ASN GLU LEU PRO LEU ILE TYR HIS VAL ASP VAL ALA SER MET TYR PRO ASN ILE MET THR THR ASN ARG LEU GLN PRO ASP SER ILE LYS

ALA GLU ARG ASP CYS ALA SER CYS ASP PHE ASN ARG PRO GLY LYS THR CYS ALA ARG LYS LEU LYS TRP ALA TRP ARG GLY GLU PHE PHE PRO SER LYS MET ASP GLU TYR ASN MET ILE LYS ARG ALA LEU GLN ASN GLU THR PHE PRO ASN LYS ASN LYS PHE SER LYS LYS LYS VAL

LEU THR PHE ASP GLU LEU SER TYR ALA ASP GLN VAL ILE HIS ILE LYS LYS ARG LEU THR GLU TYR SER ARG LYS VAL TYR HIS ARG VAL LYS VAL SER GLU ILE VAL GLU ARG GLU ALA ILE VAL CYS GLN ARG GLU ASN PRO PHE TYR VAL ASP THR VAL LYS SER PHE ARG ASP ARG

ARG TYR GLU PHE LYS GLY LEU ALA LYS THR TRP LYS GLY ASN LEU SER LYS ILE ASP PRO SER ASP LYS HIS ALA ARG ASP GLU ALA LYS LYS MET ILE VAL LEU TYR ASP SER LEU GLN LEU ALA HIS LYS VAL ILE LEU ASN SER PHE TYR GLY TYR VAL MET ARG LYS GLY SER ARG

TRP TYR SER MET GLU MET ALA GLY ILE THR CYS LEU THR GLY ALA THR ILE ILE GLN MET ALA ARG ALA LEU VAL GLU ARG VAL GLY ARG PRO LEU GLU LEU ASP THR ASP GLY ILE TRP CYS ILE LEU PRO LYS SER PHE PRO GLU THR TYR PHE PHE THR LEU GLU ASN GLY LYS LYS

LEU TYR LEU SER TYR PRO CYS SER MET LEU ASN TYR ARG VAL HIS GLN LYS PHE THR ASN HIS GLN TYR GLN GLU LEU LYS ASP PRO LEU ASN TYR ILE TYR GLU THR HIS SER GLU ASN THR ILE PHE PHE GLU VAL ASP GLY PRO TYR LYS ALA MET ILE LEU PRO SER SER LYS GLU

GLU GLY LYS GLY ILE LYS LYS ARG TYR ALA ALA VAL PHE ASN GLU ASP GLY SER LEU ALA GLU LEU LYS GLY PHE GLU LEU LYS ARG ARG GLY GLU LEU GLN LEU ILE LYS ASN PHE GLN SER ASP ILE PHE LYS VAL PHE LEU GLU GLY ASP THR LEU GLU GLY CYS TYR SER ALA VAL ALA

SER VAL CYS ASN ARG TRP LEU ASP VAL LEU ASP SER HIS GLY LEU MET LEU GLU ASP GLU ASP LEU VAL SER LEU ILE CYS GLU ASN ARG SER MET SER LYS THR LEU LYS GLU TYR GLU GLY GLN LYS SER THR SER ILE THR THR ALA ARG ARG LEU GLY ASP PHE LEU GLY GLU ASP

MET VAL LYS ASP LYS GLY LEU GLN CYS LYS TYR ILE ILE SER SER LYS PRO PHE ASN ALA PRO VAL THR GLU ARG ALA ALA ILE PRO VAL ALA ILE PHE SER ALA ASP ILE PRO ILE LYS ARG SER PHE LEU ARG ARG TRP THR LEU ASP PRO SER LEU GLU ASP LEU ASP ILE ARG THR ILE

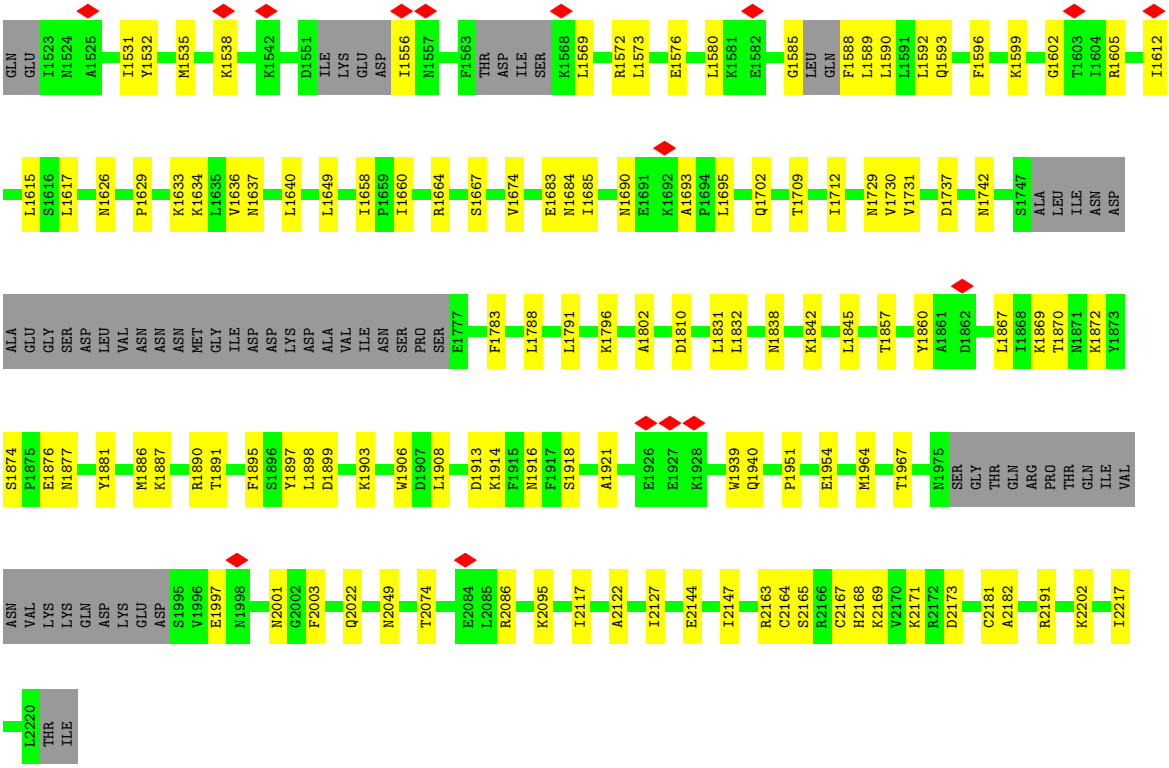
ILE ASP TRP GLY TYR TYR ARG GLU ARG LEU GLY SER ALA ILE GLN LYS ILE ILE THR ILE PRO ALA ALA LEU GLN GLY VAL SER ASN PRO VAL PRO ARG VAL GLU HIS PRO ASP TRP LEU LYS ARG LYS ILE ALA THR LYS GLU ASP LYS PHE LYS GLN THR SER LEU THR LYS PHE PHE

SER LYS THR LYS ASN VAL PRO THR MET GLY LYS ILE LYS ASP ILE GLU ASP LEU PHE GLU PRO THR VAL GLU GLU ASP ASN ALA LYS ILE LYS ILE ALA ARG THR THR LYS LYS LYS ALA VAL SER LYS ARG LYS ARG ASN GLN LEU THR ASN GLU GLU ASP PRO LEU VAL LEU PRO SER

GLU ILE PRO SER MET ASP GLU ASP TYR VAL GLY TRP LEU ASN TYR GLN LYS ILE LYS TRP LYS ILE GLN ALA ARG ASP ARG LYS ARG ARG ASP GLN LEU PHE GLY ASN THR ASN SER SER ARG GLU ARG SER ALA LEU GLY SER MET ILE ARG LYS GLN ALA GLU SER TYR ALA ASN SER

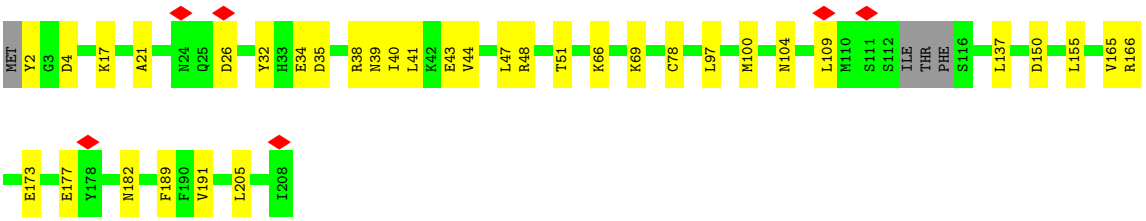
T1321 W1322 E1323 V1324 Y1327 G1331 G1334 V1338 F1339 V1340 T1341 I1342 N1343 G1344 K1345 V1346 Q1347 N1348 I1353 Y1358 F1361 M1366 P1367 L1368 Q1369 K1370 I1371 K1372 N1373 C1374 S1382 P1387 S1390 G1395 L1402 P1403 E1404 S1405 V1406 E1409 E1412 N1413 F1427

P1433 H1434 Q1435 I1438 M1439 D1440 L1441 V1445 T1446 F1447 R1448 S1449 K1450 ALA MET GLY A1454 L1455 G1456 Q1460 Q1461 M1465 K1466 D1467 L1468 S1469 N1473 L1477 I1484 G1485 Y1486 L1487 L1488 H1489 F1490 P1491 THR SER ILE GLY TYR E1497 D1507 V1513 LEU LYS PRO SER ASN GLN ALA



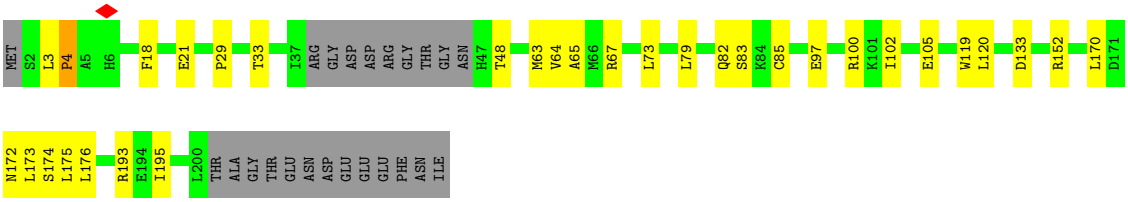
• Molecule 13: DNA replication complex GINS protein PSF1

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	87445	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.67	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3300	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.035	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	453.6, 453.6, 453.6	wwPDB
Map dimensions	420, 420, 420	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: ZN, ADP, ATP, MG

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	0.25	0/5321	0.52	0/7184
2	3	0.24	0/5154	0.50	0/6989
3	4	0.24	0/4769	0.50	0/6439
4	5	0.25	0/5523	0.49	0/7461
5	6	0.25	0/5113	0.50	0/6897
6	7	0.25	0/5306	0.52	0/7170
7	A	0.54	0/215	0.73	0/329
8	C	0.25	0/1441	0.45	0/1950
9	D	0.25	0/2056	0.46	0/2783
10	E	0.26	0/4358	0.46	0/5929
11	F	0.25	0/4474	0.48	0/6053
12	G	0.25	0/6770	0.45	0/9159
13	H	0.25	0/1683	0.48	0/2264
14	I	0.25	0/1624	0.49	0/2197
All	All	0.25	0/53807	0.49	0/72804

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

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	5235	0	5274	71	0
2	3	5067	0	5134	60	0
3	4	4702	0	4791	76	0
4	5	5447	0	5496	73	0
5	6	5032	0	5066	71	0
6	7	5223	0	5314	89	0
7	A	189	0	100	3	0
8	C	1408	0	1415	15	0
9	D	2014	0	2011	25	0
10	E	4276	0	4135	58	0
11	F	4379	0	4427	75	0
12	G	6628	0	6629	108	0
13	H	1663	0	1658	25	0
14	I	1591	0	1642	19	0
15	2	31	0	12	1	0
15	3	31	0	12	2	0
15	5	31	0	12	1	0
15	7	31	0	12	3	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	3	1	0	0	0	0
17	5	1	0	0	0	0
17	7	1	0	0	0	0
18	4	27	0	12	3	0
18	6	27	0	12	1	0
All	All	53042	0	53164	714	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 7.

All (714) 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)
4:5:755:LEU:HD21	4:5:763:LEU:HD23	1.48	0.92
1:2:789:VAL:HG11	1:2:838:ILE:HD11	1.65	0.78
12:G:1532:TYR:HH	12:G:1556:ILE:N	1.83	0.76
4:5:529:ARG:HD3	4:5:531:ASP:H	1.50	0.76
12:G:2167:CYS:SG	12:G:2169:LYS:NZ	2.59	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:744:VAL:HG12	3:4:745:GLU:H	1.52	0.73
12:G:1918:SER:HB2	12:G:1939:TRP:HE1	1.52	0.73
11:F:13:GLN:HG2	11:F:15:PRO:HD2	1.68	0.73
4:5:451:ALA:HB1	4:5:464:LEU:HD11	1.70	0.73
1:2:343:LYS:HD3	1:2:371:GLY:HA3	1.70	0.72
3:4:197:PHE:HE2	3:4:253:GLN:HB2	1.54	0.72
8:C:25:PRO:HA	8:C:37:PRO:HB3	1.72	0.71
5:6:143:MET:HG3	5:6:148:LEU:HB2	1.71	0.70
11:F:486:GLY:N	11:F:489:ASP:OD2	2.23	0.70
4:5:178:TYR:HB3	4:5:249:LYS:HE2	1.74	0.69
2:3:687:ARG:HA	2:3:697:ILE:HD11	1.75	0.69
11:F:308:ASP:HB3	11:F:340:HIS:HA	1.75	0.68
5:6:115:PHE:HA	5:6:118:PHE:CE2	2.29	0.68
12:G:1730:VAL:HG23	12:G:1870:THR:HB	1.75	0.68
6:7:540:VAL:HG12	6:7:546:ILE:HD11	1.76	0.68
13:H:32:TYR:HD2	13:H:34:GLU:H	1.41	0.68
2:3:700:ARG:NH2	15:7:901:ATP:O1A	2.27	0.67
6:7:101:ASP:OD2	6:7:217:LYS:NZ	2.27	0.67
11:F:538:GLU:HG2	11:F:636:PRO:HB3	1.75	0.67
5:6:294:VAL:HG21	5:6:389:ALA:HB1	1.77	0.67
2:3:583:ARG:HE	2:3:584:GLU:H	1.41	0.67
3:4:375:ASP:O	5:6:98:ASN:ND2	2.27	0.67
1:2:813:ILE:HG12	1:2:841:VAL:HG21	1.77	0.66
6:7:526:PHE:HB3	6:7:567:ALA:HB2	1.78	0.66
6:7:291:GLN:NE2	6:7:292:ASN:OD1	2.29	0.66
8:C:170:GLU:HB3	8:C:173:GLU:HG3	1.78	0.65
3:4:573:SER:H	18:4:1001:ADP:H5'1	1.62	0.65
12:G:2181:CYS:SG	12:G:2182:ALA:N	2.69	0.65
5:6:311:CYS:O	5:6:315:ARG:N	2.30	0.65
6:7:440:VAL:HG12	6:7:694:ARG:HG2	1.79	0.65
8:C:109:ILE:HD11	14:I:195:ILE:HG12	1.79	0.65
4:5:710:GLU:OE1	4:5:713:ARG:NH1	2.30	0.65
4:5:276:MET:HG2	4:5:328:ILE:HB	1.79	0.65
4:5:495:GLU:HA	4:5:498:GLU:HG2	1.76	0.65
12:G:1321:THR:N	12:G:1446:THR:HG1	1.94	0.65
2:3:442:LEU:HD21	2:3:462:MET:HE3	1.78	0.64
4:5:630:ARG:NH1	4:5:648:ILE:O	2.30	0.64
6:7:650:PRO:HD2	6:7:701:LYS:HG2	1.78	0.64
4:5:498:GLU:HG3	4:5:499:GLN:HG2	1.79	0.64
11:F:549:ARG:HH12	11:F:620:ARG:HD3	1.62	0.64
11:F:405:ASN:H	11:F:436:GLY:HA3	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:333:GLN:NE2	4:5:321:VAL:O	2.30	0.64
12:G:1857:THR:HB	12:G:1869:LYS:HB3	1.79	0.64
3:4:838:THR:HG23	3:4:840:PRO:HD2	1.78	0.64
12:G:1488:LEU:HG	12:G:1593:GLN:HB3	1.80	0.64
3:4:785:ARG:HE	3:4:786:SER:H	1.46	0.63
1:2:576:LEU:HA	1:2:595:ALA:HB3	1.80	0.63
9:D:195:ASN:HA	9:D:199:LEU:HB2	1.79	0.63
12:G:1342:ILE:HG23	12:G:1344:GLY:H	1.64	0.63
2:3:294:VAL:HG22	2:3:326:VAL:HG22	1.81	0.63
12:G:1347:GLN:NE2	12:G:1348:ASN:O	2.32	0.63
3:4:565:LEU:HD22	3:4:702:PHE:HE2	1.63	0.63
10:E:244:GLY:HA3	10:E:602:LEU:HB3	1.79	0.63
12:G:1742:ASN:HD22	12:G:1898:LEU:HG	1.64	0.63
12:G:1887:LYS:O	12:G:1891:THR:HG23	1.98	0.63
1:2:791:ALA:HB1	4:5:562:GLU:HG3	1.81	0.63
6:7:414:LEU:HD22	6:7:638:MET:HG3	1.80	0.63
11:F:172:VAL:HG23	11:F:532:ILE:HG22	1.80	0.62
6:7:368:ALA:HB1	6:7:371:LEU:HB3	1.81	0.62
10:E:93:GLU:HG2	10:E:98:ILE:HB	1.82	0.62
1:2:343:LYS:NZ	1:2:367:CYS:SG	2.72	0.62
1:2:422:GLU:OE1	1:2:458:ARG:NH1	2.33	0.62
2:3:455:ARG:NH1	2:3:500:ALA:O	2.31	0.62
10:E:411:ARG:NH2	10:E:486:ASP:OD2	2.33	0.62
12:G:1590:LEU:HB2	12:G:1612:ILE:HG12	1.81	0.62
12:G:1908:LEU:HD21	12:G:1964:MET:HG2	1.81	0.62
12:G:1690:ASN:ND2	12:G:1695:LEU:O	2.28	0.62
1:2:866:LEU:HD21	12:G:2074:THR:HG22	1.81	0.61
10:E:48:LEU:HD12	10:E:259:LEU:HD21	1.80	0.61
6:7:456:VAL:HG22	6:7:596:ILE:HB	1.82	0.61
10:E:312:THR:HG22	10:E:315:THR:HG23	1.81	0.61
5:6:310:THR:OG1	5:6:345:THR:OG1	2.18	0.61
6:7:150:ASN:OD1	6:7:151:GLU:N	2.32	0.61
8:C:104:PHE:N	8:C:170:GLU:OE2	2.31	0.61
11:F:430:THR:HG22	11:F:431:LEU:HD12	1.82	0.61
4:5:498:GLU:OE1	4:5:549:ARG:NH2	2.27	0.61
12:G:1322:TRP:HE1	12:G:1342:ILE:HG13	1.66	0.61
3:4:767:LYS:HG3	5:6:732:VAL:HG11	1.82	0.61
12:G:2117:ILE:HD11	12:G:2127:ILE:HG23	1.82	0.61
2:3:636:ALA:HA	8:C:43:LYS:HE2	1.82	0.60
12:G:1535:MET:HA	12:G:1538:LYS:HB2	1.83	0.60
5:6:695:LEU:H	5:6:838:VAL:HG23	1.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:559:THR:HA	1:2:764:MET:HE1	1.84	0.60
4:5:725:GLY:HA3	12:G:1838:ASN:HD21	1.66	0.60
3:4:425:ASP:OD2	5:6:280:ARG:NH2	2.34	0.60
3:4:527:ALA:HB3	3:4:537:LYS:HD3	1.84	0.60
12:G:1997:GLU:O	12:G:2001:ASN:ND2	2.34	0.60
3:4:774:TYR:HE2	5:6:724:ASP:HB2	1.67	0.59
13:H:104:ASN:HB2	13:H:109:LEU:HD13	1.83	0.59
11:F:89:GLN:HA	11:F:92:LYS:HG2	1.84	0.59
4:5:446:ALA:HB2	4:5:489:ASP:HA	1.83	0.59
14:I:64:VAL:HG13	14:I:67:ARG:HG3	1.83	0.59
1:2:527:VAL:HB	1:2:531:HIS:HB3	1.85	0.59
2:3:51:ASN:O	2:3:55:ASN:ND2	2.29	0.59
2:3:705:LEU:HD21	2:3:733:LEU:HD22	1.83	0.59
10:E:105:ILE:O	10:E:115:SER:N	2.36	0.59
12:G:1602:GLY:O	12:G:1605:ARG:NH1	2.35	0.59
6:7:67:LEU:HD21	6:7:121:ILE:HD12	1.85	0.58
12:G:2171:LYS:NZ	12:G:2173:ASP:O	2.24	0.58
9:D:232:VAL:HA	9:D:291:VAL:HG12	1.84	0.58
4:5:760:THR:HG23	4:5:761:ILE:HG12	1.85	0.58
11:F:554:ARG:NH1	11:F:555:LEU:O	2.36	0.58
1:2:211:LEU:HD22	1:2:271:PHE:HE1	1.68	0.58
2:3:97:ILE:HG12	2:3:156:SER:HB2	1.85	0.58
4:5:279:ASP:OD2	4:5:329:LYS:NZ	2.30	0.58
12:G:1448:ARG:H	12:G:1468:LEU:HD21	1.68	0.58
2:3:391:LYS:HB2	2:3:399:LEU:HB2	1.86	0.58
2:3:640:GLY:HA2	2:3:652:THR:HG23	1.85	0.58
5:6:575:GLY:O	5:6:581:LYS:NZ	2.34	0.58
11:F:55:GLN:HE22	11:F:58:ALA:H	1.51	0.58
2:3:411:PRO:HG3	4:5:545:THR:HG22	1.86	0.58
9:D:121:GLU:O	14:I:48:THR:OG1	2.22	0.58
11:F:379:LEU:HD21	11:F:382:ASP:HB2	1.86	0.58
12:G:1366:MET:SD	12:G:1366:MET:N	2.76	0.58
13:H:165:VAL:HG11	13:H:205:LEU:HD13	1.85	0.58
4:5:53:ASN:ND2	4:5:60:SER:O	2.37	0.57
9:D:148:LEU:HD13	9:D:151:ILE:HD11	1.85	0.57
11:F:668:ARG:O	11:F:669:ARG:NH1	2.37	0.57
10:E:316:LEU:HD13	10:E:413:LEU:HD13	1.86	0.57
11:F:640:VAL:HG22	11:F:659:ILE:HD11	1.86	0.57
1:2:202:ASN:HA	1:2:205:ARG:HH21	1.68	0.57
1:2:211:LEU:HD13	1:2:271:PHE:HD1	1.70	0.57
5:6:816:VAL:HG12	5:6:818:GLU:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:1683:GLU:HG3	12:G:1684:ASN:H	1.68	0.57
2:3:640:GLY:HA3	2:3:651:VAL:HA	1.86	0.57
5:6:589:VAL:HG21	5:6:597:TYR:HB2	1.86	0.57
6:7:225:LEU:HD23	6:7:229:GLN:HB3	1.85	0.57
6:7:575:ASN:HB3	6:7:577:ARG:HE	1.69	0.57
10:E:93:GLU:OE1	10:E:137:SER:OG	2.20	0.57
12:G:1737:ASP:HB2	12:G:1899:ASP:HB3	1.86	0.57
12:G:2202:LYS:HD3	12:G:2217:ILE:HG21	1.85	0.57
1:2:525:LYS:HB2	1:2:533:ILE:HB	1.85	0.57
12:G:1358:TYR:HB2	12:G:1427:PHE:HB2	1.86	0.57
6:7:98:GLN:NE2	6:7:100:ASP:O	2.34	0.57
10:E:68:ARG:NH2	10:E:97:GLU:OE2	2.38	0.57
12:G:1649:LEU:HB3	12:G:1660:ILE:HD11	1.86	0.57
3:4:638:SER:O	3:4:642:ARG:NE	2.29	0.57
4:5:532:ASP:OD1	4:5:694:GLN:NE2	2.31	0.57
14:I:170:LEU:HD13	14:I:173:LEU:HD22	1.85	0.57
2:3:496:THR:HG22	2:3:505:THR:HG22	1.86	0.56
1:2:335:LYS:HB3	1:2:381:VAL:HG13	1.87	0.56
4:5:337:VAL:HG13	4:5:339:THR:H	1.70	0.56
9:D:201:TYR:O	13:H:48:ARG:NH1	2.36	0.56
10:E:553:ILE:HD11	10:E:584:LEU:HB3	1.86	0.56
12:G:1658:ILE:HD11	12:G:1674:VAL:HG11	1.88	0.56
12:G:1913:ASP:OD1	12:G:1914:LYS:N	2.38	0.56
4:5:415:LEU:HD21	4:5:540:ILE:HD12	1.86	0.56
10:E:380:MET:SD	10:E:385:LYS:HG3	2.46	0.56
6:7:717:LEU:O	6:7:721:ARG:HG2	2.06	0.56
7:A:16:DA:H2"	7:A:17:DA:C8	2.40	0.56
10:E:39:LEU:HD21	10:E:484:LEU:HD11	1.87	0.56
4:5:300:ILE:HD12	4:5:324:ARG:HD3	1.87	0.56
1:2:792:ASP:OD1	1:2:795:ARG:NH1	2.39	0.55
3:4:744:VAL:HG12	3:4:745:GLU:N	2.20	0.55
2:3:542:ARG:NH2	15:7:901:ATP:O3G	2.37	0.55
12:G:1729:ASN:ND2	12:G:1872:LYS:O	2.38	0.55
14:I:82:GLN:HG3	14:I:83:SER:H	1.72	0.55
11:F:490:LEU:O	11:F:494:MET:HB2	2.07	0.55
2:3:331:ALA:O	2:3:339:ARG:NH2	2.39	0.55
2:3:448:THR:HA	2:3:455:ARG:HA	1.89	0.55
6:7:190:GLU:HG2	6:7:267:TYR:CZ	2.42	0.55
3:4:190:CYS:HB3	3:4:257:LEU:HD12	1.88	0.55
10:E:572:ILE:HD13	10:E:579:TYR:HE1	1.71	0.55
11:F:516:ILE:HG22	11:F:523:VAL:HG11	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:H:189:PHE:HB3	13:H:191:VAL:HG13	1.88	0.55
1:2:271:PHE:CE2	1:2:295:VAL:HG11	2.41	0.55
11:F:351:ARG:H	11:F:354:ILE:HD11	1.72	0.55
14:I:79:LEU:HB3	14:I:85:CYS:HB2	1.87	0.55
5:6:734:LEU:HD11	5:6:742:ILE:HD13	1.89	0.55
11:F:650:ASP:HB2	11:F:681:LYS:HE3	1.89	0.55
12:G:2163:ARG:NH1	12:G:2168:HIS:O	2.40	0.55
15:3:1002:ATP:O1A	4:5:651:ARG:NH2	2.40	0.54
5:6:177:PHE:HA	5:6:180:PHE:HD2	1.71	0.54
13:H:173:GLU:HA	13:H:182:ASN:HA	1.89	0.54
4:5:413:LEU:HB3	4:5:553:ILE:HG22	1.88	0.54
3:4:808:HIS:ND1	3:4:821:ASP:OD1	2.34	0.54
5:6:260:GLU:O	5:6:352:ARG:NH1	2.41	0.54
7:A:14:DA:H2"	7:A:15:DA:C8	2.42	0.54
11:F:214:LYS:HB3	11:F:624:TRP:CD1	2.42	0.54
5:6:173:GLN:HB2	5:6:176:ARG:HB3	1.88	0.54
13:H:97:LEU:HA	13:H:100:MET:SD	2.48	0.54
1:2:310:ARG:HH21	5:6:300:VAL:HG11	1.72	0.54
11:F:434:TRP:HZ3	11:F:465:LEU:HD21	1.72	0.54
6:7:654:GLU:OE2	6:7:657:ASN:ND2	2.40	0.54
10:E:249:ASN:OD1	10:E:250:SER:N	2.40	0.54
12:G:1634:LYS:HA	12:G:1637:ASN:HD21	1.73	0.54
14:I:152:ARG:NH2	14:I:172:ASN:O	2.40	0.54
5:6:140:ILE:HA	5:6:143:MET:HE2	1.90	0.53
10:E:51:LYS:NZ	10:E:264:GLU:OE1	2.32	0.53
12:G:1593:GLN:NE2	12:G:1615:LEU:O	2.41	0.53
6:7:286:SER:O	6:7:290:SER:N	2.34	0.53
1:2:508:HIS:HB3	1:2:511:ILE:HD12	1.90	0.53
4:5:166:ILE:HG13	4:5:286:VAL:HG11	1.90	0.53
10:E:510:GLY:HA3	10:E:551:TRP:CZ3	2.43	0.53
11:F:272:LYS:HB2	11:F:302:SER:HB2	1.89	0.53
4:5:172:LEU:HB2	4:5:252:ASP:OD1	2.08	0.53
3:4:435:VAL:HB	3:4:463:VAL:HG11	1.91	0.53
10:E:30:PHE:HB2	10:E:83:LEU:HD23	1.90	0.53
12:G:1345:LYS:HZ3	12:G:1585:GLY:HA3	1.74	0.53
1:2:419:LYS:NZ	4:5:267:VAL:O	2.41	0.53
9:D:285:LEU:HG	9:D:290:LYS:HD2	1.89	0.53
12:G:2022:GLN:NE2	12:G:2049:ASN:OD1	2.41	0.53
1:2:300:PHE:O	1:2:319:ARG:NH1	2.42	0.52
2:3:330:HIS:O	2:3:339:ARG:NH2	2.33	0.52
12:G:1916:ASN:HD21	12:G:1940:GLN:HE21	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:635:ASP:N	3:4:635:ASP:OD1	2.43	0.52
5:6:820:THR:HG22	5:6:822:SER:H	1.74	0.52
6:7:223:LYS:O	6:7:225:LEU:HD12	2.09	0.52
6:7:577:ARG:HG3	6:7:581:LEU:HD12	1.91	0.52
6:7:578:LEU:HG	6:7:580:PRO:HD2	1.90	0.52
11:F:352:ARG:NH2	11:F:538:GLU:OE1	2.38	0.52
3:4:361:ASP:OD2	3:4:362:ARG:NH1	2.39	0.52
6:7:384:HIS:CG	6:7:385:LYS:H	2.27	0.52
10:E:281:ASP:OD2	10:E:406:ARG:NH1	2.43	0.52
10:E:429:THR:O	10:E:433:GLU:HG2	2.10	0.52
1:2:581:ARG:HH12	1:2:583:ASP:HA	1.75	0.52
1:2:850:LYS:O	1:2:854:ARG:HG3	2.09	0.52
3:4:408:ASP:OD1	3:4:408:ASP:N	2.43	0.52
10:E:89:VAL:HG23	10:E:90:ILE:HG23	1.91	0.52
11:F:45:VAL:HG13	11:F:52:ASN:ND2	2.25	0.52
11:F:291:ASN:OD1	11:F:295:ASN:N	2.38	0.52
1:2:783:MET:SD	4:5:570:ASN:ND2	2.83	0.52
2:3:480:ASP:O	2:3:483:ARG:HB2	2.10	0.52
3:4:535:ASP:OD1	3:4:535:ASP:N	2.42	0.52
3:4:799:GLU:OE1	3:4:803:ARG:NH1	2.37	0.52
4:5:426:LEU:HD12	4:5:478:CYS:HB3	1.92	0.52
10:E:88:GLY:O	10:E:129:TRP:HB2	2.09	0.52
1:2:688:ASP:HB3	1:2:691:ALA:HB3	1.92	0.52
11:F:596:VAL:HG12	11:F:649:PHE:HZ	1.74	0.52
1:2:814:LEU:HD13	4:5:576:HIS:NE2	2.24	0.52
5:6:308:SER:HA	5:6:319:ASP:HA	1.91	0.52
5:6:707:SER:OG	5:6:798:ARG:NH1	2.43	0.52
9:D:198:ILE:HG22	9:D:202:MET:HE1	1.91	0.52
4:5:183:CYS:SG	4:5:184:ARG:N	2.83	0.51
5:6:689:TYR:HB3	5:6:716:LEU:HD11	1.92	0.51
6:7:584:ILE:HG22	6:7:586:LEU:HD23	1.91	0.51
10:E:381:ASP:HB3	10:E:384:ILE:HG12	1.91	0.51
10:E:507:PHE:HA	10:E:551:TRP:CZ3	2.45	0.51
13:H:2:TYR:N	13:H:78:CYS:HG	2.08	0.51
6:7:404:LEU:HG	6:7:637:LYS:HE3	1.93	0.51
1:2:341:CYS:SG	1:2:343:LYS:HG2	2.51	0.51
4:5:22:ASP:OD1	4:5:22:ASP:N	2.44	0.51
11:F:84:VAL:O	11:F:88:ILE:HG13	2.10	0.51
12:G:1531:ILE:HD11	12:G:1633:LYS:HG2	1.92	0.51
12:G:1572:ARG:NH2	12:G:1576:GLU:OE2	2.42	0.51
1:2:271:PHE:CD2	1:2:295:VAL:HG11	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:573:SER:HB2	18:4:1001:ADP:H2'	1.92	0.51
12:G:1596:PHE:HB3	12:G:1599:LYS:HB3	1.92	0.51
6:7:257:VAL:HG22	6:7:272:GLU:HB3	1.93	0.51
6:7:685:THR:HG22	6:7:687:ARG:H	1.76	0.51
10:E:326:LEU:HB3	10:E:337:SER:OG	2.11	0.51
11:F:633:CYS:HB3	11:F:634:PRO:HD3	1.92	0.51
4:5:486:ARG:NH2	4:5:488:GLU:OE1	2.44	0.51
2:3:462:MET:SD	2:3:489:VAL:HG11	2.51	0.51
6:7:254:ALA:N	6:7:308:SER:O	2.40	0.51
9:D:185:THR:HG21	13:H:137:LEU:HD21	1.93	0.51
12:G:2164:CYS:SG	12:G:2165:SER:N	2.84	0.51
14:I:21:GLU:HA	14:I:73:LEU:HD23	1.91	0.51
11:F:439:THR:HG22	11:F:441:VAL:H	1.75	0.51
12:G:1441:LEU:HD12	12:G:1445:VAL:HG23	1.92	0.50
1:2:289:ILE:HD11	10:E:367:GLY:HA2	1.92	0.50
10:E:572:ILE:HD13	10:E:579:TYR:CE1	2.45	0.50
4:5:211:CYS:SG	4:5:212:LEU:N	2.84	0.50
4:5:763:LEU:HD13	4:5:769:ASN:O	2.11	0.50
6:7:428:VAL:HG22	6:7:598:PHE:HD2	1.76	0.50
6:7:622:HIS:HB3	6:7:624:LYS:HG2	1.94	0.50
6:7:409:ASP:O	6:7:413:ARG:NH1	2.44	0.50
13:H:35:ASP:OD1	13:H:35:ASP:N	2.44	0.50
12:G:1334:GLY:N	12:G:1404:GLU:OE1	2.44	0.50
6:7:322:VAL:HG21	6:7:328:PRO:HG3	1.94	0.50
12:G:1387:PRO:HD3	12:G:1831:LEU:HD11	1.92	0.50
8:C:28:GLY:HA3	8:C:38:ILE:HD11	1.93	0.50
9:D:176:SER:O	9:D:180:ILE:HG13	2.11	0.50
10:E:105:ILE:H	10:E:115:SER:N	2.10	0.50
11:F:321:VAL:HG21	11:F:550:PHE:HD1	1.76	0.49
9:D:184:ASP:OD1	9:D:185:THR:N	2.45	0.49
10:E:149:ASP:N	10:E:149:ASP:OD1	2.46	0.49
11:F:398:LYS:NZ	11:F:427:ASP:OD2	2.34	0.49
13:H:47:LEU:O	13:H:51:THR:HG23	2.12	0.49
11:F:298:LEU:HG	11:F:307:ILE:HD11	1.94	0.49
12:G:1664:ARG:NH1	12:G:1667:SER:OG	2.46	0.49
14:I:102:ILE:HA	14:I:105:GLU:OE1	2.12	0.49
1:2:763:LEU:O	1:2:767:ILE:HG12	2.12	0.49
15:3:1002:ATP:O3G	4:5:549:ARG:NH2	2.43	0.49
3:4:437:GLY:HA3	3:4:463:VAL:HA	1.94	0.49
4:5:763:LEU:HD11	4:5:770:ILE:HD13	1.93	0.49
6:7:501:PRO:HG2	6:7:505:GLU:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:1593:GLN:HE22	12:G:1617:LEU:HB2	1.77	0.49
6:7:262:CYS:N	6:7:268:GLU:OE1	2.46	0.49
10:E:620:VAL:HG12	10:E:632:ILE:HG13	1.95	0.49
13:H:38:ARG:HA	13:H:41:LEU:HD12	1.95	0.49
12:G:1874:SER:OG	12:G:1876:GLU:OE1	2.31	0.49
3:4:281:VAL:HA	3:4:284:ILE:HG12	1.94	0.49
10:E:579:TYR:CD2	10:E:637:LEU:HD22	2.47	0.49
11:F:477:GLU:HA	11:F:521:LYS:HZ3	1.77	0.49
2:3:481:VAL:O	2:3:484:VAL:HG12	2.13	0.49
3:4:553:THR:OG1	5:6:740:GLU:OE2	2.31	0.49
6:7:434:LEU:HD11	6:7:699:LEU:HG	1.95	0.49
12:G:1580:LEU:HB3	12:G:1588:PHE:CZ	2.48	0.49
6:7:262:CYS:SG	6:7:265:CYS:HB2	2.53	0.48
6:7:115:GLU:HA	6:7:118:CYS:SG	2.52	0.48
11:F:401:ILE:HG22	11:F:433:ILE:HB	1.95	0.48
11:F:443:VAL:HG23	11:F:454:SER:HB2	1.95	0.48
3:4:637:MET:O	3:4:641:THR:OG1	2.31	0.48
4:5:421:ALA:HB2	15:5:1701:ATP:C8	2.48	0.48
6:7:400:ARG:HB3	6:7:637:LYS:NZ	2.29	0.48
9:D:230:ILE:HD13	9:D:282:ILE:HD11	1.95	0.48
11:F:531:ARG:HG2	11:F:540:VAL:HG12	1.95	0.48
11:F:638:THR:HG23	11:F:657:LYS:HG3	1.94	0.48
2:3:668:ILE:HG13	2:3:668:ILE:O	2.13	0.48
3:4:368:PRO:HG2	3:4:382:MET:SD	2.54	0.48
6:7:210:ASN:O	6:7:214:ARG:HG2	2.14	0.48
6:7:460:GLY:O	6:7:466:LYS:NZ	2.45	0.48
7:A:18:DA:H2"	7:A:19:DA:N7	2.29	0.48
12:G:1908:LEU:HD11	12:G:1964:MET:HE2	1.95	0.48
12:G:1913:ASP:HB3	12:G:1916:ASN:HB2	1.95	0.48
3:4:762:ILE:HG22	3:4:817:VAL:HG11	1.96	0.48
10:E:12:TYR:HA	10:E:15:ILE:HD12	1.95	0.48
3:4:712:VAL:HG13	6:7:668:ARG:HB3	1.96	0.48
12:G:1353:ILE:HB	12:G:1433:PRO:HB3	1.95	0.48
1:2:678:ASP:HB3	1:2:812:SER:HB2	1.96	0.48
2:3:314:LEU:HD13	4:5:255:PHE:HE2	1.78	0.48
3:4:744:VAL:CG1	3:4:745:GLU:H	2.25	0.48
6:7:62:LYS:HG2	6:7:66:MET:HE1	1.96	0.48
10:E:103:TYR:HA	10:E:117:ARG:HD3	1.95	0.48
10:E:353:GLU:O	10:E:357:LYS:HG2	2.13	0.48
11:F:167:ARG:HB2	11:F:397:HIS:CD2	2.49	0.48
14:I:18:PHE:HA	14:I:21:GLU:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:652:GLN:O	4:5:656:ILE:HG13	2.13	0.48
5:6:833:GLN:HA	5:6:836:ILE:HB	1.94	0.48
9:D:169:ILE:HD11	9:D:174:LEU:HD21	1.96	0.48
11:F:77:LEU:H	11:F:77:LEU:HD23	1.79	0.48
11:F:489:ASP:O	11:F:493:SER:OG	2.27	0.48
12:G:1435:GLN:HA	12:G:1438:ILE:HG22	1.96	0.48
4:5:630:ARG:HH12	4:5:649:THR:HA	1.78	0.48
12:G:1842:LYS:O	12:G:1845:LEU:HG	2.14	0.48
3:4:329:LYS:HG2	3:4:434:GLU:HB3	1.96	0.47
4:5:339:THR:HG22	4:5:339:THR:O	2.14	0.47
11:F:648:GLN:HA	11:F:660:ASN:O	2.14	0.47
2:3:671:LEU:HA	2:3:721:VAL:HB	1.96	0.47
3:4:435:VAL:HG12	3:4:466:VAL:HG22	1.97	0.47
3:4:531:TYR:HB2	3:4:723:HIS:CD2	2.49	0.47
5:6:516:LEU:HD13	5:6:519:MET:HE3	1.96	0.47
6:7:677:SER:HA	6:7:680:SER:OG	2.14	0.47
2:3:420:ARG:NH2	4:5:495:GLU:OE2	2.47	0.47
5:6:137:ARG:O	5:6:140:ILE:HG22	2.14	0.47
9:D:256:TYR:CZ	9:D:290:LYS:HD3	2.50	0.47
14:I:174:SER:OG	14:I:175:LEU:N	2.48	0.47
3:4:641:THR:O	3:4:644:VAL:HB	2.15	0.47
4:5:186:CYS:SG	4:5:188:HIS:ND1	2.81	0.47
5:6:144:LYS:HZ1	5:6:196:LEU:HB2	1.78	0.47
5:6:517:LYS:O	5:6:521:LYS:HG2	2.14	0.47
11:F:58:ALA:HA	11:F:61:LYS:HE3	1.96	0.47
3:4:601:LEU:HB3	3:4:621:LEU:HD23	1.96	0.47
4:5:263:GLU:OE1	4:5:263:GLU:N	2.46	0.47
3:4:456:LEU:HD23	6:7:252:LYS:HE2	1.96	0.47
3:4:565:LEU:HD22	3:4:702:PHE:CE2	2.48	0.47
5:6:309:PHE:HB3	5:6:344:TRP:HB3	1.97	0.47
8:C:46:LEU:HD22	8:C:50:LEU:HD11	1.97	0.47
11:F:208:LEU:O	12:G:2191:ARG:NH2	2.36	0.47
12:G:1465:MET:O	12:G:1469:SER:OG	2.26	0.47
1:2:416:ASP:OD2	4:5:272:ARG:NH2	2.43	0.47
1:2:743:ARG:O	1:2:746:GLN:HG2	2.14	0.47
3:4:569:ASP:OD1	3:4:569:ASP:N	2.46	0.47
4:5:45:ILE:HG22	8:C:144:ILE:HD11	1.97	0.47
5:6:689:TYR:O	5:6:691:ARG:NH1	2.48	0.47
6:7:66:MET:O	6:7:70:VAL:HG23	2.14	0.47
1:2:191:ALA:HB3	1:2:197:TRP:HB2	1.96	0.47
1:2:774:ILE:HG13	1:2:825:LEU:HG	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:573:ILE:HA	4:5:576:HIS:HD1	1.80	0.47
6:7:412:ASN:OD1	6:7:413:ARG:HG3	2.14	0.47
6:7:570:LEU:HD23	6:7:585:ASN:ND2	2.30	0.47
12:G:1796:LYS:NZ	12:G:1897:TYR:OH	2.40	0.47
13:H:17:LYS:O	13:H:21:ALA:N	2.46	0.47
3:4:565:LEU:HD12	3:4:566:LEU:H	1.80	0.46
3:4:204:LYS:NZ	3:4:207:LYS:HE3	2.30	0.46
3:4:521:LEU:HA	3:4:524:ARG:HG2	1.97	0.46
6:7:411:TYR:HA	6:7:414:LEU:HD12	1.97	0.46
8:C:122:ASN:OD1	8:C:123:VAL:N	2.48	0.46
3:4:809:ALA:HB2	3:4:817:VAL:HG12	1.98	0.46
9:D:82:GLN:HG3	9:D:86:ARG:NE	2.31	0.46
12:G:1788:LEU:HD12	12:G:1791:LEU:HD11	1.96	0.46
5:6:776:LYS:HD2	5:6:828:TYR:CG	2.51	0.46
10:E:643:LYS:HA	10:E:646:LEU:HG	1.96	0.46
11:F:494:MET:HE1	12:G:2147:ILE:HG22	1.97	0.46
14:I:3:LEU:N	14:I:4:PRO:HD2	2.30	0.46
2:3:646:GLU:HB3	2:3:648:PRO:HD2	1.98	0.46
11:F:271:ILE:HG23	11:F:305:VAL:HG13	1.96	0.46
1:2:307:ARG:NH2	1:2:402:LEU:O	2.49	0.46
1:2:782:ASP:OD1	12:G:2086:ARG:NE	2.44	0.46
2:3:352:LYS:O	2:3:355:LYS:HG2	2.16	0.46
2:3:679:ILE:HA	2:3:682:ASN:HD21	1.80	0.46
13:H:4:ASP:OD1	13:H:4:ASP:N	2.47	0.46
2:3:410:ASP:OD1	2:3:410:ASP:N	2.48	0.46
6:7:114:THR:HG22	6:7:204:PHE:HE2	1.81	0.46
11:F:87:VAL:O	11:F:91:MET:HG2	2.15	0.46
12:G:1382:SER:HB2	12:G:1685:ILE:HG12	1.97	0.46
12:G:1886:MET:HG3	12:G:1890:ARG:HE	1.80	0.46
1:2:335:LYS:HB2	1:2:383:ARG:HG3	1.98	0.46
1:2:613:ASN:ND2	1:2:614:ASP:OD1	2.49	0.46
3:4:245:ALA:O	3:4:249:LEU:N	2.48	0.46
11:F:22:TYR:CD2	13:H:177:GLU:HB2	2.51	0.46
11:F:278:ASP:N	11:F:278:ASP:OD1	2.48	0.46
12:G:1535:MET:HE2	12:G:1640:LEU:HD12	1.98	0.46
12:G:1634:LYS:HA	12:G:1637:ASN:ND2	2.31	0.46
9:D:231:HIS:HB2	9:D:294:ILE:HD11	1.98	0.45
10:E:278:THR:HG21	10:E:421:ALA:HB1	1.97	0.45
10:E:478:TRP:HB3	13:H:166:ARG:HH12	1.81	0.45
12:G:1633:LYS:O	12:G:1637:ASN:ND2	2.49	0.45
3:4:645:LEU:HA	3:4:648:VAL:HG12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:392:LEU:HD11	4:5:429:VAL:HG13	1.97	0.45
4:5:752:LEU:HA	4:5:755:LEU:HD12	1.98	0.45
1:2:838:ILE:HG23	1:2:865:THR:HG22	1.98	0.45
5:6:525:ILE:HD12	5:6:525:ILE:H	1.81	0.45
5:6:612:VAL:HG12	5:6:623:ILE:HG22	1.98	0.45
12:G:1406:VAL:HA	12:G:1409:GLU:CD	2.37	0.45
2:3:375:ASP:OD1	2:3:375:ASP:N	2.49	0.45
2:3:722:ASN:HB3	2:3:724:VAL:HG22	1.99	0.45
2:3:201:HIS:NE2	2:3:232:PRO:HD2	2.32	0.45
3:4:743:PRO:HB2	3:4:747:LEU:HG	1.99	0.45
2:3:56:TYR:HD1	6:7:218:LYS:HE2	1.80	0.45
2:3:198:ARG:HD3	2:3:211:TYR:HD2	1.81	0.45
5:6:140:ILE:HD11	5:6:189:VAL:HG23	1.97	0.45
5:6:276:ILE:HB	5:6:363:GLU:HG2	1.99	0.45
10:E:615:GLU:HG3	10:E:616:THR:HG23	1.98	0.45
11:F:169:TYR:HB3	11:F:386:ARG:HH12	1.81	0.45
3:4:644:VAL:O	3:4:647:GLU:HG3	2.16	0.45
5:6:182:GLN:HG3	5:6:186:ARG:HE	1.82	0.45
6:7:428:VAL:HG22	6:7:598:PHE:CD2	2.51	0.45
1:2:620:ILE:HG13	1:2:624:MET:HE2	1.99	0.45
2:3:673:GLN:NE2	2:3:674:GLU:OE2	2.50	0.45
2:3:687:ARG:HH22	6:7:602:ASP:CG	2.20	0.45
10:E:571:SER:OG	10:E:572:ILE:N	2.50	0.45
12:G:1602:GLY:HA2	12:G:1605:ARG:HH22	1.81	0.45
12:G:1860:TYR:HB3	12:G:1867:LEU:HD12	1.98	0.45
12:G:2122:ALA:HB3	12:G:2127:ILE:HD11	1.98	0.45
2:3:198:ARG:HD3	2:3:211:TYR:CD2	2.52	0.45
3:4:607:ARG:HH22	3:4:612:LYS:HA	1.82	0.45
5:6:304:LEU:HD21	5:6:307:ALA:HB2	1.98	0.45
9:D:79:TYR:CE2	9:D:176:SER:HB2	2.52	0.45
11:F:400:VAL:HG13	11:F:432:LEU:HD13	1.98	0.45
1:2:326:ARG:NH1	1:2:583:ASP:OD1	2.50	0.45
2:3:278:LEU:HD13	2:3:282:LEU:HD12	1.99	0.45
4:5:99:LYS:HG2	4:5:132:LEU:HD12	1.99	0.45
5:6:186:ARG:HA	5:6:189:VAL:HG12	1.98	0.45
5:6:653:HIS:O	5:6:708:ARG:NH2	2.38	0.45
12:G:1488:LEU:HD23	12:G:1490:PHE:CZ	2.52	0.45
1:2:232:ARG:O	1:2:236:GLU:HG2	2.16	0.44
2:3:662:TYR:CE1	2:3:666:ARG:HG3	2.52	0.44
3:4:573:SER:N	18:4:1001:ADP:H5'1	2.29	0.44
5:6:515:GLU:OE2	5:6:750:GLN:NE2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:F:503:LEU:HD21	11:F:620:ARG:HE	1.82	0.44
6:7:134:TYR:OH	6:7:144:ASN:ND2	2.36	0.44
12:G:1895:PHE:HB3	12:G:1898:LEU:HD12	1.99	0.44
13:H:41:LEU:HA	13:H:44:VAL:HG12	1.98	0.44
1:2:211:LEU:HD22	1:2:271:PHE:CE1	2.50	0.44
1:2:806:THR:OG1	1:2:807:VAL:N	2.51	0.44
6:7:529:MET:O	6:7:534:ARG:NH2	2.50	0.44
6:7:679:PHE:HB2	6:7:727:LEU:HD13	2.00	0.44
9:D:203:PRO:O	9:D:207:GLN:HG3	2.17	0.44
10:E:608:ALA:O	10:E:612:ILE:HG12	2.18	0.44
12:G:1615:LEU:O	12:G:1615:LEU:HD23	2.17	0.44
12:G:2095:LYS:HD2	12:G:2095:LYS:HA	1.78	0.44
13:H:26:ASP:OD1	13:H:26:ASP:N	2.46	0.44
5:6:525:ILE:O	5:6:529:LEU:N	2.48	0.44
12:G:1361:PHE:CD2	12:G:1366:MET:HB2	2.52	0.44
12:G:1870:THR:HG23	12:G:1881:TYR:HE2	1.82	0.44
1:2:769:TYR:CE1	1:2:773:LYS:HD2	2.53	0.44
4:5:737:PHE:HA	4:5:740:THR:OG1	2.18	0.44
1:2:551:GLN:NE2	5:6:658:GLN:HE22	2.15	0.44
2:3:535:LEU:HB3	2:3:539:LEU:HD11	2.00	0.44
3:4:406:VAL:HG13	3:4:410:GLN:HB2	1.99	0.44
3:4:655:SER:HB3	3:4:664:THR:HG22	2.00	0.44
6:7:70:VAL:HG22	6:7:75:LEU:HB3	2.00	0.44
11:F:544:ASP:N	11:F:544:ASP:OD1	2.51	0.44
1:2:474:PHE:O	1:2:768:HIS:ND1	2.46	0.44
1:2:589:TRP:NE1	4:5:454:GLN:OE1	2.48	0.44
5:6:153:ILE:HB	5:6:267:PHE:CD1	2.53	0.44
5:6:551:MET:O	5:6:759:ARG:NH2	2.51	0.44
11:F:167:ARG:HB2	11:F:397:HIS:NE2	2.32	0.44
6:7:21:ILE:HG12	6:7:117:PHE:HE1	1.83	0.44
11:F:55:GLN:NE2	11:F:58:ALA:H	2.15	0.44
12:G:1435:GLN:HB3	12:G:1439:MET:HE3	1.99	0.44
12:G:1484:ILE:HD12	12:G:1589:LEU:HB2	1.99	0.44
1:2:614:ASP:OD1	1:2:614:ASP:N	2.51	0.43
3:4:261:LEU:HD12	3:4:265:PRO:HA	1.99	0.43
5:6:189:VAL:HG13	5:6:197:LEU:HD11	1.99	0.43
6:7:705:ALA:O	6:7:707:MET:N	2.48	0.43
10:E:358:ARG:O	10:E:362:MET:HG2	2.18	0.43
3:4:428:ARG:HD3	3:4:431:ASP:OD2	2.19	0.43
6:7:579:SER:OG	6:7:580:PRO:HD3	2.19	0.43
5:6:645:ASP:O	5:6:649:GLN:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:107:GLN:NE2	6:7:238:LEU:O	2.37	0.43
12:G:1742:ASN:ND2	12:G:1898:LEU:HG	2.31	0.43
2:3:56:TYR:CD1	6:7:218:LYS:HE2	2.53	0.43
2:3:673:GLN:HA	2:3:676:ILE:HB	2.00	0.43
3:4:607:ARG:HH12	3:4:612:LYS:HA	1.83	0.43
3:4:819:LEU:O	3:4:822:VAL:HG22	2.18	0.43
4:5:529:ARG:NH1	4:5:532:ASP:H	2.16	0.43
5:6:718:ASP:OD1	5:6:718:ASP:N	2.51	0.43
6:7:13:ASP:N	6:7:13:ASP:OD1	2.50	0.43
5:6:113:GLU:O	5:6:116:GLU:HG2	2.19	0.43
5:6:149:ASN:HB3	5:6:261:ARG:NH2	2.33	0.43
6:7:651:VAL:HG22	6:7:706:ASP:OD1	2.19	0.43
9:D:199:LEU:HA	9:D:202:MET:HE1	1.99	0.43
10:E:540:ARG:HE	10:E:540:ARG:HB2	1.61	0.43
10:E:578:THR:HG22	10:E:633:ARG:HD2	2.00	0.43
3:4:338:VAL:HG23	5:6:452:ILE:HD12	1.99	0.43
6:7:574:TYR:HB2	6:7:601:LEU:HD22	2.01	0.43
5:6:652:ILE:O	5:6:655:ALA:N	2.52	0.43
6:7:410:VAL:O	6:7:414:LEU:HG	2.19	0.43
12:G:1342:ILE:HG22	12:G:1345:LYS:O	2.18	0.43
1:2:206:THR:HA	1:2:209:ARG:HG2	2.01	0.43
3:4:432:ARG:HB3	3:4:469:VAL:HG22	1.99	0.43
3:4:687:PRO:HG2	3:4:690:GLU:OE1	2.19	0.43
5:6:580:SER:HA	18:6:1101:ADP:H5'2	2.01	0.43
10:E:406:ARG:NH2	10:E:422:SER:OG	2.52	0.43
12:G:1802:ALA:HB1	12:G:1810:ASP:OD1	2.19	0.43
4:5:84:SER:HB3	4:5:199:SER:HB3	2.00	0.43
6:7:695:LEU:HD21	6:7:719:LEU:HD23	2.01	0.43
11:F:409:ASP:OD1	11:F:409:ASP:N	2.51	0.43
12:G:1513:VAL:HG12	12:G:1569:LEU:HD23	2.00	0.43
12:G:1690:ASN:HD21	12:G:1693:ALA:HB3	1.84	0.43
2:3:279:ASP:OD1	2:3:279:ASP:N	2.51	0.43
2:3:544:ASP:OD2	2:3:704:THR:OG1	2.22	0.43
4:5:392:LEU:HB3	4:5:603:ILE:CD1	2.49	0.43
4:5:392:LEU:HB3	4:5:603:ILE:HD11	2.00	0.43
4:5:480:ASP:OD1	4:5:480:ASP:N	2.49	0.43
4:5:541:ASP:OD1	4:5:541:ASP:N	2.50	0.43
6:7:396:ASP:O	6:7:400:ARG:HG2	2.19	0.43
6:7:414:LEU:O	6:7:418:ILE:HG13	2.19	0.43
11:F:287:LEU:HD23	11:F:287:LEU:HA	1.93	0.43
12:G:1374:CYS:SG	12:G:1402:LEU:HD12	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:1626:ASN:O	12:G:1629:PRO:HD2	2.18	0.43
3:4:195:ARG:NH1	3:4:196:ASN:OD1	2.51	0.42
3:4:826:VAL:HA	3:4:829:ILE:HG22	2.01	0.42
5:6:144:LYS:HZ1	5:6:193:ALA:HB1	1.84	0.42
9:D:141:ARG:NE	13:H:150:ASP:O	2.52	0.42
2:3:703:GLU:O	2:3:707:ARG:HG2	2.18	0.42
3:4:230:LEU:HD11	3:4:280:MET:CE	2.49	0.42
4:5:278:CYS:HB3	4:5:330:ILE:HD12	2.01	0.42
10:E:148:VAL:HG13	10:E:152:LEU:HD12	2.01	0.42
11:F:314:PRO:HB2	11:F:320:TYR:CE2	2.53	0.42
11:F:359:ILE:O	11:F:378:ARG:NH1	2.51	0.42
14:I:33:THR:HG22	14:I:63:MET:SD	2.59	0.42
3:4:349:CYS:SG	3:4:381:SER:OG	2.70	0.42
5:6:576:ASP:O	5:6:579:THR:HG22	2.20	0.42
6:7:221:SER:OG	6:7:222:SER:N	2.50	0.42
9:D:203:PRO:HB3	13:H:48:ARG:HD3	2.00	0.42
1:2:783:MET:HE1	4:5:573:ILE:HB	2.01	0.42
6:7:529:MET:HB2	6:7:533:ASP:HB3	2.01	0.42
10:E:29:ILE:HG12	10:E:82:LEU:HD12	2.02	0.42
14:I:29:PRO:HG2	14:I:65:ALA:HA	2.02	0.42
3:4:183:THR:HG23	3:4:185:VAL:H	1.85	0.42
3:4:343:LYS:HA	3:4:343:LYS:HD3	1.86	0.42
6:7:364:LYS:HD3	6:7:364:LYS:HA	1.79	0.42
6:7:465:ALA:HB2	15:7:901:ATP:C8	2.55	0.42
6:7:651:VAL:N	6:7:706:ASP:OD1	2.49	0.42
9:D:145:ARG:HD3	13:H:155:LEU:HD21	2.02	0.42
10:E:127:ARG:O	10:E:129:TRP:CE3	2.72	0.42
1:2:391:GLN:HG2	1:2:405:HIS:CD2	2.54	0.42
1:2:641:GLN:OE1	1:2:643:ARG:NH1	2.52	0.42
2:3:40:ASP:HA	2:3:43:ARG:NE	2.34	0.42
2:3:299:LYS:HD3	2:3:322:LEU:HD11	2.02	0.42
3:4:230:LEU:HD23	3:4:283:LEU:HG	2.01	0.42
3:4:608:ASP:OD1	3:4:609:VAL:N	2.53	0.42
5:6:694:SER:HB2	5:6:838:VAL:HG22	2.02	0.42
14:I:97:GLU:O	14:I:100:ARG:HG2	2.20	0.42
1:2:191:ALA:HB1	1:2:196:GLU:HG3	2.02	0.42
1:2:581:ARG:HE	5:6:621:TYR:HE2	1.68	0.42
2:3:277:ILE:HB	2:3:320:LEU:HD21	2.00	0.42
5:6:155:TYR:CD2	5:6:271:PRO:HD3	2.54	0.42
6:7:100:ASP:N	6:7:100:ASP:OD1	2.52	0.42
8:C:6:ILE:HD13	13:H:17:LYS:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:243:ASP:HB2	9:D:246:LEU:HD23	2.01	0.42
11:F:40:ALA:O	11:F:43:GLU:HG3	2.19	0.42
12:G:1709:THR:HA	12:G:1712:ILE:HG12	2.00	0.42
12:G:1967:THR:HG21	12:G:2003:PHE:HB3	2.00	0.42
14:I:176:LEU:HD23	14:I:176:LEU:HA	1.92	0.42
3:4:545:PHE:O	3:4:755:LYS:HE2	2.20	0.42
6:7:203:TYR:HE2	6:7:338:THR:HG22	1.85	0.42
6:7:709:ASP:OD1	6:7:710:ILE:N	2.53	0.42
9:D:76:LEU:HD21	9:D:175:LEU:HD21	2.01	0.42
10:E:422:SER:O	10:E:426:GLU:HG2	2.20	0.42
11:F:477:GLU:HA	11:F:521:LYS:NZ	2.34	0.42
12:G:2202:LYS:HD2	12:G:2202:LYS:HA	1.84	0.42
1:2:506:TYR:H	15:2:901:ATP:HN61	1.68	0.42
6:7:439:GLY:N	6:7:452:GLY:O	2.38	0.42
10:E:8:PHE:HB3	10:E:258:LEU:HD13	2.01	0.42
11:F:466:ALA:HB1	11:F:519:VAL:HG21	2.02	0.42
12:G:1477:LEU:HD23	12:G:1477:LEU:HA	1.94	0.42
12:G:1485:GLY:N	12:G:1589:LEU:O	2.41	0.42
5:6:321:VAL:HG21	5:6:330:PRO:HG3	2.02	0.42
6:7:385:LYS:C	6:7:386:LYS:HD3	2.40	0.42
13:H:66:LYS:O	13:H:69:LYS:HG2	2.20	0.42
1:2:510:ASP:OD1	1:2:510:ASP:N	2.53	0.41
3:4:839:ASP:HB3	3:4:840:PRO:HD3	2.02	0.41
5:6:319:ASP:OD1	5:6:319:ASP:N	2.53	0.41
6:7:608:ASP:OD1	6:7:609:ASP:N	2.52	0.41
6:7:668:ARG:HH11	6:7:684:ALA:HB1	1.85	0.41
10:E:28:VAL:HB	10:E:81:LEU:HD13	2.02	0.41
10:E:318:LEU:HD23	10:E:318:LEU:HA	1.89	0.41
11:F:77:LEU:HG	11:F:78:PHE:CD2	2.55	0.41
11:F:664:PHE:CD2	11:F:665:ILE:HG23	2.54	0.41
1:2:336:TYR:HD1	1:2:350:PRO:HB2	1.85	0.41
2:3:559:ARG:NH1	4:5:623:SER:OG	2.53	0.41
4:5:144:ASN:ND2	10:E:375:GLU:HA	2.35	0.41
4:5:498:GLU:HB2	4:5:651:ARG:NH2	2.35	0.41
9:D:118:MET:HG3	9:D:120:ASN:H	1.85	0.41
10:E:532:ASP:OD1	10:E:533:GLY:N	2.52	0.41
12:G:1573:LEU:HD23	12:G:1573:LEU:HA	1.95	0.41
2:3:313:THR:HG22	4:5:201:THR:O	2.20	0.41
2:3:649:LYS:HE2	2:3:649:LYS:HB3	1.82	0.41
3:4:796:ARG:O	3:4:799:GLU:HG3	2.20	0.41
5:6:139:GLN:HG2	5:6:143:MET:HE1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:F:482:ILE:HD13	11:F:524:VAL:HB	2.01	0.41
12:G:1324:VAL:HG11	12:G:1327:TYR:CE2	2.55	0.41
12:G:1535:MET:HE1	12:G:1636:VAL:C	2.41	0.41
12:G:1535:MET:HE1	12:G:1637:ASN:HA	2.02	0.41
12:G:1788:LEU:HD12	12:G:1788:LEU:HA	1.92	0.41
3:4:349:CYS:O	3:4:353:ASP:N	2.52	0.41
8:C:119:GLU:HG2	8:C:120:LEU:HD12	2.03	0.41
10:E:542:PRO:O	10:E:546:LEU:HD23	2.20	0.41
11:F:89:GLN:HA	11:F:92:LYS:HE2	2.01	0.41
11:F:546:LEU:HD12	11:F:550:PHE:HE2	1.85	0.41
12:G:1702:GLN:H	12:G:1702:GLN:HG3	1.71	0.41
12:G:1874:SER:HB3	12:G:1877:ASN:ND2	2.36	0.41
2:3:712:HIS:CD2	2:3:728:VAL:HG11	2.55	0.41
4:5:158:LYS:HA	4:5:158:LYS:HD3	1.81	0.41
6:7:404:LEU:HD23	6:7:404:LEU:HA	1.95	0.41
10:E:75:ASP:O	10:E:118:ARG:NH2	2.47	0.41
11:F:404:ALA:HB2	11:F:642:CYS:SG	2.61	0.41
11:F:481:MET:HB2	11:F:523:VAL:HG12	2.02	0.41
11:F:539:ILE:HA	11:F:638:THR:O	2.20	0.41
1:2:596:LEU:HD11	1:2:620:ILE:HG22	2.02	0.41
2:3:314:LEU:HD13	4:5:277:THR:HG21	2.02	0.41
2:3:725:ASP:HA	2:3:728:VAL:HG12	2.03	0.41
4:5:415:LEU:O	4:5:555:ILE:HA	2.21	0.41
5:6:105:ASP:O	5:6:109:GLU:HG2	2.20	0.41
5:6:272:THR:O	5:6:289:SER:OG	2.37	0.41
6:7:668:ARG:O	6:7:672:LYS:HG3	2.20	0.41
6:7:685:THR:HB	6:7:688:THR:HG23	2.02	0.41
1:2:400:GLY:O	3:4:660:GLY:HA2	2.20	0.41
2:3:327:TYR:HA	2:3:328:PRO:HD3	1.94	0.41
5:6:782:LYS:HD2	5:6:782:LYS:HA	1.83	0.41
10:E:326:LEU:HD12	10:E:329:LEU:HD22	2.03	0.41
2:3:181:SER:HB2	2:3:295:VAL:HG22	2.02	0.41
3:4:743:PRO:HG2	3:4:747:LEU:HD21	2.01	0.41
6:7:217:LYS:HB2	6:7:217:LYS:HE3	1.91	0.41
6:7:665:ILE:HD13	6:7:665:ILE:HA	1.93	0.41
11:F:359:ILE:HD12	11:F:362:LEU:HD12	2.03	0.41
12:G:1906:TRP:CE3	12:G:1921:ALA:HB2	2.56	0.41
13:H:40:ILE:O	13:H:43:GLU:HG3	2.20	0.41
1:2:189:VAL:HG12	1:2:197:TRP:CE3	2.56	0.41
2:3:370:SER:HB2	4:5:404:MET:SD	2.61	0.41
2:3:374:HIS:O	2:3:378:LYS:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:242:ASN:HB3	3:4:306:TYR:HE2	1.86	0.41
4:5:455:ARG:HH22	4:5:460:ARG:HB3	1.86	0.41
6:7:254:ALA:HB2	6:7:310:PHE:HB2	2.03	0.41
6:7:670:ASP:HA	6:7:673:ARG:HH21	1.86	0.41
8:C:27:LEU:HD23	8:C:27:LEU:HA	1.85	0.41
11:F:527:SER:OG	11:F:529:PRO:O	2.34	0.41
12:G:1535:MET:HE3	12:G:1640:LEU:HB2	2.03	0.41
1:2:410:LEU:HD23	1:2:453:ALA:HB3	2.03	0.41
1:2:573:ALA:N	1:2:616:ASP:OD1	2.54	0.41
1:2:783:MET:HE1	4:5:570:ASN:HA	2.02	0.41
2:3:99:SER:HB2	2:3:158:LYS:HE3	2.03	0.41
10:E:40:CYS:O	10:E:44:MET:HG3	2.21	0.41
12:G:1731:VAL:HB	12:G:1906:TRP:HB2	2.02	0.41
12:G:1742:ASN:HD21	12:G:1895:PHE:HA	1.86	0.41
3:4:829:ILE:O	3:4:833:ILE:HG12	2.20	0.40
4:5:39:ARG:HB3	4:5:44:PHE:CD2	2.56	0.40
5:6:377:LEU:HD11	5:6:452:ILE:HG22	2.03	0.40
5:6:638:ILE:HD12	5:6:678:ILE:HD11	2.02	0.40
9:D:225:ASN:HB3	14:I:193:ARG:HD2	2.03	0.40
11:F:666:HIS:CE1	11:F:671:ARG:HH21	2.39	0.40
1:2:792:ASP:OD2	1:2:864:TYR:OH	2.24	0.40
5:6:261:ARG:HE	5:6:261:ARG:HB2	1.72	0.40
6:7:210:ASN:HB2	6:7:214:ARG:NH2	2.36	0.40
11:F:445:ALA:HA	12:G:2144:GLU:HG2	2.03	0.40
12:G:1338:VAL:HG12	12:G:1340:VAL:HB	2.02	0.40
1:2:835:ASP:O	1:2:838:ILE:HG22	2.22	0.40
3:4:230:LEU:HD11	3:4:280:MET:HE3	2.02	0.40
5:6:313:MET:SD	5:6:313:MET:N	2.95	0.40
8:C:15:GLU:OE1	8:C:15:GLU:N	2.53	0.40
8:C:180:SER:O	8:C:184:TYR:HD2	2.03	0.40
11:F:58:ALA:HA	11:F:61:LYS:HG2	2.03	0.40
11:F:517:ASN:HA	11:F:523:VAL:HG21	2.03	0.40
14:I:119:TRP:CE2	14:I:120:LEU:HG	2.56	0.40
1:2:551:GLN:HE22	5:6:658:GLN:HE22	1.70	0.40
3:4:186:SER:HB3	3:4:260:GLN:CD	2.42	0.40
5:6:118:PHE:CE2	5:6:166:LEU:HD21	2.56	0.40
6:7:415:ALA:O	6:7:429:LYS:HD3	2.21	0.40
8:C:32:ASN:HD21	8:C:38:ILE:HD11	1.85	0.40
10:E:622:ILE:HG23	10:E:630:ILE:HG22	2.03	0.40
12:G:1435:GLN:HB3	12:G:1439:MET:CE	2.51	0.40
12:G:1903:LYS:HB2	12:G:1903:LYS:HE2	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:H:35:ASP:O	13:H:39:ASN:ND2	2.46	0.40
14:I:133:ASP:OD1	14:I:133:ASP:N	2.54	0.40
1:2:398:PRO:HA	1:2:399:PRO:HD3	1.95	0.40
1:2:438:LEU:HD23	1:2:438:LEU:HA	1.87	0.40
3:4:456:LEU:HD21	6:7:310:PHE:CD2	2.56	0.40
4:5:562:GLU:HA	4:5:565:ASP:HB2	2.03	0.40
5:6:189:VAL:O	5:6:193:ALA:N	2.48	0.40
10:E:494:ARG:O	10:E:497:GLN:HG2	2.20	0.40
11:F:82:SER:O	11:F:85:LYS:N	2.54	0.40
12:G:1487:LEU:O	12:G:1592:LEU:HA	2.22	0.40
12:G:1783:PHE:CZ	12:G:1832:LEU:HB2	2.56	0.40
12:G:1951:PRO:HA	12:G:1954:GLU:HG2	2.02	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%)	637 (97%)	21 (3%)	0	100	100
2	3	641/1006 (64%)	625 (98%)	16 (2%)	0	100	100
3	4	580/933 (62%)	555 (96%)	25 (4%)	0	100	100
4	5	681/775 (88%)	651 (96%)	30 (4%)	0	100	100
5	6	628/1017 (62%)	602 (96%)	26 (4%)	0	100	100
6	7	657/845 (78%)	617 (94%)	39 (6%)	1 (0%)	47	79
8	C	169/229 (74%)	165 (98%)	4 (2%)	0	100	100
9	D	243/294 (83%)	232 (96%)	11 (4%)	0	100	100
10	E	539/657 (82%)	528 (98%)	11 (2%)	0	100	100
11	F	540/689 (78%)	509 (94%)	31 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
12	G	807/2222 (36%)	773 (96%)	34 (4%)	0	100 100
13	H	200/208 (96%)	191 (96%)	9 (4%)	0	100 100
14	I	186/213 (87%)	173 (93%)	12 (6%)	1 (0%)	29 67
All	All	6529/9956 (66%)	6258 (96%)	269 (4%)	2 (0%)	100 100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	I	4	PRO
6	7	583	ASN

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	576/770 (75%)	575 (100%)	1 (0%)	93 96
2	3	557/864 (64%)	556 (100%)	1 (0%)	93 96
3	4	533/848 (63%)	529 (99%)	4 (1%)	81 89
4	5	615/688 (89%)	614 (100%)	1 (0%)	93 96
5	6	555/886 (63%)	555 (100%)	0	100 100
6	7	584/753 (78%)	583 (100%)	1 (0%)	93 96
8	C	158/199 (79%)	157 (99%)	1 (1%)	86 91
9	D	235/279 (84%)	234 (100%)	1 (0%)	91 94
10	E	452/592 (76%)	451 (100%)	1 (0%)	93 96
11	F	492/629 (78%)	492 (100%)	0	100 100
12	G	742/2014 (37%)	742 (100%)	0	100 100
13	H	189/193 (98%)	189 (100%)	0	100 100
14	I	180/198 (91%)	180 (100%)	0	100 100
All	All	5868/8913 (66%)	5857 (100%)	11 (0%)	93 96

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	743	ARG
2	3	188	LYS
3	4	228	LYS
3	4	252	LYS
3	4	428	ARG
3	4	510	ARG
4	5	184	ARG
6	7	673	ARG
8	C	43	LYS
9	D	86	ARG
10	E	300	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	405	HIS
1	2	551	GLN
12	G	1940	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 10 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	ADP	6	1101	-	24,29,29	0.95	1 (4%)	29,45,45	1.52	4 (13%)
15	ATP	5	1701	17	26,33,33	0.61	0	31,52,52	0.80	2 (6%)
15	ATP	7	901	17	26,33,33	0.59	0	31,52,52	0.79	1 (3%)
18	ADP	4	1001	-	24,29,29	0.95	1 (4%)	29,45,45	1.49	4 (13%)
15	ATP	2	901	-	26,33,33	0.60	0	31,52,52	0.79	2 (6%)
15	ATP	3	1002	17	26,33,33	0.61	0	31,52,52	0.81	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	ADP	6	1101	-	-	6/12/32/32	0/3/3/3
15	ATP	5	1701	17	-	4/18/38/38	0/3/3/3
15	ATP	7	901	17	-	6/18/38/38	0/3/3/3
18	ADP	4	1001	-	-	4/12/32/32	0/3/3/3
15	ATP	2	901	-	-	5/18/38/38	0/3/3/3
15	ATP	3	1002	17	-	2/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	1001	ADP	C5-C4	2.54	1.47	1.40
18	6	1101	ADP	C5-C4	2.47	1.47	1.40

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	6	1101	ADP	PA-O3A-PB	-3.89	119.47	132.83
18	4	1001	ADP	C3'-C2'-C1'	3.63	106.44	100.98
18	4	1001	ADP	PA-O3A-PB	-3.61	120.45	132.83
18	6	1101	ADP	C3'-C2'-C1'	3.39	106.08	100.98
18	6	1101	ADP	N3-C2-N1	-3.15	123.76	128.68
18	4	1001	ADP	N3-C2-N1	-3.09	123.85	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	6	1101	ADP	C4-C5-N7	-2.70	106.59	109.40
18	4	1001	ADP	C4-C5-N7	-2.58	106.71	109.40
15	3	1002	ATP	C5-C6-N6	2.33	123.89	120.35
15	2	901	ATP	C5-C6-N6	2.29	123.84	120.35
15	5	1701	ATP	C5-C6-N6	2.27	123.81	120.35
15	7	901	ATP	C5-C6-N6	2.26	123.79	120.35
15	3	1002	ATP	PB-O3B-PG	2.05	139.88	132.83
15	2	901	ATP	PB-O3B-PG	2.05	139.86	132.83
15	5	1701	ATP	PB-O3B-PG	2.01	139.74	132.83

There are no chirality outliers.

All (27) torsion outliers are listed below:

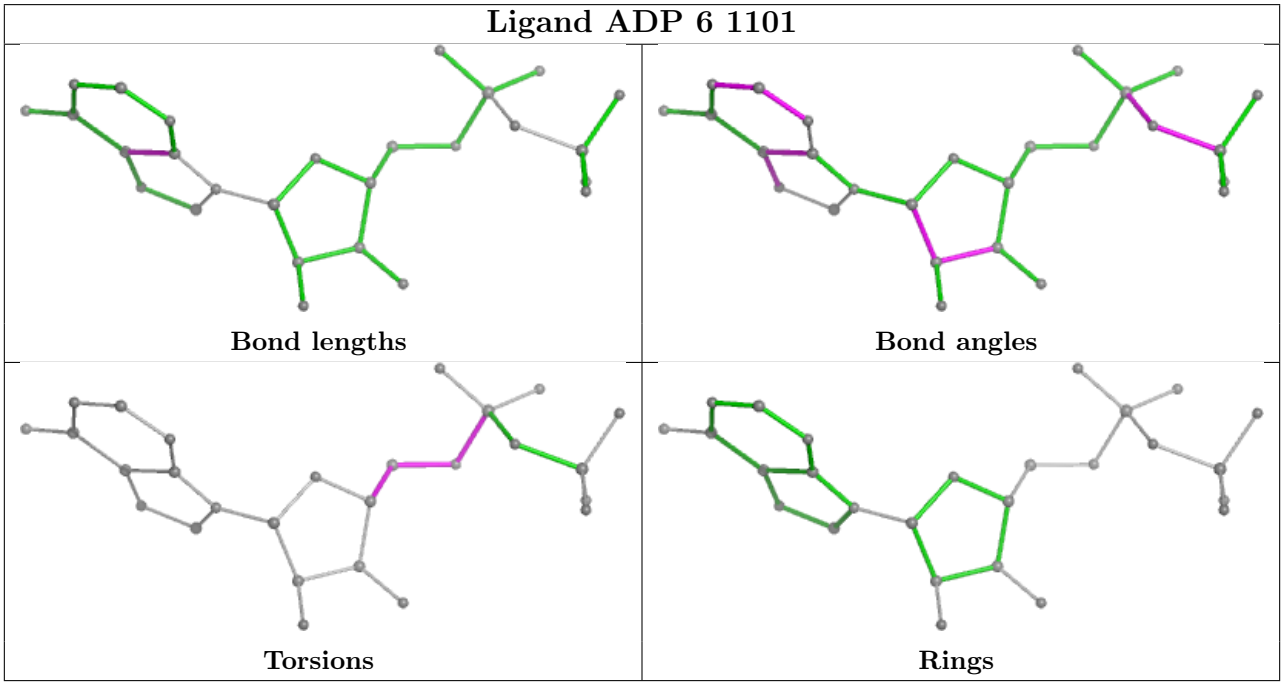
Mol	Chain	Res	Type	Atoms
15	2	901	ATP	PB-O3B-PG-O2G
15	5	1701	ATP	C5'-O5'-PA-O1A
18	4	1001	ADP	C5'-O5'-PA-O3A
18	6	1101	ADP	C5'-O5'-PA-O2A
15	3	1002	ATP	C3'-C4'-C5'-O5'
18	6	1101	ADP	O4'-C4'-C5'-O5'
15	3	1002	ATP	O4'-C4'-C5'-O5'
18	6	1101	ADP	C3'-C4'-C5'-O5'
18	4	1001	ADP	PA-O3A-PB-O1B
18	6	1101	ADP	C4'-C5'-O5'-PA
15	2	901	ATP	O4'-C4'-C5'-O5'
15	5	1701	ATP	C5'-O5'-PA-O3A
15	7	901	ATP	C5'-O5'-PA-O3A
18	6	1101	ADP	C5'-O5'-PA-O3A
15	5	1701	ATP	C5'-O5'-PA-O2A
15	7	901	ATP	C5'-O5'-PA-O1A
15	7	901	ATP	C5'-O5'-PA-O2A
18	4	1001	ADP	C5'-O5'-PA-O2A
18	6	1101	ADP	C5'-O5'-PA-O1A
15	7	901	ATP	C4'-C5'-O5'-PA
15	2	901	ATP	PA-O3A-PB-O3B
15	5	1701	ATP	PA-O3A-PB-O1B
15	7	901	ATP	PA-O3A-PB-O3B
15	2	901	ATP	PB-O3B-PG-O3G
18	4	1001	ADP	O4'-C4'-C5'-O5'
15	2	901	ATP	PA-O3A-PB-O1B
15	7	901	ATP	PA-O3A-PB-O1B

There are no ring outliers.

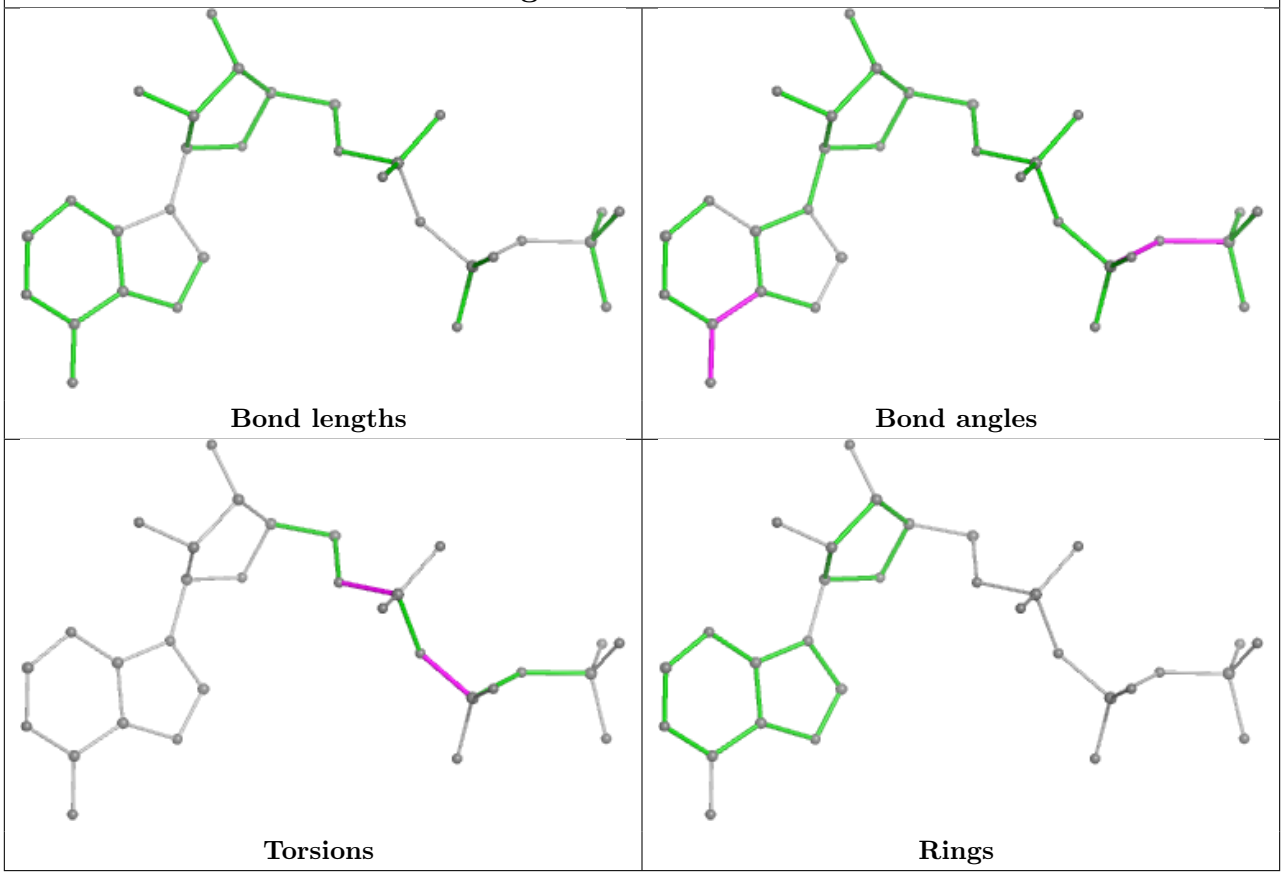
6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	6	1101	ADP	1	0
15	5	1701	ATP	1	0
15	7	901	ATP	3	0
18	4	1001	ADP	3	0
15	2	901	ATP	1	0
15	3	1002	ATP	2	0

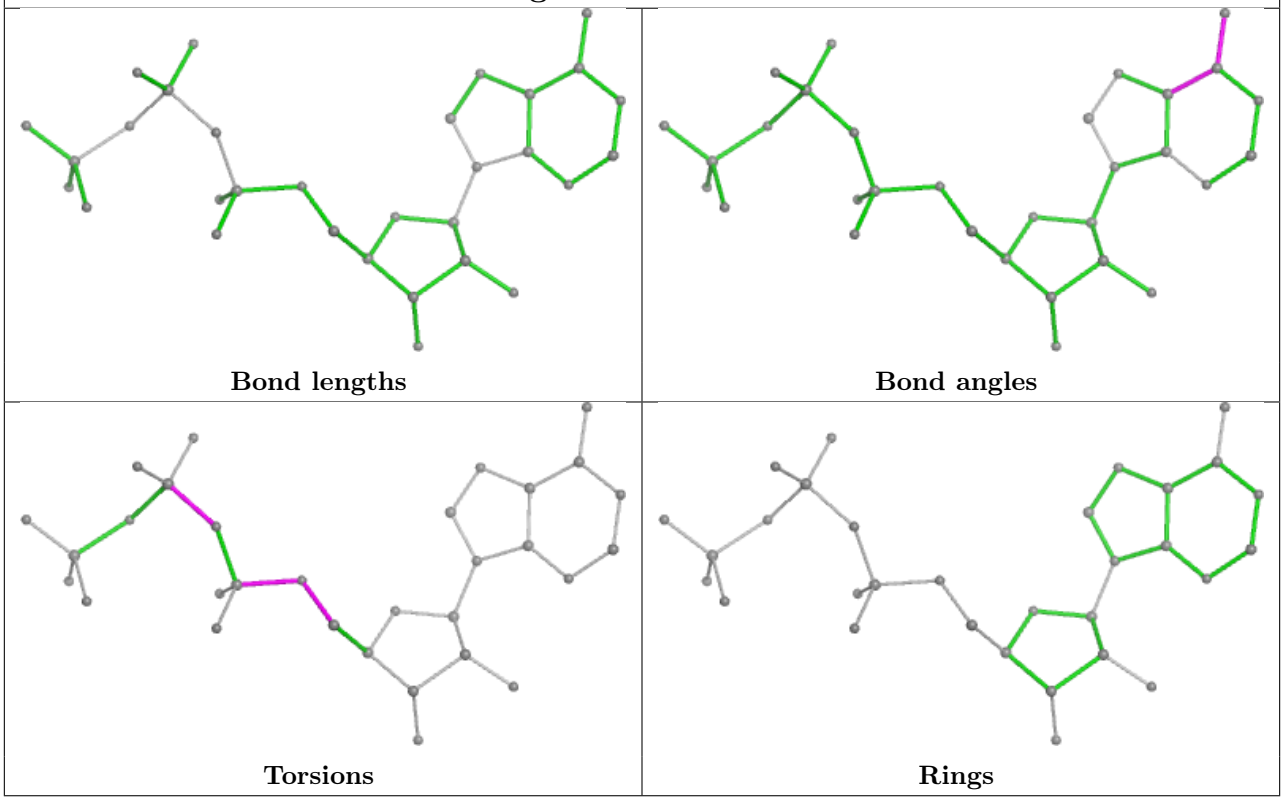
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



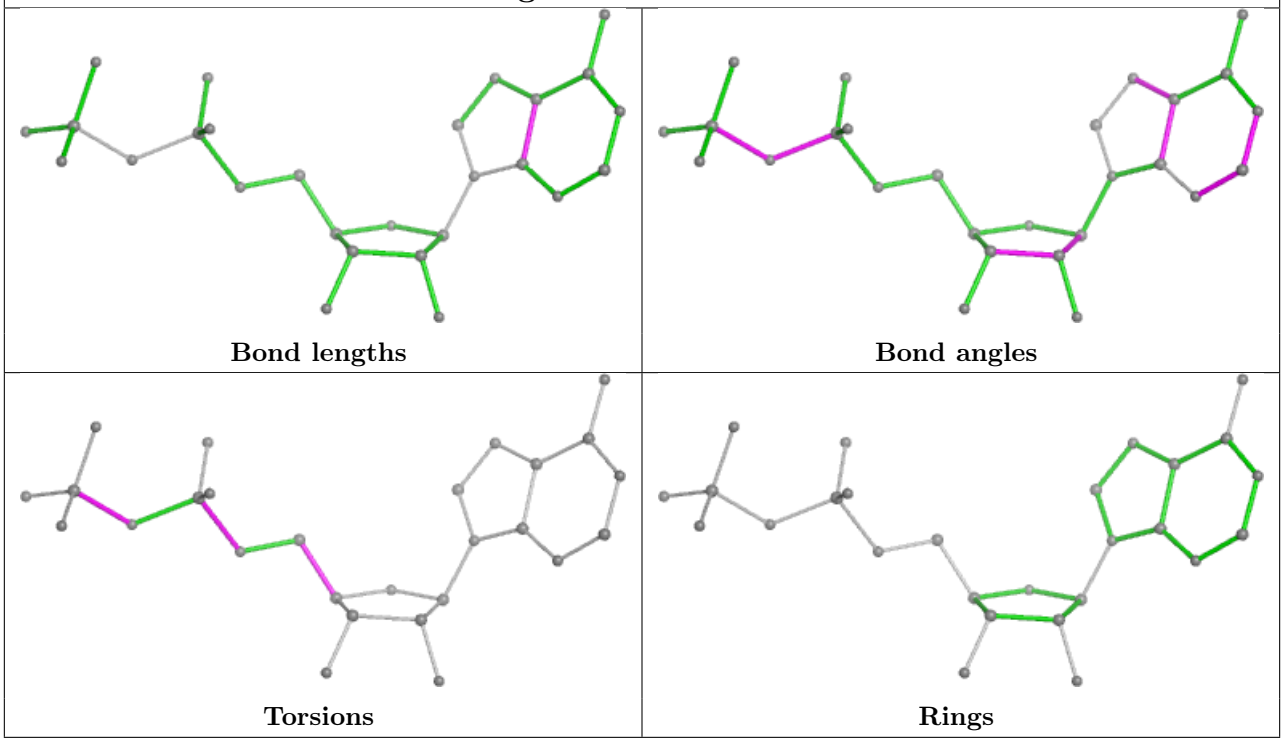
Ligand ATP 5 1701



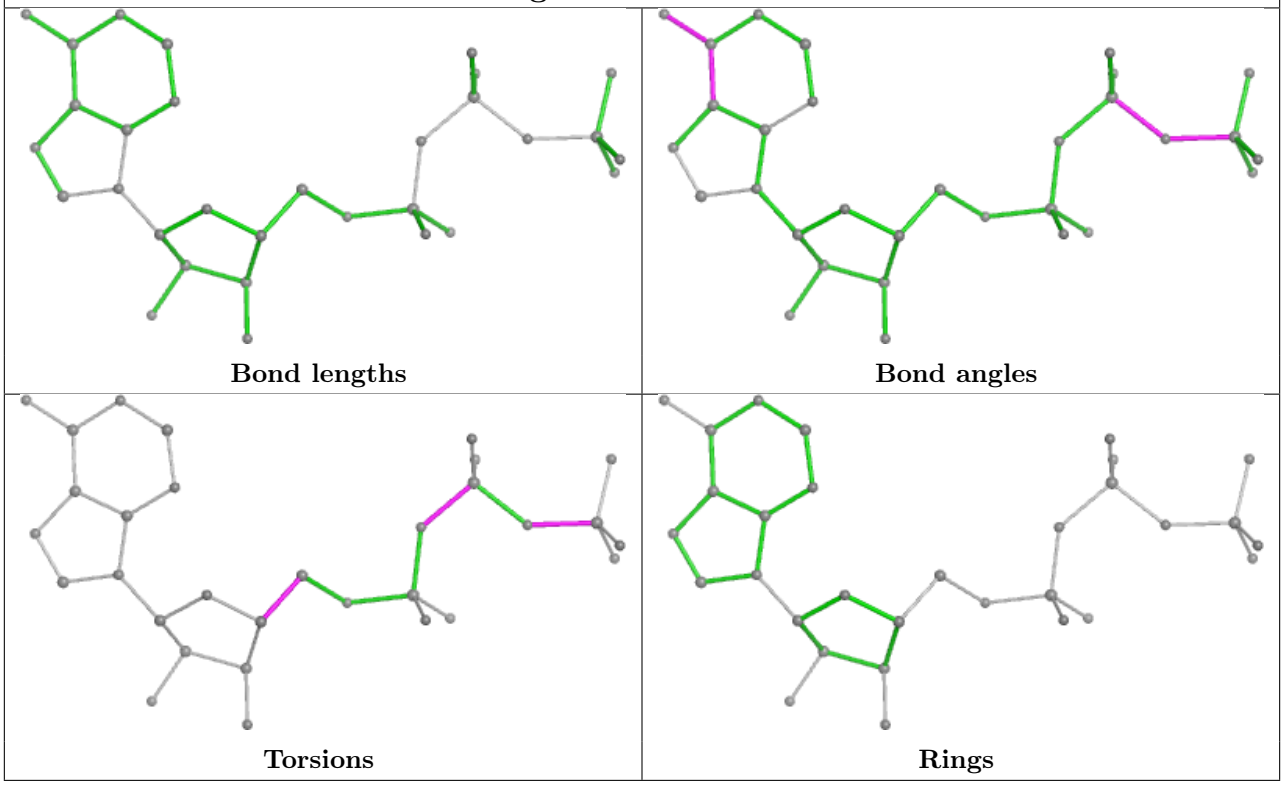
Ligand ATP 7 901



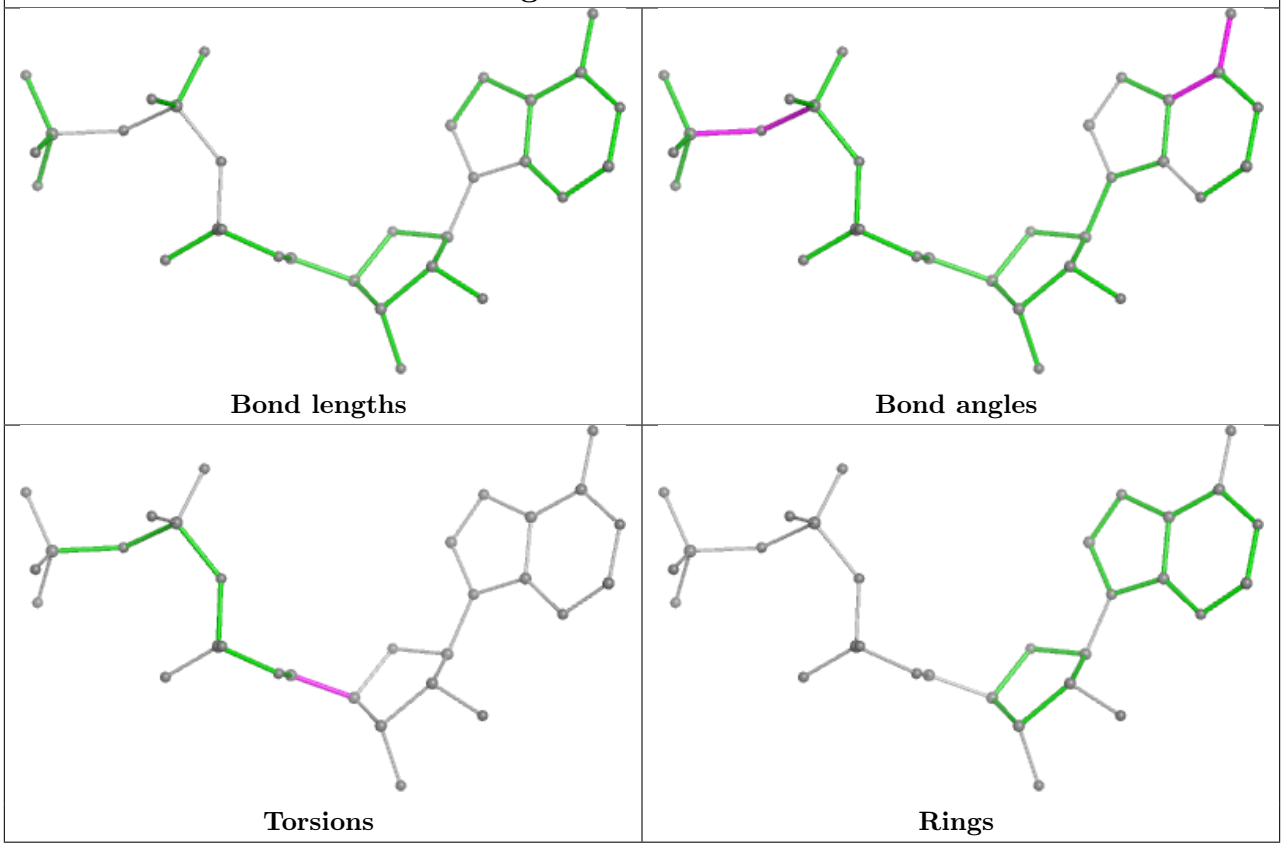
Ligand ADP 4 1001



Ligand ATP 2 901



Ligand ATP 3 1002



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

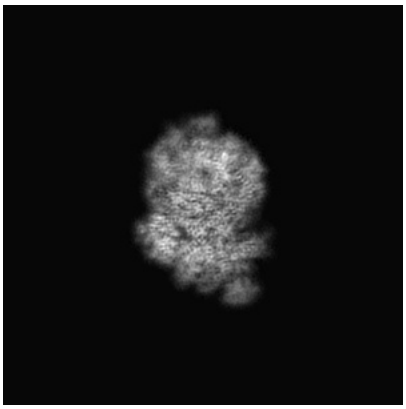
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17458. These allow visual inspection of the internal detail of the map and identification of artifacts.

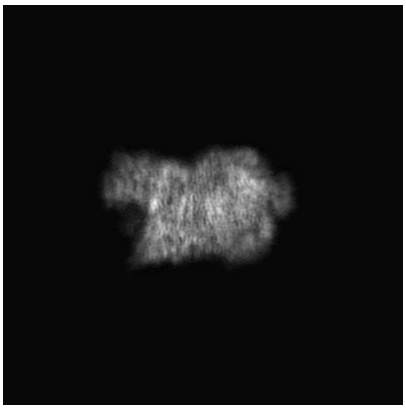
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

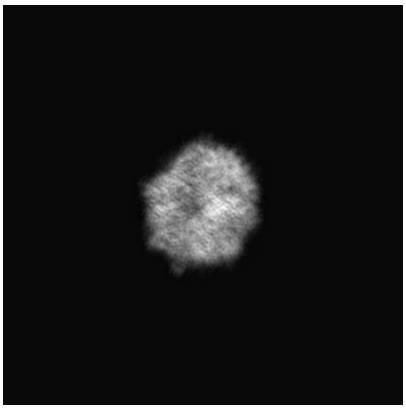
6.1.1 Primary map



X

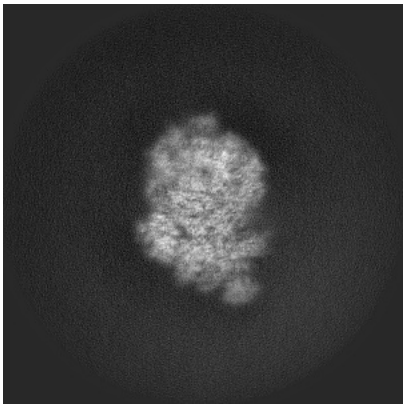


Y

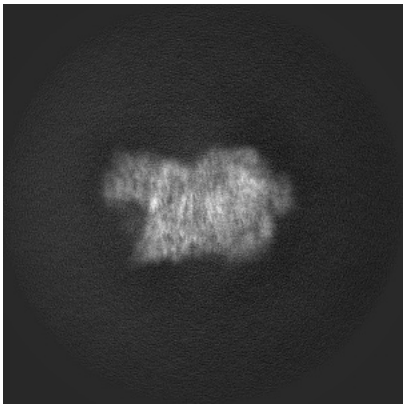


Z

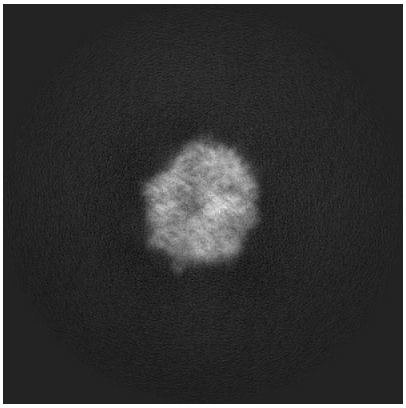
6.1.2 Raw map



X



Y

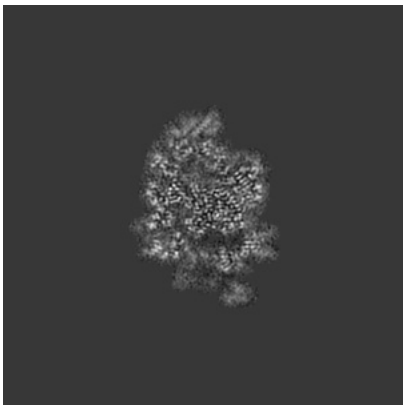


Z

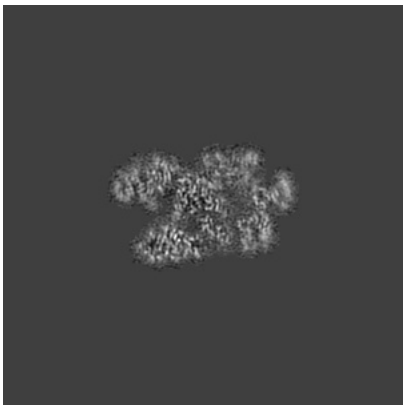
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

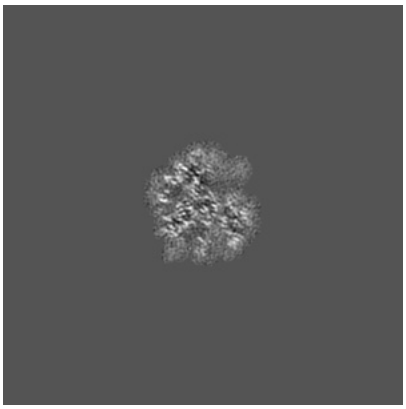
6.2.1 Primary map



X Index: 210

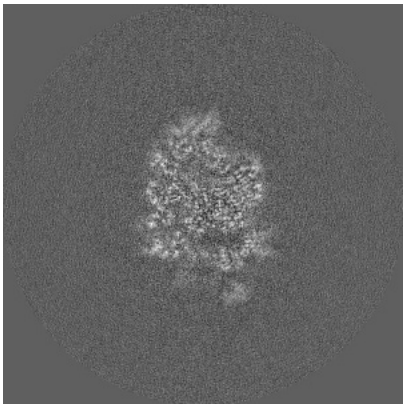


Y Index: 210

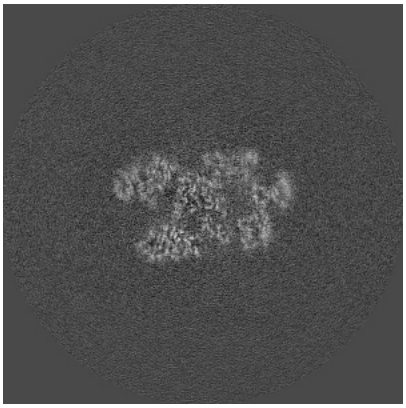


Z Index: 210

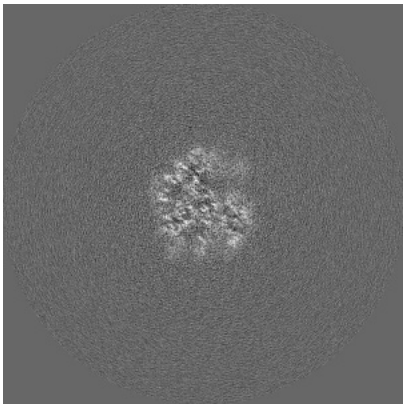
6.2.2 Raw map



X Index: 210



Y Index: 210

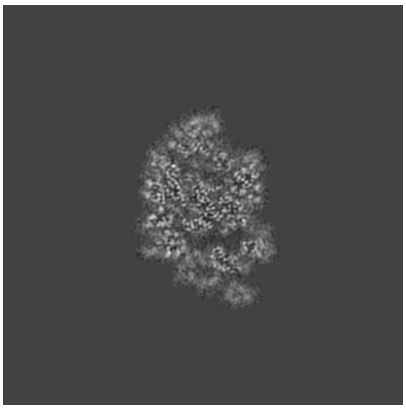


Z Index: 210

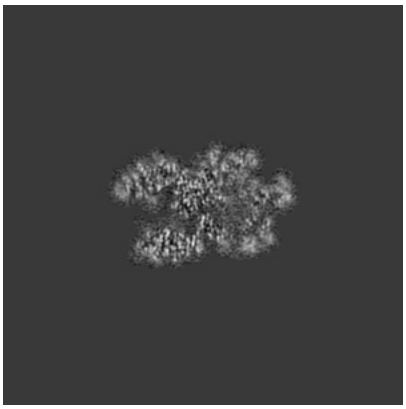
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

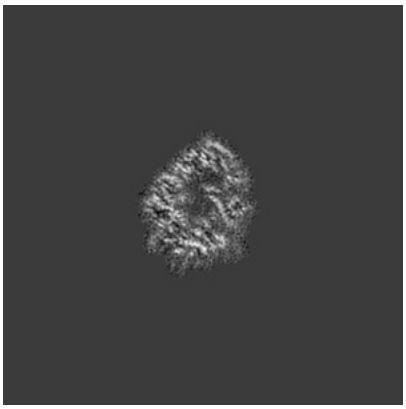
6.3.1 Primary map



X Index: 214

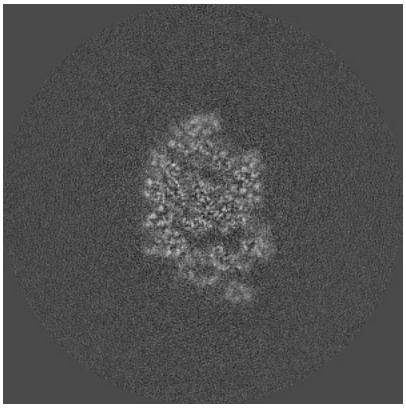


Y Index: 206

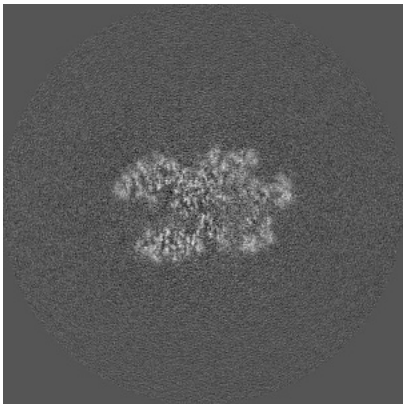


Z Index: 165

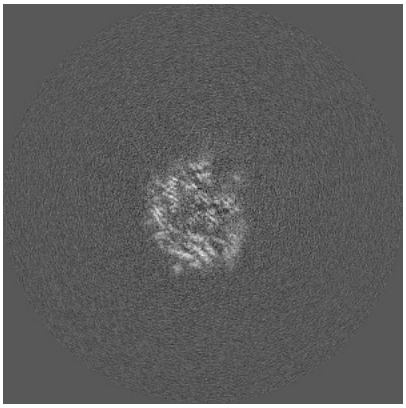
6.3.2 Raw map



X Index: 214



Y Index: 206

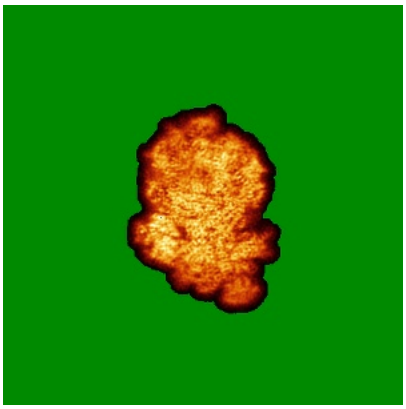


Z Index: 188

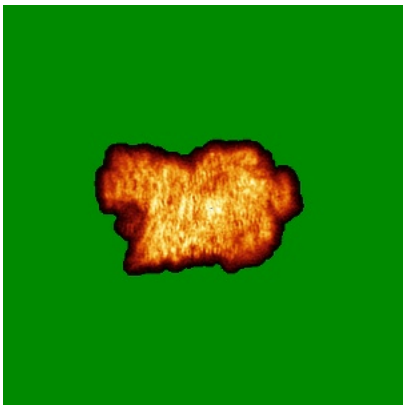
The images above show the largest variance slices of the map in three orthogonal directions.

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

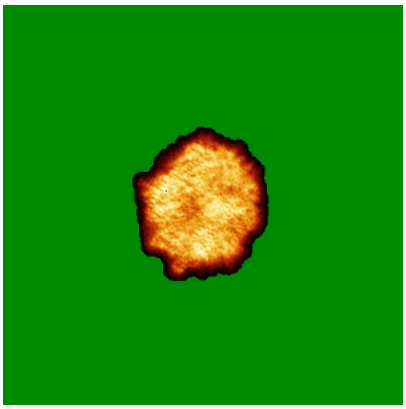
6.4.1 Primary map



X

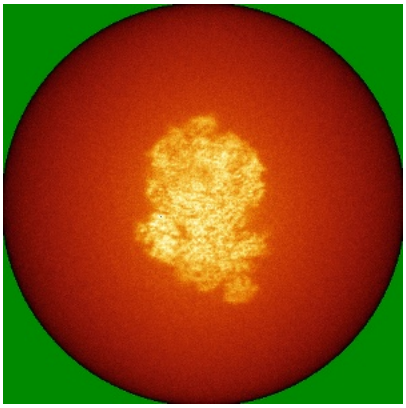


Y

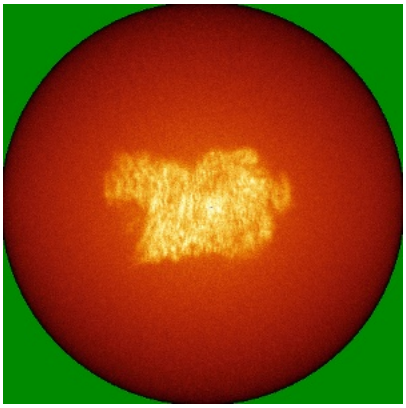


Z

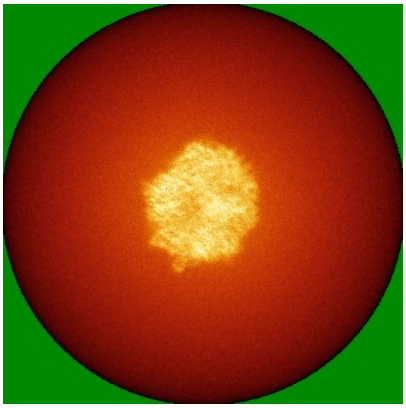
6.4.2 Raw map



X



Y

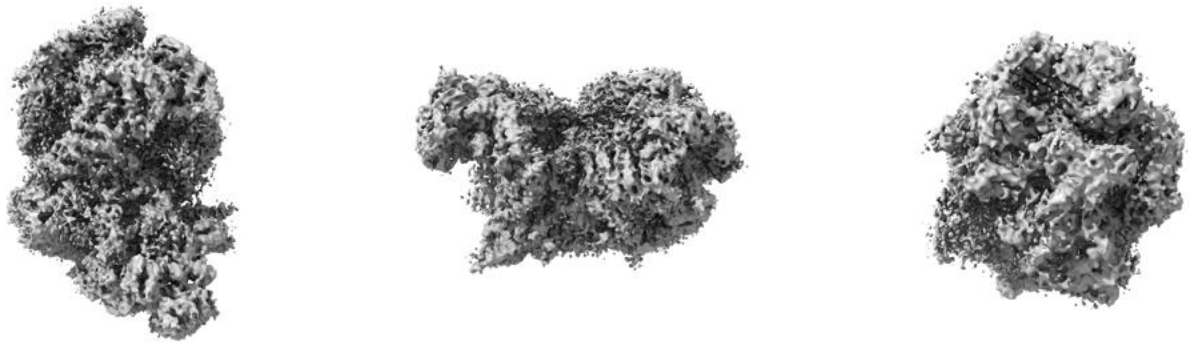


Z

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 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

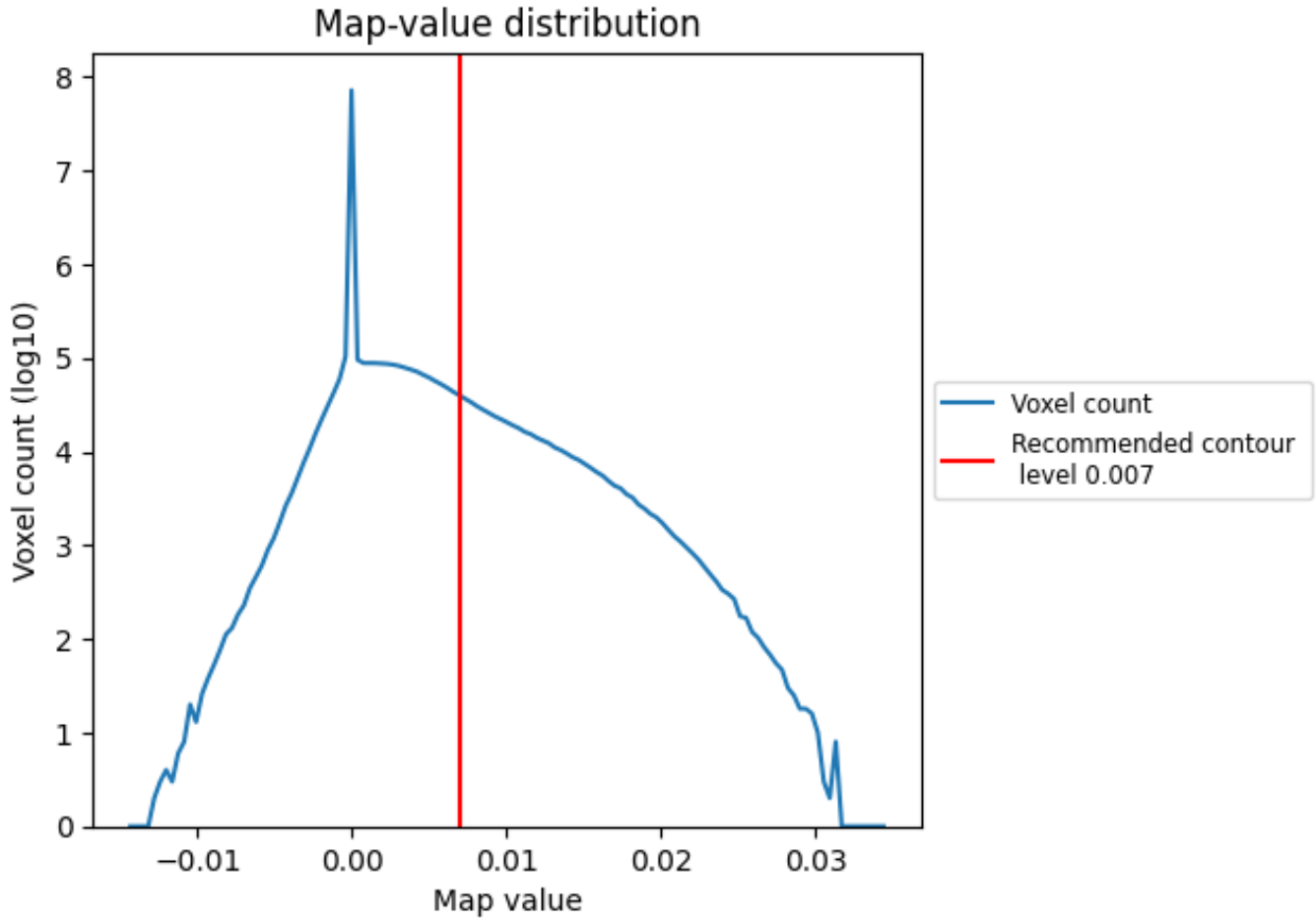
6.6 Mask visualisation (i)

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

7 Map analysis

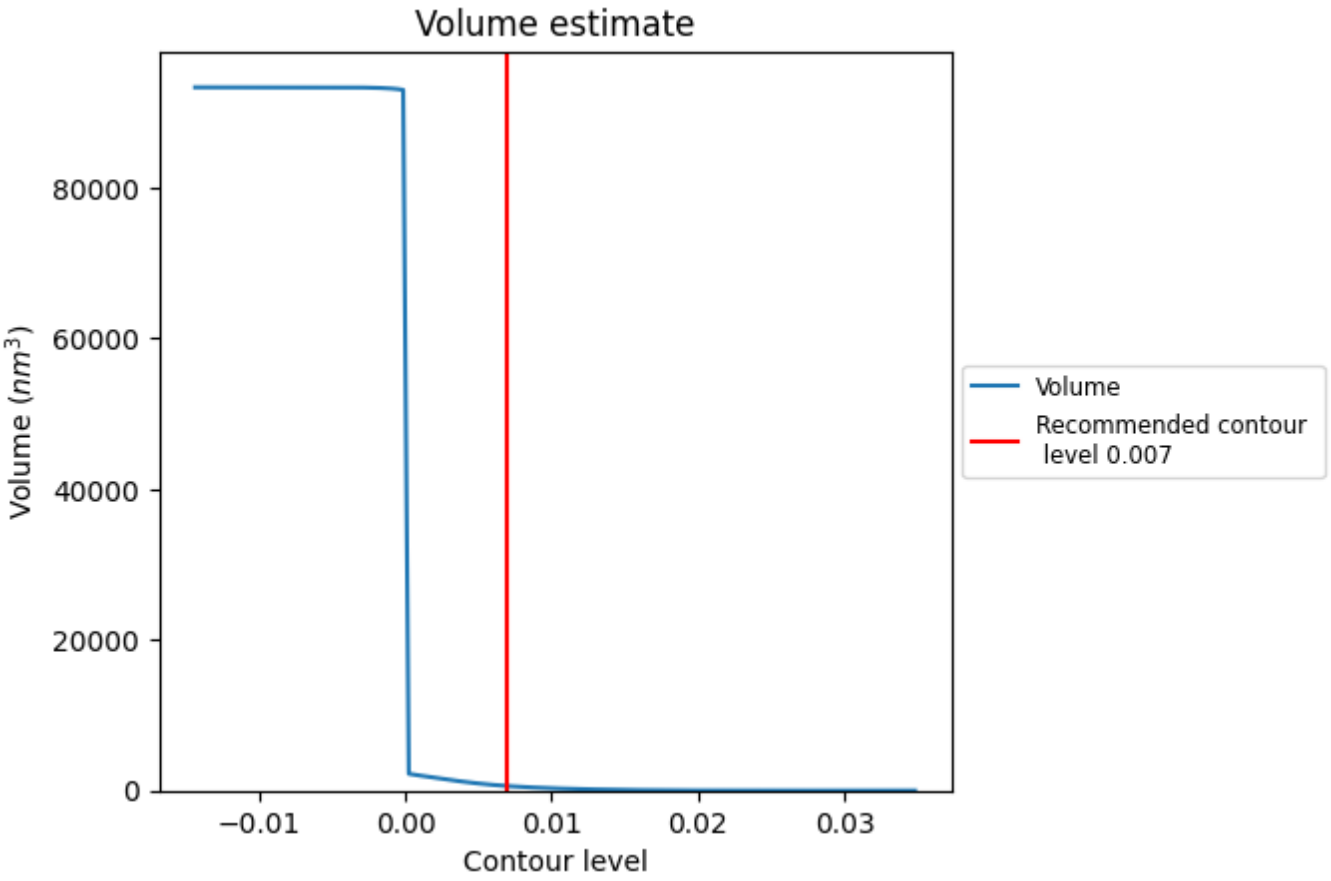
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

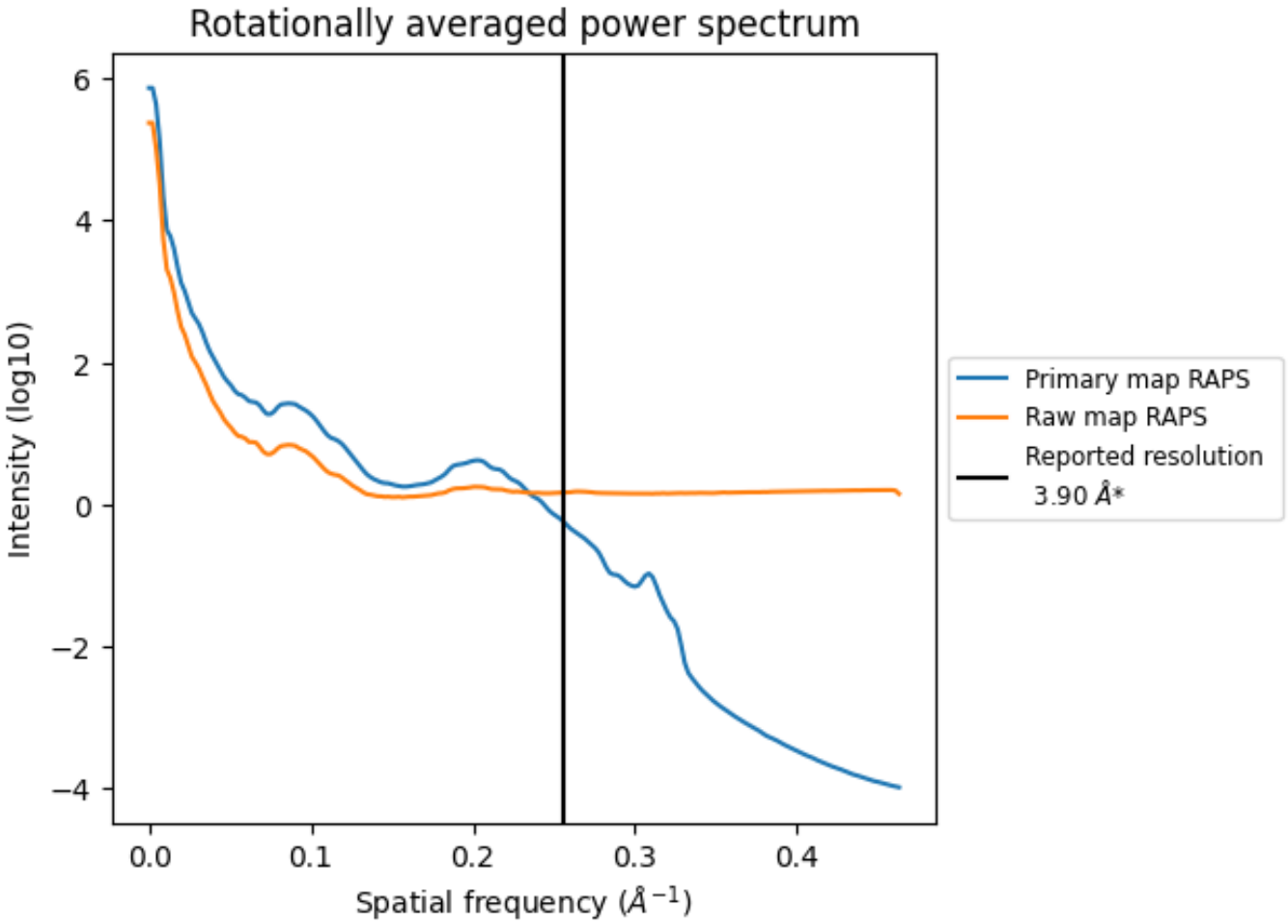
7.2 Volume estimate



The volume at the recommended contour level is 602 nm^3; this corresponds to an approximate mass of 544 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)

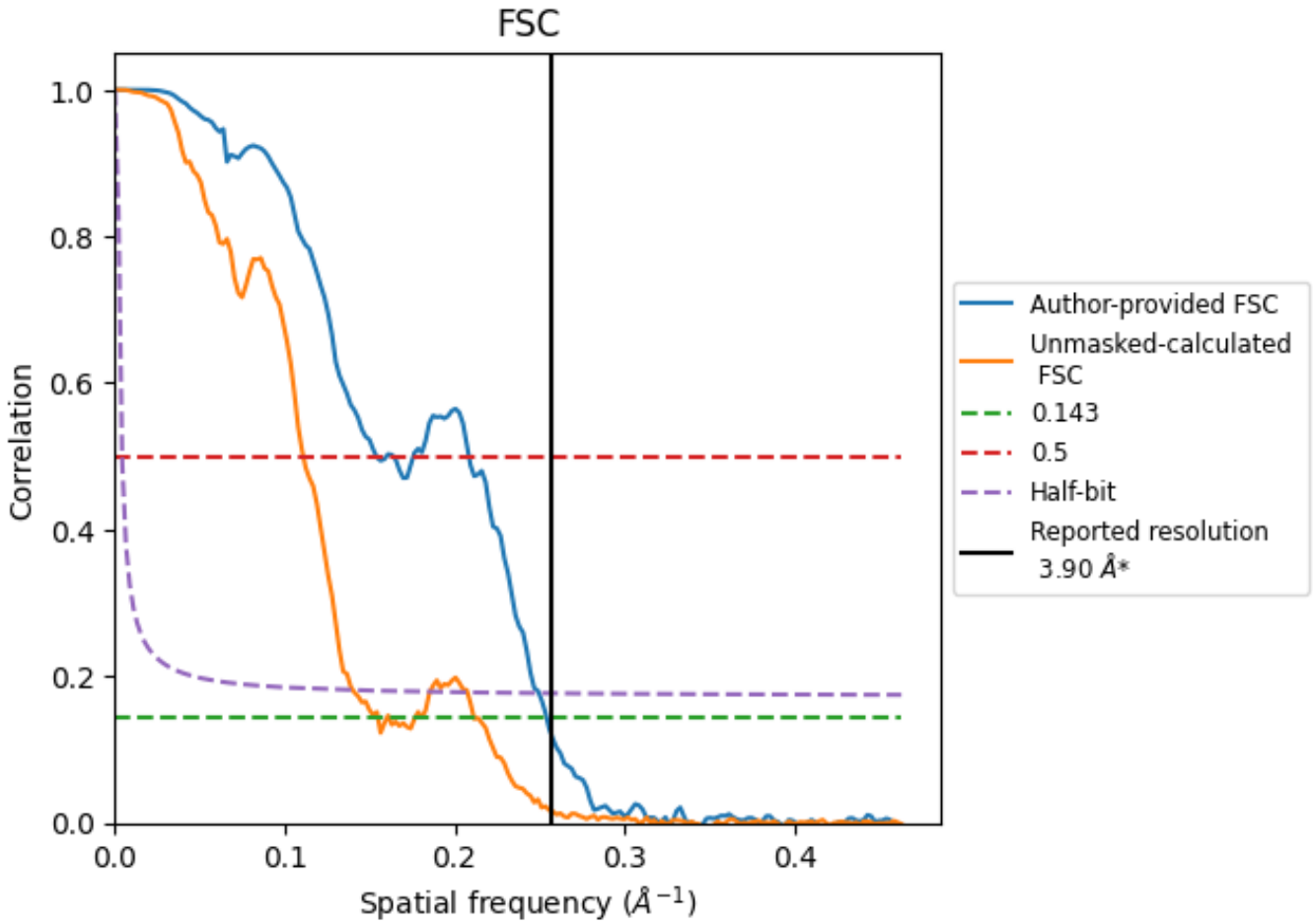


*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8.2 Resolution estimates (i)

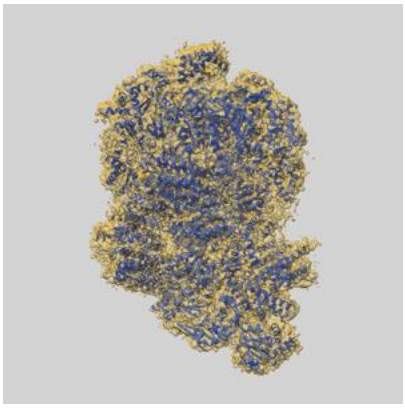
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.93	6.49	4.01
Unmasked-calculated*	6.46	9.01	7.13

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.46 differs from the reported value 3.9 by more than 10 %

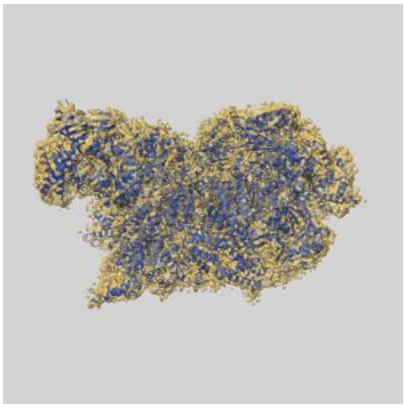
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-17458 and PDB model 8P62. Per-residue inclusion information can be found in section 3 on page 11.

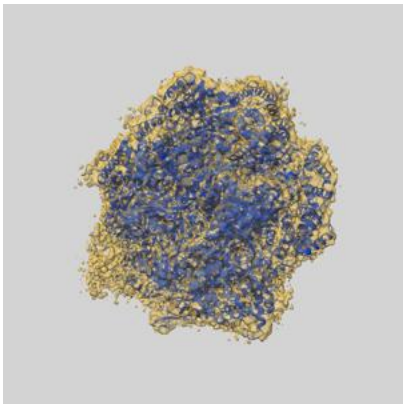
9.1 Map-model overlay



X



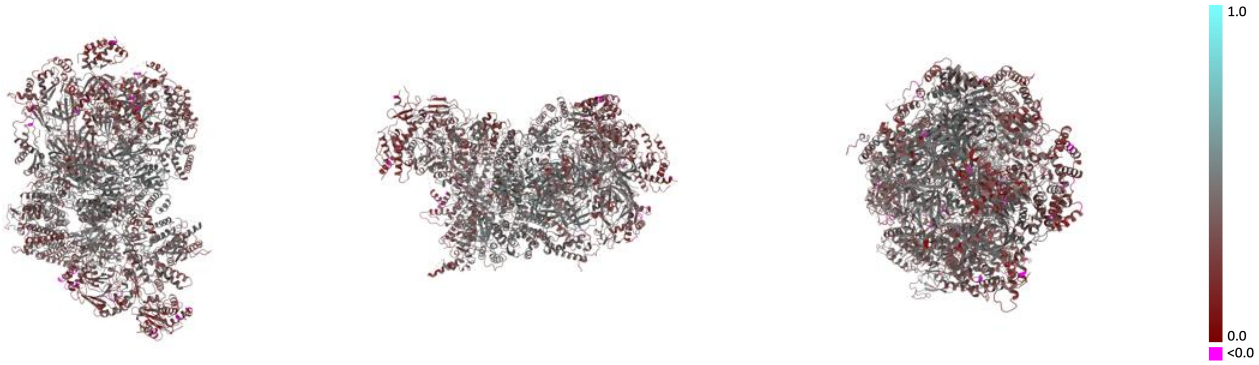
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.007 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.

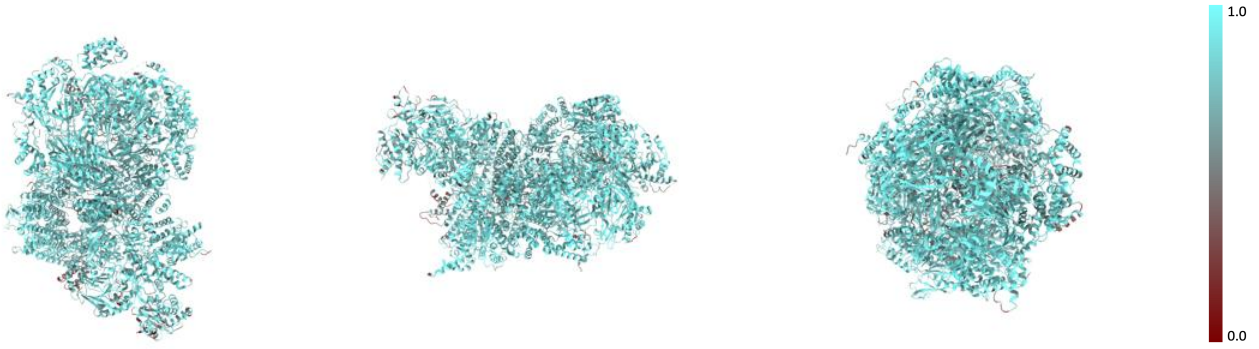
9.2 Q-score mapped to coordinate model (i)



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.

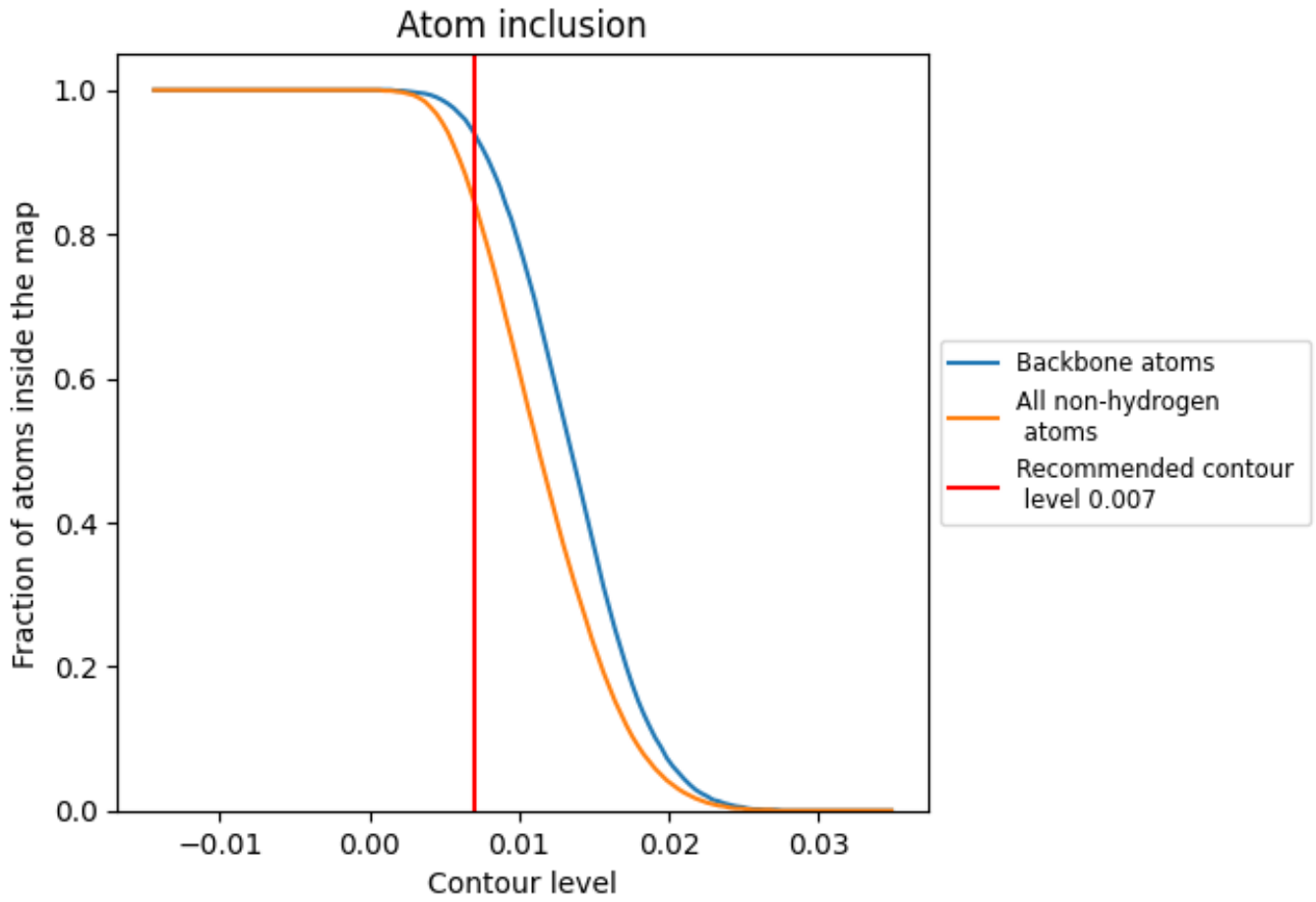
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.007).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 84% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8450	0.3820
2	0.8710	0.4340
3	0.8590	0.4070
4	0.8520	0.3300
5	0.8340	0.4290
6	0.8630	0.3860
7	0.8170	0.3200
A	0.8990	0.4330
C	0.8750	0.3960
D	0.8810	0.3710
E	0.9060	0.4290
F	0.7760	0.3500
G	0.8090	0.3570
H	0.8180	0.3510
I	0.8790	0.3940