



## Full wwPDB EM Validation Report ⓘ

May 5, 2026 – 02:59 pm BST

PDB ID : 9RHI / pdb\_00009rhi  
EMDB ID : EMD-53970  
Title : pre-Initiation Complex on ARS1 DNA (monomer)  
Authors : Puehringer, T.; Butryn, A.; Couves, E.C.; Costa, A.  
Deposited on : 2025-06-09  
Resolution : 3.20 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](mailto: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>.

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

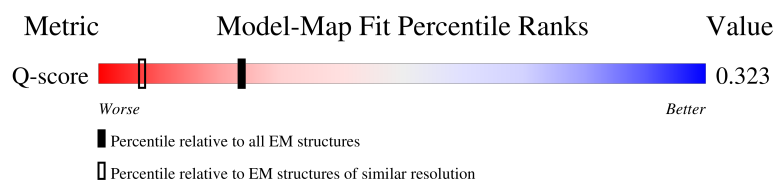
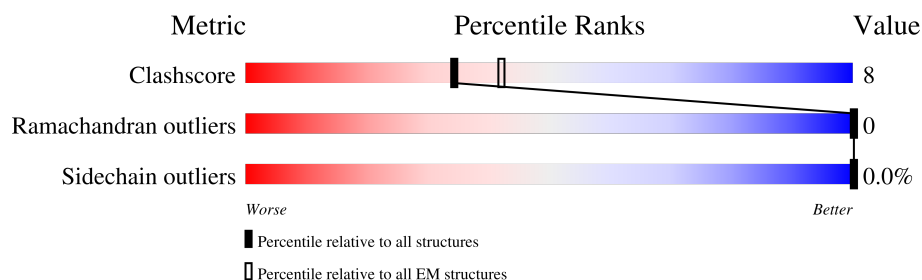
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using 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) : 2.49

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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	15020 ( 2.70 - 3.70 )

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	868	<div> <div>14%</div> <div>64%</div> <div>10%</div> <div>25%</div> </div>
2	3	1006	<div> <div>9%</div> <div>48%</div> <div>11%</div> <div>41%</div> </div>
3	4	933	<div> <div>9%</div> <div>44%</div> <div>17%</div> <div>38%</div> </div>
4	5	775	<div> <div>11%</div> <div>59%</div> <div>14%</div> <div>27%</div> </div>

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Mol	Chain	Length	Quality of chain
5	6	1017	
6	7	845	
6	f	845	
7	A	31	
8	B	31	
9	C	217	
10	D	294	
11	E	657	
12	F	689	
13	H	208	
14	I	213	
15	Q	704	
15	T	704	
16	R	257	
17	S	801	

## 2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 45961 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	648	Total	C	N	O	S	0	0
			5147	3237	923	968	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	593	Total	C	N	O	S	0	0
			4655	2940	829	873	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	576	Total	C	N	O	S	0	0
			4597	2900	791	878	28		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	566	Total	C	N	O	S	0	0
			4455	2815	759	858	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	580	Total	C	N	O	S	0	0
			4601	2905	800	871	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	616	Total	C	N	O	S	0	0
			4862	3073	842	921	26		
6	f	44	Total	C	N	O	S	0	0
			355	208	63	80	4		

- Molecule 7 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	31	Total	C	N	O	P	0	0
			635	304	119	181	31		

- Molecule 8 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	31	Total	C	N	O	P	0	0
			636	306	108	191	31		

- Molecule 9 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	183	Total	C	N	O	S	0	0
			1472	954	234	277	7		

There are 23 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

- Molecule 10 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	222	Total	C	N	O	S	0	0
			1842	1175	304	351	12		

- Molecule 11 is a protein called Cell division control protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	505	Total	C	N	O	S	0	0
			4114	2640	693	767	14		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	198	ASP	-	linker	UNP Q08032
E	199	TYR	-	linker	UNP Q08032
E	200	LYS	-	linker	UNP Q08032
E	201	ASP	-	linker	UNP Q08032
E	202	ASP	-	linker	UNP Q08032
E	203	ASP	-	linker	UNP Q08032
E	204	GLY	-	linker	UNP Q08032
E	205	ASP	-	linker	UNP Q08032
E	206	TYR	-	linker	UNP Q08032
E	207	LYS	-	linker	UNP Q08032
E	208	ASP	-	linker	UNP Q08032
E	209	ASP	-	linker	UNP Q08032
E	210	ASP	-	linker	UNP Q08032

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	86	Total	C	N	O	S	0	0
			688	446	119	122	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	208	Total	C	N	O	S	0	0
			1697	1065	290	332	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	191	Total	C	N	O	S	0	0
			1589	1021	279	284	5		

- Molecule 15 is a protein called DNA replication regulator SLD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	201	Total	C	N	O	S	0	0
			1644	1066	271	301	6		
15	T	30	Total	C	N	O	S	0	0
			246	150	44	51	1		

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	669	GLU	-	expression tag	UNP P53135
Q	670	ASN	-	expression tag	UNP P53135
Q	671	LEU	-	expression tag	UNP P53135
Q	672	TYR	-	expression tag	UNP P53135
Q	673	PHE	-	expression tag	UNP P53135
Q	674	GLN	-	expression tag	UNP P53135
Q	675	GLY	-	expression tag	UNP P53135
Q	676	TRP	-	expression tag	UNP P53135
Q	677	SER	-	expression tag	UNP P53135
Q	678	HIS	-	expression tag	UNP P53135
Q	679	PRO	-	expression tag	UNP P53135
Q	680	GLN	-	expression tag	UNP P53135
Q	681	PHE	-	expression tag	UNP P53135
Q	682	GLU	-	expression tag	UNP P53135
Q	683	LYS	-	expression tag	UNP P53135
Q	684	GLY	-	expression tag	UNP P53135
Q	685	GLY	-	expression tag	UNP P53135
Q	686	GLY	-	expression tag	UNP P53135
Q	687	SER	-	expression tag	UNP P53135
Q	688	GLY	-	expression tag	UNP P53135
Q	689	GLY	-	expression tag	UNP P53135
Q	690	GLY	-	expression tag	UNP P53135
Q	691	SER	-	expression tag	UNP P53135
Q	692	GLY	-	expression tag	UNP P53135
Q	693	GLY	-	expression tag	UNP P53135
Q	694	SER	-	expression tag	UNP P53135
Q	695	SER	-	expression tag	UNP P53135
Q	696	ALA	-	expression tag	UNP P53135
Q	697	TRP	-	expression tag	UNP P53135

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	698	SER	-	expression tag	UNP P53135
Q	699	HIS	-	expression tag	UNP P53135
Q	700	PRO	-	expression tag	UNP P53135
Q	701	GLN	-	expression tag	UNP P53135
Q	702	PHE	-	expression tag	UNP P53135
Q	703	GLU	-	expression tag	UNP P53135
Q	704	LYS	-	expression tag	UNP P53135
T	669	GLU	-	expression tag	UNP P53135
T	670	ASN	-	expression tag	UNP P53135
T	671	LEU	-	expression tag	UNP P53135
T	672	TYR	-	expression tag	UNP P53135
T	673	PHE	-	expression tag	UNP P53135
T	674	GLN	-	expression tag	UNP P53135
T	675	GLY	-	expression tag	UNP P53135
T	676	TRP	-	expression tag	UNP P53135
T	677	SER	-	expression tag	UNP P53135
T	678	HIS	-	expression tag	UNP P53135
T	679	PRO	-	expression tag	UNP P53135
T	680	GLN	-	expression tag	UNP P53135
T	681	PHE	-	expression tag	UNP P53135
T	682	GLU	-	expression tag	UNP P53135
T	683	LYS	-	expression tag	UNP P53135
T	684	GLY	-	expression tag	UNP P53135
T	685	GLY	-	expression tag	UNP P53135
T	686	GLY	-	expression tag	UNP P53135
T	687	SER	-	expression tag	UNP P53135
T	688	GLY	-	expression tag	UNP P53135
T	689	GLY	-	expression tag	UNP P53135
T	690	GLY	-	expression tag	UNP P53135
T	691	SER	-	expression tag	UNP P53135
T	692	GLY	-	expression tag	UNP P53135
T	693	GLY	-	expression tag	UNP P53135
T	694	SER	-	expression tag	UNP P53135
T	695	SER	-	expression tag	UNP P53135
T	696	ALA	-	expression tag	UNP P53135
T	697	TRP	-	expression tag	UNP P53135
T	698	SER	-	expression tag	UNP P53135
T	699	HIS	-	expression tag	UNP P53135
T	700	PRO	-	expression tag	UNP P53135
T	701	GLN	-	expression tag	UNP P53135
T	702	PHE	-	expression tag	UNP P53135
T	703	GLU	-	expression tag	UNP P53135

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Chain	Residue	Modelled	Actual	Comment	Reference
T	704	LYS	-	expression tag	UNP P53135

- Molecule 16 is a protein called Mitochondrial morphogenesis protein SLD7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	111	Total	C	N	O	S	0	0
			898	564	157	176	1		

- Molecule 17 is a protein called DNA replication regulator DPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	221	Total	C	N	O	S	0	0
			1795	1180	296	311	8		

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	765	GLY	-	expression tag	UNP P47027
S	766	SER	-	expression tag	UNP P47027
S	767	SER	-	expression tag	UNP P47027
S	768	LEU	-	expression tag	UNP P47027
S	769	GLU	-	expression tag	UNP P47027
S	770	VAL	-	expression tag	UNP P47027
S	771	LEU	-	expression tag	UNP P47027
S	772	PHE	-	expression tag	UNP P47027
S	773	GLN	-	expression tag	UNP P47027
S	774	GLY	-	expression tag	UNP P47027
S	775	PRO	-	expression tag	UNP P47027
S	776	GLU	-	expression tag	UNP P47027
S	777	GLY	-	expression tag	UNP P47027
S	778	SER	-	expression tag	UNP P47027
S	779	SER	-	expression tag	UNP P47027
S	780	ASP	-	expression tag	UNP P47027
S	781	TYR	-	expression tag	UNP P47027
S	782	LYS	-	expression tag	UNP P47027
S	783	ASP	-	expression tag	UNP P47027
S	784	HIS	-	expression tag	UNP P47027
S	785	ASP	-	expression tag	UNP P47027
S	786	GLY	-	expression tag	UNP P47027
S	787	ASP	-	expression tag	UNP P47027
S	788	TYR	-	expression tag	UNP P47027
S	789	LYS	-	expression tag	UNP P47027

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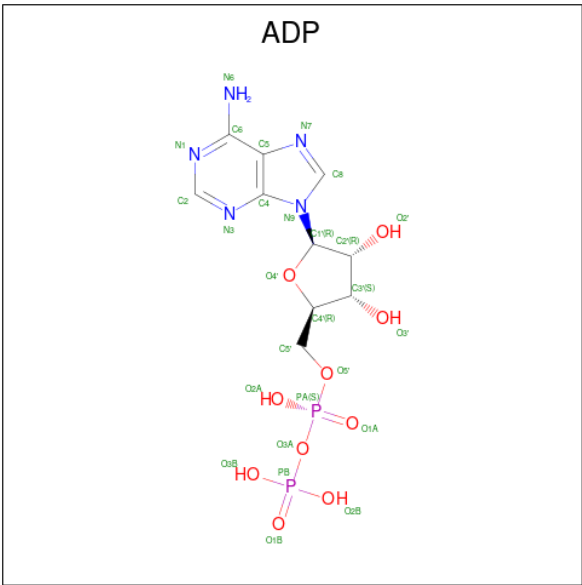
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Chain	Residue	Modelled	Actual	Comment	Reference
S	790	ASP	-	expression tag	UNP P47027
S	791	HIS	-	expression tag	UNP P47027
S	792	ASP	-	expression tag	UNP P47027
S	793	ILE	-	expression tag	UNP P47027
S	794	ASP	-	expression tag	UNP P47027
S	795	TYR	-	expression tag	UNP P47027
S	796	LYS	-	expression tag	UNP P47027
S	797	ASP	-	expression tag	UNP P47027
S	798	ASP	-	expression tag	UNP P47027
S	799	ASP	-	expression tag	UNP P47027
S	800	ASP	-	expression tag	UNP P47027
S	801	LYS	-	expression tag	UNP P47027

- Molecule 18 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
18	2	1	Total Zn 1 1	0
18	4	1	Total Zn 1 1	0
18	5	1	Total Zn 1 1	0
18	6	1	Total Zn 1 1	0
18	7	1	Total Zn 1 1	0

- Molecule 19 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).

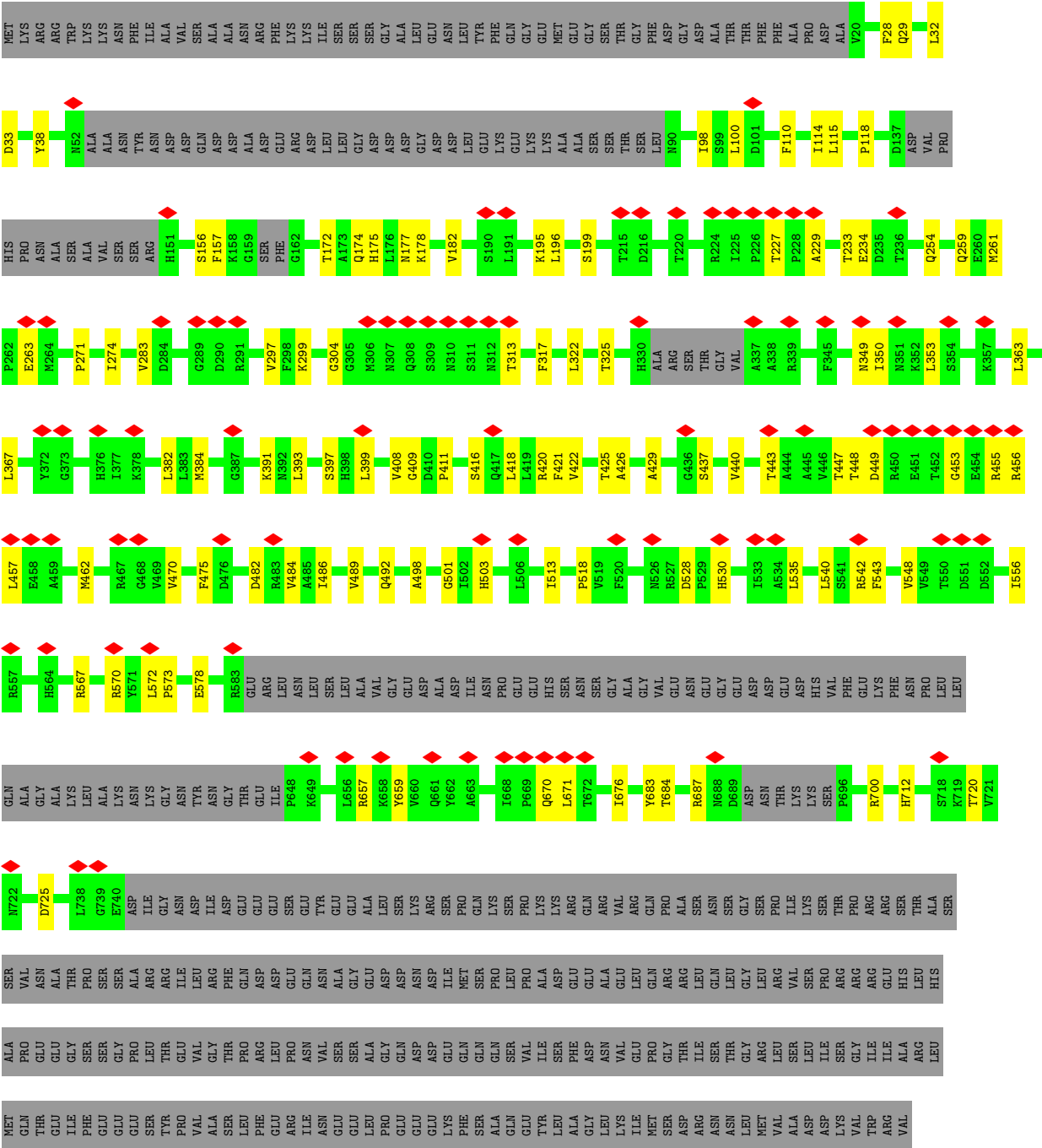


Mol	Chain	Residues	Atoms					AltConf
19	7	1	Total	C	N	O	P	0
			27	10	5	10	2	

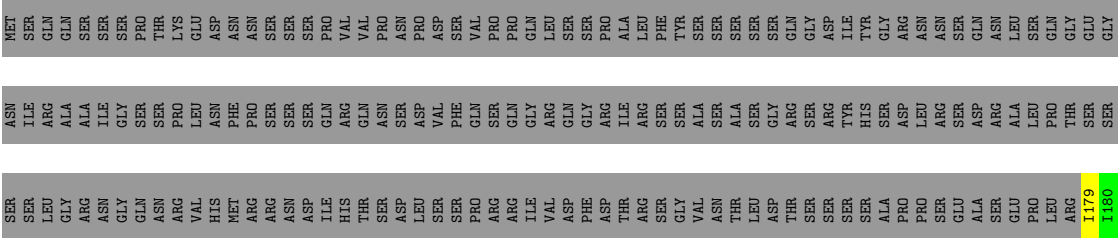
- Molecule 20 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
20	7	1	Total	Mg	0
			1	1	





● Molecule 3: DNA replication licensing factor MCM4











[illegible]

- Molecule 6: DNA replication licensing factor MCM7

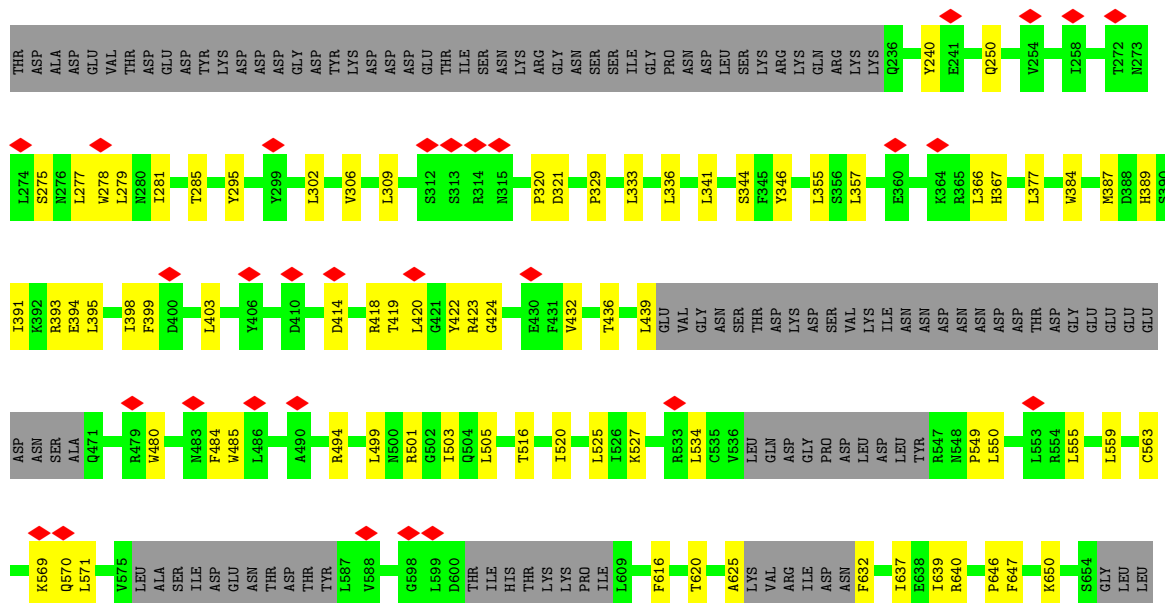
Chain f:  95%

[illegible]

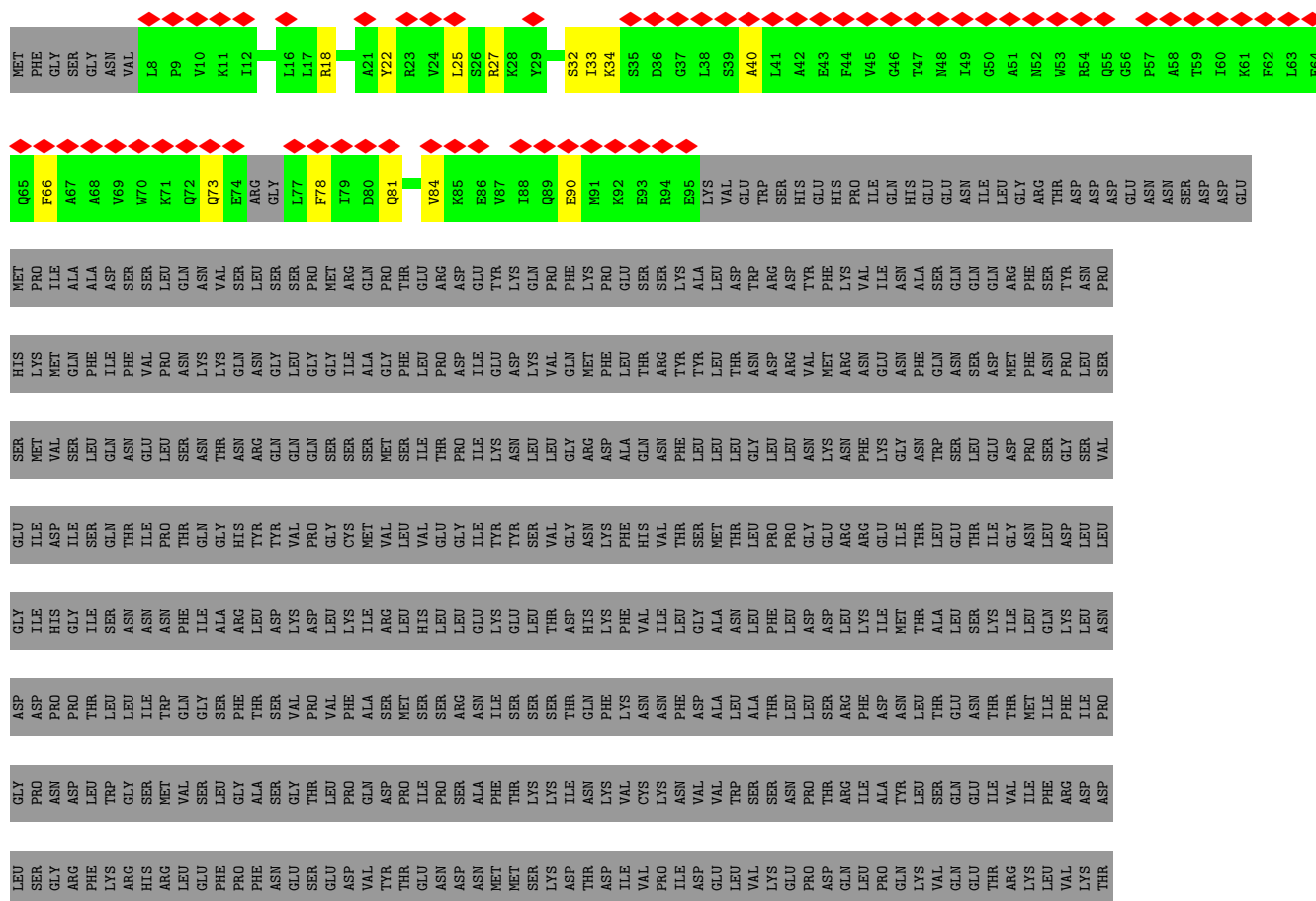
- Molecule 7: DNA (31-MER)

Chain A:  32% 55% 45%

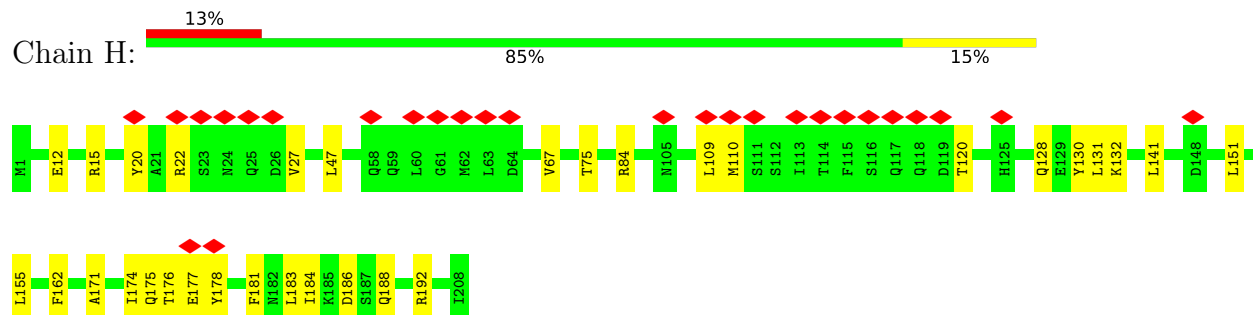




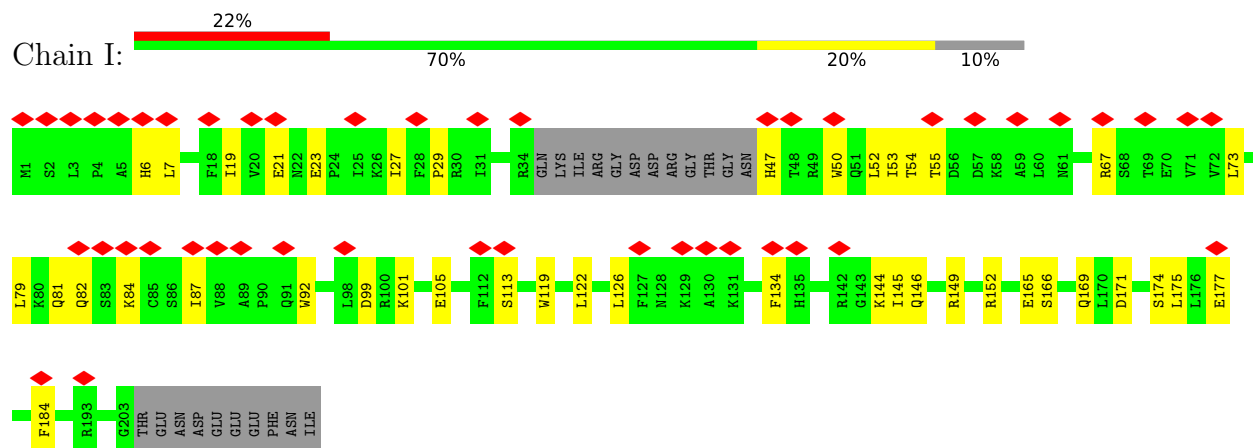
• Molecule 12: DNA polymerase epsilon subunit B



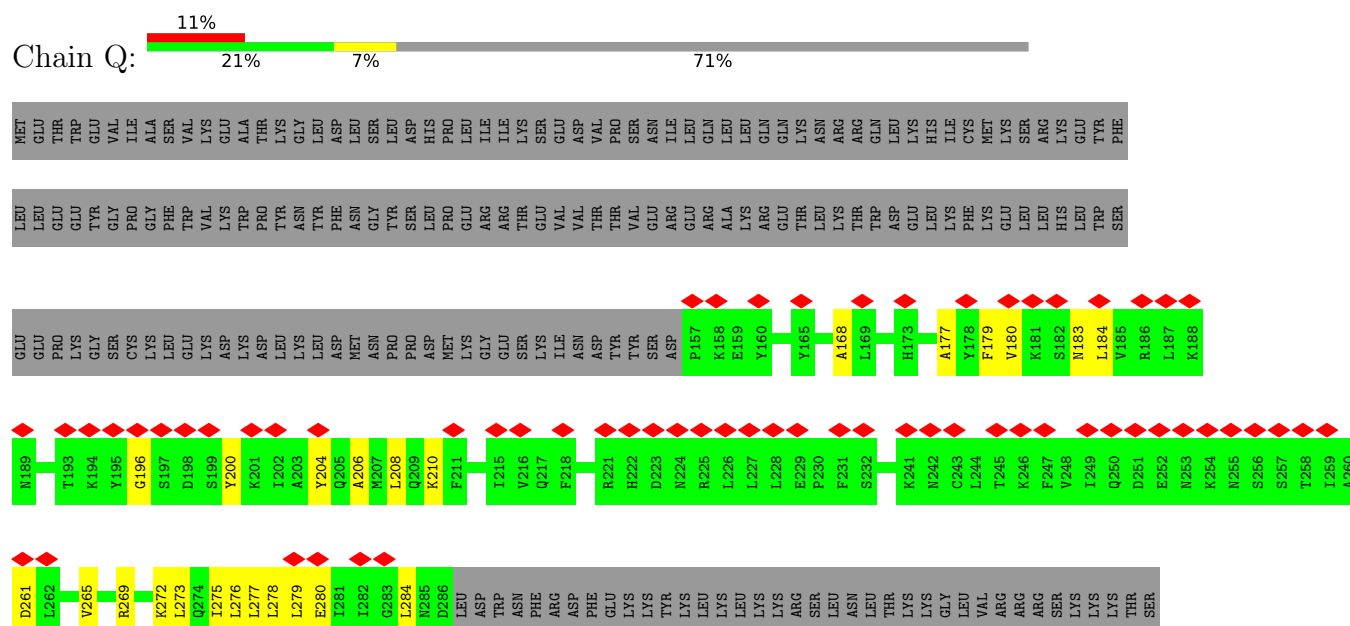
- Molecule 13: DNA replication complex GINS protein PSF1

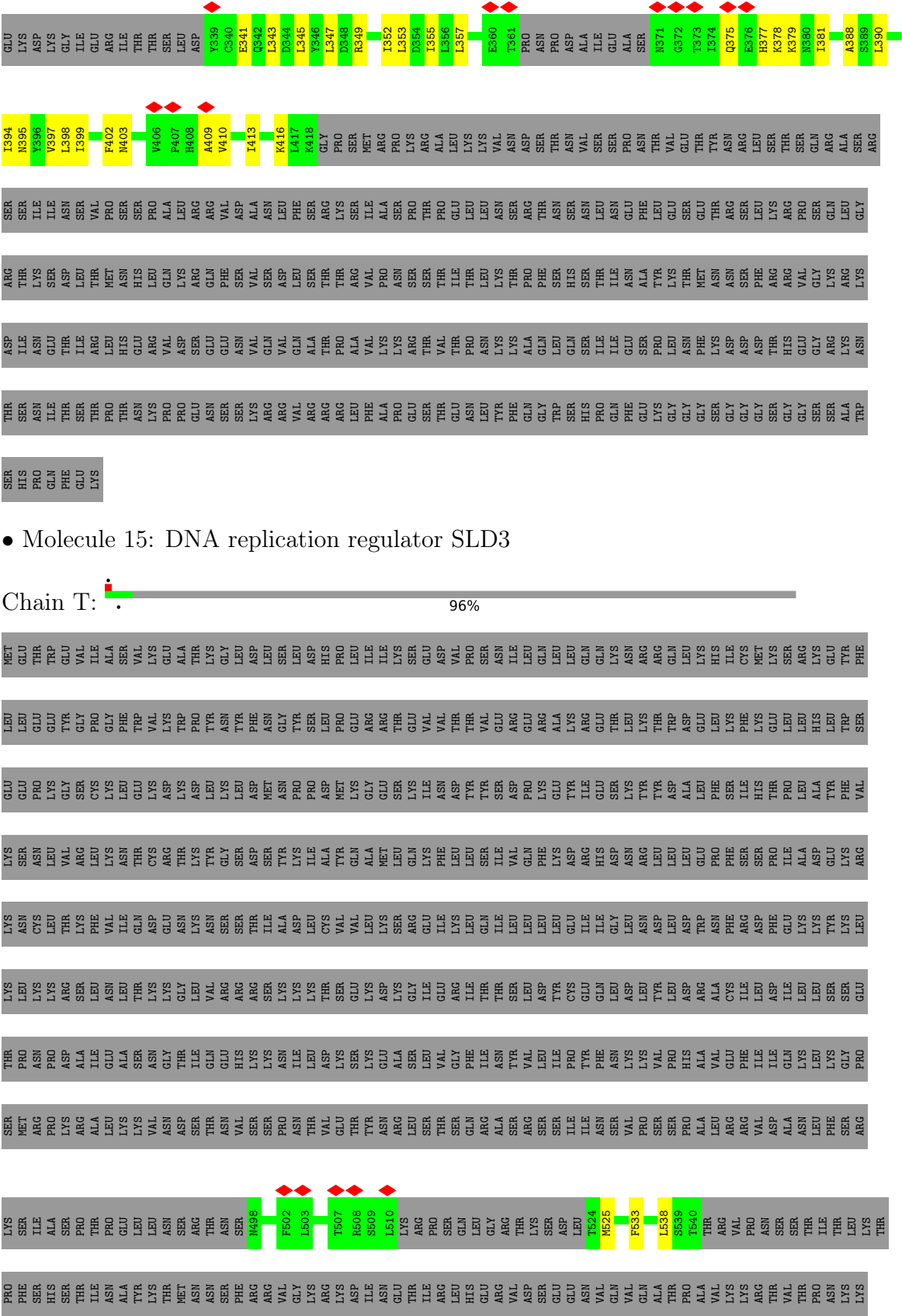


- Molecule 14: DNA replication complex GINS protein PSF2



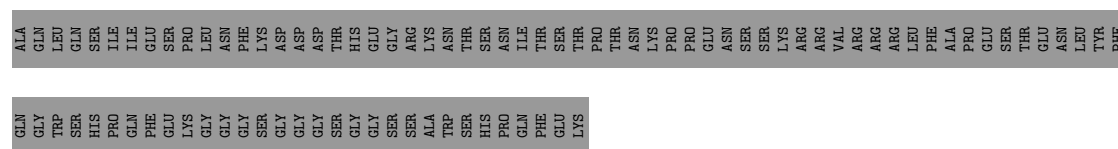
- Molecule 15: DNA replication regulator SLD3



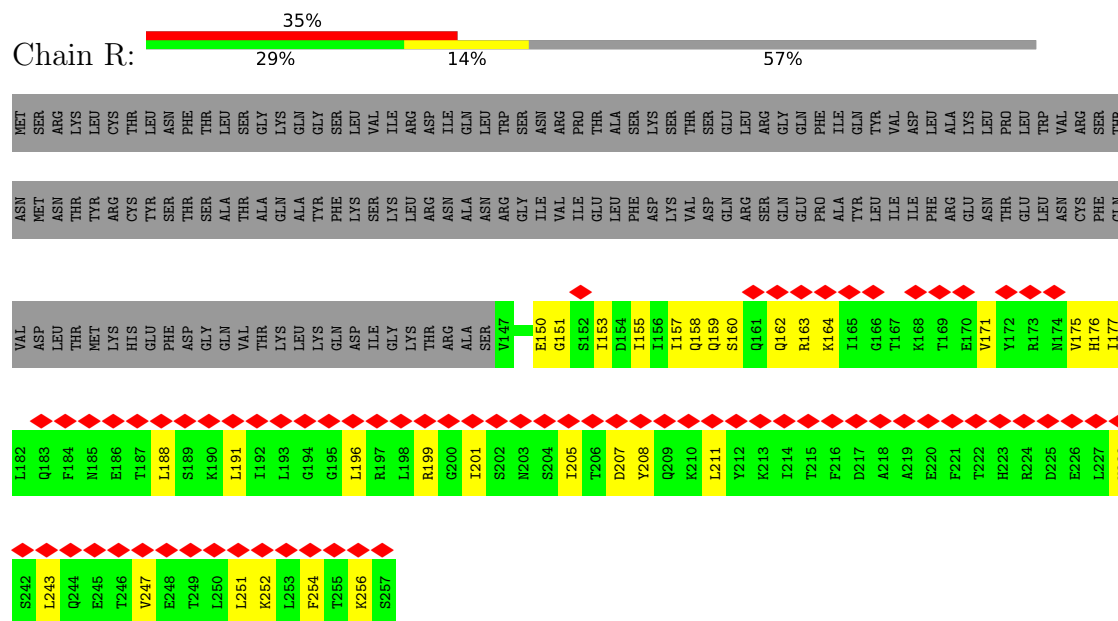


● Molecule 15: DNA replication regulator SLD3

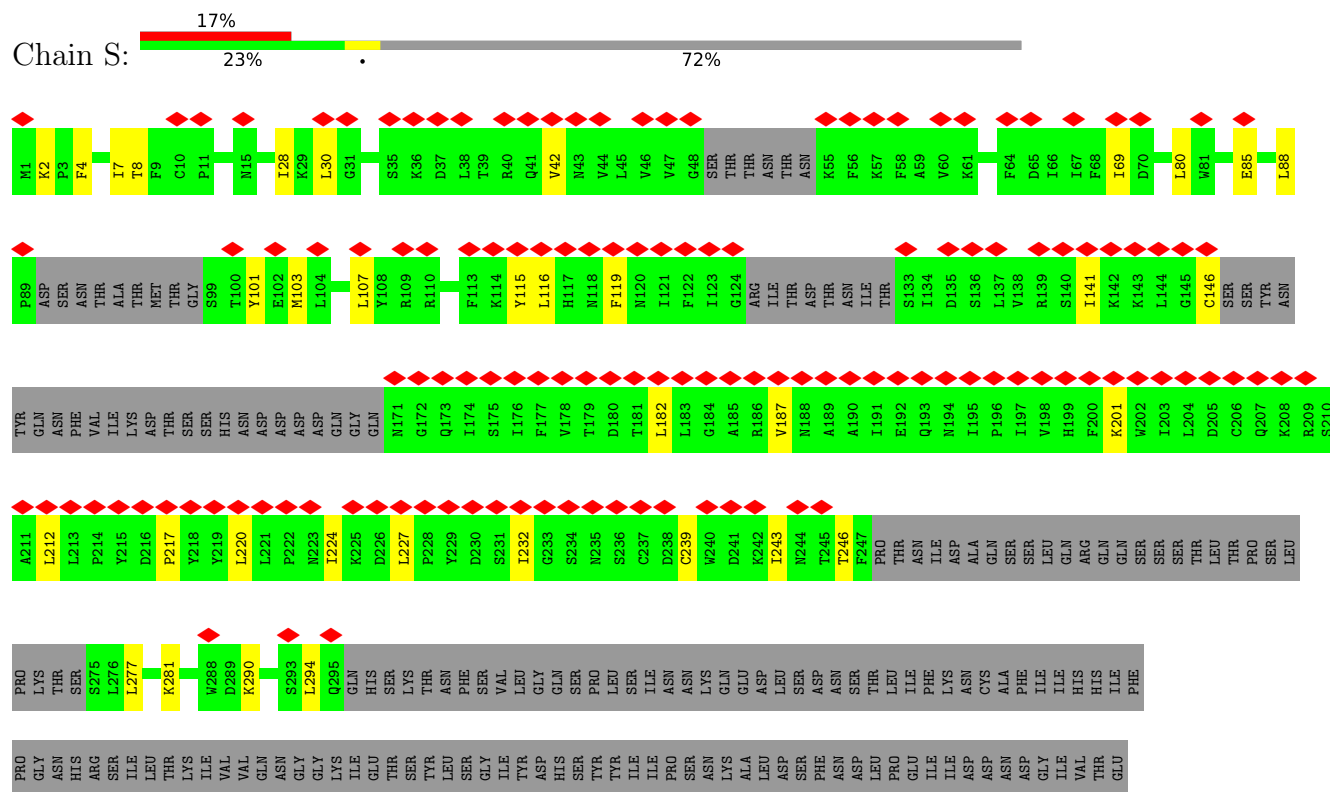
Chain T:  96%



### • Molecule 16: Mitochondrial morphogenesis protein SLD7



### • Molecule 17: DNA replication regulator DPB11



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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	302350	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 ( $e^-/\text{\AA}^2$ )	39	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.264	Depositor
Minimum map value	-0.647	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.26	Depositor
Map size (Å)	570.0, 570.0, 570.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	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, 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	0.10	0/5235	0.29	0/7067
2	3	0.11	0/4734	0.30	0/6414
3	4	0.12	0/4665	0.34	0/6301
4	5	0.12	0/4516	0.30	0/6097
5	6	0.11	0/4671	0.31	0/6293
6	7	0.12	0/4932	0.31	0/6663
6	f	0.11	0/356	0.34	0/479
7	A	0.16	0/713	0.36	0/1097
8	B	0.19	0/711	0.41	0/1096
9	C	0.12	0/1506	0.29	0/2038
10	D	0.12	0/1876	0.31	0/2531
11	E	0.11	0/4190	0.28	0/5665
12	F	0.11	0/701	0.31	0/944
13	H	0.10	0/1719	0.25	0/2314
14	I	0.11	0/1622	0.32	0/2195
15	Q	0.08	0/1671	0.23	0/2248
15	T	0.07	0/247	0.22	0/329
16	R	0.08	0/907	0.22	0/1212
17	S	0.09	0/1832	0.25	0/2465
All	All	0.11	0/46804	0.30	0/63448

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	5147	0	5207	64	0
2	3	4655	0	4730	80	0
3	4	4597	0	4660	116	0
4	5	4455	0	4543	77	0
5	6	4601	0	4621	86	0
6	7	4862	0	4944	121	0
6	f	355	0	337	4	0
7	A	635	0	350	9	0
8	B	636	0	355	16	0
9	C	1472	0	1479	20	0
10	D	1842	0	1854	36	0
11	E	4114	0	4114	86	0
12	F	688	0	712	10	0
13	H	1697	0	1698	27	0
14	I	1589	0	1637	35	0
15	Q	1644	0	1708	30	0
15	T	246	0	237	2	0
16	R	898	0	922	24	0
17	S	1795	0	1860	22	0
18	2	1	0	0	0	0
18	4	1	0	0	0	0
18	5	1	0	0	0	0
18	6	1	0	0	0	0
18	7	1	0	0	0	0
19	7	27	0	12	2	0
20	7	1	0	0	0	0
All	All	45961	0	45980	744	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 8.

All (744) 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)
11:E:329:PRO:HA	11:E:414:ASP:HA	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:451:ARG:HB2	5:6:445:VAL:HB	1.71	0.71
2:3:156:SER:HB2	2:3:325:THR:HB	1.72	0.70
6:7:247:ARG:HB3	6:7:314:LYS:HB3	1.75	0.69
2:3:448:THR:HA	6:7:502:VAL:HA	1.75	0.68
3:4:721:ALA:HB3	6:7:661:VAL:HG22	1.75	0.68
6:7:693:ILE:HG22	6:7:697:GLN:HE21	1.58	0.68
2:3:542:ARG:NH1	19:7:901:ADP:O2A	2.26	0.67
5:6:589:VAL:HG21	5:6:597:TYR:HD2	1.60	0.67
1:2:234:LEU:HG	1:2:239:SER:HB3	1.76	0.66
1:2:372:PRO:HD3	8:B:46:DA:H5''	1.77	0.65
4:5:168:SER:HB3	4:5:257:LYS:HB2	1.78	0.65
11:E:158:ALA:HB1	11:E:240:TYR:HA	1.78	0.65
14:I:21:GLU:HA	14:I:73:LEU:HD22	1.79	0.65
6:7:265:CYS:HB3	6:7:289:CYS:SG	2.37	0.65
2:3:437:SER:HB3	2:3:440:VAL:HB	1.80	0.64
3:4:368:PRO:HG2	3:4:382:MET:HG3	1.78	0.64
6:7:529:MET:HE3	6:7:534:ARG:HG2	1.80	0.64
6:7:147:ARG:NH2	6:7:150:ASN:OD1	2.29	0.64
1:2:613:ASN:HB2	1:2:616:ASP:HB2	1.79	0.63
17:S:8:THR:HB	17:S:42:VAL:HA	1.80	0.63
10:D:145:ARG:NH2	13:H:151:LEU:O	2.31	0.63
14:I:79:LEU:HB3	14:I:84:LYS:HB2	1.81	0.62
2:3:670:GLN:H	2:3:720:THR:HA	1.64	0.62
3:4:561:ASP:OD1	3:4:562:ILE:N	2.33	0.62
5:6:143:MET:HA	5:6:148:LEU:HB2	1.82	0.62
2:3:671:LEU:HD21	2:3:676:ILE:HD11	1.81	0.62
3:4:559:ARG:HD2	3:4:668:ARG:HB3	1.80	0.62
5:6:721:GLU:HA	5:6:724:ASP:HB2	1.82	0.62
2:3:462:MET:HE1	2:3:470:VAL:HG11	1.80	0.62
5:6:141:GLU:HB2	16:R:171:VAL:HG13	1.81	0.62
11:E:30:PHE:HB3	11:E:86:PHE:HZ	1.65	0.62
2:3:456:ARG:H	6:7:502:VAL:HG11	1.64	0.62
3:4:224:LEU:HD13	3:4:227:ILE:HD12	1.82	0.61
4:5:183:CYS:HB3	4:5:188:HIS:H	1.65	0.61
6:7:333:ILE:HD13	6:7:351:VAL:HG11	1.81	0.61
2:3:712:HIS:ND1	2:3:725:ASP:OD1	2.31	0.61
3:4:634:PHE:HE2	3:4:698:LEU:HD21	1.64	0.61
11:E:277:LEU:HD22	11:E:309:LEU:HD12	1.82	0.61
11:E:439:LEU:HB2	11:E:550:LEU:HD12	1.83	0.61
17:S:182:LEU:HA	17:S:187:VAL:HG11	1.83	0.61
3:4:704:LEU:HD21	3:4:800:SER:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:137:ARG:NH1	16:R:179:ASP:OD2	2.33	0.60
4:5:166:ILE:HG23	4:5:288:PRO:HA	1.82	0.60
2:3:683:TYR:OH	2:3:687:ARG:NH2	2.34	0.60
1:2:402:LEU:HB2	5:6:623:ILE:HD11	1.84	0.60
3:4:565:LEU:HD21	3:4:705:VAL:HG12	1.83	0.60
3:4:367:GLU:HB3	5:6:441:ARG:HB2	1.84	0.59
3:4:543:GLN:HA	3:4:562:ILE:HD12	1.82	0.59
11:E:50:LYS:O	14:I:81:GLN:NE2	2.32	0.59
5:6:612:VAL:HG22	5:6:623:ILE:HG22	1.84	0.59
6:7:205:LYS:HD2	6:7:206:PRO:HD2	1.82	0.59
6:7:618:TYR:HB3	6:7:626:PRO:HG3	1.85	0.59
10:D:56:PRO:HB3	14:I:53:ILE:O	2.03	0.59
4:5:184:ARG:N	4:5:240:PRO:O	2.29	0.59
11:E:395:LEU:HG	11:E:399:PHE:HE1	1.66	0.59
14:I:27:ILE:HG22	14:I:87:ILE:HG12	1.83	0.59
9:C:131:ARG:HH21	9:C:169:LEU:HD23	1.67	0.59
13:H:176:THR:HG21	13:H:181:PHE:CD2	2.38	0.59
1:2:439:ASN:OD1	1:2:446:VAL:N	2.33	0.59
2:3:453:GLY:HA3	6:7:503:THR:HA	1.84	0.59
4:5:447:ALA:HB1	4:5:452:SER:HB3	1.85	0.58
3:4:652:GLN:HB3	3:4:668:ARG:HA	1.85	0.58
10:D:205:GLU:HG2	17:S:294:LEU:HD22	1.84	0.58
3:4:198:LEU:HD23	3:4:230:LEU:HD11	1.84	0.58
3:4:687:PRO:O	3:4:691:ASN:ND2	2.37	0.58
10:D:178:ASP:HB3	13:H:141:LEU:HD11	1.86	0.58
15:Q:180:VAL:HG13	15:Q:184:LEU:HD22	1.85	0.58
17:S:224:ILE:HG21	17:S:232:ILE:HG12	1.84	0.58
2:3:455:ARG:O	6:7:316:GLN:NE2	2.37	0.58
15:Q:265:VAL:HG22	15:Q:381:ILE:HD11	1.85	0.58
2:3:425:THR:HA	2:3:657:ARG:HH21	1.68	0.57
6:7:621:MET:HE3	6:7:622:HIS:HE1	1.69	0.57
5:6:107:THR:HG23	5:6:109:GLU:H	1.69	0.57
7:A:2:DG:N2	8:B:48:DT:O2	2.37	0.57
3:4:543:GLN:HG3	3:4:562:ILE:HB	1.85	0.57
6:7:495:ALA:HA	6:7:510:GLY:HA3	1.85	0.57
4:5:50:LEU:O	4:5:54:ILE:HG13	2.04	0.57
13:H:47:LEU:HD22	13:H:75:THR:HG23	1.85	0.57
14:I:101:LYS:HD2	14:I:113:SER:HB2	1.85	0.57
6:7:81:ASP:HA	6:7:205:LYS:HB3	1.87	0.57
8:B:40:DT:H2"	8:B:41:DA:C8	2.40	0.56
4:5:39:ARG:CZ	11:E:320:PRO:HB2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:450:THR:HG21	4:5:492:ALA:HB1	1.87	0.56
2:3:482:ASP:O	2:3:486:ILE:HG12	2.06	0.56
8:B:23:DT:H2"	8:B:24:DA:C8	2.40	0.56
11:E:357:LEU:HD21	11:E:366:LEU:HD22	1.87	0.56
17:S:115:TYR:HB3	17:S:212:LEU:HB2	1.88	0.56
4:5:460:ARG:HH12	8:B:37:DT:H5"	1.69	0.56
5:6:154:ASP:HB3	5:6:157:HIS:HB3	1.87	0.56
10:D:125:PRO:HG3	14:I:50:TRP:NE1	2.20	0.56
4:5:90:PHE:CE2	4:5:94:ILE:HD11	2.40	0.56
2:3:259:GLN:HE21	2:3:271:PRO:HB2	1.69	0.56
2:3:350:ILE:HG12	2:3:659:TYR:HD1	1.70	0.56
11:E:24:SER:OG	13:H:178:TYR:O	2.23	0.56
2:3:416:SER:O	2:3:420:ARG:HG2	2.05	0.56
10:D:189:ILE:HG22	13:H:130:TYR:CD2	2.40	0.56
1:2:832:TYR:O	1:2:836:ARG:HG3	2.07	0.55
3:4:196:ASN:ND2	3:4:253:GLN:OE1	2.37	0.55
11:E:391:ILE:HG22	11:E:395:LEU:HD13	1.89	0.55
12:F:34:LYS:HE3	12:F:78:PHE:HB3	1.88	0.55
2:3:455:ARG:HA	6:7:502:VAL:HB	1.87	0.55
3:4:635:ASP:HA	3:4:694:LEU:HD21	1.87	0.55
5:6:665:LYS:HE2	7:A:19:DG:H5"	1.87	0.55
6:7:147:ARG:O	6:7:151:GLU:HG3	2.05	0.55
3:4:566:LEU:HB3	3:4:574:LYS:HD2	1.89	0.55
5:6:526:TYR:O	5:6:530:VAL:HG23	2.06	0.55
6:7:420:PRO:HB2	6:7:625:GLN:HG2	1.89	0.55
15:Q:177:ALA:HB2	15:Q:397:VAL:HG22	1.88	0.55
1:2:215:LEU:HD12	1:2:274:VAL:HG12	1.88	0.55
4:5:28:ILE:O	4:5:32:LYS:HG3	2.07	0.55
1:2:707:HIS:HE1	5:6:555:VAL:HG11	1.72	0.55
2:3:700:ARG:NH1	6:7:462:PRO:O	2.40	0.55
4:5:456:ASP:HB3	4:5:459:THR:HB	1.89	0.55
14:I:29:PRO:HD2	14:I:67:ARG:O	2.07	0.54
13:H:12:GLU:OE2	13:H:15:ARG:NH1	2.40	0.54
4:5:40:LEU:HD11	4:5:45:ILE:HD13	1.87	0.54
11:E:2:TYR:OH	11:E:137:SER:O	2.24	0.54
1:2:806:THR:HG22	1:2:807:VAL:H	1.73	0.54
11:E:499:LEU:O	11:E:503:ILE:HG12	2.08	0.54
17:S:141:ILE:HG23	17:S:146:CYS:HB3	1.88	0.54
3:4:796:ARG:HH12	5:6:578:SER:HA	1.73	0.54
5:6:829:ASP:O	5:6:833:GLN:HG2	2.08	0.54
1:2:746:GLN:HG2	1:2:749:ARG:HH21	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:87:LEU:HD22	10:D:136:LEU:HD11	1.90	0.54
12:F:40:ALA:HB2	12:F:81:GLN:HG3	1.89	0.54
16:R:159:GLN:O	16:R:163:ARG:HG3	2.07	0.54
4:5:476:VAL:HG22	4:5:518:SER:HB2	1.88	0.54
10:D:94:GLN:HG2	10:D:133:LEU:HD13	1.89	0.54
3:4:526:ILE:HD13	3:4:541:LEU:HB2	1.90	0.54
16:R:176:HIS:CE1	16:R:180:LYS:HE2	2.43	0.54
1:2:402:LEU:HD22	5:6:623:ILE:HG13	1.90	0.54
5:6:311:CYS:SG	5:6:340:ASN:ND2	2.80	0.54
5:6:589:VAL:HG21	5:6:597:TYR:CD2	2.43	0.54
6:7:414:LEU:HG	6:7:433:LEU:HD11	1.90	0.54
2:3:313:THR:O	4:5:175:ARG:NH1	2.39	0.54
6:7:66:MET:O	6:7:70:VAL:HG23	2.08	0.54
9:C:105:PHE:H	9:C:170:GLU:CD	2.16	0.54
14:I:52:LEU:HD13	14:I:55:THR:HB	1.90	0.54
2:3:449:ASP:HB3	2:3:453:GLY:HA2	1.90	0.53
3:4:360:ILE:HD11	3:4:363:GLY:HA2	1.88	0.53
2:3:393:LEU:HB2	2:3:397:SER:HB3	1.89	0.53
3:4:181:TRP:HE1	6:7:147:ARG:NH2	2.06	0.53
2:3:426:ALA:HB3	2:3:429:ALA:HB2	1.90	0.53
12:F:73:GLN:NE2	12:F:90:GLU:OE1	2.40	0.53
1:2:591:LEU:HD11	1:2:636:ILE:HG21	1.91	0.53
10:D:90:ARG:HD3	14:I:53:ILE:HG23	1.90	0.53
2:3:29:GLN:NE2	2:3:33:ASP:OD2	2.41	0.53
11:E:281:ILE:HG12	11:E:302:LEU:HD22	1.91	0.53
3:4:438:THR:N	3:4:462:ASP:O	2.40	0.53
4:5:39:ARG:HB2	4:5:44:PHE:CD1	2.44	0.53
5:6:161:ARG:NH1	5:6:162:GLU:OE2	2.42	0.53
13:H:120:THR:O	13:H:128:GLN:NE2	2.40	0.53
15:Q:275:ILE:O	15:Q:279:LEU:HG	2.08	0.53
10:D:135:ARG:O	10:D:139:VAL:HG23	2.08	0.53
11:E:29:ILE:HG12	11:E:82:LEU:HB2	1.90	0.53
4:5:504:ILE:HD11	4:5:506:LYS:HE3	1.91	0.53
4:5:685:GLN:HA	4:5:689:MET:HG2	1.91	0.53
1:2:534:ARG:HG2	1:2:536:ASP:H	1.73	0.52
1:2:625:GLU:HB2	1:2:676:ARG:HE	1.73	0.52
2:3:475:PHE:HE2	2:3:543:PHE:HZ	1.57	0.52
2:3:456:ARG:NH1	6:7:327:ILE:HG22	2.25	0.52
3:4:245:ALA:HB1	3:4:258:TYR:HE1	1.73	0.52
4:5:568:ILE:O	4:5:572:VAL:HG23	2.10	0.52
15:Q:168:ALA:O	15:Q:269:ARG:NE	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:492:GLN:HE21	6:7:467:SER:HB3	1.74	0.52
3:4:768:THR:HB	3:4:772:ARG:HH12	1.74	0.52
15:T:533:PHE:HE2	15:T:538:LEU:HB2	1.74	0.52
10:D:94:GLN:HE22	10:D:129:MET:HE3	1.75	0.52
11:E:555:LEU:O	11:E:559:LEU:HG	2.09	0.52
12:F:18:ARG:NE	13:H:175:GLN:OE1	2.43	0.52
6:7:527:ASP:O	6:7:534:ARG:NH2	2.42	0.52
15:Q:377:HIS:O	15:Q:381:ILE:HG13	2.10	0.52
4:5:527:TYR:OH	4:5:534:LYS:NZ	2.43	0.52
2:3:448:THR:OG1	6:7:501:PRO:O	2.24	0.52
3:4:340:PRO:HG3	5:6:452:ILE:HG13	1.92	0.52
5:6:543:VAL:O	5:6:547:ILE:HG12	2.09	0.51
5:6:775:GLU:O	5:6:779:GLU:HG2	2.10	0.51
5:6:608:LEU:HD12	5:6:627:ALA:HB3	1.92	0.51
6:7:130:LYS:HG2	6:7:132:ILE:HG23	1.92	0.51
15:Q:280:GLU:O	15:Q:284:LEU:HG	2.11	0.51
1:2:518:SER:HA	1:2:537:ILE:HB	1.90	0.51
2:3:456:ARG:NH1	6:7:328:PRO:O	2.37	0.51
9:C:12:ASP:O	9:C:49:TRP:N	2.44	0.51
9:C:88:ILE:HG23	9:C:127:LEU:HD12	1.92	0.51
2:3:535:LEU:HB2	2:3:540:LEU:HD21	1.93	0.51
3:4:650:GLU:HG2	5:6:582:SER:HB2	1.91	0.51
5:6:608:LEU:HA	5:6:627:ALA:HB3	1.92	0.51
8:B:19:DT:H2"	8:B:20:DA:C8	2.46	0.51
8:B:25:DT:H2"	8:B:26:DG:H8	1.76	0.51
11:E:336:LEU:HD11	11:E:341:LEU:HA	1.92	0.51
3:4:724:LEU:HD11	6:7:690:LEU:HD23	1.93	0.51
16:R:188:LEU:HD13	16:R:243:LEU:HD11	1.93	0.51
1:2:339:PHE:HB2	1:2:348:LEU:HD12	1.92	0.51
3:4:181:TRP:HE1	6:7:147:ARG:HH22	1.59	0.51
6:7:142:ILE:HG13	6:7:143:LEU:N	2.26	0.51
11:E:333:LEU:HD12	11:E:336:LEU:HD22	1.92	0.51
15:Q:395:ASN:HA	15:Q:399:ILE:HD12	1.91	0.51
3:4:315:ARG:O	6:7:341:ARG:NH2	2.44	0.51
1:2:514:ALA:HB2	1:2:679:ILE:HG21	1.93	0.51
6:7:542:GLU:OE2	6:7:593:ARG:NH1	2.44	0.51
15:Q:394:ILE:HG12	15:Q:398:LEU:HD12	1.93	0.51
2:3:175:HIS:HA	2:3:178:LYS:HD2	1.93	0.51
9:C:23:ASP:OD1	9:C:40:LYS:N	2.44	0.51
3:4:778:ARG:HD3	3:4:793:ALA:HB3	1.93	0.50
3:4:199:MET:HE1	3:4:283:LEU:HG	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:44:DT:H2"	8:B:45:DG:C8	2.46	0.50
3:4:560:GLY:HA2	3:4:803:ARG:HD2	1.92	0.50
10:D:145:ARG:HD2	13:H:155:LEU:HD11	1.94	0.50
5:6:500:ASP:HB3	5:6:503:VAL:HG12	1.94	0.50
6:7:501:PRO:HG2	6:7:507:ILE:HD11	1.92	0.50
17:S:201:LYS:HD3	17:S:232:ILE:HB	1.93	0.50
5:6:139:GLN:NE2	5:6:151:ILE:HG13	2.26	0.50
9:C:134:GLU:HG3	9:C:138:HIS:CD2	2.46	0.50
10:D:262:ASP:HB2	10:D:278:ARG:HH12	1.77	0.50
1:2:746:GLN:HG2	1:2:749:ARG:NH2	2.26	0.50
3:4:818:GLU:HB2	3:4:820:GLU:HG2	1.93	0.50
5:6:553:GLY:O	5:6:812:ARG:NH1	2.45	0.50
9:C:12:ASP:HA	9:C:48:LEU:HD23	1.92	0.50
14:I:105:GLU:OE2	14:I:113:SER:N	2.40	0.50
1:2:792:ASP:HA	1:2:795:ARG:HH12	1.76	0.50
4:5:90:PHE:O	4:5:94:ILE:HG13	2.11	0.50
5:6:614:ARG:NH2	8:B:34:DA:H8	2.10	0.50
8:B:45:DG:H2"	8:B:46:DA:C8	2.47	0.50
16:R:243:LEU:O	16:R:247:VAL:HG23	2.12	0.50
2:3:118:PRO:HD2	2:3:177:ASN:O	2.12	0.49
6:7:411:TYR:HB2	6:7:702:LEU:HD21	1.94	0.49
11:E:103:TYR:HD1	11:E:117:ARG:HE	1.60	0.49
11:E:341:LEU:HB2	11:E:387:MET:HE1	1.93	0.49
2:3:38:TYR:CE1	2:3:98:ILE:HA	2.48	0.49
4:5:559:ASP:O	4:5:564:ARG:HD2	2.12	0.49
5:6:136:TYR:HE2	5:6:153:ILE:HG23	1.77	0.49
10:D:138:PHE:HD1	10:D:141:ARG:HH21	1.61	0.49
14:I:99:ASP:OD1	14:I:144:LYS:NZ	2.39	0.49
1:2:300:PHE:HB3	1:2:319:ARG:HD2	1.95	0.49
6:7:635:PRO:HA	6:7:638:MET:HG2	1.93	0.49
6:7:651:VAL:N	6:7:706:ASP:O	2.42	0.49
15:Q:204:TYR:O	15:Q:208:LEU:HG	2.13	0.49
3:4:251:TYR:CE2	3:4:253:GLN:HB2	2.48	0.49
6:7:654:GLU:HA	6:7:657:ASN:OD1	2.13	0.49
5:6:179:PRO:HA	5:6:182:GLN:NE2	2.28	0.49
6:7:151:GLU:O	6:7:155:SER:HB2	2.13	0.49
6:7:457:CYS:HB3	6:7:597:LEU:HD13	1.94	0.49
6:7:466:LYS:N	19:7:901:ADP:O3B	2.45	0.49
13:H:171:ALA:HB3	13:H:183:LEU:HB2	1.94	0.49
15:Q:179:PHE:HD1	15:Q:183:ASN:HD22	1.59	0.49
2:3:227:THR:HG22	2:3:229:ALA:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:521:LEU:O	3:4:524:ARG:HG2	2.12	0.49
10:D:97:LEU:O	10:D:101:ILE:HG12	2.12	0.49
17:S:88:LEU:HD21	17:S:103:MET:HB2	1.94	0.49
2:3:484:VAL:HG13	6:7:486:LYS:HD3	1.94	0.49
4:5:177:THR:O	4:5:194:ILE:N	2.43	0.49
5:6:657:GLU:HB2	5:6:708:ARG:HH21	1.78	0.49
11:E:128:PRO:HG3	11:E:250:GLN:HB2	1.95	0.49
11:E:133:ASN:HA	11:E:137:SER:HB3	1.94	0.49
11:E:485:TRP:HZ3	13:H:188:GLN:HE21	1.59	0.49
2:3:501:GLY:HA2	6:7:509:GLU:OE1	2.12	0.49
4:5:446:ALA:N	4:5:489:ASP:OD1	2.45	0.49
4:5:90:PHE:CD2	4:5:137:LEU:HD22	2.48	0.49
6:7:151:GLU:O	6:7:155:SER:CB	2.60	0.49
5:6:120:GLU:O	5:6:137:ARG:NH2	2.46	0.48
6:7:497:VAL:HG22	6:7:508:LEU:HD11	1.94	0.48
10:D:265:GLU:OE1	14:I:166:SER:HB2	2.13	0.48
11:E:34:LEU:H	11:E:484:PHE:HD1	1.61	0.48
16:R:205:ILE:HG22	16:R:207:ASP:H	1.77	0.48
4:5:166:ILE:HG21	4:5:286:VAL:HG12	1.94	0.48
3:4:637:MET:O	3:4:642:ARG:NH2	2.46	0.48
6:7:102:LEU:O	6:7:106:ILE:HG13	2.13	0.48
2:3:498:ALA:HA	2:3:503:HIS:CE1	2.48	0.48
1:2:682:VAL:HG12	1:2:684:ARG:HG2	1.96	0.48
1:2:812:SER:O	1:2:816:ILE:HG13	2.14	0.48
3:4:439:PHE:CZ	3:4:459:THR:HB	2.48	0.48
5:6:405:PRO:HA	5:6:450:TYR:HA	1.95	0.48
5:6:614:ARG:HH22	8:B:34:DA:H2'	1.78	0.48
9:C:136:ASN:HB2	14:I:184:PHE:CZ	2.47	0.48
16:R:228:LYS:HG2	16:R:232:MET:HE3	1.95	0.48
4:5:526:ILE:HD11	4:5:541:ASP:H	1.78	0.48
4:5:351:GLU:OE1	13:H:22:ARG:NH1	2.47	0.48
1:2:803:PHE:CD1	1:2:804:PRO:HD2	2.47	0.48
3:4:750:TYR:OH	3:4:811:MET:O	2.32	0.48
11:E:639:ILE:HD12	11:E:640:ARG:H	1.78	0.48
6:f:149:ARG:HE	6:f:153:MET:HE3	1.79	0.48
14:I:169:GLN:NE2	14:I:171:ASP:OD2	2.46	0.48
17:S:224:ILE:HG23	17:S:227:LEU:HB2	1.95	0.48
1:2:760:GLN:O	1:2:764:MET:HG3	2.14	0.48
2:3:297:VAL:HG12	2:3:299:LYS:HG3	1.95	0.48
3:4:393:ASP:OD1	3:4:394:LYS:N	2.46	0.48
6:7:261:THR:HG22	6:7:268:GLU:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:285:THR:HA	11:E:295:TYR:CE2	2.49	0.48
11:E:480:TRP:CE2	11:E:549:PRO:HD3	2.49	0.47
16:R:176:HIS:ND1	16:R:180:LYS:HE2	2.29	0.47
1:2:814:LEU:O	1:2:818:GLU:HG3	2.14	0.47
2:3:233:THR:HG23	2:3:234:GLU:HG3	1.95	0.47
5:6:525:ILE:O	5:6:529:LEU:HG	2.14	0.47
8:B:25:DT:H2''	8:B:26:DG:C8	2.49	0.47
10:D:94:GLN:NE2	10:D:129:MET:HB3	2.29	0.47
11:E:66:GLU:HB3	11:E:70:HIS:CD2	2.49	0.47
11:E:70:HIS:NE2	13:H:184:ILE:HG21	2.29	0.47
14:I:126:LEU:HB3	14:I:134:PHE:HZ	1.78	0.47
17:S:4:PHE:HA	17:S:7:ILE:HD12	1.95	0.47
3:4:584:ILE:O	3:4:584:ILE:HG22	2.14	0.47
4:5:39:ARG:HG3	4:5:43:GLN:H	1.79	0.47
5:6:750:GLN:HG2	5:6:753:ARG:HH22	1.78	0.47
10:D:94:GLN:HE21	10:D:98:ILE:HD11	1.79	0.47
10:D:143:TYR:CZ	10:D:147:ARG:HD2	2.49	0.47
12:F:27:ARG:HH21	13:H:177:GLU:HG3	1.78	0.47
5:6:688:ARG:HA	5:6:688:ARG:HH11	1.79	0.47
15:Q:272:LYS:NZ	15:Q:388:ALA:O	2.46	0.47
3:4:681:ARG:NH1	6:7:683:GLN:HG3	2.29	0.47
5:6:402:ILE:HD13	5:6:455:LEU:HB2	1.97	0.47
5:6:721:GLU:O	5:6:725:THR:HG23	2.14	0.47
15:Q:206:ALA:O	15:Q:210:LYS:HG3	2.14	0.47
2:3:687:ARG:HG2	6:7:609:ASP:OD2	2.14	0.47
3:4:648:VAL:HG13	3:4:649:MET:HE2	1.95	0.47
1:2:534:ARG:HD2	1:2:536:ASP:HB2	1.96	0.47
2:3:572:LEU:HD12	2:3:573:PRO:HD2	1.96	0.47
3:4:322:ILE:HA	3:4:439:PHE:HD2	1.80	0.47
3:4:452:VAL:HG13	6:7:277:THR:HB	1.97	0.47
3:4:712:VAL:HG21	6:7:672:LYS:HA	1.96	0.47
4:5:44:PHE:CD2	14:I:146:GLN:HG2	2.50	0.47
4:5:57:LYS:NZ	9:C:134:GLU:OE1	2.40	0.47
5:6:581:LYS:HD2	5:6:681:ALA:HB1	1.96	0.47
5:6:717:ASP:N	5:6:717:ASP:OD1	2.43	0.47
3:4:277:LYS:HE3	3:4:297:GLU:HA	1.97	0.47
4:5:489:ASP:O	4:5:493:ILE:HG12	2.14	0.47
3:4:799:GLU:HB3	3:4:803:ARG:NH2	2.29	0.47
4:5:72:ASN:HB3	4:5:75:ILE:HD12	1.96	0.47
5:6:513:ILE:HG22	5:6:517:LYS:HE3	1.96	0.47
5:6:601:LYS:HD2	5:6:601:LYS:HA	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:92:LYS:HB3	6:7:97:THR:OG1	2.15	0.47
10:D:126:LEU:HD23	11:E:22:HIS:HE2	1.79	0.47
1:2:802:SER:O	4:5:529:ARG:NH2	2.48	0.47
3:4:371:CYS:HB3	3:4:376:CYS:O	2.15	0.47
14:I:6:HIS:CD2	14:I:7:LEU:HG	2.50	0.47
16:R:211:LEU:HD11	16:R:254:PHE:HB3	1.97	0.47
1:2:806:THR:HG22	1:2:807:VAL:N	2.30	0.46
4:5:622:LEU:HD23	4:5:681:ILE:HD11	1.97	0.46
5:6:357:GLN:OE1	5:6:387:GLU:N	2.49	0.46
6:7:402:MET:O	6:7:406:THR:HG23	2.16	0.46
6:7:652:MET:HA	6:7:708:VAL:HG22	1.97	0.46
11:E:570:GLN:HG2	11:E:571:LEU:H	1.80	0.46
15:Q:261:ASP:OD1	15:Q:378:LYS:NZ	2.47	0.46
6:7:693:ILE:HG22	6:7:697:GLN:NE2	2.28	0.46
9:C:62:ALA:HB2	9:C:68:PRO:HA	1.97	0.46
16:R:151:GLY:O	16:R:155:ILE:HG13	2.15	0.46
2:3:182:VAL:HG21	2:3:274:ILE:HD11	1.97	0.46
3:4:593:GLY:N	3:4:632:ASP:O	2.48	0.46
4:5:45:ILE:HG13	4:5:46:TYR:N	2.30	0.46
5:6:794:ARG:HD3	5:6:838:VAL:HG21	1.97	0.46
6:7:18:PHE:HB2	6:7:116:LEU:HD11	1.97	0.46
6:7:286:SER:HB2	6:7:289:CYS:HB2	1.97	0.46
7:A:10:DC:H2"	7:A:11:DC:C6	2.50	0.46
7:A:25:DT:H2"	7:A:26:DA:C8	2.51	0.46
11:E:480:TRP:NE1	11:E:549:PRO:HD3	2.31	0.46
11:E:534:LEU:HD22	15:Q:352:ILE:HG12	1.97	0.46
1:2:798:ILE:HD13	4:5:560:HIS:HE1	1.80	0.46
2:3:304:GLY:HA3	2:3:317:PHE:HD1	1.80	0.46
2:3:411:PRO:HB3	4:5:545:THR:HG22	1.97	0.46
3:4:335:SER:HB3	3:4:397:ILE:HG23	1.96	0.46
4:5:91:GLU:O	4:5:95:THR:HG23	2.14	0.46
5:6:695:LEU:HD23	5:6:794:ARG:NH2	2.31	0.46
5:6:835:ILE:O	5:6:838:VAL:HG22	2.15	0.46
6:7:481:VAL:HG11	6:7:512:ALA:HB1	1.98	0.46
11:E:616:PHE:O	11:E:620:THR:OG1	2.27	0.46
3:4:702:PHE:HD1	3:4:702:PHE:H	1.59	0.46
6:7:323:PRO:HB2	6:7:326:HIS:CE1	2.49	0.46
6:7:569:PRO:HA	6:7:584:ILE:HG12	1.97	0.46
2:3:367:LEU:HD11	2:3:382:LEU:HB2	1.98	0.46
4:5:182:MET:HE2	4:5:242:ILE:HD11	1.97	0.46
4:5:356:GLU:O	4:5:359:GLN:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:695:LEU:O	6:7:699:LEU:HG	2.15	0.46
11:E:302:LEU:O	11:E:306:VAL:HG23	2.15	0.46
11:E:367:HIS:HD2	11:E:377:LEU:HD21	1.79	0.46
15:Q:273:LEU:O	15:Q:277:LEU:HG	2.15	0.46
2:3:304:GLY:HA3	2:3:317:PHE:CD1	2.50	0.46
3:4:826:VAL:O	3:4:830:ARG:HG2	2.13	0.46
7:A:11:DC:H2''	7:A:12:DA:C8	2.51	0.46
17:S:217:PRO:HA	17:S:220:LEU:HD12	1.98	0.46
3:4:322:ILE:HD11	3:4:441:SER:HB3	1.96	0.46
6:7:661:VAL:O	6:7:665:ILE:HG12	2.16	0.46
11:E:67:LEU:C	11:E:69:ARG:H	2.23	0.46
3:4:182:GLY:H	6:7:146:ARG:CZ	2.28	0.46
3:4:550:LYS:HE3	3:4:552:PHE:CE1	2.51	0.46
3:4:657:ALA:HA	3:4:662:ILE:HA	1.97	0.46
4:5:37:GLU:O	11:E:422:TYR:HE2	1.99	0.46
6:7:83:ASP:O	6:7:87:GLN:HG3	2.16	0.46
6:7:622:HIS:HB3	6:7:624:LYS:HE2	1.98	0.46
11:E:53:LEU:HD12	14:I:82:GLN:NE2	2.31	0.46
5:6:124:VAL:HG11	5:6:157:HIS:NE2	2.30	0.46
11:E:2:TYR:HE2	11:E:134:ILE:HG12	1.81	0.46
11:E:62:PHE:O	11:E:632:PHE:N	2.48	0.46
17:S:28:ILE:HG12	6:f:177:MET:HG3	1.98	0.46
2:3:443:THR:HG22	2:3:489:VAL:HG21	1.98	0.45
4:5:148:LEU:HD23	4:5:260:GLU:HB3	1.97	0.45
4:5:166:ILE:HD11	4:5:256:LEU:HD22	1.98	0.45
5:6:262:VAL:HG13	5:6:352:ARG:HE	1.81	0.45
5:6:517:LYS:O	5:6:521:LYS:HG3	2.16	0.45
6:7:439:GLY:HA3	6:7:452:GLY:HA2	1.98	0.45
10:D:193:LEU:HD22	13:H:130:TYR:CG	2.51	0.45
11:E:27:LEU:HD23	11:E:56:SER:HB2	1.97	0.45
16:R:160:SER:O	16:R:164:LYS:HG3	2.16	0.45
1:2:803:PHE:HB3	1:2:845:PHE:HE1	1.82	0.45
3:4:435:VAL:HG12	3:4:466:VAL:HG22	1.97	0.45
4:5:90:PHE:HD2	4:5:137:LEU:HD22	1.82	0.45
17:S:101:TYR:OH	17:S:246:THR:O	2.34	0.45
1:2:803:PHE:HB3	1:2:845:PHE:CE1	2.51	0.45
2:3:254:GLN:HB2	2:3:283:VAL:HG22	1.97	0.45
3:4:774:TYR:CG	3:4:798:LEU:HD11	2.52	0.45
14:I:23:GLU:O	14:I:73:LEU:HB2	2.16	0.45
16:R:177:ILE:HG12	16:R:230:ILE:O	2.17	0.45
8:B:41:DA:H2''	8:B:42:DG:H8	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:94:GLN:HE22	10:D:129:MET:HB3	1.80	0.45
15:Q:390:LEU:O	15:Q:394:ILE:HG13	2.17	0.45
3:4:451:ARG:O	3:4:451:ARG:HG2	2.17	0.45
4:5:39:ARG:HD2	4:5:42:SER:HA	1.98	0.45
6:f:166:LEU:O	6:f:166:LEU:HD23	2.17	0.45
5:6:397:PHE:HD2	5:6:459:VAL:HG22	1.81	0.45
6:7:73:ARG:HA	6:7:73:ARG:HD3	1.62	0.45
6:7:662:GLN:O	6:7:666:ARG:HG3	2.17	0.45
10:D:294:ILE:HB	14:I:175:LEU:HD11	1.99	0.45
17:S:69:ILE:HD13	17:S:107:LEU:HD22	1.99	0.45
1:2:364:CYS:O	1:2:368:LYS:N	2.49	0.45
3:4:308:VAL:HG11	3:4:325:LEU:HD23	1.99	0.45
3:4:808:HIS:HE1	3:4:812:LYS:HE3	1.82	0.45
4:5:378:ILE:O	4:5:385:LYS:NZ	2.41	0.45
11:E:389:HIS:CE1	11:E:393:ARG:HH21	2.34	0.45
11:E:637:ILE:HD12	11:E:647:PHE:HZ	1.82	0.45
16:R:158:GLN:O	16:R:162:GLN:HG3	2.17	0.45
1:2:442:ASN:HD22	1:2:446:VAL:HG11	1.81	0.45
9:C:146:LEU:HD22	9:C:189:ARG:HA	1.98	0.45
13:H:20:TYR:HD1	13:H:27:VAL:HG11	1.82	0.45
2:3:100:LEU:HD21	2:3:115:LEU:HD21	1.99	0.45
2:3:418:LEU:O	2:3:422:VAL:HG23	2.17	0.45
2:3:455:ARG:NH2	6:7:505:GLU:HB3	2.32	0.45
3:4:241:LEU:HD23	3:4:276:ILE:HD13	1.99	0.45
3:4:396:VAL:HA	3:4:417:LEU:O	2.17	0.45
10:D:171:LEU:HD21	10:D:175:LEU:HD12	1.99	0.45
14:I:149:ARG:NH1	14:I:177:GLU:HG2	2.32	0.45
17:S:277:LEU:O	17:S:281:LYS:HG3	2.17	0.45
1:2:792:ASP:HA	1:2:795:ARG:NH1	2.32	0.45
15:Q:180:VAL:HA	15:Q:184:LEU:HD13	1.98	0.45
1:2:348:LEU:HD21	1:2:364:CYS:SG	2.57	0.44
5:6:526:TYR:HE2	5:6:545:LYS:HE3	1.82	0.44
6:7:343:LEU:HD22	6:7:349:VAL:HG11	2.00	0.44
6:7:621:MET:HE3	6:7:622:HIS:CE1	2.51	0.44
11:E:22:HIS:O	13:H:192:ARG:NH2	2.48	0.44
1:2:557:GLU:HB2	1:2:605:LEU:HD12	1.99	0.44
4:5:452:SER:HB2	4:5:454:GLN:OE1	2.17	0.44
5:6:122:PHE:HZ	5:6:157:HIS:CD2	2.35	0.44
2:3:363:LEU:O	2:3:367:LEU:HG	2.18	0.44
2:3:384:MET:HE2	2:3:513:ILE:HB	1.99	0.44
3:4:333:LEU:HD11	3:4:400:GLN:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:334:ARG:HH22	5:6:375:ARG:CZ	2.31	0.44
8:B:47:DC:H2"	8:B:48:DT:C6	2.53	0.44
9:C:3:TYR:CE2	10:D:218:MET:HE3	2.52	0.44
11:E:275:SER:O	11:E:279:LEU:HG	2.17	0.44
11:E:336:LEU:HD12	11:E:336:LEU:HA	1.82	0.44
15:Q:196:GLY:O	15:Q:200:TYR:HB3	2.18	0.44
15:Q:403:ASN:HA	15:Q:410:VAL:HG21	1.99	0.44
1:2:687:VAL:HA	5:6:781:ARG:HH21	1.83	0.44
2:3:578:GLU:HG3	4:5:670:PRO:HB2	2.00	0.44
3:4:535:ASP:O	3:4:706:TYR:OH	2.29	0.44
5:6:513:ILE:HD13	16:R:157:ILE:HD13	1.99	0.44
11:E:71:TYR:HA	11:E:74:LEU:HG	1.98	0.44
11:E:485:TRP:HE1	13:H:186:ASP:HB3	1.81	0.44
13:H:110:MET:SD	13:H:132:LYS:HD2	2.57	0.44
17:S:116:LEU:HA	17:S:119:PHE:HD2	1.82	0.44
4:5:450:THR:HA	4:5:502:ILE:HD13	1.99	0.44
11:E:103:TYR:HB3	11:E:117:ARG:HG2	1.99	0.44
12:F:22:TYR:HE2	12:F:27:ARG:HE	1.65	0.44
15:Q:278:LEU:HD13	15:Q:343:LEU:HA	1.98	0.44
2:3:408:VAL:O	2:3:548:VAL:HA	2.18	0.44
4:5:548:SER:O	4:5:651:ARG:HD3	2.16	0.44
6:7:457:CYS:HA	6:7:565:ALA:HB3	1.99	0.44
6:7:680:SER:HB2	6:7:727:LEU:HD23	1.99	0.44
3:4:199:MET:HA	3:4:227:ILE:HD11	2.00	0.44
3:4:774:TYR:HA	3:4:777:MET:HG2	2.00	0.44
6:7:309:ALA:O	6:7:336:ASN:HA	2.17	0.44
6:7:317:GLU:CD	6:7:329:ARG:H	2.26	0.44
6:7:525:GLU:HB3	6:7:528:LYS:HG2	2.00	0.44
2:3:420:ARG:HH22	4:5:499:GLN:HG3	1.82	0.44
4:5:146:ILE:HD13	4:5:160:VAL:HB	2.00	0.43
16:R:191:LEU:HD21	16:R:240:PHE:CZ	2.52	0.43
16:R:196:LEU:HD22	16:R:201:ILE:HD12	2.00	0.43
2:3:456:ARG:HA	6:7:316:GLN:NE2	2.32	0.43
3:4:536:VAL:HG22	3:4:706:TYR:CD2	2.53	0.43
5:6:333:CYS:HA	5:6:344:TRP:HH2	1.84	0.43
5:6:641:PHE:HD2	5:6:682:ALA:HB2	1.82	0.43
5:6:822:SER:O	5:6:826:GLU:HG3	2.18	0.43
6:7:459:MET:HB2	6:7:599:LEU:HD13	1.99	0.43
8:B:45:DG:H2"	8:B:46:DA:N7	2.34	0.43
14:I:149:ARG:HH12	14:I:177:GLU:HG2	1.83	0.43
3:4:315:ARG:HH22	3:4:410:GLN:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:117:PHE:O	6:7:121:ILE:HG13	2.19	0.43
6:7:252:LYS:O	6:7:310:PHE:N	2.47	0.43
3:4:356:MET:SD	3:4:368:PRO:HG3	2.59	0.43
3:4:697:PRO:HB2	5:6:577:PRO:HG2	2.01	0.43
3:4:721:ALA:HA	6:7:689:LEU:HD21	1.99	0.43
5:6:534:ALA:HB2	5:6:587:TYR:CD2	2.53	0.43
6:7:404:LEU:HD23	6:7:641:TYR:CD2	2.53	0.43
6:7:473:ILE:HD13	6:7:564:LEU:HD22	2.01	0.43
15:Q:398:LEU:HA	15:Q:402:PHE:HD1	1.83	0.43
1:2:695:LEU:O	1:2:699:VAL:HG23	2.19	0.43
5:6:650:VAL:HA	5:6:653:HIS:NE2	2.32	0.43
6:7:634:GLU:HG2	6:7:637:LYS:H	1.83	0.43
12:F:33:ILE:HB	13:H:175:GLN:HB2	1.99	0.43
1:2:474:PHE:CD1	1:2:561:HIS:HD2	2.36	0.43
3:4:669:SER:OG	3:4:670:SER:N	2.52	0.43
8:B:27:DT:H2"	8:B:28:DA:C8	2.53	0.43
9:C:159:ASN:OD1	9:C:160:ILE:N	2.51	0.43
10:D:119:PRO:HB2	14:I:47:HIS:CE1	2.53	0.43
11:E:520:ILE:HG23	11:E:525:LEU:HB2	1.99	0.43
1:2:181:LEU:HD11	1:2:203:VAL:HG22	2.01	0.43
1:2:795:ARG:HA	4:5:560:HIS:HD2	1.84	0.43
3:4:437:GLY:HA2	3:4:464:VAL:HG22	1.99	0.43
3:4:579:GLN:OE1	6:7:543:GLN:HA	2.19	0.43
10:D:263:LEU:HD11	14:I:165:GLU:HG2	1.99	0.43
11:E:646:PRO:O	11:E:650:LYS:HG3	2.19	0.43
6:7:451:ARG:HH11	6:7:542:GLU:HA	1.84	0.43
6:7:668:ARG:HA	6:7:668:ARG:HD2	1.84	0.43
1:2:862:ALA:HB1	1:2:866:LEU:HD12	2.00	0.43
6:7:432:LEU:O	6:7:435:LEU:HB2	2.19	0.43
10:D:68:LYS:HE2	14:I:19:ILE:HD13	2.01	0.43
11:E:278:TRP:CE2	11:E:418:ARG:HD3	2.54	0.43
11:E:355:LEU:HB2	11:E:357:LEU:HD12	2.01	0.43
11:E:394:GLU:O	11:E:398:ILE:HG13	2.19	0.43
3:4:264:TYR:OH	6:7:142:ILE:HD13	2.18	0.43
3:4:750:TYR:HE1	3:4:813:LEU:HD11	1.84	0.43
4:5:370:LEU:HD22	4:5:666:LEU:HD21	1.99	0.43
6:7:142:ILE:HG13	6:7:143:LEU:H	1.84	0.43
6:7:607:ASP:O	6:7:611:LYS:HG3	2.18	0.43
10:D:132:GLU:OE2	14:I:54:THR:OG1	2.31	0.43
11:E:11:ALA:O	11:E:15:ILE:HG13	2.18	0.43
11:E:31:VAL:HG22	11:E:84:VAL:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:66:PHE:CZ	12:F:84:VAL:HG22	2.54	0.43
2:3:367:LEU:HD22	2:3:421:PHE:HE2	1.84	0.42
3:4:255:GLU:O	3:4:258:TYR:HB3	2.19	0.42
9:C:129:LEU:O	9:C:133:GLN:HG2	2.18	0.42
14:I:92:TRP:HZ2	14:I:122:LEU:HD23	1.83	0.42
3:4:566:LEU:HB2	3:4:674:SER:HA	2.01	0.42
5:6:340:ASN:OD1	5:6:343:PHE:HB2	2.20	0.42
6:7:323:PRO:HB2	6:7:326:HIS:ND1	2.34	0.42
6:7:537:ILE:HG23	6:7:563:ILE:HG13	2.00	0.42
10:D:123:LYS:NZ	11:E:20:SER:O	2.52	0.42
10:D:203:PRO:O	10:D:207:GLN:HG3	2.19	0.42
1:2:809:HIS:O	1:2:813:ILE:HG13	2.19	0.42
2:3:350:ILE:HG23	2:3:659:TYR:CE1	2.54	0.42
3:4:182:GLY:HA2	6:7:143:LEU:HD21	2.00	0.42
4:5:631:LYS:HE2	4:5:631:LYS:HB3	1.90	0.42
5:6:559:THR:HB	5:6:563:ILE:H	1.83	0.42
6:7:69:LYS:O	6:7:74:GLU:N	2.42	0.42
10:D:125:PRO:HG3	14:I:50:TRP:CE2	2.53	0.42
12:F:32:SER:HB3	13:H:174:ILE:HD12	2.01	0.42
17:S:2:LYS:HB3	17:S:30:LEU:O	2.19	0.42
17:S:290:LYS:O	17:S:294:LEU:HG	2.19	0.42
6:7:314:LYS:HZ2	6:7:503:THR:HG21	1.85	0.42
11:E:10:GLU:O	11:E:14:LYS:N	2.41	0.42
11:E:55:GLN:HB2	13:H:162:PHE:CE1	2.53	0.42
11:E:123:LEU:HD13	11:E:143:PHE:HD2	1.84	0.42
11:E:336:LEU:HD13	11:E:344:SER:HB3	2.00	0.42
3:4:187:ILE:HD11	15:T:525:MET:HE1	2.00	0.42
3:4:442:ILE:HG23	3:4:460:TYR:HE1	1.83	0.42
5:6:781:ARG:NH1	5:6:795:ILE:O	2.43	0.42
9:C:194:LYS:HB2	11:E:494:ARG:HD3	2.00	0.42
11:E:516:THR:O	11:E:520:ILE:HG13	2.19	0.42
1:2:233:THR:O	1:2:237:MET:HG2	2.19	0.42
1:2:559:THR:HG23	1:2:764:MET:HG2	2.02	0.42
3:4:696:PRO:N	3:4:697:PRO:HD2	2.35	0.42
3:4:721:ALA:HB1	6:7:660:VAL:HG12	2.00	0.42
4:5:38:PHE:HE1	4:5:71:TYR:HB2	1.85	0.42
4:5:278:CYS:HB3	4:5:330:ILE:HD12	2.01	0.42
4:5:426:LEU:HD23	4:5:478:CYS:HB3	2.02	0.42
5:6:517:LYS:HD3	16:R:150:GLU:OE2	2.20	0.42
6:7:472:ALA:O	6:7:476:ILE:HG12	2.20	0.42
7:A:4:DC:H2"	7:A:5:DA:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:28:PHE:CE1	2:3:32:LEU:HD21	2.54	0.42
2:3:455:ARG:N	6:7:503:THR:OG1	2.53	0.42
6:7:656:VAL:HG22	6:7:710:ILE:HG12	2.02	0.42
11:E:384:TRP:HA	11:E:387:MET:HE3	2.01	0.42
11:E:640:ARG:HA	11:E:640:ARG:HD3	1.91	0.42
14:I:119:TRP:CZ3	14:I:145:ILE:HG23	2.54	0.42
1:2:810:LEU:HD12	1:2:813:ILE:HB	2.00	0.42
2:3:195:LYS:HA	6:7:370:LEU:O	2.19	0.42
3:4:245:ALA:HB2	3:4:308:VAL:HG22	2.02	0.42
4:5:31:PHE:O	4:5:35:ILE:HG12	2.19	0.42
4:5:39:ARG:HH21	11:E:321:ASP:CG	2.28	0.42
4:5:561:ASN:HB3	4:5:564:ARG:HG2	2.01	0.42
4:5:564:ARG:O	4:5:568:ILE:HG13	2.20	0.42
11:E:63:GLY:HA2	11:E:632:PHE:CD2	2.54	0.42
11:E:84:VAL:HG22	11:E:123:LEU:HG	2.02	0.42
15:Q:347:LEU:HB2	15:Q:416:LYS:HE2	2.02	0.42
15:Q:353:LEU:O	15:Q:357:LEU:HG	2.19	0.42
1:2:624:MET:HE1	1:2:677:PHE:CD2	2.55	0.42
2:3:409:GLY:O	2:3:518:PRO:HD3	2.20	0.42
4:5:285:LYS:HE2	4:5:285:LYS:HB2	1.90	0.42
9:C:18:CYS:HB3	9:C:72:VAL:HG13	2.02	0.42
11:E:501:ARG:O	11:E:505:LEU:HG	2.20	0.42
2:3:98:ILE:HD11	2:3:157:PHE:CE1	2.54	0.42
4:5:145:GLN:HG2	4:5:161:ARG:HG2	2.01	0.42
11:E:53:LEU:HD12	14:I:82:GLN:HE21	1.85	0.42
11:E:527:LYS:HB2	15:Q:355:ILE:HD11	2.02	0.42
1:2:519:LEU:HD12	1:2:519:LEU:HA	1.88	0.41
1:2:674:LEU:HA	1:2:677:PHE:HD2	1.85	0.41
3:4:527:ALA:HB3	3:4:537:LYS:HZ3	1.85	0.41
11:E:389:HIS:O	11:E:393:ARG:HG3	2.20	0.41
11:E:432:VAL:O	11:E:436:THR:HG23	2.20	0.41
15:Q:375:GLN:O	15:Q:379:LYS:HG3	2.20	0.41
16:R:252:LYS:O	16:R:256:LYS:HG3	2.20	0.41
1:2:438:LEU:HB3	1:2:446:VAL:HG13	2.01	0.41
2:3:299:LYS:HD3	2:3:322:LEU:HD13	2.02	0.41
6:7:664:TYR:O	6:7:668:ARG:HG2	2.20	0.41
9:C:47:PRO:HG2	9:C:50:LEU:HB3	2.01	0.41
13:H:109:LEU:HD12	13:H:131:LEU:HD11	2.02	0.41
15:Q:409:ALA:O	15:Q:413:ILE:HG13	2.20	0.41
1:2:678:ASP:HB2	1:2:812:SER:OG	2.19	0.41
2:3:110:PHE:O	2:3:114:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:337:PRO:HG3	5:6:375:ARG:HD3	2.02	0.41
3:4:403:PRO:O	3:4:406:VAL:HG22	2.20	0.41
3:4:645:LEU:O	3:4:649:MET:HG2	2.20	0.41
5:6:137:ARG:HG2	16:R:175:VAL:HG21	2.02	0.41
5:6:643:LYS:HE3	5:6:643:LYS:HB3	1.85	0.41
11:E:395:LEU:HA	11:E:398:ILE:HD12	2.03	0.41
16:R:199:ARG:HH12	16:R:251:LEU:C	2.29	0.41
1:2:190:LYS:HE2	1:2:190:LYS:HB3	1.93	0.41
2:3:349:ASN:O	2:3:353:LEU:HD23	2.21	0.41
2:3:503:HIS:CD2	6:7:515:LEU:HG	2.54	0.41
3:4:582:HIS:O	3:4:585:THR:HG22	2.19	0.41
5:6:689:TYR:CD2	5:6:716:LEU:HD11	2.56	0.41
12:F:25:LEU:HB2	12:F:33:ILE:HD11	2.02	0.41
14:I:82:GLN:HB2	14:I:84:LYS:HG2	2.03	0.41
1:2:430:TYR:CE1	1:2:449:THR:HB	2.55	0.41
1:2:564:VAL:HG12	1:2:599:ALA:HB2	2.03	0.41
1:2:813:ILE:HG12	1:2:841:VAL:HG21	2.02	0.41
2:3:196:LEU:HD21	2:3:199:SER:HB3	2.02	0.41
2:3:567:ARG:HG2	2:3:570:ARG:HH22	1.84	0.41
3:4:437:GLY:HA3	3:4:463:VAL:HA	2.03	0.41
3:4:703:ASP:O	3:4:705:VAL:N	2.52	0.41
4:5:39:ARG:HB2	4:5:44:PHE:CE1	2.55	0.41
4:5:162:LEU:HD23	4:5:294:ILE:O	2.21	0.41
5:6:184:GLY:O	5:6:188:VAL:HG23	2.20	0.41
5:6:644:MET:HE3	5:6:649:GLN:HG2	2.02	0.41
7:A:8:DT:H2"	7:A:9:DA:C8	2.56	0.41
15:Q:345:LEU:O	15:Q:349:ARG:HG2	2.20	0.41
1:2:634:ALA:HA	4:5:457:PRO:HG2	2.03	0.41
3:4:622:VAL:HG21	3:4:665:LEU:HD23	2.03	0.41
6:7:558:ASN:HB3	6:7:560:ARG:NE	2.36	0.41
10:D:216:VAL:HG11	13:H:84:ARG:NH2	2.35	0.41
11:E:70:HIS:CE1	13:H:184:ILE:HD13	2.55	0.41
11:E:625:ALA:C	11:E:640:ARG:HG2	2.46	0.41
1:2:820:PHE:CE2	1:2:836:ARG:HB2	2.55	0.41
2:3:391:LYS:HB2	2:3:399:LEU:HB2	2.03	0.41
2:3:572:LEU:HD13	4:5:613:ARG:HD3	2.01	0.41
2:3:684:THR:HB	6:7:606:ARG:HH11	1.85	0.41
3:4:217:ASN:N	3:4:221:ASP:OD2	2.49	0.41
3:4:242:ASN:HB3	3:4:306:TYR:CE1	2.55	0.41
3:4:581:VAL:O	3:4:585:THR:N	2.54	0.41
3:4:761:ILE:O	3:4:817:VAL:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:153:MET:HE3	6:7:153:MET:HB3	1.95	0.41
6:7:615:HIS:O	6:7:619:VAL:HG23	2.21	0.41
7:A:1:DA:H2"	7:A:2:DG:C8	2.55	0.41
11:E:419:THR:OG1	11:E:424:GLY:O	2.23	0.41
6:f:162:ARG:HG2	6:f:167:MET:SD	2.60	0.41
3:4:365:ILE:H	5:6:439:GLY:HA3	1.86	0.41
3:4:526:ILE:HG21	3:4:541:LEU:HD13	2.02	0.41
6:7:628:LEU:HD22	6:7:630:PHE:CE2	2.56	0.41
9:C:25:PRO:HD2	13:H:67:VAL:HG12	2.03	0.41
11:E:346:TYR:CD1	11:E:357:LEU:HD23	2.56	0.41
14:I:126:LEU:HB3	14:I:134:PHE:CZ	2.55	0.41
1:2:769:TYR:CE1	1:2:773:LYS:HG3	2.55	0.41
1:2:788:ARG:HH11	4:5:566:ILE:HD11	1.86	0.41
2:3:261:MET:HB3	2:3:263:GLU:OE1	2.21	0.41
2:3:456:ARG:O	6:7:502:VAL:HG21	2.21	0.41
2:3:457:LEU:HD23	2:3:457:LEU:H	1.85	0.41
3:4:277:LYS:HB2	3:4:301:TYR:HD2	1.85	0.41
3:4:531:TYR:CG	3:4:532:GLU:N	2.88	0.41
3:4:536:VAL:O	3:4:540:ILE:HG12	2.20	0.41
3:4:657:ALA:HB3	5:6:603:SER:HB3	2.02	0.41
3:4:834:LYS:HE2	3:4:834:LYS:HB2	1.88	0.41
4:5:158:LYS:O	4:5:297:ILE:HA	2.20	0.41
4:5:413:LEU:HB2	4:5:550:PHE:CE1	2.55	0.41
5:6:107:THR:OG1	5:6:108:GLY:N	2.51	0.41
5:6:152:TYR:HB3	5:6:266:SER:HB2	2.03	0.41
5:6:575:GLY:HA3	5:6:715:ILE:HG13	2.02	0.41
5:6:657:GLU:OE2	5:6:798:ARG:NH2	2.49	0.41
5:6:750:GLN:HG2	5:6:753:ARG:NH2	2.36	0.41
6:7:28:PHE:CZ	6:7:84:ASP:HB3	2.55	0.41
11:E:395:LEU:HG	11:E:399:PHE:CE1	2.53	0.41
11:E:399:PHE:HD2	11:E:403:LEU:HD11	1.85	0.41
14:I:152:ARG:NH2	14:I:174:SER:H	2.19	0.41
15:Q:272:LYS:O	15:Q:276:LEU:HG	2.21	0.41
17:S:69:ILE:HD11	17:S:107:LEU:HB3	2.03	0.41
17:S:80:LEU:HD22	17:S:85:GLU:OE1	2.21	0.41
1:2:796:GLU:HG3	1:2:861:PHE:CE2	2.56	0.41
5:6:770:ARG:O	5:6:774:VAL:HG23	2.20	0.41
6:7:206:PRO:HB3	6:7:352:THR:HG21	2.03	0.41
9:C:97:LEU:HD11	9:C:127:LEU:HD21	2.02	0.41
10:D:126:LEU:HD23	11:E:22:HIS:NE2	2.36	0.41
11:E:34:LEU:HD22	11:E:439:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:341:GLU:O	15:Q:345:LEU:HG	2.20	0.41
1:2:211:LEU:HD22	1:2:271:PHE:CD1	2.56	0.40
1:2:707:HIS:CD2	1:2:709:GLU:HB2	2.56	0.40
2:3:447:THR:O	6:7:502:VAL:HG22	2.21	0.40
2:3:528:ASP:HB3	2:3:530:HIS:CE1	2.56	0.40
2:3:556:ILE:HD12	2:3:556:ILE:H	1.86	0.40
3:4:804:LEU:O	3:4:807:ALA:HB3	2.21	0.40
5:6:192:TYR:HD1	16:R:178:ASN:HB3	1.86	0.40
6:7:638:MET:O	6:7:642:ILE:HG13	2.21	0.40
11:E:68:ARG:HA	11:E:71:TYR:HB3	2.02	0.40
16:R:153:ILE:O	16:R:157:ILE:HG13	2.20	0.40
16:R:201:ILE:HG22	16:R:208:TYR:HD2	1.86	0.40
1:2:707:HIS:HD2	1:2:709:GLU:HB2	1.87	0.40
3:4:179:ILE:HG22	3:4:186:SER:HB2	2.02	0.40
3:4:323:ASP:HA	3:4:439:PHE:O	2.22	0.40
4:5:497:MET:HE1	4:5:550:PHE:CZ	2.56	0.40
6:7:709:ASP:O	6:7:713:VAL:HG23	2.21	0.40
9:C:163:SER:HA	9:C:166:LEU:HD12	2.03	0.40
2:3:172:THR:OG1	2:3:174:GLN:HG2	2.21	0.40
4:5:415:LEU:HD21	4:5:540:ILE:HG12	2.03	0.40
5:6:339:GLU:N	5:6:339:GLU:OE1	2.54	0.40
6:7:663:ALA:HA	6:7:666:ARG:NE	2.37	0.40
7:A:21:DT:H2"	7:A:22:DA:C8	2.56	0.40
10:D:77:LEU:O	10:D:147:ARG:NH1	2.44	0.40
11:E:420:LEU:O	11:E:423:ARG:HG2	2.20	0.40
17:S:239:CYS:O	17:S:243:ILE:HG13	2.20	0.40
1:2:500:SER:HB2	1:2:757:PRO:HD2	2.04	0.40
3:4:219:THR:O	3:4:223:GLU:HG3	2.22	0.40
3:4:565:LEU:HB3	3:4:702:PHE:CD2	2.57	0.40
3:4:571:SER:HA	6:7:687:ARG:CZ	2.52	0.40
4:5:38:PHE:O	4:5:44:PHE:HD1	2.05	0.40
4:5:179:LEU:HD23	4:5:179:LEU:HA	1.95	0.40
4:5:562:GLU:HA	4:5:565:ASP:HB2	2.03	0.40
5:6:120:GLU:HA	5:6:137:ARG:HH21	1.85	0.40
5:6:155:TYR:CZ	5:6:167:ALA:HB1	2.56	0.40
6:7:593:ARG:NH1	6:7:687:ARG:HH12	2.19	0.40
11:E:563:CYS:HA	11:E:569:LYS:HD2	2.04	0.40
17:S:116:LEU:HA	17:S:119:PHE:CD2	2.57	0.40
3:4:393:ASP:OD2	3:4:424:VAL:HG21	2.22	0.40
3:4:643:SER:HA	3:4:646:HIS:ND1	2.36	0.40
3:4:705:VAL:O	3:4:832:ALA:HB1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:747:LEU:HD12	3:4:748:THR:N	2.37	0.40
6:7:252:LYS:HD3	6:7:252:LYS:HA	1.86	0.40
6:7:537:ILE:CG2	6:7:563:ILE:HG21	2.52	0.40
6:7:618:TYR:CD1	6:7:626:PRO:HB3	2.57	0.40
10:D:121:GLU:HB2	14:I:47:HIS:ND1	2.36	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	642/868 (74%)	630 (98%)	12 (2%)	0	100	100
2	3	579/1006 (58%)	554 (96%)	25 (4%)	0	100	100
3	4	564/933 (60%)	535 (95%)	29 (5%)	0	100	100
4	5	550/775 (71%)	539 (98%)	11 (2%)	0	100	100
5	6	562/1017 (55%)	544 (97%)	18 (3%)	0	100	100
6	7	596/845 (70%)	584 (98%)	12 (2%)	0	100	100
6	f	42/845 (5%)	42 (100%)	0	0	100	100
9	C	179/217 (82%)	175 (98%)	4 (2%)	0	100	100
10	D	216/294 (74%)	213 (99%)	3 (1%)	0	100	100
11	E	487/657 (74%)	472 (97%)	15 (3%)	0	100	100
12	F	82/689 (12%)	80 (98%)	2 (2%)	0	100	100
13	H	206/208 (99%)	202 (98%)	4 (2%)	0	100	100
14	I	187/213 (88%)	182 (97%)	5 (3%)	0	100	100
15	Q	195/704 (28%)	194 (100%)	1 (0%)	0	100	100
15	T	26/704 (4%)	26 (100%)	0	0	100	100
16	R	109/257 (42%)	108 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	S	209/801 (26%)	207 (99%)	2 (1%)	0	100	100
All	All	5431/11033 (49%)	5287 (97%)	144 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	570/770 (74%)	570 (100%)	0	100	100
2	3	514/864 (60%)	514 (100%)	0	100	100
3	4	523/848 (62%)	522 (100%)	1 (0%)	87	89
4	5	510/688 (74%)	510 (100%)	0	100	100
5	6	507/886 (57%)	507 (100%)	0	100	100
6	7	546/753 (72%)	546 (100%)	0	100	100
6	f	43/753 (6%)	43 (100%)	0	100	100
9	C	165/192 (86%)	165 (100%)	0	100	100
10	D	216/279 (77%)	216 (100%)	0	100	100
11	E	457/592 (77%)	457 (100%)	0	100	100
12	F	73/629 (12%)	73 (100%)	0	100	100
13	H	193/193 (100%)	193 (100%)	0	100	100
14	I	179/198 (90%)	179 (100%)	0	100	100
15	Q	188/654 (29%)	188 (100%)	0	100	100
15	T	30/654 (5%)	30 (100%)	0	100	100
16	R	102/234 (44%)	102 (100%)	0	100	100
17	S	201/749 (27%)	201 (100%)	0	100	100
All	All	5017/9936 (50%)	5016 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	4	702	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
2	3	175	HIS
2	3	177	ASN
2	3	259	GLN
2	3	269	GLN
2	3	340	GLN
2	3	374	HIS
2	3	503	HIS
2	3	532	ASN
2	3	564	HIS
3	4	242	ASN
3	4	387	ASN
3	4	395	GLN
4	5	254	GLN
4	5	539	ASN
5	6	364	ASN
5	6	659	GLN
5	6	673	ASN
6	7	9	GLN
6	7	19	ASN
6	7	72	ASN
6	7	98	GLN
6	7	264	GLN
6	7	379	GLN
6	7	425	ASN
6	7	622	HIS
6	7	697	GLN
9	C	103	HIS
9	C	181	HIS
10	D	94	GLN
10	D	162	ASN
11	E	77	ASN
11	E	101	GLN
11	E	141	GLN
11	E	328	GLN
11	E	409	GLN
11	E	617	GLN
13	H	182	ASN
13	H	188	GLN

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Mol	Chain	Res	Type
13	H	193	GLN
14	I	82	GLN
15	Q	183	ASN
16	R	176	HIS
16	R	223	HIS
17	S	278	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 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	$\# Z  > 2$
19	ADP	7	901	20	27,29,29	1.36	4 (14%)	42,45,45	1.97	10 (23%)

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
19	ADP	7	901	20	-	4/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	7	901	ADP	C5-C4	4.59	1.47	1.39
19	7	901	ADP	C5-C6	2.70	1.48	1.41
19	7	901	ADP	C8-N7	2.35	1.36	1.31
19	7	901	ADP	C5-N7	-2.17	1.34	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	7	901	ADP	C5-C4-N3	-6.22	118.64	126.75
19	7	901	ADP	N3-C4-N9	4.92	135.19	127.08
19	7	901	ADP	C2-N3-C4	3.84	120.81	111.75
19	7	901	ADP	PA-O3A-PB	-3.46	120.96	132.83
19	7	901	ADP	C4-C5-N7	-3.18	106.75	110.62
19	7	901	ADP	N3-C2-N1	-3.08	123.79	128.60
19	7	901	ADP	C3'-C2'-C1'	2.71	106.58	101.43
19	7	901	ADP	C5-N7-C8	2.68	107.31	103.51
19	7	901	ADP	C4-N9-C8	2.52	108.46	105.73
19	7	901	ADP	C6-C5-N7	2.07	135.87	132.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	7	901	ADP	C5'-O5'-PA-O1A
19	7	901	ADP	C5'-O5'-PA-O3A
19	7	901	ADP	C5'-O5'-PA-O2A
19	7	901	ADP	O4'-C4'-C5'-O5'

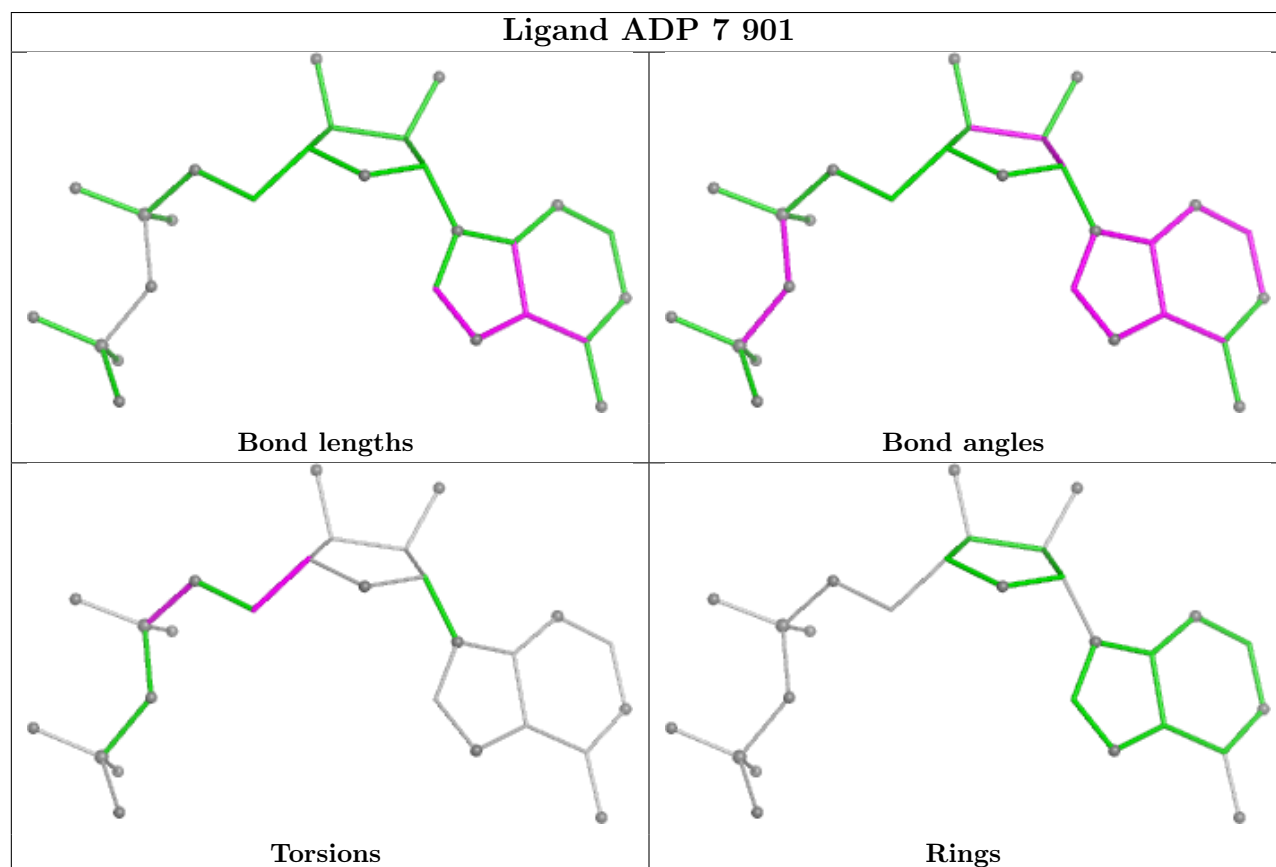
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	7	901	ADP	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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.

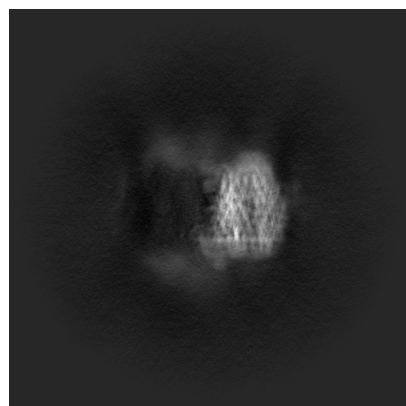
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53970. These allow visual inspection of the internal detail of the map and identification of artifacts.

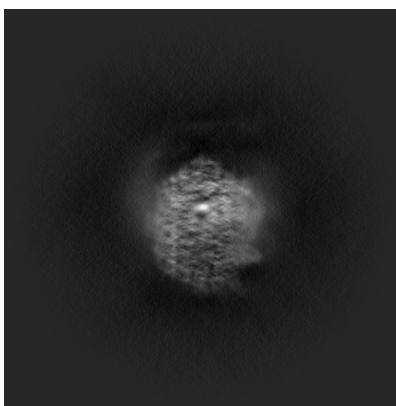
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

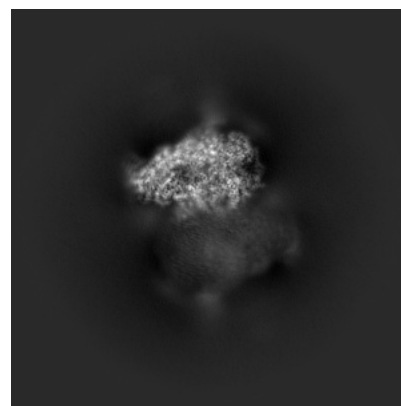
#### 6.1.1 Primary map



X

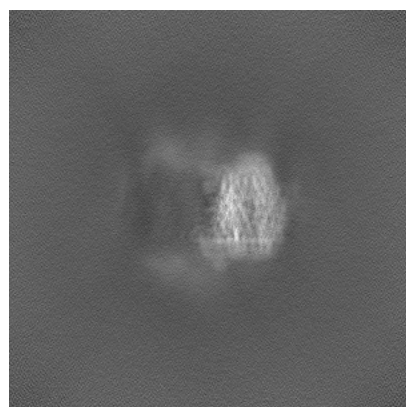


Y

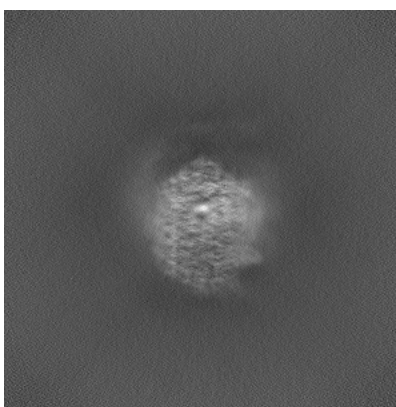


Z

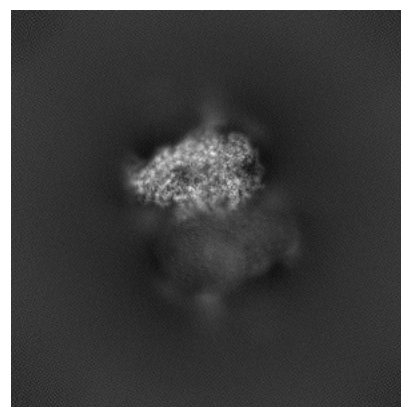
#### 6.1.2 Raw map



X



Y

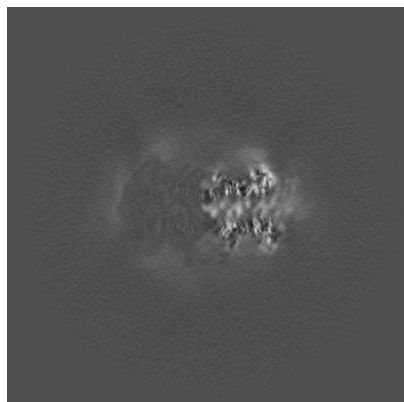


Z

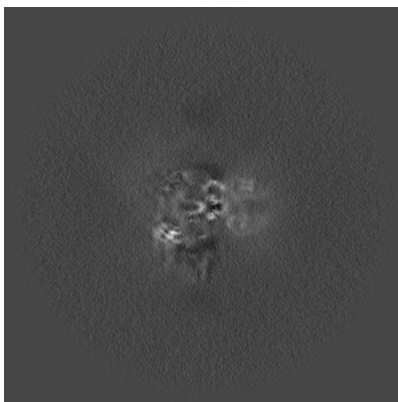
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

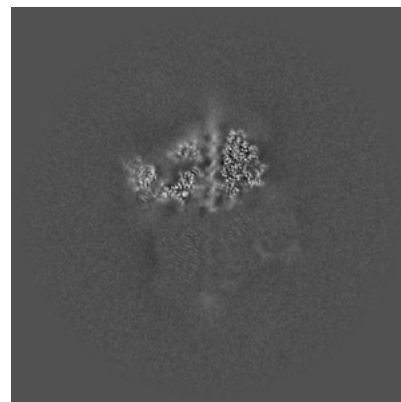
### 6.2.1 Primary map



X Index: 300

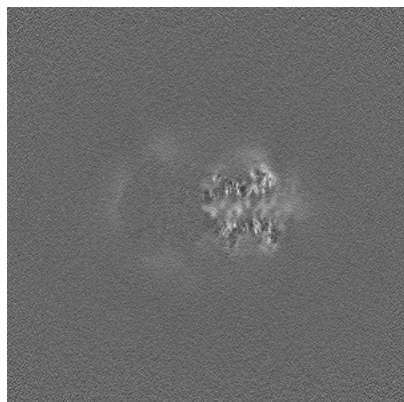


Y Index: 300

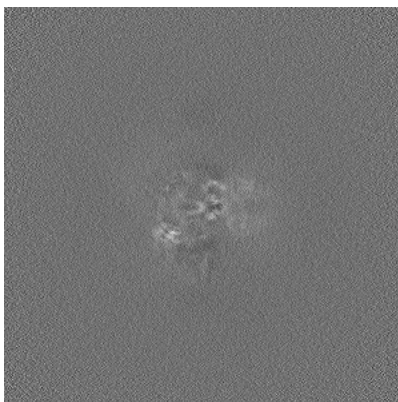


Z Index: 300

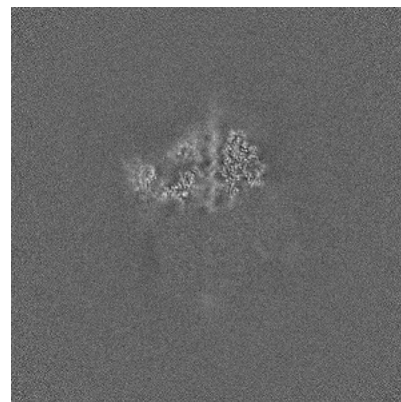
### 6.2.2 Raw map



X Index: 300



Y Index: 300



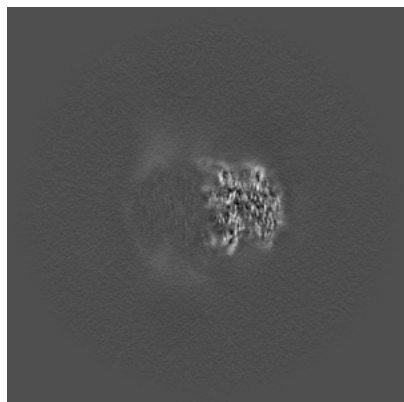
Z Index: 300

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

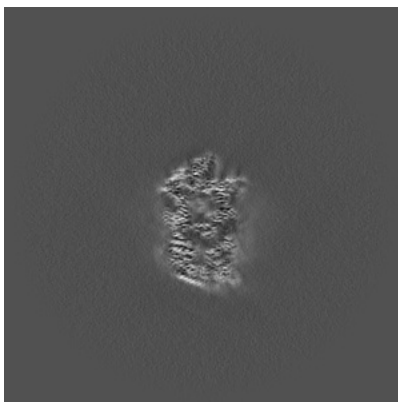


## 6.3 Largest variance slices [i](#)

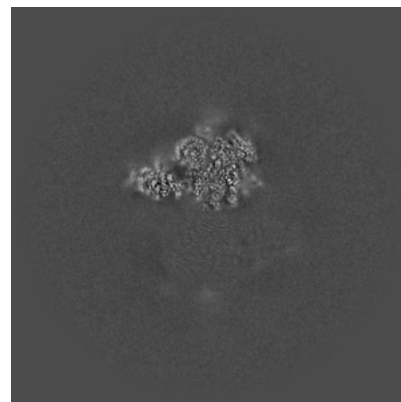
### 6.3.1 Primary map



X Index: 328

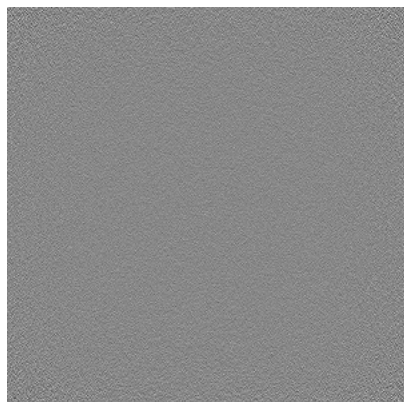


Y Index: 339

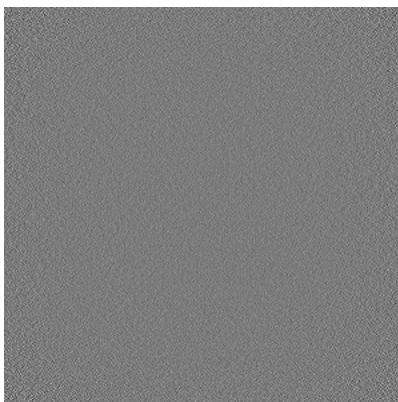


Z Index: 319

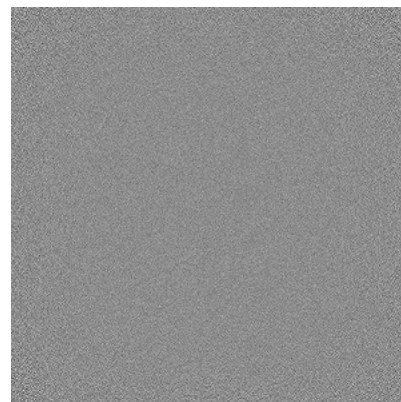
### 6.3.2 Raw map



X Index: 0



Y Index: 0

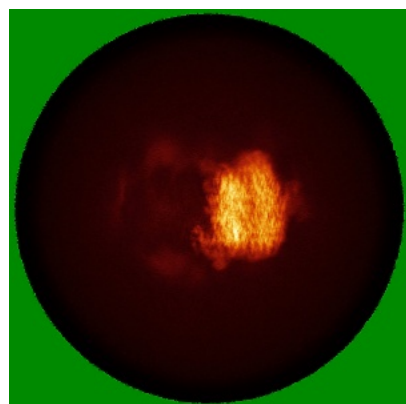


Z Index: 0

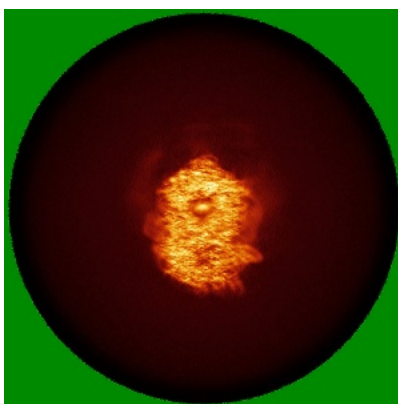
The images above show the largest variance slices of the map in three orthogonal directions.

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

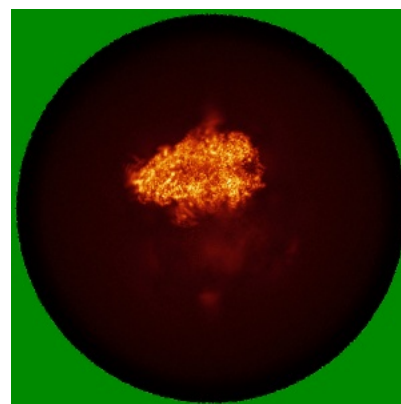
### 6.4.1 Primary map



X

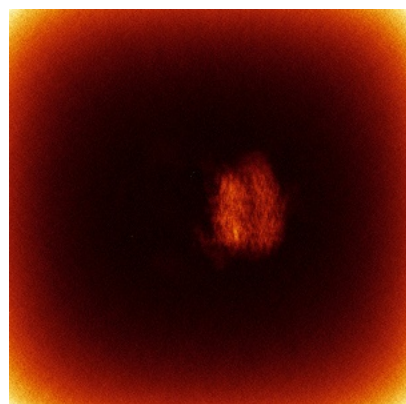


Y

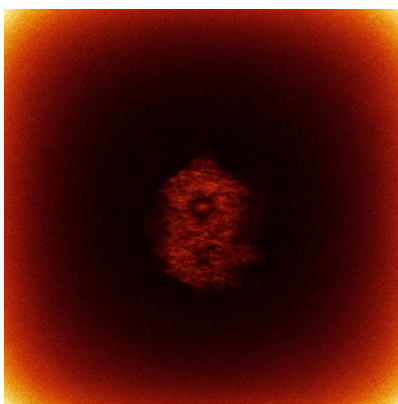


Z

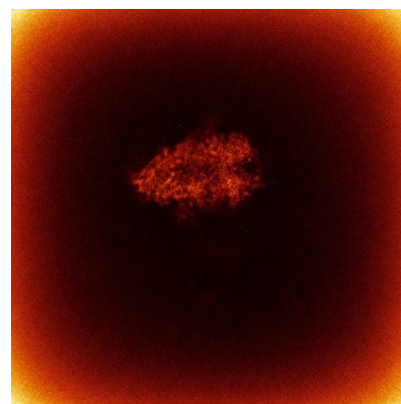
### 6.4.2 Raw map



X



Y



Z

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

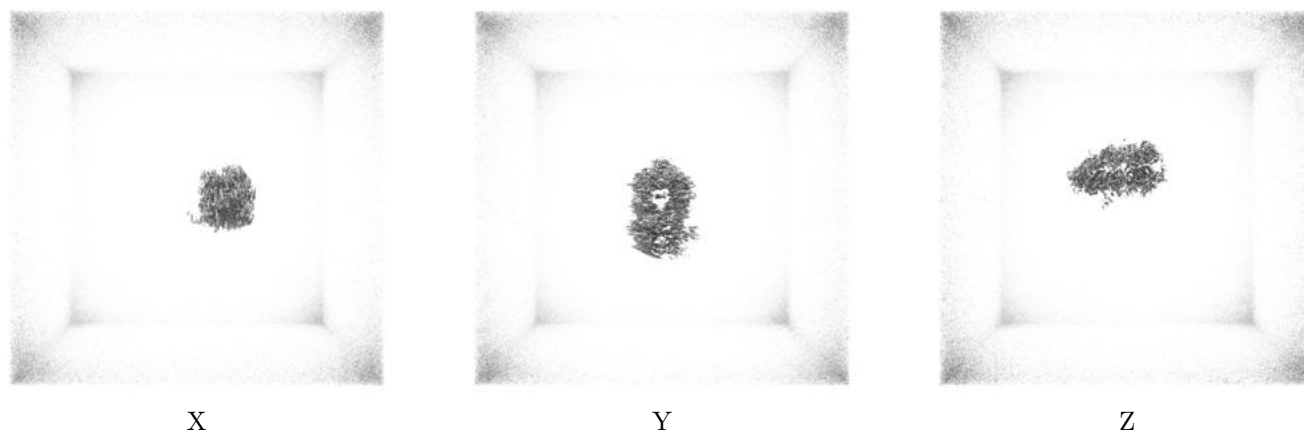
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.26. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

## 6.6 Mask visualisation [i](#)

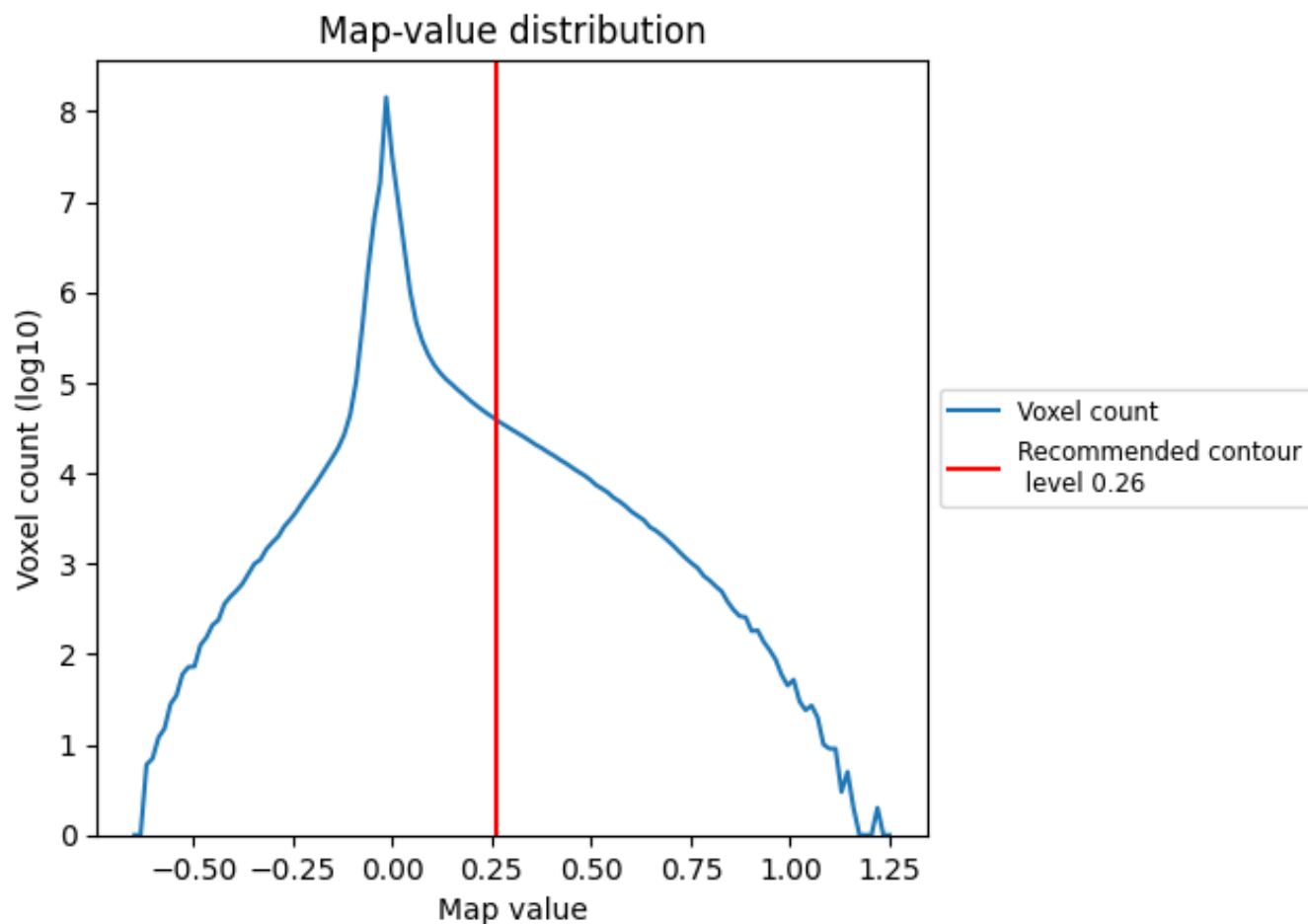
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

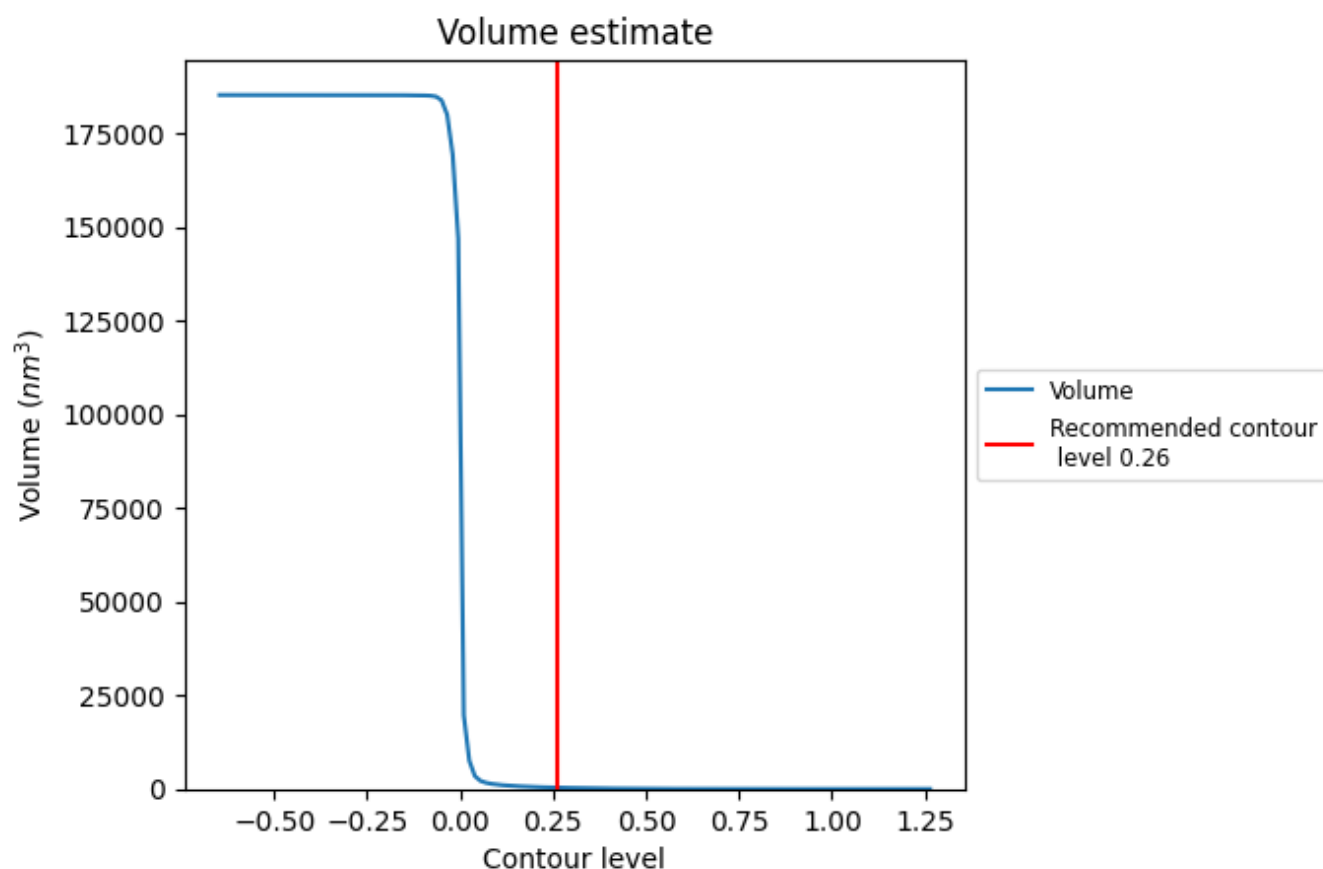
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

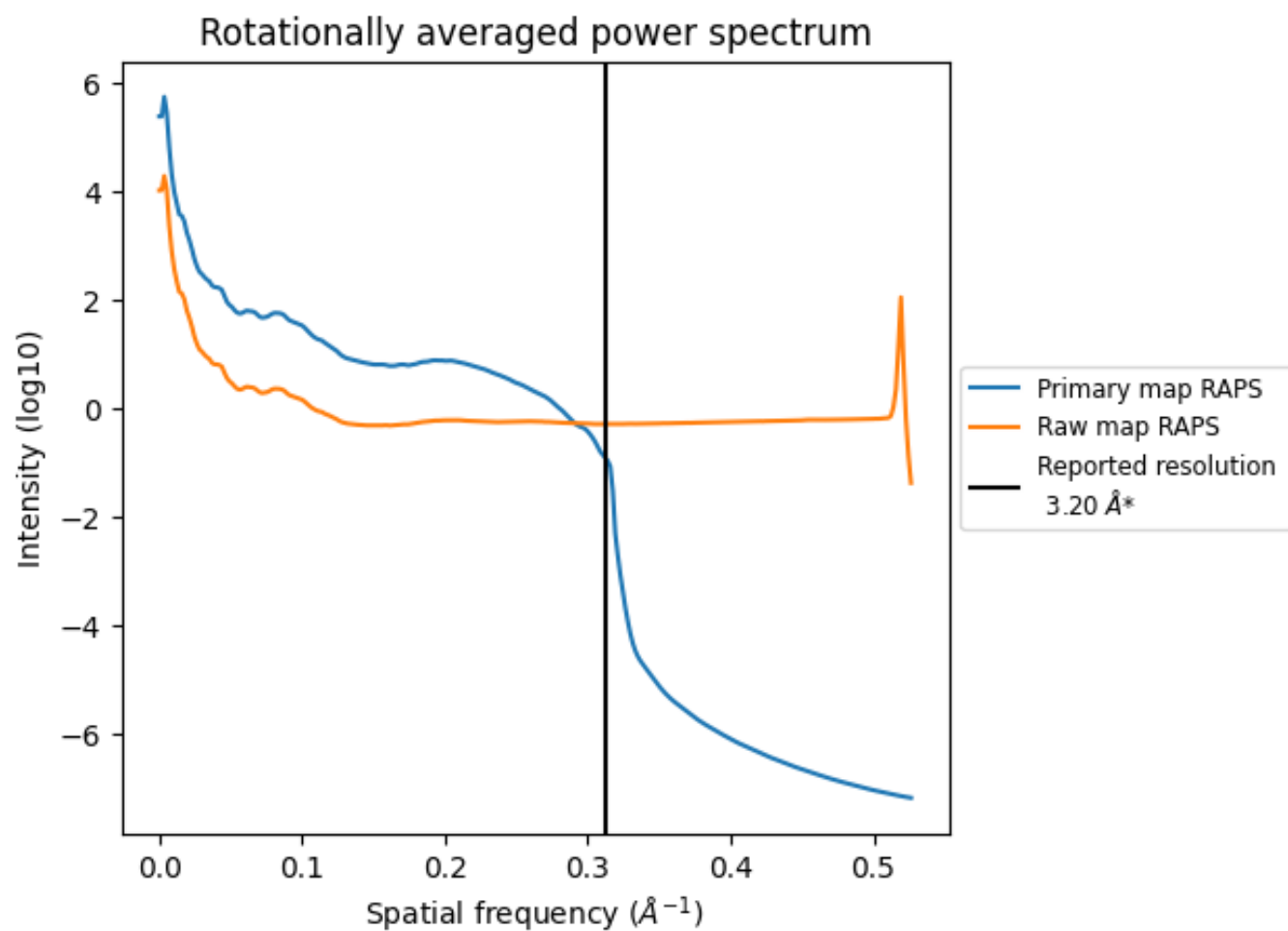
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 350  $\text{nm}^3$ ; this corresponds to an approximate mass of 316 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

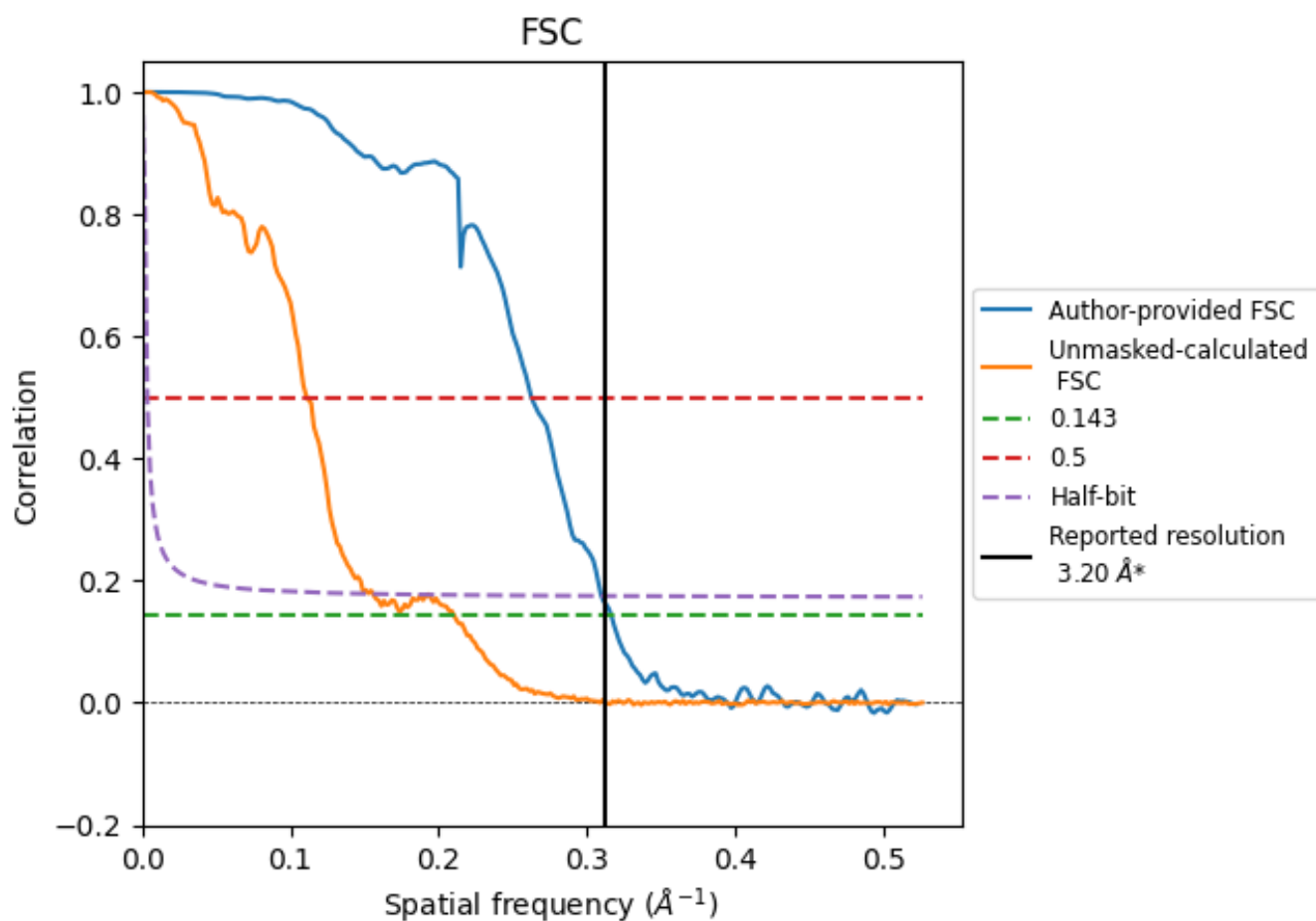


\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 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 0.312  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

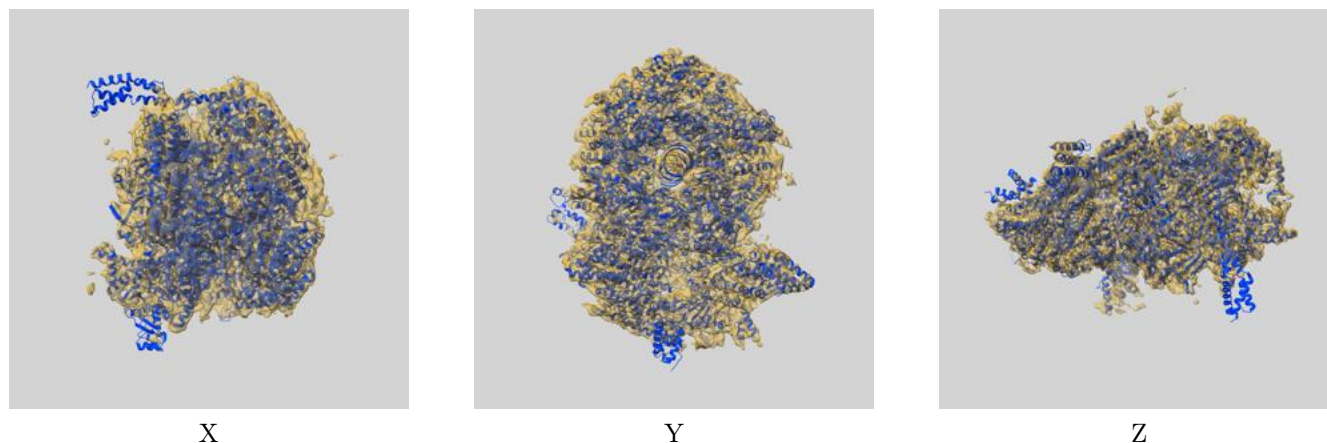
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.16	3.81	3.23
Unmasked-calculated*	4.75	8.98	6.42

\*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 4.75 differs from the reported value 3.2 by more than 10 %

## 9 Map-model fit [i](#)

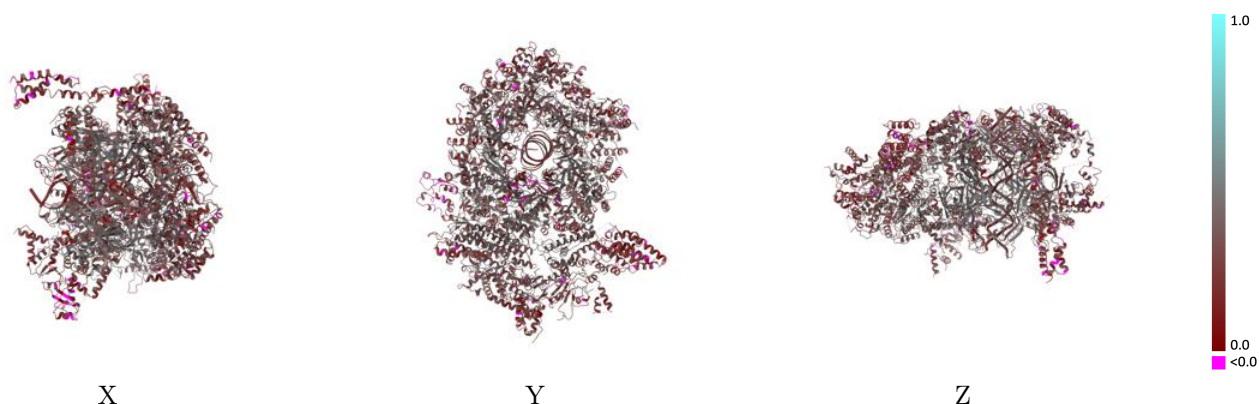
This section contains information regarding the fit between EMDB map EMD-53970 and PDB model 9RHI. Per-residue inclusion information can be found in section [3](#) on page [13](#).

### 9.1 Map-model overlay [i](#)



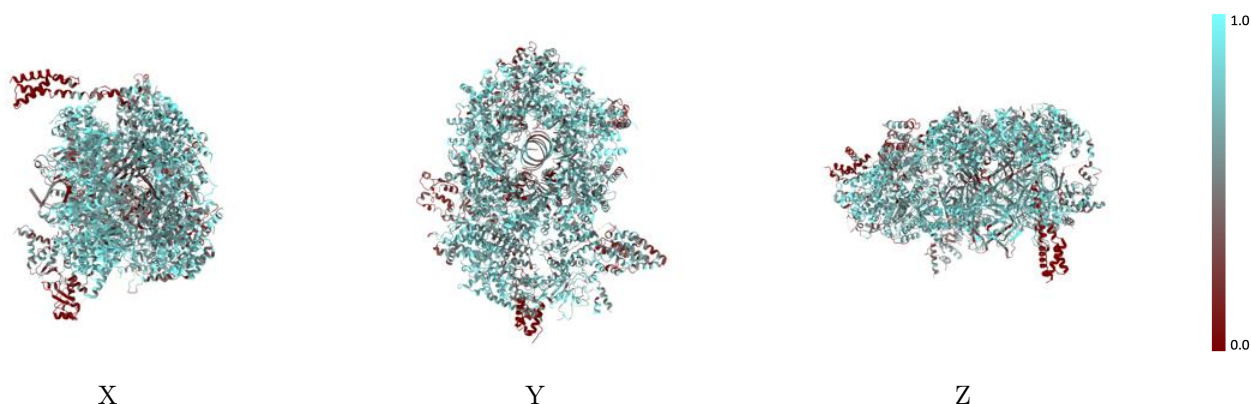
The images above show the 3D surface view of the map at the recommended contour level 0.26 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



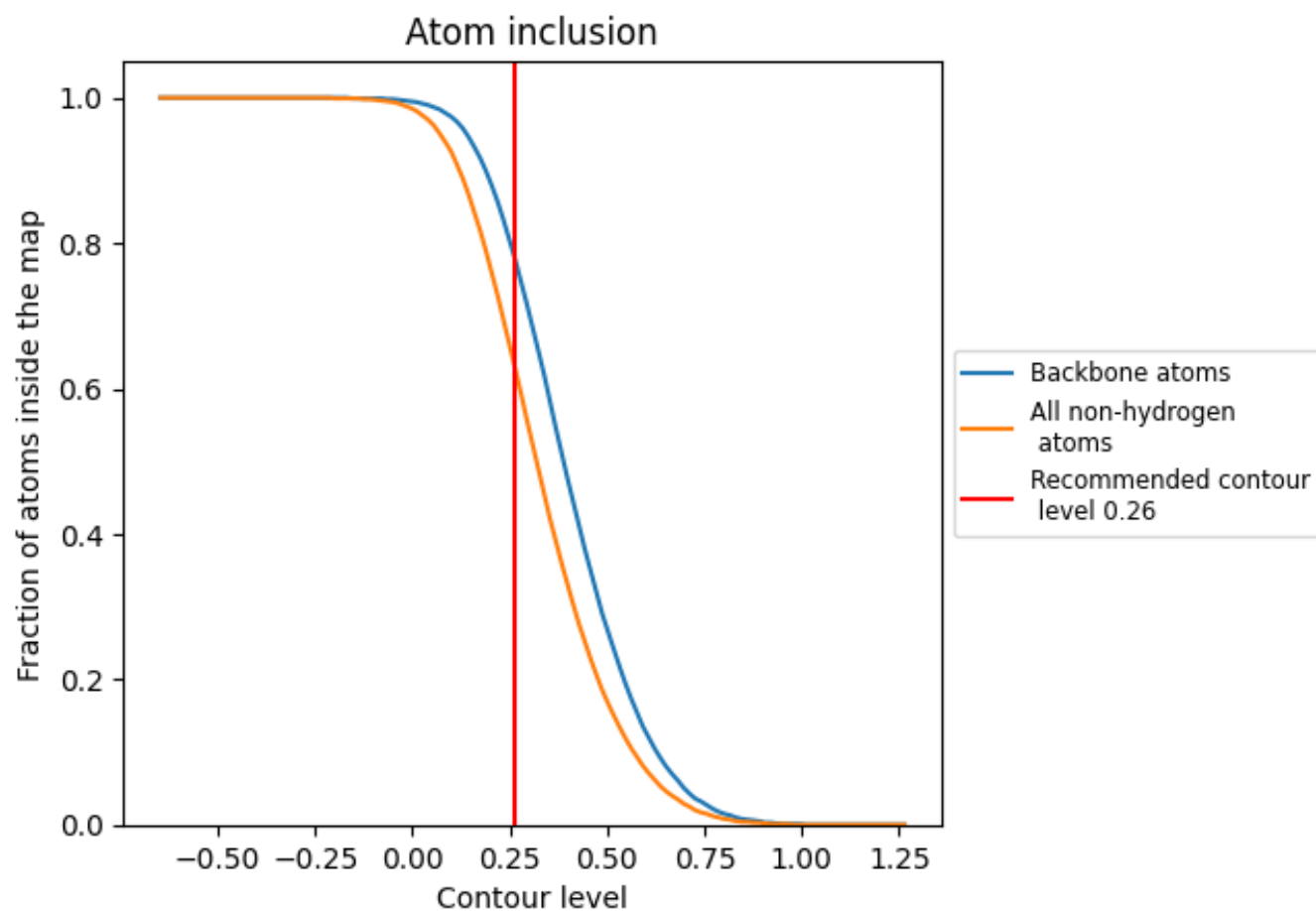
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.26).

## 9.4 Atom inclusion [i](#)











































At the recommended contour level, 78% of all backbone atoms, 64% 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 (0.26) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6370	 0.3230
2	 0.6650	 0.3670
3	 0.6620	 0.3650
4	 0.6560	 0.3180
5	 0.6720	 0.3610
6	 0.7110	 0.3460
7	 0.7050	 0.3450
A	 0.5730	 0.2380
B	 0.5760	 0.2470
C	 0.6940	 0.3630
D	 0.7310	 0.3260
E	 0.7150	 0.3180
F	 0.2120	 0.2390
H	 0.6690	 0.2940
I	 0.5890	 0.3160
Q	 0.4760	 0.1980
R	 0.1570	 0.1830
S	 0.3110	 0.1980
T	 0.5870	 0.2620
f	 0.4090	 0.1620

