



Full wwPDB EM Validation Report ⓘ

Aug 27, 2026 – 06:27 am BST

PDB ID : 9FSS / pdb_00009fss
EMDB ID : EMD-50734
Title : RNA Polymerase III Class III Open Mini Pre-Initiation complex 2 (OC2-mini)
Authors : Shah, S.Z.; Ramsay, E.P.; Cecatiello, V.; Perry, T.N.; Vannini, A.
Deposited on : 2024-06-21
Resolution : 4.14 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.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

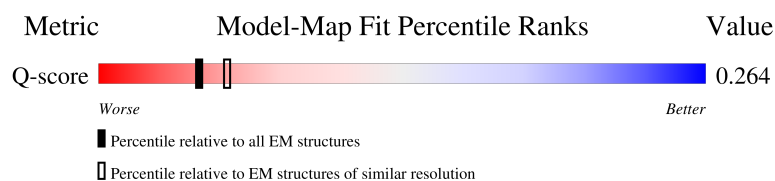
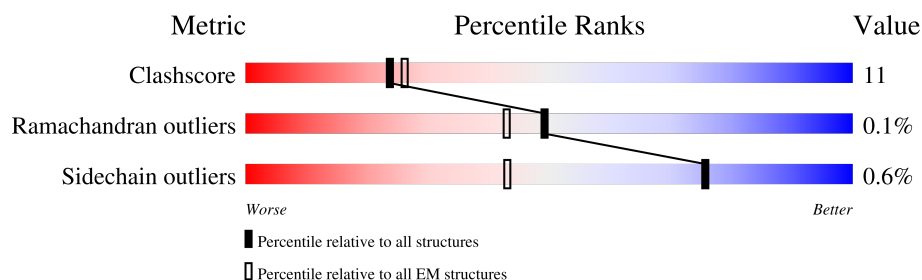
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.14 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	5577 (3.64 - 4.64)

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

Mol	Chain	Length	Quality of chain
1	A	1390	
2	B	1133	
3	C	534	
4	D	398	

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Mol	Chain	Length	Quality of chain
5	E	708	
6	F	316	
7	G	223	
8	H	204	
9	I	148	
10	J	108	
11	K	346	
12	L	133	
13	M	210	
14	N	127	
15	O	150	
16	P	58	
17	Q	67	
18	R	200	
19	S	419	
20	T	484	
21	U	368	
22	W	1519	
23	X	98	
24	Y	98	
25	Z	411	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	SF4	F	401	-	-	X	-

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 56344 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-directed RNA polymerase III subunit RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1381	Total	C	N	O	S	0	0
			10848	6876	1891	2008	73		

- Molecule 2 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1097	Total	C	N	O	S	0	0
			8680	5499	1516	1597	68		

- Molecule 3 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	512	Total	C	N	O	S	0	0
			4075	2565	712	774	24		

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	174	Total	C	N	O	S	0	0
			1347	843	233	262	9		

- Molecule 5 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	400	Total	C	N	O	S	0	0
			3211	2038	557	596	20		

- Molecule 6 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	303	Total	C	N	O	S	0	0
			2403	1516	411	460	16		

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	82	Total	C	N	O	S	0	0
			717	463	121	127	6		

- Molecule 8 is a protein called DNA-directed RNA polymerase III subunit RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	189	Total	C	N	O	S	0	0
			1509	979	237	286	7		

- Molecule 9 is a protein called DNA-directed RNA polymerase III subunit RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	124	Total	C	N	O	S	0	0
			1001	626	174	198	3		

- Molecule 10 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	56	Total	C	N	O	S	0	0
			436	272	81	77	6		

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	343	Total	C	N	O	S	0	0
			2736	1723	488	514	11		

- Molecule 12 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	107	Total	C	N	O	S	0	0
			856	531	153	165	7		

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	209	Total	C	N	O	S	0	0
			1715	1083	300	324	8		

- Molecule 14 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	78	Total	C	N	O	S	0	0
			627	402	106	114	5		

- Molecule 15 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 16 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	46	Total	C	N	O	S	0	0
			388	241	75	66	6		

- Molecule 17 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	66	Total	C	N	O	S	0	0
			524	339	88	91	6		

- Molecule 18 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	178	Total	C	N	O	S	0	0
			1402	909	246	240	7		

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	140	MET	-	initiating methionine	UNP P20226
R	141	ALA	-	expression tag	UNP P20226
R	142	HIS	-	expression tag	UNP P20226
R	143	HIS	-	expression tag	UNP P20226
R	144	HIS	-	expression tag	UNP P20226
R	145	HIS	-	expression tag	UNP P20226
R	146	HIS	-	expression tag	UNP P20226
R	147	HIS	-	expression tag	UNP P20226
R	148	VAL	-	expression tag	UNP P20226
R	149	GLY	-	expression tag	UNP P20226
R	150	THR	-	expression tag	UNP P20226
R	151	LEU	-	expression tag	UNP P20226

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Chain	Residue	Modelled	Actual	Comment	Reference
R	152	GLU	-	expression tag	UNP P20226
R	153	VAL	-	expression tag	UNP P20226
R	154	LEU	-	expression tag	UNP P20226
R	155	PHE	-	expression tag	UNP P20226
R	156	GLN	-	expression tag	UNP P20226
R	157	GLY	-	expression tag	UNP P20226
R	158	PRO	-	expression tag	UNP P20226

- Molecule 19 is a protein called Transcription factor IIIB 50 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	359	Total	C	N	O	S	0	0
			2813	1766	500	525	22		

- Molecule 20 is a protein called Transcription factor TFIIB component B'' homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	97	Total	C	N	O	S	0	0
			825	533	143	146	3		

- Molecule 21 is a protein called snRNA-activating protein complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	141	Total	C	N	O	S	0	0
			1183	770	203	202	8		

- Molecule 22 is a protein called snRNA-activating protein complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	242	Total	C	N	O	S	0	0
			2018	1264	370	378	6		

There are 51 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	-38	MET	-	initiating methionine	UNP Q5SXM2
W	-37	ALA	-	expression tag	UNP Q5SXM2
W	-36	SER	-	expression tag	UNP Q5SXM2
W	-35	TRP	-	expression tag	UNP Q5SXM2
W	-34	SER	-	expression tag	UNP Q5SXM2
W	-33	HIS	-	expression tag	UNP Q5SXM2

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Chain	Residue	Modelled	Actual	Comment	Reference
W	-32	PRO	-	expression tag	UNP Q5SXM2
W	-31	GLN	-	expression tag	UNP Q5SXM2
W	-30	PHE	-	expression tag	UNP Q5SXM2
W	-29	GLU	-	expression tag	UNP Q5SXM2
W	-28	LYS	-	expression tag	UNP Q5SXM2
W	-27	GLY	-	expression tag	UNP Q5SXM2
W	-26	GLY	-	expression tag	UNP Q5SXM2
W	-25	GLY	-	expression tag	UNP Q5SXM2
W	-24	SER	-	expression tag	UNP Q5SXM2
W	-23	GLY	-	expression tag	UNP Q5SXM2
W	-22	GLY	-	expression tag	UNP Q5SXM2
W	-21	GLY	-	expression tag	UNP Q5SXM2
W	-20	SER	-	expression tag	UNP Q5SXM2
W	-19	TRP	-	expression tag	UNP Q5SXM2
W	-18	SER	-	expression tag	UNP Q5SXM2
W	-17	HIS	-	expression tag	UNP Q5SXM2
W	-16	PRO	-	expression tag	UNP Q5SXM2
W	-15	GLN	-	expression tag	UNP Q5SXM2
W	-14	PHE	-	expression tag	UNP Q5SXM2
W	-13	GLU	-	expression tag	UNP Q5SXM2
W	-12	LYS	-	expression tag	UNP Q5SXM2
W	-11	GLY	-	expression tag	UNP Q5SXM2
W	-10	GLY	-	expression tag	UNP Q5SXM2
W	-9	GLY	-	expression tag	UNP Q5SXM2
W	-8	SER	-	expression tag	UNP Q5SXM2
W	-7	GLU	-	expression tag	UNP Q5SXM2
W	-6	ASN	-	expression tag	UNP Q5SXM2
W	-5	LEU	-	expression tag	UNP Q5SXM2
W	-4	TYR	-	expression tag	UNP Q5SXM2
W	-3	PHE	-	expression tag	UNP Q5SXM2
W	-2	GLN	-	expression tag	UNP Q5SXM2
W	-1	GLY	-	expression tag	UNP Q5SXM2
W	0	SER	-	expression tag	UNP Q5SXM2
W	1	ALA	-	expression tag	UNP Q5SXM2
W	1470	ALA	-	expression tag	UNP Q5SXM2
W	1471	HIS	-	expression tag	UNP Q5SXM2
W	1472	HIS	-	expression tag	UNP Q5SXM2
W	1473	HIS	-	expression tag	UNP Q5SXM2
W	1474	HIS	-	expression tag	UNP Q5SXM2
W	1475	HIS	-	expression tag	UNP Q5SXM2
W	1476	HIS	-	expression tag	UNP Q5SXM2
W	1477	HIS	-	expression tag	UNP Q5SXM2

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Chain	Residue	Modelled	Actual	Comment	Reference
W	1478	HIS	-	expression tag	UNP Q5SXM2
W	1479	HIS	-	expression tag	UNP Q5SXM2
W	1480	HIS	-	expression tag	UNP Q5SXM2

- Molecule 23 is a DNA chain called U6_2_Template.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	69	Total	C	N	O	P	0	0
			1403	672	246	416	69		

- Molecule 24 is a DNA chain called U6_2_Non template.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	63	Total	C	N	O	P	0	0
			1300	619	242	376	63		

- Molecule 25 is a protein called snRNA-activating protein complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	385	Total	C	N	O	S	0	0
			3123	1977	533	591	22		

- Molecule 26 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

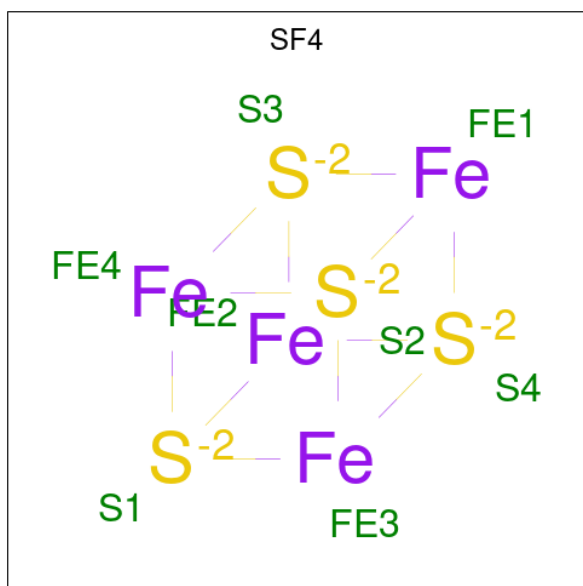
Mol	Chain	Residues	Atoms		AltConf
26	A	2	Total	Zn	0
			2	2	
26	B	1	Total	Zn	0
			1	1	
26	J	1	Total	Zn	0
			1	1	
26	P	1	Total	Zn	0
			1	1	
26	Q	1	Total	Zn	0
			1	1	
26	S	1	Total	Zn	0
			1	1	
26	Z	2	Total	Zn	0
			2	2	

- Molecule 27 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of

Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
27	A	1	Total	Mg	0
			1	1	

- Molecule 28 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).

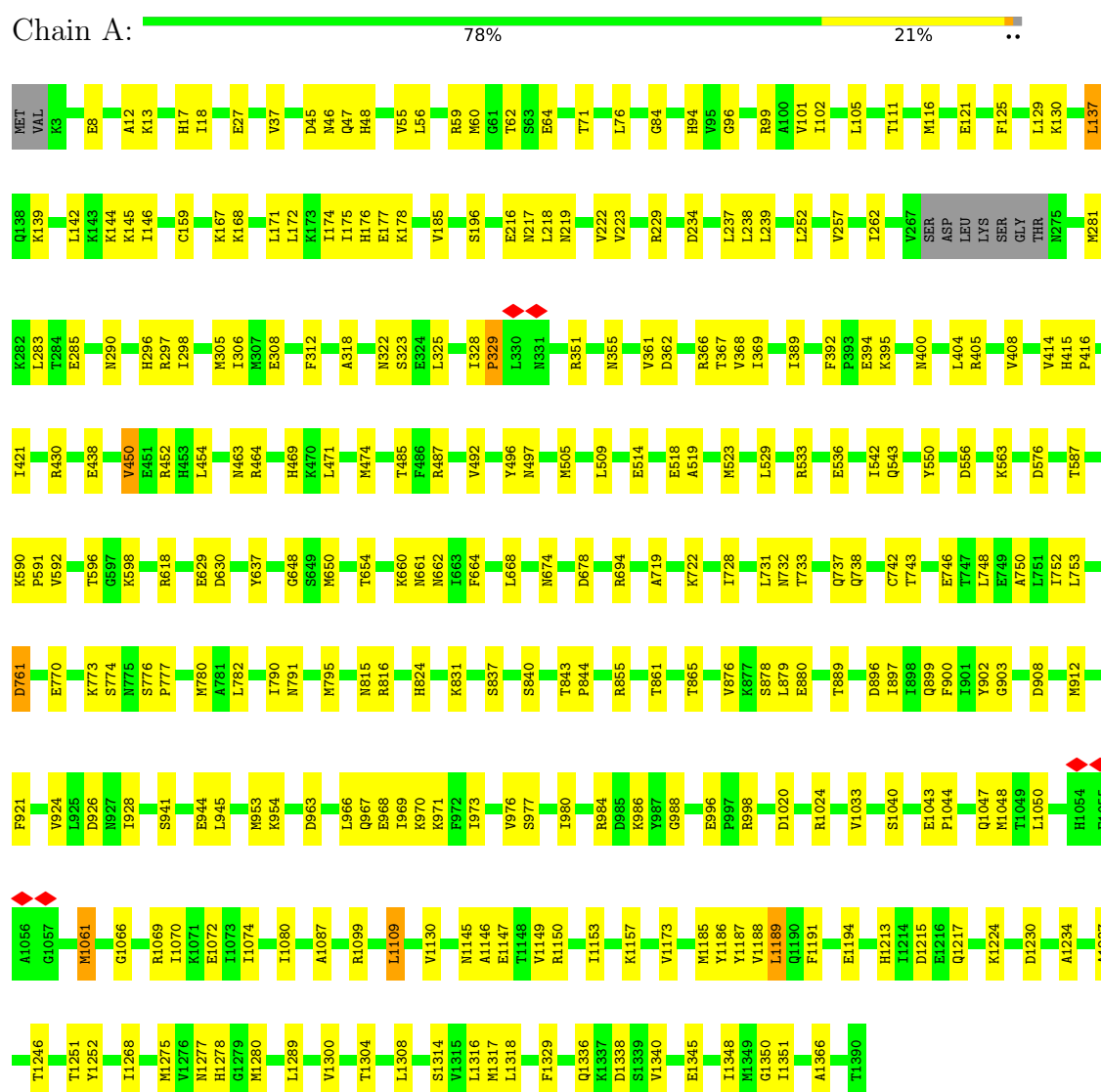


Mol	Chain	Residues	Atoms			AltConf
28	F	1	Total	Fe	S	0
			8	4	4	

3 Residue-property plots

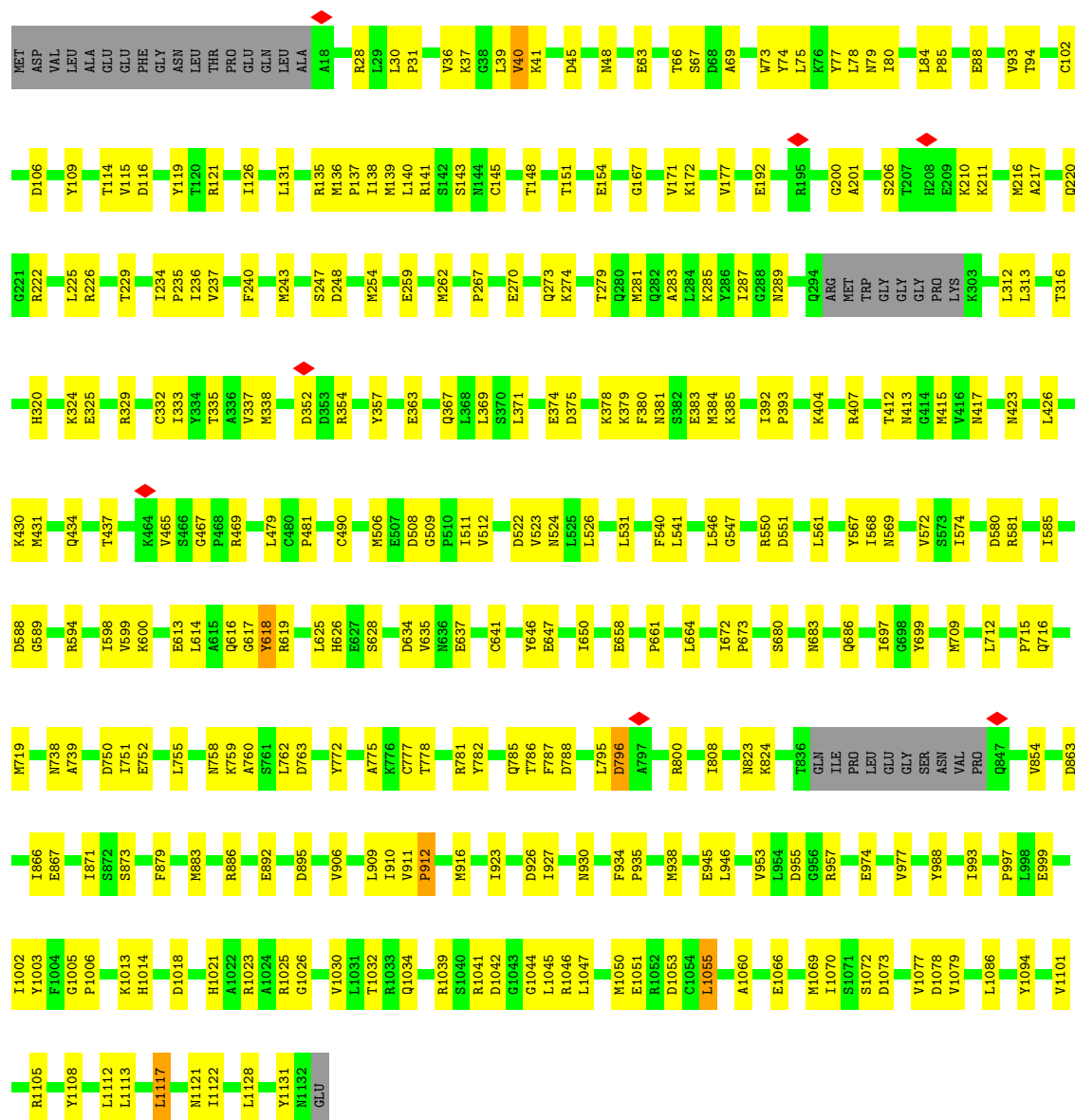
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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-directed RNA polymerase III subunit RPC1

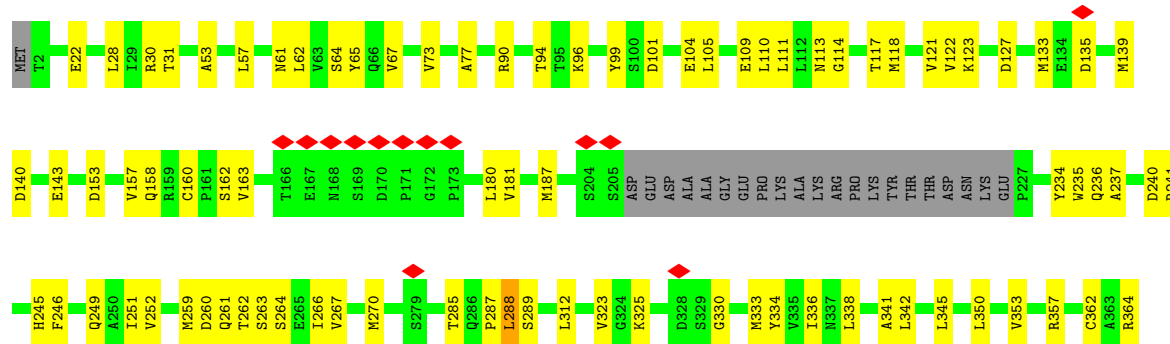


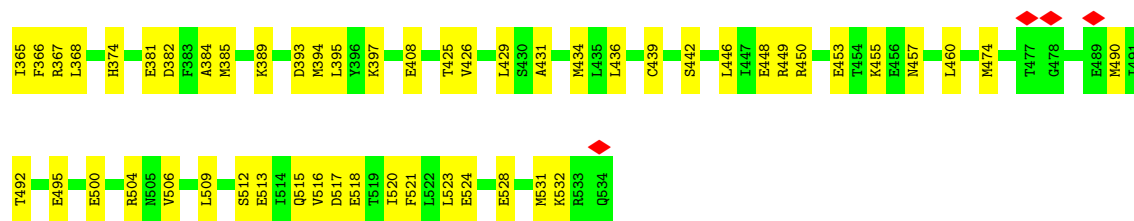
• Molecule 2: DNA-directed RNA polymerase III subunit RPC2



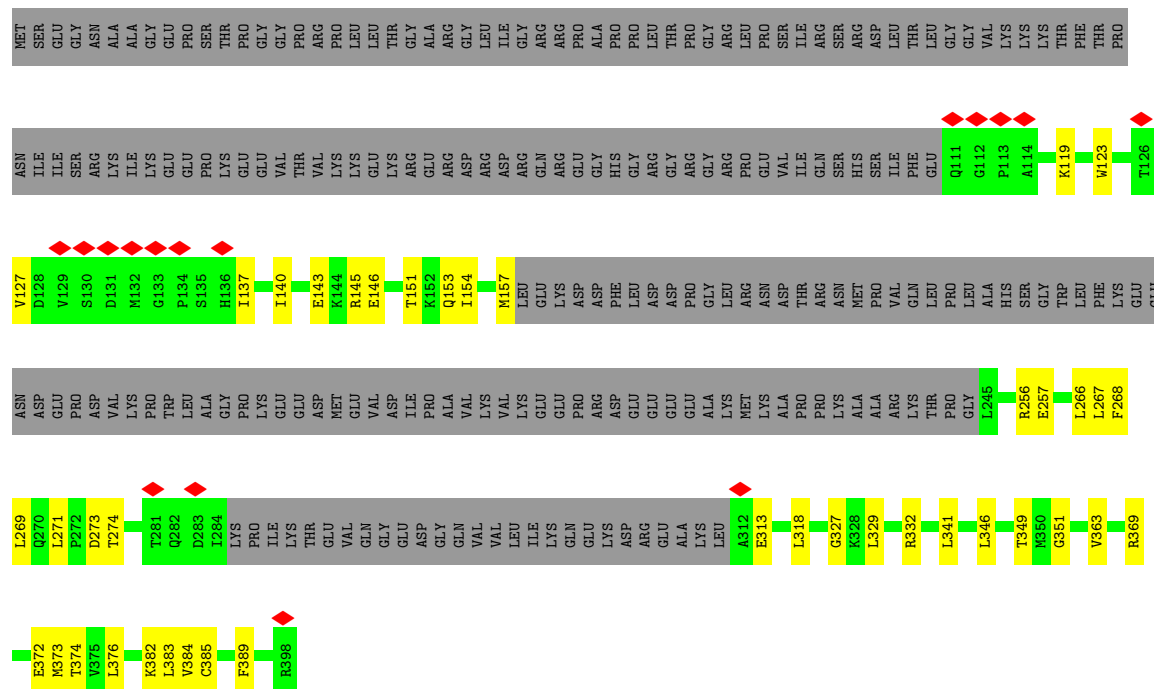
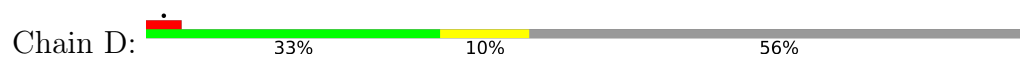


• Molecule 3: DNA-directed RNA polymerase III subunit RPC3

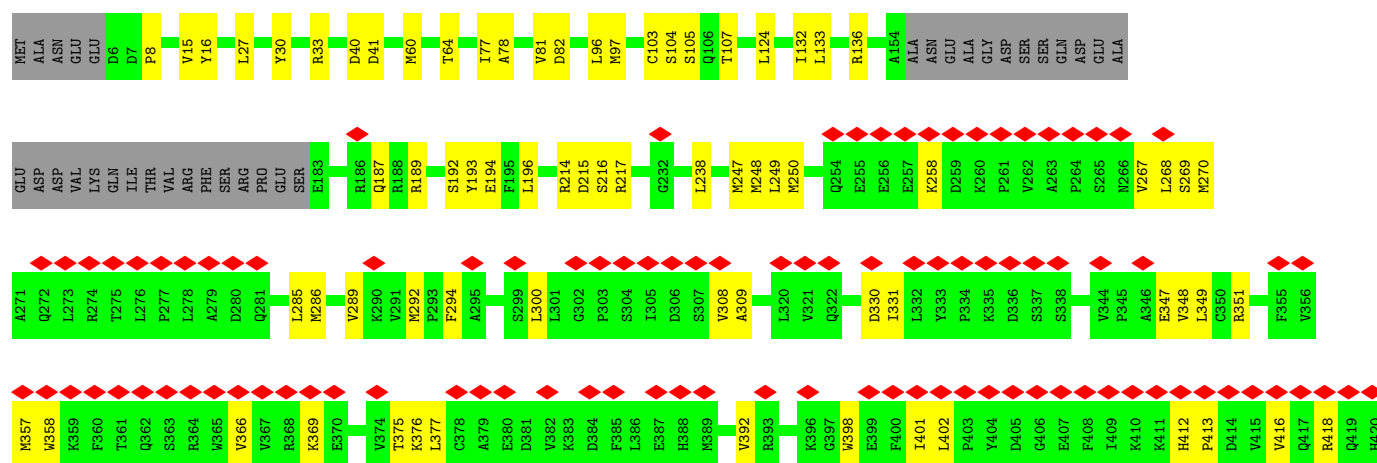




• Molecule 4: DNA-directed RNA polymerase III subunit RPC4

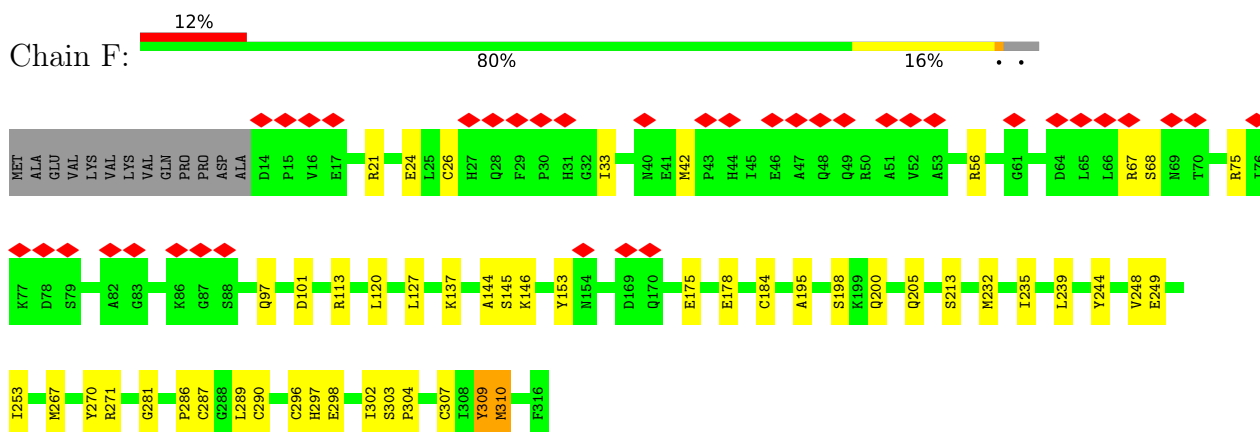


• Molecule 5: DNA-directed RNA polymerase III subunit RPC5

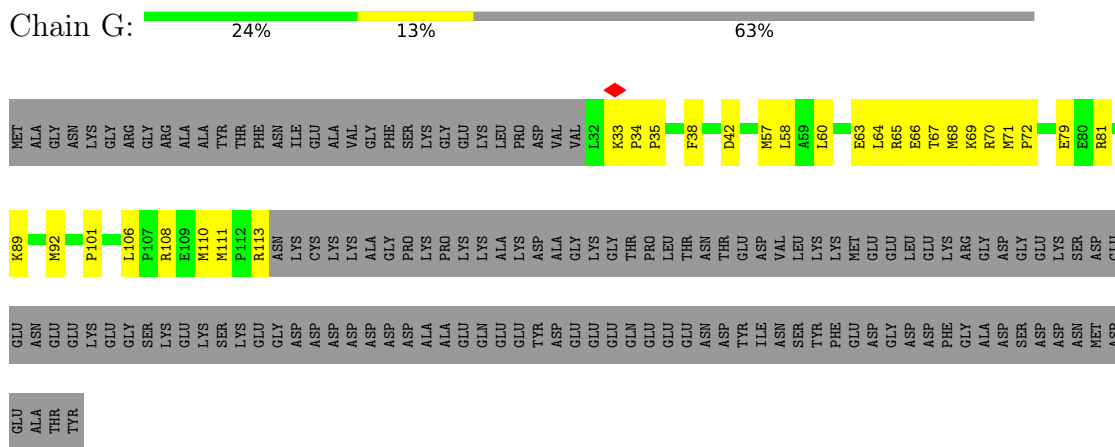




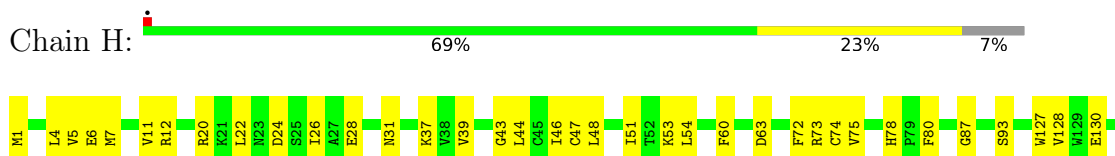
- Molecule 6: DNA-directed RNA polymerase III subunit RPC6



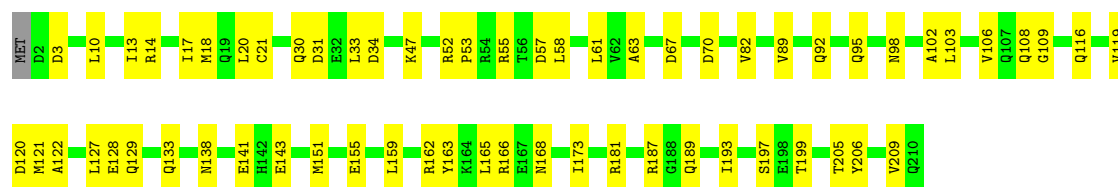
- Molecule 7: DNA-directed RNA polymerase III subunit RPC7



- Molecule 8: DNA-directed RNA polymerase III subunit RPC8

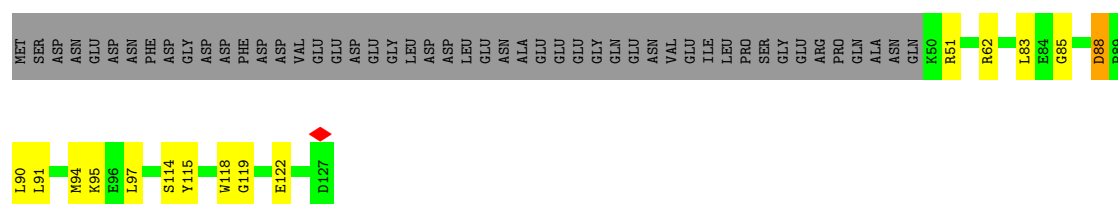


Chain M:  70% 30%



- Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain N:  50% 11% 39%



- Molecule 15: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain O:  83% 15%



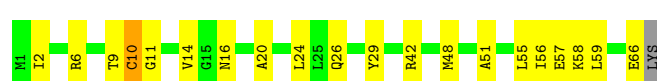
- Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain P:  50% 29% 21%



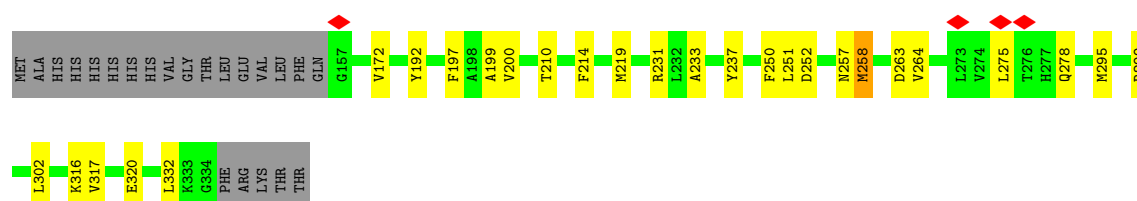
- Molecule 17: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain Q:  69% 28%

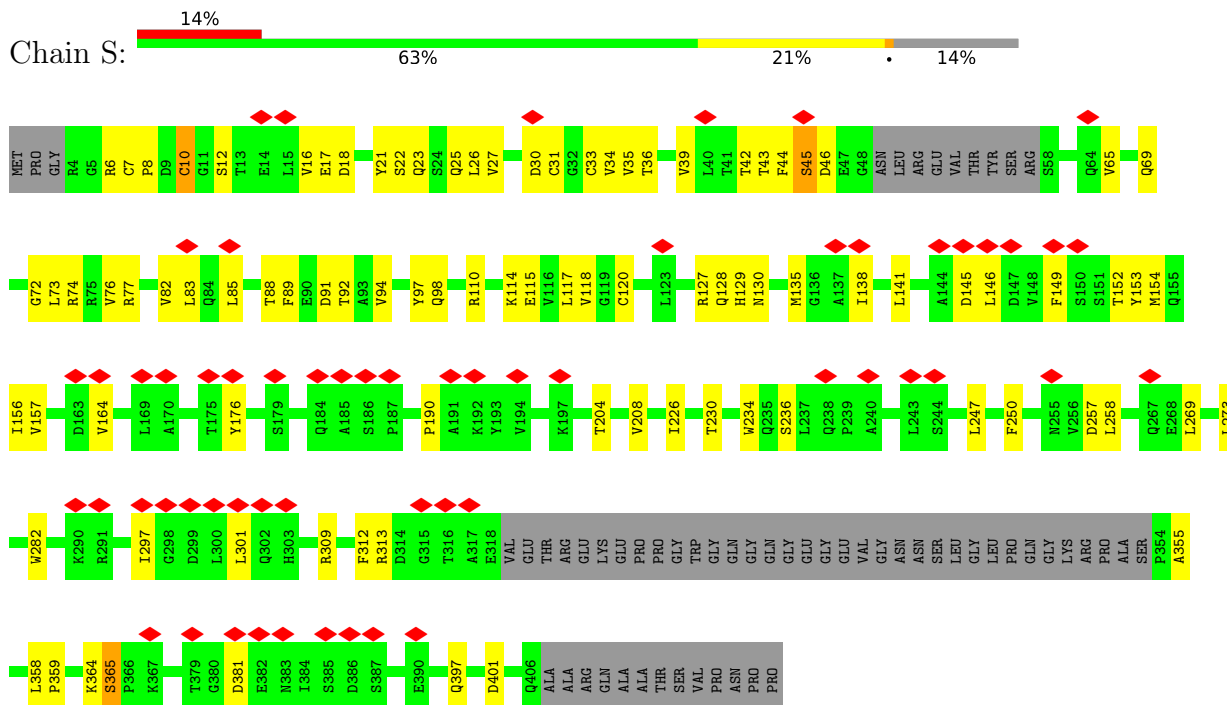


- Molecule 18: TATA-box-binding protein

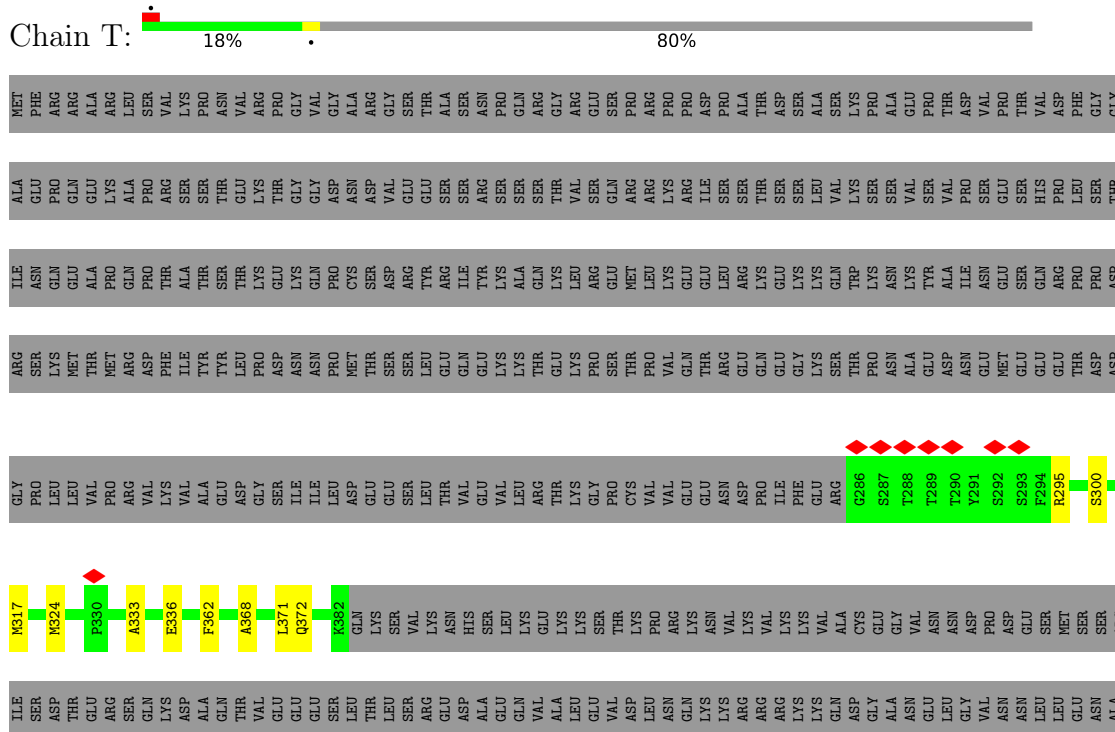
Chain R:  76% 13% 11%



Chain S:

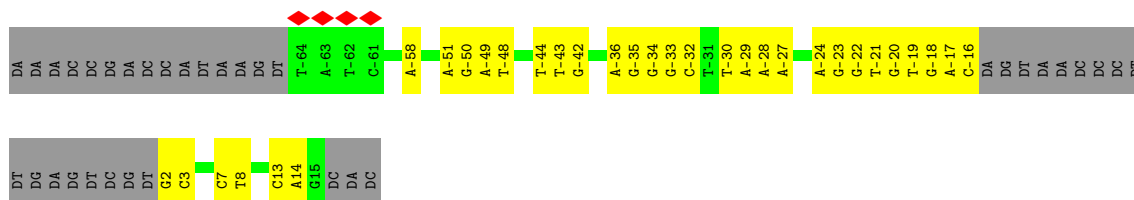


Chain T:



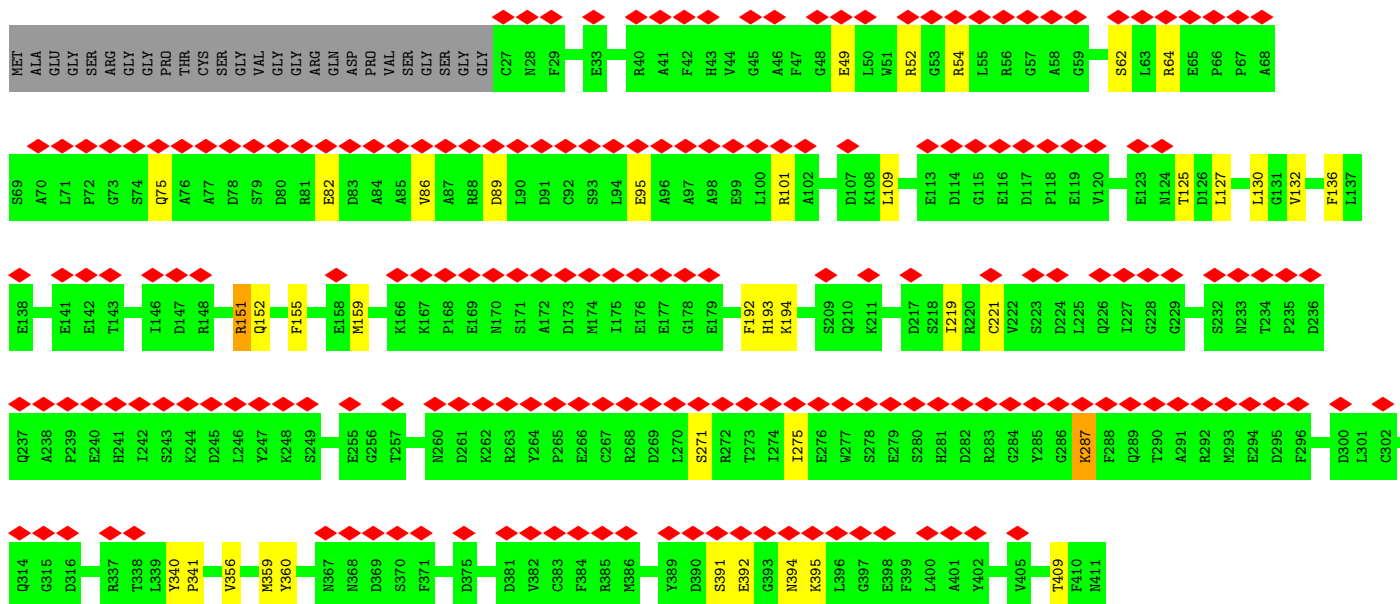
Chain U:





• Molecule 25: snRNA-activating protein complex subunit 3

Chain Z: 47% 84% 9% 6%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	13256	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.063	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	401.1, 401.1, 401.1	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95500004, 0.95500004, 0.95500004	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.23	0/11044	0.47	2/14893 (0.0%)
2	B	0.25	1/8845 (0.0%)	0.47	1/11930 (0.0%)
3	C	0.17	0/4141	0.41	0/5592
4	D	0.19	0/1362	0.42	0/1831
5	E	0.13	0/3282	0.38	0/4439
6	F	0.18	0/2446	0.42	1/3301 (0.0%)
7	G	0.22	0/739	0.46	0/996
8	H	0.16	0/1551	0.39	0/2110
9	I	0.16	0/1013	0.44	2/1365 (0.1%)
10	J	0.17	0/444	0.40	0/597
11	K	0.21	0/2790	0.41	0/3782
12	L	0.21	0/871	0.42	0/1174
13	M	0.17	0/1745	0.38	0/2358
14	N	0.24	0/637	0.46	0/861
15	O	0.16	0/1207	0.38	0/1628
16	P	0.23	0/394	0.44	0/524
17	Q	0.27	0/533	0.50	0/719
18	R	0.15	0/1428	0.31	0/1924
19	S	0.15	0/2863	0.42	0/3883
20	T	0.14	0/847	0.30	0/1131
21	U	0.12	0/1215	0.30	0/1640
22	W	0.15	0/2058	0.37	2/2760 (0.1%)
23	X	0.25	0/1569	0.99	3/2414 (0.1%)
24	Y	0.25	0/1459	0.95	1/2249 (0.0%)
25	Z	0.10	0/3203	0.30	0/4335
All	All	0.20	1/57686 (0.0%)	0.47	12/78436 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
19	S	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	716	GLN	C-N	5.34	1.44	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	329	PRO	CA-N-CD	-10.37	97.48	112.00
9	I	91	PRO	CA-N-CD	-8.97	99.45	112.00
22	W	148	PRO	CA-N-CD	-8.71	99.31	111.50
23	X	24	DC	N1-C1'-C2'	8.22	125.83	113.50
1	A	329	PRO	N-CD-CG	-7.18	92.42	103.20
2	B	912	PRO	CA-N-CD	-6.82	102.45	112.00
22	W	148	PRO	N-CD-CG	-6.25	96.30	103.80
24	Y	-32	DC	O4'-C1'-N1	5.85	117.18	108.40
9	I	91	PRO	N-CD-CG	-5.81	94.48	103.20
23	X	23	DC	N1-C1'-C2'	5.79	122.19	113.50
23	X	36	DC	N1-C1'-C2'	5.60	121.90	113.50
6	F	310	MET	CB-CG-SD	-5.48	96.27	112.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1157	LYS	Peptide
19	S	10	CYS	Peptide

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10848	0	11088	243	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	8680	0	8805	263	0
3	C	4075	0	4149	119	0
4	D	1347	0	1392	36	0
5	E	3211	0	3227	66	0
6	F	2403	0	2405	42	0
7	G	717	0	719	28	0
8	H	1509	0	1461	38	0
9	I	1001	0	1028	17	0
10	J	436	0	439	7	0
11	K	2736	0	2712	56	0
12	L	856	0	840	25	0
13	M	1715	0	1733	45	0
14	N	627	0	659	11	0
15	O	1186	0	1147	18	0
16	P	388	0	393	16	0
17	Q	524	0	540	20	0
18	R	1402	0	1489	22	0
19	S	2813	0	2847	82	0
20	T	825	0	812	10	0
21	U	1183	0	1175	21	0
22	W	2018	0	1997	27	0
23	X	1403	0	782	44	0
24	Y	1300	0	712	28	0
25	Z	3123	0	2986	32	0
26	A	2	0	0	0	0
26	B	1	0	0	0	0
26	J	1	0	0	0	0
26	P	1	0	0	0	0
26	Q	1	0	0	0	0
26	S	1	0	0	0	0
26	Z	2	0	0	0	0
27	A	1	0	0	0	0
28	F	8	0	0	7	0
All	All	56344	0	55537	1216	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 11.

All (1216) 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)
19:S:16:VAL:O	19:S:27:VAL:N	1.97	0.97
1:A:1366:ALA:HB1	8:H:22:LEU:HD21	1.50	0.94
1:A:1317:MET:HE1	1:A:1318:LEU:HD23	1.52	0.91
2:B:647:GLU:N	2:B:647:GLU:OE1	2.03	0.91
13:M:138:ASN:ND2	13:M:141:GLU:OE2	2.04	0.89
1:A:257:VAL:HG12	1:A:283:LEU:HD11	1.51	0.89
1:A:176:HIS:ND1	1:A:216:GLU:OE2	2.07	0.88
7:G:92:MET:HE2	7:G:92:MET:O	1.73	0.88
2:B:109:TYR:HH	2:B:145:CYS:HG	0.93	0.86
2:B:588:ASP:OD1	2:B:589:GLY:N	2.11	0.84
2:B:782:TYR:OH	2:B:788:ASP:OD1	1.96	0.83
2:B:506:MET:SD	2:B:569:ASN:ND2	2.51	0.83
2:B:1072:SER:OG	2:B:1073:ASP:OD2	1.96	0.82
2:B:613:GLU:OE1	2:B:619:ARG:NE	2.11	0.81
4:D:146:GLU:N	4:D:146:GLU:OE1	2.13	0.81
7:G:57:MET:HE3	7:G:57:MET:O	1.81	0.81
3:C:114:GLY:O	3:C:236:GLN:NE2	2.15	0.80
1:A:62:THR:OG1	1:A:64:GLU:OE2	2.01	0.79
17:Q:10:CYS:SG	17:Q:11:GLY:N	2.55	0.78
2:B:1069:MET:SD	2:B:1070:ILE:HD13	2.24	0.78
1:A:485:THR:O	1:A:487:ARG:NH1	2.16	0.78
8:H:138:HIS:O	8:H:138:HIS:ND1	2.17	0.77
5:E:97:MET:N	5:E:97:MET:HE2	2.00	0.77
18:R:172:VAL:HG12	18:R:219:MET:HE2	1.66	0.77
3:C:436:LEU:HD21	3:C:523:LEU:HD22	1.68	0.76
2:B:854:VAL:HG13	2:B:854:VAL:O	1.83	0.76
2:B:1041:ARG:NH1	19:S:46:ASP:OD1	2.19	0.74
1:A:732:ASN:OD1	1:A:733:THR:N	2.20	0.74
14:N:88:ASP:OD1	14:N:90:LEU:N	2.20	0.74
16:P:38:GLU:N	16:P:38:GLU:OE1	2.21	0.74
17:Q:26:GLN:OE1	17:Q:26:GLN:O	2.05	0.74
2:B:1032:THR:OG1	2:B:1034:GLN:OE1	2.06	0.73
2:B:135:ARG:H	2:B:412:THR:HG22	1.52	0.73
23:X:37:DT:H2'	23:X:38:DT:H71	1.68	0.73
19:S:115:GLU:O	19:S:118:VAL:HG22	1.87	0.73
19:S:33:CYS:SG	19:S:34:VAL:N	2.61	0.73
1:A:529:LEU:HD12	1:A:668:LEU:HD12	1.70	0.73
1:A:899:GLN:N	1:A:899:GLN:OE1	2.22	0.73
2:B:216:MET:HE2	2:B:216:MET:HA	1.70	0.73
19:S:135:MET:N	19:S:135:MET:HE2	2.02	0.73
19:S:226:ILE:O	19:S:230:THR:HG23	1.89	0.73
3:C:385:MET:HE2	3:C:385:MET:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:365:ILE:HG21	3:C:395:LEU:HD21	1.70	0.72
1:A:55:VAL:HG12	1:A:56:LEU:HD12	1.72	0.71
3:C:104:GLU:OE1	3:C:105:LEU:HD12	1.90	0.71
1:A:1280:MET:HE3	1:A:1280:MET:HA	1.71	0.71
9:I:93:THR:OG1	9:I:96:GLU:OE1	2.06	0.71
2:B:211:LYS:O	2:B:211:LYS:HD3	1.91	0.71
2:B:1050:MET:SD	2:B:1050:MET:N	2.63	0.71
2:B:74:TYR:C	2:B:75:LEU:HD23	2.16	0.71
3:C:393:ASP:OD1	3:C:394:MET:N	2.24	0.71
1:A:27:GLU:OE1	2:B:1094:TYR:OH	2.08	0.71
5:E:347:GLU:OE1	5:E:347:GLU:N	2.21	0.70
14:N:94:MET:SD	14:N:95:LYS:N	2.64	0.70
19:S:34:VAL:HG12	19:S:34:VAL:O	1.90	0.70
2:B:524:ASN:ND2	5:E:107:THR:O	2.25	0.70
7:G:108:ARG:O	7:G:108:ARG:NE	2.25	0.70
1:A:1366:ALA:HB1	8:H:22:LEU:CD2	2.22	0.69
3:C:53:ALA:O	3:C:57:LEU:HD22	1.92	0.69
2:B:220:GLN:OE1	2:B:220:GLN:N	2.25	0.69
4:D:154:ILE:HG23	4:D:154:ILE:O	1.91	0.69
1:A:283:LEU:HD23	1:A:283:LEU:O	1.92	0.69
2:B:281:MET:HE3	2:B:281:MET:H	1.58	0.69
2:B:324:LYS:NZ	2:B:325:GLU:OE2	2.25	0.68
2:B:67:SER:OG	2:B:69:ALA:O	2.05	0.68
1:A:238:LEU:C	1:A:239:LEU:HD12	2.18	0.68
8:H:93:SER:O	8:H:127:TRP:NE1	2.25	0.68
2:B:795:LEU:HD13	2:B:800:ARG:HA	1.76	0.67
9:I:92:VAL:HG13	9:I:93:THR:HG23	1.76	0.67
13:M:197:SER:OG	13:M:199:THR:O	2.13	0.67
1:A:325:LEU:HD12	1:A:325:LEU:H	1.59	0.67
18:R:299:ARG:O	18:R:299:ARG:HG3	1.95	0.67
22:W:205:LEU:HD22	22:W:242:ILE:HD12	1.77	0.67
5:E:96:LEU:C	5:E:97:MET:HE2	2.20	0.66
2:B:384:MET:HE2	2:B:384:MET:C	2.21	0.66
2:B:274:LYS:HA	2:B:274:LYS:HE2	1.77	0.66
2:B:955:ASP:OD2	2:B:957:ARG:NH1	2.27	0.66
7:G:79:GLU:N	7:G:79:GLU:OE1	2.26	0.66
3:C:140:ASP:N	3:C:143:GLU:OE2	2.27	0.66
19:S:258:LEU:O	19:S:258:LEU:HD12	1.96	0.66
7:G:65:ARG:NH1	7:G:66:GLU:OE2	2.29	0.66
1:A:598:LYS:NZ	1:A:648:GLY:O	2.29	0.65
8:H:20:ARG:NH1	8:H:28:GLU:OE2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:300:SER:OG	24:Y:-33:DG:OP1	2.06	0.65
18:R:210:THR:OG1	23:X:28:DT:OP2	2.07	0.65
3:C:162:SER:N	3:C:181:VAL:O	2.30	0.64
3:C:367:ARG:NE	6:F:244:TYR:O	2.28	0.64
25:Z:394:ASN:OD1	25:Z:395:LYS:N	2.30	0.64
2:B:216:MET:SD	2:B:217:ALA:N	2.70	0.64
5:E:366:VAL:HG13	5:E:366:VAL:O	1.97	0.64
22:W:256:ASN:OD1	22:W:257:ARG:N	2.29	0.64
1:A:111:THR:OG1	1:A:159:CYS:SG	2.55	0.64
1:A:1072:GLU:OE2	1:A:1080:ILE:HD11	1.96	0.64
1:A:84:GLY:C	1:A:257:VAL:HG22	2.22	0.64
6:F:137:LYS:NZ	6:F:153:TYR:O	2.31	0.64
15:O:81:ARG:NH1	15:O:82:PRO:O	2.30	0.64
3:C:118:MET:O	3:C:122:VAL:HG22	1.97	0.64
16:P:26:ASN:OD1	16:P:37:ARG:N	2.30	0.64
1:A:912:MET:HE2	1:A:912:MET:N	2.13	0.64
7:G:63:GLU:O	7:G:67:THR:OG1	2.14	0.64
23:X:54:DT:H2'	23:X:55:DT:H71	1.80	0.64
2:B:755:LEU:HD12	2:B:755:LEU:O	1.97	0.64
1:A:876:VAL:HG21	2:B:1053:ASP:OD1	1.98	0.63
1:A:880:GLU:OE2	1:A:880:GLU:N	2.29	0.63
3:C:118:MET:HE3	3:C:118:MET:HA	1.80	0.63
3:C:365:ILE:HA	3:C:368:LEU:HD12	1.79	0.63
8:H:48:LEU:HD12	8:H:48:LEU:O	1.97	0.63
2:B:254:MET:HE2	2:B:333:ILE:HD13	1.81	0.63
24:Y:-49:DA:OP2	25:Z:194:LYS:NZ	2.29	0.63
3:C:158:GLN:HB2	3:C:187:MET:SD	2.38	0.63
6:F:248:VAL:HG21	6:F:270:TYR:CE1	2.33	0.63
6:F:113:ARG:HE	6:F:120:LEU:HD13	1.63	0.63
1:A:1061:MET:SD	1:A:1061:MET:N	2.72	0.63
4:D:373:MET:SD	4:D:374:THR:N	2.71	0.63
5:E:40:ASP:OD2	5:E:214:ARG:NH2	2.32	0.63
1:A:1329:PHE:CD1	2:B:1122:ILE:HD11	2.34	0.62
19:S:257:ASP:OD1	19:S:258:LEU:N	2.32	0.62
1:A:463:ASN:OD1	1:A:464:ARG:N	2.31	0.62
6:F:286:PRO:O	6:F:290:CYS:N	2.32	0.62
1:A:471:LEU:HD22	1:A:474:MET:HE2	1.82	0.62
11:K:87:MET:SD	11:K:87:MET:N	2.73	0.62
23:X:57:DG:C2'	23:X:58:DT:H71	2.30	0.62
3:C:460:LEU:HD23	3:C:495:GLU:OE2	1.99	0.62
1:A:908:ASP:O	1:A:912:MET:HE3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:895:ASP:O	2:B:906:VAL:HG23	2.00	0.62
1:A:37:VAL:O	1:A:37:VAL:HG22	1.99	0.62
2:B:73:TRP:CH2	2:B:75:LEU:HD21	2.35	0.61
8:H:5:VAL:HG23	8:H:7:MET:SD	2.39	0.61
2:B:758:ASN:OD1	2:B:759:LYS:N	2.33	0.61
2:B:531:LEU:HD23	2:B:531:LEU:O	2.01	0.61
2:B:923:ILE:HG22	17:Q:42:ARG:HD3	1.81	0.61
3:C:429:LEU:HD22	3:C:429:LEU:H	1.65	0.61
1:A:305:MET:SD	1:A:305:MET:N	2.72	0.61
4:D:269:LEU:HD11	4:D:271:LEU:HD11	1.82	0.61
18:R:316:LYS:N	18:R:320:GLU:OE1	2.34	0.61
1:A:1317:MET:C	1:A:1317:MET:HE2	2.25	0.61
5:E:270:MET:SD	5:E:270:MET:N	2.73	0.61
11:K:115:ILE:O	11:K:315:VAL:HG12	2.00	0.61
25:Z:151:ARG:HG3	25:Z:152:GLN:N	2.16	0.61
1:A:1278:HIS:CE1	1:A:1280:MET:SD	2.94	0.61
2:B:561:LEU:C	2:B:561:LEU:HD23	2.26	0.61
1:A:394:GLU:CD	1:A:404:LEU:HD11	2.25	0.61
2:B:102:CYS:O	2:B:106:ASP:N	2.34	0.61
2:B:508:ASP:OD1	2:B:508:ASP:O	2.19	0.61
3:C:531:MET:SD	3:C:531:MET:N	2.74	0.61
12:L:87:ARG:NE	15:O:76:ASN:OD1	2.33	0.61
19:S:31:CYS:O	19:S:33:CYS:N	2.34	0.61
11:K:51:VAL:HG11	12:L:114:PHE:HA	1.83	0.60
6:F:26:CYS:O	6:F:75:ARG:NH1	2.33	0.60
1:A:1317:MET:SD	1:A:1318:LEU:N	2.74	0.60
1:A:563:LYS:HE2	1:A:563:LYS:HA	1.84	0.60
2:B:407:ARG:NH1	19:S:82:VAL:HG22	2.15	0.60
1:A:463:ASN:ND2	2:B:1051:GLU:OE2	2.28	0.60
1:A:668:LEU:HD23	1:A:668:LEU:C	2.27	0.60
3:C:333:MET:HE2	3:C:333:MET:HA	1.83	0.60
3:C:450:ARG:HD3	3:C:509:LEU:HD21	1.84	0.60
3:C:518:GLU:OE1	3:C:518:GLU:N	2.26	0.60
2:B:247:SER:OG	2:B:248:ASP:N	2.34	0.59
3:C:455:LYS:HE3	3:C:455:LYS:HA	1.84	0.59
1:A:1186:TYR:O	1:A:1189:LEU:HD22	2.02	0.59
2:B:109:TYR:OH	2:B:145:CYS:SG	2.36	0.59
2:B:151:THR:HG22	2:B:154:GLU:OE2	2.02	0.59
2:B:946:LEU:HD23	2:B:1003:TYR:CE2	2.38	0.59
3:C:90:ARG:O	3:C:94:THR:OG1	2.21	0.59
3:C:449:ARG:NH1	6:F:304:PRO:O	2.26	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:151:MET:HE1	13:M:159:LEU:HD22	1.84	0.59
2:B:1030:VAL:HG23	19:S:43:THR:O	2.03	0.59
3:C:104:GLU:OE1	3:C:105:LEU:N	2.36	0.59
19:S:30:ASP:OD1	19:S:31:CYS:N	2.35	0.59
3:C:500:GLU:OE1	3:C:504:ARG:NH1	2.34	0.58
6:F:232:MET:HE3	6:F:232:MET:HA	1.85	0.58
5:E:401:ILE:HG23	5:E:402:LEU:HG	1.84	0.58
22:W:155:THR:HG22	22:W:157:VAL:HG13	1.85	0.58
1:A:367:THR:HG22	1:A:368:VAL:N	2.18	0.58
9:I:33:ASN:OD1	9:I:34:LYS:N	2.36	0.58
5:E:348:VAL:HG13	5:E:348:VAL:O	2.02	0.58
8:H:149:ARG:HG3	8:H:149:ARG:HH11	1.68	0.58
1:A:125:PHE:CE2	1:A:146:ILE:HG22	2.37	0.58
1:A:737:GLN:OE1	1:A:737:GLN:N	2.26	0.58
21:U:140:MET:SD	21:U:140:MET:N	2.74	0.58
1:A:237:LEU:HD12	1:A:237:LEU:H	1.67	0.58
1:A:438:GLU:OE2	1:A:438:GLU:N	2.37	0.58
5:E:248:MET:C	5:E:248:MET:HE2	2.29	0.58
13:M:159:LEU:HD21	13:M:206:TYR:CE1	2.39	0.58
22:W:331:PHE:CE2	25:Z:356:VAL:HG22	2.39	0.58
1:A:45:ASP:OD1	1:A:47:GLN:N	2.37	0.57
2:B:465:VAL:O	2:B:467:GLY:N	2.37	0.57
2:B:946:LEU:HD23	2:B:1003:TYR:CZ	2.38	0.57
2:B:1077:VAL:HG22	2:B:1078:ASP:H	1.68	0.57
1:A:116:MET:SD	1:A:116:MET:N	2.77	0.57
1:A:1213:HIS:N	1:A:1224:LYS:O	2.37	0.57
6:F:248:VAL:HG21	6:F:270:TYR:CZ	2.38	0.57
2:B:854:VAL:O	2:B:854:VAL:CG1	2.51	0.57
4:D:151:THR:HG22	4:D:151:THR:O	2.03	0.57
19:S:72:GLY:O	19:S:76:VAL:HG23	2.04	0.57
24:Y:-34:DG:H2'	24:Y:-33:DG:C8	2.39	0.57
3:C:450:ARG:HD3	3:C:509:LEU:HD11	1.86	0.57
6:F:310:MET:HB2	28:F:401:SF4:S4	2.45	0.57
14:N:91:LEU:O	14:N:94:MET:SD	2.63	0.57
6:F:248:VAL:HG21	6:F:270:TYR:OH	2.05	0.56
18:R:263:ASP:OD1	18:R:264:VAL:N	2.38	0.56
1:A:218:LEU:HD12	1:A:218:LEU:O	2.05	0.56
8:H:31:ASN:OD1	8:H:48:LEU:HG	2.05	0.56
1:A:76:LEU:HD12	1:A:76:LEU:O	2.06	0.56
2:B:335:THR:O	2:B:338:MET:SD	2.62	0.56
2:B:1113:LEU:O	2:B:1117:LEU:HD22	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:103:CYS:N	5:E:136:ARG:O	2.33	0.56
5:E:376:LYS:O	5:E:376:LYS:HD3	2.04	0.56
12:L:58:MET:HE2	12:L:102:GLU:C	2.29	0.56
19:S:269:LEU:O	19:S:273:LEU:HG	2.05	0.56
1:A:967:GLN:OE1	1:A:967:GLN:O	2.23	0.56
3:C:135:ASP:CG	3:C:135:ASP:O	2.47	0.56
9:I:62:SER:OG	9:I:64:GLU:OE2	2.24	0.56
2:B:867:GLU:OE1	2:B:886:ARG:NH1	2.37	0.56
3:C:64:SER:OG	3:C:65:TYR:N	2.39	0.56
1:A:252:LEU:O	1:A:252:LEU:HD12	2.06	0.56
2:B:312:LEU:HD12	2:B:316:THR:HB	1.87	0.56
2:B:407:ARG:CZ	19:S:82:VAL:HG22	2.36	0.56
2:B:1030:VAL:HG22	19:S:42:THR:OG1	2.06	0.56
2:B:1121:ASN:CG	2:B:1121:ASN:O	2.48	0.56
8:H:151:ARG:O	8:H:189:SER:N	2.39	0.56
17:Q:9:THR:O	17:Q:11:GLY:N	2.39	0.56
20:T:368:ALA:O	20:T:372:GLN:NE2	2.39	0.56
1:A:661:ASN:OD1	1:A:661:ASN:C	2.49	0.56
1:A:404:LEU:HD13	1:A:450:VAL:CG2	2.36	0.56
16:P:18:ILE:HG13	16:P:23:HIS:HA	1.88	0.56
19:S:21:TYR:N	19:S:23:GLN:OE1	2.38	0.56
1:A:1186:TYR:CE2	1:A:1189:LEU:HD21	2.41	0.55
3:C:450:ARG:HD2	3:C:506:VAL:HG13	1.86	0.55
6:F:296:CYS:CB	28:F:401:SF4:S2	2.85	0.55
24:Y:-28:DA:H2'	24:Y:-27:DA:C8	2.41	0.55
1:A:596:THR:HG21	15:O:119:GLY:O	2.05	0.55
2:B:363:GLU:OE1	2:B:367:GLN:NE2	2.34	0.55
2:B:1013:LYS:HE3	2:B:1014:HIS:CE1	2.41	0.55
3:C:509:LEU:O	3:C:512:SER:OG	2.21	0.55
4:D:266:LEU:C	4:D:267:LEU:HD22	2.31	0.55
6:F:298:GLU:N	6:F:298:GLU:OE1	2.40	0.55
17:Q:20:ALA:O	17:Q:24:LEU:HD23	2.06	0.55
1:A:731:LEU:HD13	1:A:748:LEU:HD22	1.87	0.55
1:A:1087:ALA:HB2	1:A:1246:THR:HG22	1.88	0.55
12:L:29:MET:SD	12:L:30:VAL:N	2.78	0.55
19:S:154:MET:SD	19:S:154:MET:C	2.90	0.55
1:A:105:LEU:HD21	1:A:223:VAL:HG13	1.88	0.55
1:A:1146:ALA:O	1:A:1149:VAL:HG22	2.07	0.55
2:B:426:LEU:N	2:B:431:MET:O	2.40	0.55
3:C:389:LYS:HG3	3:C:389:LYS:O	2.06	0.55
5:E:330:ASP:OD2	5:E:331:ILE:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:53:LYS:C	8:H:54:LEU:HD12	2.31	0.55
11:K:97:ASN:ND2	11:K:103:ASP:OD1	2.38	0.55
11:K:125:ARG:NH1	11:K:137:THR:OG1	2.39	0.55
23:X:57:DG:H2"	23:X:58:DT:H71	1.88	0.55
11:K:10:MET:C	11:K:10:MET:HE2	2.32	0.55
23:X:52:DT:H2"	23:X:53:DT:H72	1.88	0.55
1:A:367:THR:HG22	1:A:368:VAL:H	1.71	0.55
3:C:30:ARG:O	3:C:30:ARG:HG2	2.05	0.55
13:M:20:LEU:C	13:M:20:LEU:HD23	2.32	0.55
3:C:341:ALA:O	3:C:345:LEU:HD22	2.07	0.55
2:B:775:ALA:HB3	2:B:883:MET:SD	2.47	0.55
6:F:67:ARG:NH1	6:F:68:SER:O	2.40	0.55
2:B:222:ARG:NH2	2:B:267:PRO:O	2.36	0.54
19:S:152:THR:O	19:S:156:ILE:HG22	2.06	0.54
2:B:281:MET:H	2:B:281:MET:CE	2.20	0.54
2:B:335:THR:HA	2:B:338:MET:SD	2.47	0.54
4:D:313:GLU:OE1	4:D:313:GLU:HA	2.08	0.54
13:M:103:LEU:N	13:M:103:LEU:HD12	2.22	0.54
15:O:101:GLY:HA2	15:O:112:LEU:HD13	1.89	0.54
19:S:34:VAL:O	19:S:34:VAL:CG1	2.55	0.54
10:J:5:CYS:N	10:J:10:ASN:O	2.39	0.54
19:S:69:GLN:O	19:S:73:LEU:HD23	2.08	0.54
1:A:879:LEU:HD12	1:A:879:LEU:O	2.06	0.54
2:B:550:ARG:HG2	2:B:551:ASP:OD1	2.07	0.54
4:D:127:VAL:HG12	4:D:127:VAL:O	2.08	0.54
19:S:176:TYR:HE1	19:S:230:THR:HG21	1.71	0.54
2:B:39:LEU:O	2:B:40:VAL:HG12	2.08	0.54
6:F:310:MET:CA	28:F:401:SF4:S4	2.96	0.54
7:G:106:LEU:HD12	7:G:110:MET:HE2	1.87	0.54
2:B:262:MET:HE2	2:B:262:MET:C	2.33	0.54
17:Q:48:MET:HE2	17:Q:48:MET:HA	1.90	0.54
24:Y:13:DC:H2"	24:Y:14:DA:C8	2.43	0.54
2:B:426:LEU:N	2:B:426:LEU:HD12	2.22	0.54
5:E:77:ILE:O	5:E:81:VAL:HG12	2.08	0.54
13:M:121:MET:SD	13:M:122:ALA:N	2.78	0.54
1:A:171:LEU:HD23	1:A:172:LEU:HB2	1.89	0.54
2:B:77:TYR:C	2:B:78:LEU:HD22	2.32	0.54
2:B:374:GLU:OE2	2:B:375:ASP:N	2.39	0.54
5:E:249:LEU:HG	5:E:250:MET:SD	2.48	0.54
1:A:1278:HIS:ND1	1:A:1280:MET:SD	2.81	0.53
3:C:259:MET:SD	3:C:259:MET:C	2.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:108:ARG:HE	7:G:108:ARG:C	2.16	0.53
11:K:321:LEU:H	11:K:321:LEU:HD12	1.72	0.53
18:R:172:VAL:HG12	18:R:219:MET:CE	2.34	0.53
23:X:17:DG:H2'	23:X:18:DT:H72	1.89	0.53
2:B:75:LEU:HD22	2:B:119:TYR:HB2	1.90	0.53
4:D:332:ARG:HA	5:E:8:PRO:HA	1.89	0.53
8:H:146:GLU:OE1	8:H:146:GLU:N	2.41	0.53
15:O:28:LEU:HD12	15:O:28:LEU:N	2.22	0.53
1:A:963:ASP:OD1	1:A:963:ASP:N	2.42	0.53
13:M:116:GLN:O	13:M:119:VAL:HG22	2.09	0.53
19:S:7:CYS:HB2	19:S:8:PRO:CD	2.39	0.53
1:A:782:LEU:C	1:A:782:LEU:HD23	2.34	0.53
5:E:40:ASP:OD1	5:E:41:ASP:N	2.42	0.53
8:H:6:GLU:HA	8:H:6:GLU:OE1	2.08	0.53
11:K:82:ALA:HB3	11:K:83:GLU:OE2	2.08	0.53
1:A:298:ILE:HG22	1:A:298:ILE:O	2.09	0.53
1:A:1070:ILE:O	1:A:1074:ILE:HG12	2.09	0.53
4:D:382:LYS:C	4:D:383:LEU:HD22	2.33	0.53
1:A:130:LYS:HA	1:A:130:LYS:HE2	1.91	0.53
2:B:137:PRO:C	2:B:138:ILE:HD13	2.34	0.53
2:B:381:ASN:O	2:B:384:MET:SD	2.67	0.53
6:F:307:CYS:HA	7:G:38:PHE:CZ	2.44	0.53
23:X:33:DG:H2'	23:X:34:DC:C6	2.44	0.53
1:A:168:LYS:H	1:A:168:LYS:HD3	1.73	0.53
1:A:523:MET:HE1	2:B:1055:LEU:HD13	1.91	0.53
1:A:60:MET:SD	1:A:257:VAL:HG23	2.48	0.53
1:A:167:LYS:O	1:A:174:ILE:HD12	2.09	0.53
1:A:618:ARG:NE	1:A:637:TYR:OH	2.41	0.53
1:A:773:LYS:O	1:A:774:SER:OG	2.25	0.53
19:S:26:LEU:HD21	19:S:39:VAL:HG22	1.90	0.53
2:B:30:LEU:HB3	2:B:31:PRO:HD3	1.90	0.52
2:B:329:ARG:NH2	2:B:526:LEU:O	2.42	0.52
20:T:310:MET:HE3	20:T:371:LEU:HA	1.91	0.52
2:B:795:LEU:HD12	2:B:796:ASP:C	2.35	0.52
2:B:1066:GLU:HA	2:B:1070:ILE:HG12	1.90	0.52
3:C:520:ILE:O	3:C:524:GLU:HG2	2.09	0.52
6:F:304:PRO:HA	28:F:401:SF4:S1	2.49	0.52
1:A:968:GLU:OE1	1:A:969:ILE:N	2.43	0.52
6:F:97:GLN:NE2	6:F:101:ASP:OD2	2.42	0.52
7:G:58:LEU:HD23	7:G:58:LEU:C	2.35	0.52
11:K:112:LEU:HD12	17:Q:6:ARG:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1316:LEU:HD13	1:A:1348:ILE:HG21	1.91	0.52
3:C:323:VAL:HG22	3:C:336:ILE:HA	1.92	0.52
3:C:513:GLU:O	3:C:516:VAL:HG12	2.10	0.52
6:F:297:HIS:N	6:F:302:ILE:O	2.43	0.52
8:H:22:LEU:O	8:H:26:ILE:HG22	2.10	0.52
1:A:217:ASN:ND2	1:A:217:ASN:O	2.41	0.52
3:C:450:ARG:HG3	3:C:509:LEU:HD21	1.92	0.52
6:F:235:ILE:O	6:F:239:LEU:HD22	2.09	0.52
12:L:115:GLU:OE2	12:L:115:GLU:O	2.28	0.52
1:A:1099:ARG:NH2	10:J:52:VAL:O	2.43	0.52
5:E:187:GLN:OE1	5:E:189:ARG:N	2.33	0.52
25:Z:287:LYS:HD2	25:Z:287:LYS:O	2.10	0.52
2:B:777:CYS:SG	2:B:778:THR:N	2.82	0.52
23:X:32:DA:H2'	23:X:33:DG:C8	2.44	0.52
2:B:759:LYS:O	2:B:763:ASP:OD1	2.28	0.52
3:C:28:LEU:HG	3:C:77:ALA:HB2	1.91	0.52
9:I:111:GLU:CD	9:I:111:GLU:H	2.18	0.52
16:P:35:ARG:NE	16:P:39:CYS:O	2.39	0.52
1:A:662:ASN:OD1	1:A:664:PHE:N	2.43	0.52
1:A:791:ASN:OD1	2:B:938:MET:HE2	2.10	0.52
7:G:68:MET:HE2	7:G:68:MET:C	2.35	0.52
1:A:492:VAL:O	1:A:492:VAL:HG12	2.10	0.51
1:A:761:ASP:C	1:A:761:ASP:OD2	2.53	0.51
2:B:751:ILE:HG22	2:B:752:GLU:HG2	1.93	0.51
2:B:923:ILE:HG22	17:Q:42:ARG:CD	2.39	0.51
11:K:97:ASN:O	16:P:48:ARG:NE	2.43	0.51
2:B:259:GLU:OE2	2:B:259:GLU:HA	2.10	0.51
5:E:357:MET:HE3	5:E:357:MET:HA	1.92	0.51
6:F:127:LEU:C	6:F:127:LEU:HD23	2.36	0.51
11:K:293:LEU:O	11:K:296:VAL:HG22	2.11	0.51
1:A:139:LYS:NZ	1:A:1336:GLN:OE1	2.40	0.51
1:A:59:ARG:HB2	1:A:59:ARG:NH1	2.26	0.51
1:A:101:VAL:O	1:A:105:LEU:HG	2.10	0.51
1:A:369:ILE:HG21	1:A:505:MET:HG2	1.92	0.51
1:A:743:THR:HG22	1:A:746:GLU:HG2	1.92	0.51
4:D:143:GLU:OE1	4:D:143:GLU:N	2.38	0.51
23:X:36:DC:H2'	23:X:37:DT:C6	2.45	0.51
2:B:426:LEU:O	2:B:430:LYS:N	2.43	0.51
5:E:16:TYR:N	5:E:124:LEU:O	2.42	0.51
15:O:14:ASP:OD1	15:O:15:ILE:N	2.43	0.51
19:S:146:LEU:HA	19:S:149:PHE:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:316:THR:HG22	2:B:316:THR:O	2.11	0.51
2:B:1042:ASP:OD1	19:S:22:SER:HA	2.11	0.51
21:U:46:MET:HE1	21:U:54:PHE:CG	2.46	0.51
21:U:133:ARG:NH1	25:Z:64:ARG:O	2.40	0.51
1:A:305:MET:CE	1:A:305:MET:H	2.24	0.51
1:A:889:THR:HG22	1:A:900:PHE:O	2.11	0.51
4:D:154:ILE:O	4:D:154:ILE:CG2	2.58	0.51
5:E:81:VAL:HG13	5:E:82:ASP:N	2.26	0.51
9:I:73:LEU:HD12	9:I:116:LEU:HD23	1.93	0.51
3:C:67:VAL:HG22	3:C:73:VAL:HG22	1.93	0.51
7:G:108:ARG:NE	7:G:108:ARG:C	2.69	0.51
13:M:187:ARG:HA	13:M:209:VAL:HG13	1.92	0.51
16:P:20:GLY:O	16:P:21:GLU:HG3	2.10	0.51
1:A:394:GLU:OE2	1:A:400:ASN:ND2	2.44	0.51
2:B:225:LEU:HD21	2:B:236:ILE:HD12	1.93	0.51
5:E:40:ASP:OD1	5:E:40:ASP:C	2.54	0.51
8:H:185:THR:O	8:H:186:LEU:HD13	2.11	0.51
19:S:7:CYS:SG	19:S:10:CYS:SG	3.09	0.51
1:A:1130:VAL:HG12	1:A:1173:VAL:O	2.11	0.51
22:W:205:LEU:HD22	22:W:242:ILE:CD1	2.40	0.51
23:X:52:DT:C2'	23:X:53:DT:H72	2.40	0.51
1:A:454:LEU:HD21	1:A:509:LEU:HD22	1.93	0.50
2:B:1077:VAL:HG22	2:B:1078:ASP:N	2.25	0.50
3:C:450:ARG:CG	3:C:509:LEU:HD21	2.40	0.50
4:D:256:ARG:NE	4:D:257:GLU:OE2	2.39	0.50
19:S:145:ASP:OD2	19:S:146:LEU:N	2.44	0.50
1:A:229:ARG:O	1:A:229:ARG:HG2	2.11	0.50
5:E:60:MET:SD	5:E:60:MET:N	2.84	0.50
19:S:153:TYR:CE1	19:S:157:VAL:HG21	2.47	0.50
21:U:26:PHE:O	21:U:30:THR:HG23	2.10	0.50
1:A:12:ALA:HB3	2:B:1131:TYR:CD1	2.46	0.50
2:B:381:ASN:HA	2:B:384:MET:SD	2.52	0.50
2:B:469:ARG:NH1	2:B:490:CYS:O	2.42	0.50
3:C:110:LEU:HD11	3:C:157:VAL:HG23	1.93	0.50
2:B:380:PHE:O	2:B:383:GLU:OE2	2.30	0.50
2:B:1032:THR:HG22	2:B:1112:LEU:HD22	1.93	0.50
3:C:350:LEU:HD11	3:C:431:ALA:HB1	1.93	0.50
5:E:330:ASP:OD2	5:E:330:ASP:C	2.55	0.50
1:A:896:ASP:OD1	1:A:897:ILE:N	2.44	0.50
3:C:62:LEU:H	3:C:62:LEU:HD12	1.76	0.50
5:E:269:SER:OG	5:E:270:MET:SD	2.62	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:28:GLU:O	12:L:43:VAL:HG22	2.12	0.50
13:M:14:ARG:NH1	13:M:58:LEU:HD21	2.26	0.50
3:C:364:ARG:O	3:C:368:LEU:HG	2.12	0.50
16:P:40:GLY:O	16:P:42:ARG:NH1	2.45	0.50
22:W:148:PRO:HD2	22:W:148:PRO:O	2.11	0.50
2:B:760:ALA:HA	2:B:763:ASP:OD1	2.11	0.50
2:B:772:TYR:CE1	2:B:886:ARG:HG3	2.46	0.50
3:C:434:MET:SD	3:C:434:MET:C	2.94	0.50
15:O:112:LEU:N	15:O:127:GLY:O	2.34	0.50
1:A:776:SER:HB2	1:A:777:PRO:HD3	1.93	0.50
2:B:211:LYS:O	2:B:211:LYS:CD	2.58	0.50
2:B:739:ALA:O	2:B:1006:PRO:HA	2.12	0.50
2:B:1025:ARG:O	2:B:1025:ARG:HG3	2.10	0.50
19:S:364:LYS:O	19:S:365:SER:OG	2.25	0.50
2:B:378:LYS:C	2:B:378:LYS:HD2	2.37	0.49
2:B:1121:ASN:O	2:B:1121:ASN:OD1	2.29	0.49
5:E:247:MET:HE2	5:E:247:MET:HA	1.93	0.49
6:F:249:GLU:N	6:F:271:ARG:O	2.39	0.49
19:S:129:HIS:O	19:S:130:ASN:OD1	2.30	0.49
23:X:-10:DG:H2'	23:X:-9:DA:C8	2.47	0.49
1:A:177:GLU:CD	1:A:177:GLU:N	2.68	0.49
2:B:1044:GLY:O	2:B:1045:LEU:HD22	2.12	0.49
4:D:389:PHE:N	4:D:389:PHE:CD2	2.80	0.49
5:E:104:SER:HB2	5:E:133:LEU:HD12	1.93	0.49
11:K:83:GLU:N	11:K:83:GLU:CD	2.71	0.49
12:L:60:MET:O	12:L:60:MET:SD	2.70	0.49
17:Q:2:ILE:HG23	17:Q:56:ILE:HG21	1.93	0.49
1:A:167:LYS:HB2	1:A:177:GLU:OE1	2.11	0.49
1:A:252:LEU:HD12	1:A:252:LEU:C	2.37	0.49
8:H:54:LEU:HD12	8:H:54:LEU:N	2.27	0.49
11:K:161:GLU:HA	11:K:161:GLU:OE1	2.11	0.49
16:P:24:THR:OG1	16:P:38:GLU:OE2	2.26	0.49
23:X:60:DA:C2'	23:X:61:DG:H8	2.25	0.49
1:A:404:LEU:HD13	1:A:450:VAL:HG21	1.94	0.49
2:B:114:THR:OG1	2:B:131:LEU:N	2.41	0.49
4:D:145:ARG:N	4:D:153:GLN:OE1	2.45	0.49
11:K:61:LEU:HD12	11:K:62:GLU:N	2.28	0.49
13:M:53:PRO:O	13:M:55:ARG:HD2	2.12	0.49
22:W:205:LEU:HD21	22:W:245:ILE:HB	1.94	0.49
19:S:91:ASP:OD2	19:S:91:ASP:C	2.55	0.49
1:A:46:ASN:O	1:A:48:HIS:ND1	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:81:VAL:HG13	5:E:82:ASP:H	1.77	0.49
5:E:294:PHE:O	5:E:294:PHE:CD1	2.65	0.49
23:X:15:DC:H2'	23:X:16:DT:C6	2.48	0.49
1:A:1215:ASP:OD2	1:A:1217:GLN:NE2	2.39	0.49
2:B:192:GLU:O	2:B:200:GLY:N	2.42	0.49
5:E:27:LEU:HB3	5:E:132:ILE:HG12	1.95	0.49
8:H:12:ARG:NH1	8:H:63:ASP:OD2	2.45	0.49
11:K:110:LEU:HD21	11:K:212:MET:SD	2.53	0.49
12:L:29:MET:SD	12:L:29:MET:C	2.96	0.49
22:W:275:ARG:NH1	22:W:279:GLU:OE2	2.44	0.49
1:A:62:THR:HG21	1:A:76:LEU:HA	1.94	0.49
1:A:878:SER:HB2	1:A:1308:LEU:HD11	1.94	0.49
1:A:1048:MET:HE1	1:A:1070:ILE:HD12	1.94	0.49
2:B:509:GLY:O	2:B:512:VAL:HG12	2.13	0.49
2:B:1108:TYR:C	2:B:1108:TYR:CD1	2.91	0.49
3:C:240:ASP:OD1	3:C:241:ARG:N	2.45	0.49
1:A:973:ILE:HA	1:A:976:VAL:HG12	1.95	0.49
11:K:106:LEU:C	11:K:106:LEU:HD23	2.38	0.49
12:L:124:GLN:O	12:L:128:ARG:N	2.44	0.49
18:R:275:LEU:O	18:R:278:GLN:NE2	2.46	0.49
2:B:172:LYS:N	2:B:172:LYS:HD2	2.28	0.49
4:D:274:THR:HG21	5:E:248:MET:HE1	1.95	0.49
1:A:329:PRO:HD2	1:A:329:PRO:O	2.12	0.48
13:M:52:ARG:N	13:M:53:PRO:CD	2.76	0.48
16:P:23:HIS:HD1	17:Q:66:GLU:HA	1.78	0.48
25:Z:159:MET:SD	25:Z:159:MET:N	2.86	0.48
1:A:1020:ASP:OD1	1:A:1024:ARG:HD3	2.14	0.48
23:X:58:DT:H2'	23:X:59:DT:H72	1.95	0.48
3:C:111:LEU:HD12	3:C:111:LEU:H	1.78	0.48
7:G:33:LYS:HD3	7:G:34:PRO:O	2.13	0.48
19:S:44:PHE:CG	19:S:45:SER:N	2.80	0.48
19:S:397:GLN:NE2	19:S:401:ASP:OD2	2.44	0.48
1:A:770:GLU:CD	1:A:770:GLU:O	2.56	0.48
1:A:896:ASP:OD1	1:A:896:ASP:C	2.56	0.48
3:C:262:THR:O	3:C:266:ILE:HG23	2.13	0.48
8:H:5:VAL:HG22	8:H:74:CYS:O	2.13	0.48
1:A:861:THR:O	1:A:865:THR:HG23	2.13	0.48
1:A:1350:GLY:O	2:B:1069:MET:HE2	2.14	0.48
2:B:1021:HIS:CD2	2:B:1039:ARG:HG3	2.49	0.48
3:C:118:MET:SD	3:C:235:TRP:CD1	3.06	0.48
16:P:28:ILE:HD13	16:P:34:ILE:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:515:GLN:O	6:F:281:GLY:HA3	2.14	0.48
12:L:27:LEU:HD12	12:L:28:GLU:N	2.29	0.48
1:A:966:LEU:O	1:A:969:ILE:HG12	2.14	0.48
1:A:1340:VAL:HG11	1:A:1351:ILE:HD11	1.95	0.48
3:C:245:HIS:HE1	3:C:249:GLN:NE2	2.12	0.48
11:K:68:ILE:HD11	11:K:72:ILE:HG13	1.95	0.48
11:K:242:LEU:N	11:K:242:LEU:HD23	2.28	0.48
1:A:94:HIS:O	1:A:96:GLY:N	2.45	0.48
1:A:366:ARG:O	1:A:367:THR:OG1	2.29	0.48
3:C:285:THR:CG2	3:C:336:ILE:HG22	2.44	0.48
12:L:58:MET:HE2	12:L:103:LEU:N	2.29	0.48
13:M:189:GLN:H	13:M:209:VAL:HG12	1.79	0.48
22:W:152:ASP:OD1	22:W:154:VAL:N	2.47	0.48
25:Z:391:SER:OG	25:Z:392:GLU:OE2	2.26	0.48
2:B:434:GLN:OE1	2:B:434:GLN:N	2.47	0.48
2:B:522:ASP:OD1	2:B:523:VAL:N	2.47	0.48
2:B:574:ILE:O	2:B:637:GLU:HB2	2.13	0.48
10:J:1:MET:SD	10:J:1:MET:C	2.97	0.48
11:K:325:ALA:O	11:K:328:VAL:HG12	2.14	0.48
1:A:968:GLU:C	1:A:968:GLU:CD	2.82	0.48
7:G:70:ARG:HD2	7:G:70:ARG:C	2.39	0.48
11:K:89:VAL:HG12	11:K:214:CYS:SG	2.53	0.48
18:R:295:MET:HE3	18:R:302:LEU:HD11	1.96	0.48
19:S:73:LEU:HD11	19:S:98:GLN:OE1	2.13	0.48
19:S:282:TRP:HB3	22:W:201:LEU:HD23	1.95	0.48
1:A:1145:ASN:OD1	1:A:1147:GLU:N	2.47	0.47
2:B:41:LYS:O	2:B:45:ASP:HB2	2.14	0.47
2:B:1105:ARG:HG3	2:B:1105:ARG:HH11	1.79	0.47
3:C:381:GLU:O	3:C:385:MET:N	2.44	0.47
22:W:186:ASN:OD1	22:W:187:TRP:N	2.46	0.47
1:A:556:ASP:O	1:A:556:ASP:OD2	2.32	0.47
2:B:871:ILE:HD11	2:B:879:PHE:CE2	2.49	0.47
3:C:509:LEU:HA	3:C:512:SER:OG	2.13	0.47
11:K:317:PRO:O	11:K:321:LEU:HD12	2.13	0.47
15:O:66:GLU:H	15:O:66:GLU:CD	2.21	0.47
19:S:128:GLN:OE1	19:S:128:GLN:HA	2.14	0.47
23:X:54:DT:C2'	23:X:55:DT:H71	2.44	0.47
2:B:67:SER:HB3	2:B:73:TRP:CE3	2.49	0.47
7:G:57:MET:SD	7:G:60:LEU:HD22	2.54	0.47
1:A:297:ARG:HA	1:A:297:ARG:NH1	2.29	0.47
2:B:279:THR:OG1	2:B:281:MET:SD	2.66	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:267:VAL:O	3:C:270:MET:HE3	2.14	0.47
23:X:-15:DC:H1'	23:X:-14:DT:C5	2.49	0.47
3:C:393:ASP:OD1	3:C:393:ASP:C	2.55	0.47
5:E:248:MET:HE2	5:E:248:MET:O	2.14	0.47
11:K:242:LEU:HD23	11:K:242:LEU:H	1.79	0.47
1:A:1300:VAL:HG23	1:A:1300:VAL:O	2.14	0.47
3:C:442:SER:O	3:C:446:LEU:HG	2.14	0.47
13:M:95:GLN:O	13:M:98:ASN:ND2	2.47	0.47
20:T:317:MET:SD	20:T:317:MET:C	2.97	0.47
22:W:350:THR:OG1	22:W:352:GLU:OE1	2.27	0.47
25:Z:392:GLU:CD	25:Z:392:GLU:N	2.73	0.47
1:A:728:ILE:HD13	1:A:748:LEU:HD21	1.97	0.47
2:B:48:ASN:ND2	2:B:143:SER:OG	2.47	0.47
2:B:313:LEU:HD23	2:B:313:LEU:O	2.15	0.47
2:B:369:LEU:CD1	2:B:415:MET:HE2	2.44	0.47
2:B:618:TYR:OH	5:E:300:LEU:HD13	2.15	0.47
2:B:750:ASP:O	2:B:930:ASN:ND2	2.47	0.47
2:B:909:LEU:O	2:B:910:ILE:HD13	2.15	0.47
8:H:139:ASP:OD2	8:H:197:LEU:HD13	2.14	0.47
8:H:149:ARG:HG3	8:H:149:ARG:NH1	2.30	0.47
11:K:53:VAL:HG23	12:L:121:TYR:CD2	2.50	0.47
13:M:63:ALA:HB3	13:M:67:ASP:O	2.15	0.47
13:M:162:ARG:HG2	13:M:163:TYR:CD1	2.50	0.47
23:X:31:DA:H2'	23:X:32:DA:C8	2.50	0.47
23:X:41:DA:H2'	23:X:42:DT:H71	1.97	0.47
1:A:674:ASN:O	1:A:678:ASP:OD2	2.33	0.47
2:B:283:ALA:O	2:B:287:ILE:HG12	2.14	0.47
2:B:540:PHE:O	2:B:585:ILE:HD12	2.15	0.47
2:B:550:ARG:NH2	4:D:351:GLY:O	2.42	0.47
19:S:127:ARG:HG2	19:S:164:VAL:HG22	1.95	0.47
25:Z:394:ASN:OD1	25:Z:394:ASN:C	2.58	0.47
1:A:984:ARG:O	1:A:988:GLY:N	2.47	0.47
2:B:369:LEU:HD11	2:B:415:MET:HE2	1.97	0.47
2:B:588:ASP:OD1	2:B:588:ASP:C	2.57	0.47
3:C:350:LEU:HA	3:C:353:VAL:HG12	1.97	0.47
7:G:68:MET:SD	7:G:69:LYS:N	2.87	0.47
23:X:44:DA:N3	24:Y:-42:DG:N2	2.63	0.47
24:Y:-22:DG:H2''	24:Y:-21:DT:O5'	2.15	0.47
6:F:33:ILE:O	6:F:33:ILE:HG13	2.13	0.47
23:X:47:DT:H2''	23:X:48:DC:C6	2.49	0.47
2:B:1041:ARG:O	2:B:1042:ASP:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:274:THR:HG21	5:E:248:MET:CE	2.46	0.46
4:D:372:GLU:OE1	5:E:217:ARG:NH1	2.47	0.46
1:A:281:MET:O	1:A:285:GLU:HG2	2.15	0.46
2:B:131:LEU:HD23	2:B:131:LEU:C	2.40	0.46
2:B:873:SER:HB3	16:P:34:ILE:HD11	1.96	0.46
2:B:1131:TYR:HE2	8:H:60:PHE:CE2	2.34	0.46
6:F:287:CYS:HA	6:F:290:CYS:HB3	1.97	0.46
8:H:1:MET:O	8:H:78:HIS:N	2.45	0.46
24:Y:-49:DA:H4'	24:Y:-48:DT:OP1	2.14	0.46
1:A:1044:PRO:HB2	1:A:1275:MET:HE1	1.97	0.46
2:B:177:VAL:O	2:B:437:THR:HG22	2.15	0.46
2:B:1086:LEU:HD12	2:B:1086:LEU:N	2.31	0.46
3:C:350:LEU:CD1	3:C:431:ALA:HB1	2.46	0.46
3:C:517:ASP:N	3:C:517:ASP:OD1	2.45	0.46
23:X:-15:DC:H2''	23:X:-14:DT:H71	1.97	0.46
23:X:53:DT:C6	23:X:53:DT:OP2	2.68	0.46
1:A:986:LYS:NZ	15:O:103:GLU:OE2	2.45	0.46
2:B:279:THR:HB	2:B:281:MET:HE1	1.97	0.46
2:B:598:ILE:HD12	2:B:628:SER:O	2.16	0.46
3:C:338:LEU:HD12	3:C:338:LEU:H	1.79	0.46
11:K:237:PRO:O	11:K:238:ASP:OD2	2.34	0.46
14:N:62:ARG:HE	14:N:97:LEU:HD23	1.81	0.46
15:O:66:GLU:O	15:O:84:ARG:NH2	2.49	0.46
19:S:114:LYS:NZ	24:Y:-17:DA:OP1	2.42	0.46
23:X:17:DG:H2'	23:X:18:DT:C7	2.45	0.46
1:A:137:LEU:H	1:A:137:LEU:HD12	1.80	0.46
1:A:322:ASN:OD1	1:A:323:SER:N	2.49	0.46
1:A:464:ARG:HD3	1:A:496:TYR:O	2.15	0.46
1:A:590:LYS:HB3	1:A:591:PRO:HD3	1.96	0.46
1:A:1044:PRO:HA	1:A:1047:GLN:HB2	1.97	0.46
1:A:1149:VAL:O	1:A:1153:ILE:HG12	2.15	0.46
2:B:136:MET:HE2	2:B:136:MET:HA	1.97	0.46
2:B:680:SER:O	2:B:683:ASN:N	2.49	0.46
2:B:1002:ILE:HG22	2:B:1003:TYR:N	2.31	0.46
3:C:289:SER:OG	3:C:330:GLY:O	2.16	0.46
8:H:74:CYS:SG	8:H:75:VAL:N	2.88	0.46
11:K:287:ILE:HD13	11:K:297:VAL:HG11	1.97	0.46
22:W:383:ASP:OD1	22:W:383:ASP:N	2.47	0.46
23:X:61:DG:C6	24:Y:-58:DA:N6	2.84	0.46
1:A:229:ARG:O	1:A:229:ARG:CG	2.63	0.46
2:B:40:VAL:O	2:B:40:VAL:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:TYR:CD1	2:B:115:VAL:HG21	2.51	0.46
2:B:371:LEU:HD12	2:B:371:LEU:O	2.16	0.46
3:C:528:GLU:C	3:C:528:GLU:OE1	2.59	0.46
10:J:43:TYR:O	10:J:43:TYR:CG	2.68	0.46
18:R:192:TYR:CG	18:R:200:VAL:HG22	2.50	0.46
19:S:7:CYS:O	19:S:8:PRO:C	2.56	0.46
1:A:921:PHE:CE2	1:A:968:GLU:OE2	2.68	0.46
1:A:941:SER:OG	1:A:944:GLU:OE1	2.34	0.46
5:E:347:GLU:OE2	5:E:349:LEU:HD13	2.15	0.46
5:E:418:ARG:O	5:E:422:LEU:HG	2.15	0.46
10:J:5:CYS:SG	10:J:7:GLY:N	2.87	0.46
1:A:297:ARG:NH1	1:A:306:ILE:HD11	2.30	0.46
2:B:758:ASN:OD1	2:B:758:ASN:C	2.59	0.46
3:C:270:MET:C	3:C:270:MET:SD	2.99	0.46
4:D:268:PHE:CD1	4:D:269:LEU:N	2.84	0.46
8:H:24:ASP:O	8:H:28:GLU:HG3	2.16	0.46
8:H:51:ILE:HD12	8:H:54:LEU:HD11	1.98	0.46
23:X:48:DC:H2"	23:X:49:DA:C8	2.51	0.46
1:A:421:ILE:HG22	1:A:430:ARG:HB2	1.97	0.46
1:A:487:ARG:HG3	1:A:487:ARG:HH11	1.81	0.46
6:F:184:CYS:HB3	6:F:239:LEU:HD11	1.98	0.46
8:H:4:LEU:HD13	8:H:73:ARG:HD2	1.98	0.46
11:K:64:ASP:CB	11:K:306:TYR:O	2.63	0.46
11:K:98:THR:OG1	11:K:207:GLU:N	2.48	0.46
12:L:114:PHE:C	12:L:114:PHE:CD2	2.94	0.46
13:M:3:ASP:OD2	13:M:47:LYS:NZ	2.42	0.46
1:A:178:LYS:HE2	1:A:178:LYS:HA	1.97	0.46
1:A:815:ASN:OD1	1:A:824:HIS:CE1	2.69	0.46
2:B:1044:GLY:C	2:B:1045:LEU:HD22	2.41	0.46
3:C:22:GLU:N	3:C:22:GLU:OE1	2.49	0.46
3:C:261:GLN:O	3:C:264:SER:OG	2.30	0.46
3:C:532:LYS:HE3	3:C:532:LYS:HA	1.98	0.46
1:A:837:SER:O	1:A:840:SER:N	2.48	0.45
2:B:243:MET:HE3	2:B:332:CYS:SG	2.56	0.45
19:S:190:PRO:CG	22:W:155:THR:HG23	2.46	0.45
24:Y:-30:DT:H2"	24:Y:-29:DA:H8	1.81	0.45
1:A:1251:THR:HG23	1:A:1252:TYR:N	2.31	0.45
2:B:121:ARG:HB2	2:B:126:ILE:HG13	1.97	0.45
2:B:148:THR:HG23	2:B:148:THR:O	2.15	0.45
2:B:808:ILE:O	2:B:808:ILE:HD12	2.17	0.45
3:C:109:GLU:O	3:C:113:ASN:OD1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ARG:O	1:A:102:ILE:HG13	2.16	0.45
1:A:351:ARG:HH12	2:B:1032:THR:HG21	1.82	0.45
1:A:394:GLU:C	1:A:394:GLU:OE1	2.59	0.45
1:A:592:VAL:HG12	11:K:33:TYR:CD2	2.51	0.45
1:A:660:LYS:O	1:A:661:ASN:CG	2.60	0.45
1:A:738:GLN:NE2	1:A:742:CYS:O	2.40	0.45
1:A:1191:PHE:O	1:A:1194:GLU:OE2	2.34	0.45
2:B:686:GLN:O	2:B:686:GLN:NE2	2.49	0.45
11:K:195:ASP:OD1	11:K:195:ASP:O	2.34	0.45
21:U:98:ARG:NH2	21:U:140:MET:SD	2.89	0.45
22:W:361:VAL:HG13	22:W:365:ARG:HH11	1.82	0.45
23:X:32:DA:C6	23:X:33:DG:C6	3.05	0.45
2:B:333:ILE:O	2:B:337:VAL:HG12	2.17	0.45
7:G:111:MET:SD	7:G:113:ARG:N	2.89	0.45
8:H:4:LEU:HD23	8:H:74:CYS:O	2.17	0.45
11:K:118:ASP:OD1	11:K:120:ARG:N	2.42	0.45
13:M:173:ILE:HG23	13:M:209:VAL:HA	1.97	0.45
19:S:16:VAL:N	19:S:27:VAL:O	2.45	0.45
19:S:236:SER:CB	19:S:297:ILE:HD11	2.46	0.45
21:U:36:MET:CE	25:Z:127:LEU:HD23	2.46	0.45
24:Y:-18:DG:H1'	24:Y:-17:DA:N7	2.31	0.45
1:A:142:LEU:O	1:A:146:ILE:HG23	2.16	0.45
1:A:977:SER:O	1:A:980:ILE:HG22	2.17	0.45
2:B:974:GLU:O	2:B:977:VAL:HG12	2.17	0.45
3:C:101:ASP:OD1	3:C:105:LEU:HD13	2.16	0.45
8:H:37:LYS:O	8:H:44:LEU:HD12	2.16	0.45
19:S:18:ASP:HB2	19:S:27:VAL:CG2	2.46	0.45
19:S:247:LEU:HB3	19:S:258:LEU:HD22	1.99	0.45
23:X:31:DA:C2'	23:X:32:DA:C8	2.99	0.45
24:Y:-44:DT:H2''	24:Y:-43:DT:C6	2.51	0.45
1:A:8:GLU:HA	1:A:8:GLU:OE1	2.17	0.45
2:B:259:GLU:O	2:B:262:MET:SD	2.74	0.45
2:B:758:ASN:HB2	2:B:916:MET:HE2	1.98	0.45
2:B:760:ALA:O	2:B:763:ASP:N	2.50	0.45
3:C:350:LEU:HD23	3:C:350:LEU:C	2.41	0.45
5:E:192:SER:OG	5:E:194:GLU:OE1	2.33	0.45
5:E:250:MET:HE3	5:E:250:MET:HA	1.98	0.45
5:E:286:MET:N	5:E:286:MET:HE2	2.31	0.45
8:H:39:VAL:HG12	8:H:43:GLY:O	2.17	0.45
15:O:111:ARG:O	15:O:112:LEU:HD22	2.16	0.45
24:Y:-34:DG:H2''	24:Y:-33:DG:O5'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:953:MET:SD	1:A:953:MET:C	3.00	0.45
7:G:89:LYS:HA	7:G:92:MET:SD	2.57	0.45
16:P:35:ARG:NH2	16:P:39:CYS:O	2.49	0.45
2:B:171:VAL:HG12	2:B:172:LYS:HG2	1.98	0.45
2:B:614:LEU:O	2:B:617:GLY:N	2.41	0.45
2:B:912:PRO:HD2	2:B:912:PRO:O	2.17	0.45
2:B:999:GLU:O	2:B:999:GLU:HG3	2.16	0.45
3:C:160:CYS:SG	3:C:234:TYR:HB2	2.57	0.45
3:C:450:ARG:CD	3:C:509:LEU:HD21	2.44	0.45
12:L:129:ASN:HD22	12:L:129:ASN:C	2.24	0.45
19:S:85:LEU:HD11	19:S:89:PHE:CD2	2.52	0.45
22:W:210:LEU:C	22:W:210:LEU:HD23	2.42	0.45
23:X:57:DG:H2'	23:X:58:DT:H71	1.97	0.45
1:A:469:HIS:CE1	1:A:471:LEU:HB2	2.51	0.45
1:A:855:ARG:NH2	2:B:481:PRO:O	2.49	0.45
1:A:1185:MET:HG2	1:A:1187:TYR:H	1.82	0.45
2:B:84:LEU:HB2	2:B:85:PRO:HD2	1.97	0.45
2:B:338:MET:HE2	2:B:338:MET:C	2.42	0.45
3:C:96:LYS:O	3:C:99:TYR:O	2.34	0.45
6:F:213:SER:OG	6:F:267:MET:HE1	2.16	0.45
6:F:253:ILE:N	6:F:267:MET:O	2.36	0.45
11:K:285:ARG:HG3	11:K:285:ARG:HH11	1.82	0.45
13:M:103:LEU:HA	13:M:128:GLU:HG2	1.99	0.45
19:S:18:ASP:HB2	19:S:27:VAL:HG21	1.99	0.45
20:T:317:MET:SD	20:T:362:PHE:CD1	3.10	0.45
25:Z:95:GLU:CD	25:Z:95:GLU:C	2.84	0.45
1:A:219:ASN:H	1:A:222:VAL:CG1	2.30	0.45
1:A:415:HIS:HB3	1:A:416:PRO:CD	2.46	0.45
1:A:454:LEU:HD21	1:A:509:LEU:CD2	2.47	0.45
2:B:139:MET:HE3	2:B:167:GLY:O	2.17	0.45
2:B:926:ASP:O	2:B:927:ILE:HG12	2.17	0.45
3:C:495:GLU:C	3:C:495:GLU:OE1	2.59	0.45
4:D:268:PHE:O	4:D:382:LYS:HA	2.16	0.45
4:D:329:LEU:HD21	5:E:124:LEU:HD21	1.99	0.45
5:E:392:VAL:HG22	5:E:398:TRP:CE2	2.51	0.45
8:H:47:CYS:O	8:H:75:VAL:HG22	2.17	0.45
9:I:109:THR:HG23	9:I:111:GLU:OE1	2.17	0.45
11:K:281:ASP:OD1	11:K:282:THR:N	2.50	0.45
13:M:151:MET:HE3	13:M:155:GLU:HB3	1.97	0.45
19:S:25:GLN:HB3	19:S:34:VAL:HG11	1.97	0.45
19:S:73:LEU:HD22	19:S:97:TYR:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:LEU:O	2:B:41:LYS:N	2.50	0.44
2:B:201:ALA:O	2:B:216:MET:N	2.45	0.44
2:B:413:ASN:O	2:B:417:ASN:OD1	2.35	0.44
3:C:31:THR:O	3:C:31:THR:CG2	2.65	0.44
4:D:157:MET:SD	4:D:157:MET:C	3.00	0.44
4:D:369:ARG:HD2	4:D:369:ARG:O	2.17	0.44
11:K:310:VAL:HG22	11:K:311:GLU:N	2.32	0.44
14:N:51:ARG:HD3	14:N:118:TRP:CH2	2.52	0.44
14:N:88:ASP:OD1	14:N:88:ASP:C	2.60	0.44
20:T:324:MET:HE3	20:T:362:PHE:CZ	2.52	0.44
24:Y:-29:DA:H2'	24:Y:-28:DA:C8	2.52	0.44
1:A:167:LYS:HE2	1:A:167:LYS:HA	1.98	0.44
2:B:270:GLU:OE1	2:B:273:GLN:NE2	2.43	0.44
9:I:91:PRO:HD3	9:I:120:VAL:HG11	2.00	0.44
15:O:123:MET:O	15:O:123:MET:SD	2.74	0.44
19:S:27:VAL:HA	19:S:34:VAL:HA	2.00	0.44
23:X:-11:DC:H1'	23:X:-10:DG:C8	2.52	0.44
1:A:168:LYS:HD3	1:A:168:LYS:N	2.30	0.44
1:A:1187:TYR:C	1:A:1189:LEU:N	2.74	0.44
2:B:285:LYS:O	2:B:289:ASN:ND2	2.49	0.44
2:B:352:ASP:O	2:B:354:ARG:NH2	2.49	0.44
3:C:109:GLU:O	3:C:110:LEU:C	2.58	0.44
17:Q:55:LEU:O	17:Q:58:LYS:N	2.50	0.44
18:R:250:PHE:C	18:R:251:LEU:HD22	2.42	0.44
1:A:392:PHE:HB3	1:A:452:ARG:NH1	2.33	0.44
1:A:587:THR:O	15:O:92:MET:HG3	2.16	0.44
1:A:970:LYS:O	1:A:973:ILE:HG12	2.18	0.44
2:B:236:ILE:CG2	2:B:237:VAL:N	2.80	0.44
5:E:267:VAL:CG1	5:E:268:LEU:N	2.81	0.44
5:E:375:THR:HG23	5:E:377:LEU:HG	2.00	0.44
13:M:193:ILE:HG22	13:M:205:THR:O	2.17	0.44
19:S:34:VAL:C	19:S:36:THR:N	2.75	0.44
1:A:296:HIS:HD2	1:A:306:ILE:HD13	1.82	0.44
3:C:474:MET:O	3:C:474:MET:HE2	2.17	0.44
5:E:369:LYS:HD3	17:Q:26:GLN:OE1	2.16	0.44
11:K:118:ASP:OD1	11:K:118:ASP:C	2.60	0.44
17:Q:48:MET:O	17:Q:48:MET:SD	2.76	0.44
18:R:332:LEU:C	18:R:332:LEU:HD12	2.43	0.44
2:B:75:LEU:HD22	2:B:119:TYR:HA	1.99	0.44
2:B:697:ILE:CD1	2:B:709:MET:HG3	2.47	0.44
2:B:758:ASN:OD1	2:B:760:ALA:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:251:ILE:HG13	3:C:252:VAL:N	2.33	0.44
3:C:338:LEU:O	3:C:342:LEU:HG	2.17	0.44
5:E:64:THR:HG21	5:E:96:LEU:HD13	2.00	0.44
5:E:358:TRP:CD1	5:E:358:TRP:C	2.95	0.44
6:F:310:MET:N	28:F:401:SF4:S4	2.91	0.44
12:L:60:MET:HA	12:L:60:MET:HE2	2.00	0.44
17:Q:14:VAL:O	17:Q:14:VAL:CG1	2.65	0.44
1:A:1043:GLU:N	1:A:1044:PRO:CD	2.81	0.44
2:B:79:ASN:N	2:B:116:ASP:OD1	2.45	0.44
7:G:33:LYS:HD3	7:G:33:LYS:C	2.42	0.44
7:G:60:LEU:HD23	7:G:64:LEU:HD23	1.98	0.44
8:H:184:TYR:CE1	8:H:186:LEU:HD11	2.52	0.44
21:U:53:MET:HE2	21:U:53:MET:N	2.32	0.44
24:Y:2:DG:H1'	24:Y:3:DC:O4'	2.18	0.44
1:A:542:ILE:HG13	1:A:543:GLN:H	1.82	0.44
1:A:750:ALA:O	1:A:753:LEU:HG	2.17	0.44
4:D:273:ASP:OD1	4:D:274:THR:N	2.51	0.44
5:E:193:TYR:O	5:E:196:LEU:HD12	2.18	0.44
9:I:93:THR:HG1	9:I:96:GLU:CD	2.21	0.44
11:K:21:VAL:HG12	11:K:22:ARG:N	2.33	0.44
11:K:286:GLU:CD	11:K:289:ARG:HD3	2.43	0.44
23:X:19:DC:H1'	23:X:20:DA:C8	2.52	0.44
1:A:404:LEU:HD13	1:A:450:VAL:HG22	2.00	0.44
2:B:240:PHE:HE1	2:B:254:MET:SD	2.40	0.44
2:B:380:PHE:HA	2:B:383:GLU:OE2	2.17	0.44
3:C:139:MET:SD	3:C:143:GLU:OE2	2.76	0.44
3:C:285:THR:HG22	3:C:336:ILE:HG22	2.00	0.44
3:C:350:LEU:HD22	3:C:366:PHE:CE1	2.53	0.44
6:F:310:MET:CB	28:F:401:SF4:S4	3.05	0.44
11:K:241:LEU:HD23	11:K:241:LEU:H	1.83	0.44
1:A:318:ALA:HB1	1:A:325:LEU:HD21	1.99	0.43
1:A:533:ARG:HG3	1:A:1040:SER:OG	2.17	0.43
1:A:1278:HIS:ND1	1:A:1278:HIS:C	2.75	0.43
23:X:44:DA:C2	24:Y:42:DG:C2	3.06	0.43
1:A:843:THR:O	1:A:844:PRO:C	2.61	0.43
1:A:1109:LEU:N	1:A:1109:LEU:HD22	2.33	0.43
3:C:490:MET:SD	3:C:490:MET:N	2.90	0.43
8:H:46:ILE:HD12	8:H:46:ILE:N	2.33	0.43
9:I:11:LEU:HD13	9:I:16:VAL:HG13	2.00	0.43
12:L:46:GLU:N	12:L:78:SER:O	2.52	0.43
2:B:625:LEU:HD23	2:B:626:HIS:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:988:TYR:OH	2:B:997:PRO:HB3	2.18	0.43
3:C:425:THR:HG22	3:C:426:VAL:N	2.33	0.43
3:C:523:LEU:C	3:C:523:LEU:HD23	2.42	0.43
18:R:250:PHE:O	18:R:251:LEU:HD22	2.19	0.43
24:Y:-36:DA:H2'	24:Y:-35:DG:C8	2.54	0.43
25:Z:271:SER:O	25:Z:275:ILE:HG12	2.19	0.43
1:A:125:PHE:O	1:A:129:LEU:HD23	2.18	0.43
1:A:196:SER:O	3:C:374:HIS:ND1	2.52	0.43
1:A:405:ARG:HA	1:A:408:VAL:HG12	2.00	0.43
4:D:363:VAL:HG23	4:D:363:VAL:O	2.18	0.43
5:E:78:ALA:HB2	5:E:97:MET:HE1	2.00	0.43
5:E:215:ASP:OD1	5:E:216:SER:N	2.51	0.43
7:G:81:ARG:C	7:G:81:ARG:HD2	2.42	0.43
14:N:94:MET:C	14:N:94:MET:HE2	2.43	0.43
18:R:199:ALA:HB2	18:R:214:PHE:CD2	2.53	0.43
23:X:22:DA:H2''	23:X:23:DC:C6	2.54	0.43
25:Z:49:GLU:OE2	25:Z:52:ARG:NH2	2.40	0.43
1:A:389:ILE:HG12	19:S:21:TYR:CD1	2.53	0.43
2:B:36:VAL:HG13	2:B:37:LYS:HG2	2.00	0.43
2:B:259:GLU:OE2	2:B:259:GLU:CA	2.67	0.43
3:C:163:VAL:HG12	3:C:180:LEU:CD2	2.48	0.43
3:C:259:MET:SD	3:C:260:ASP:HB3	2.58	0.43
3:C:382:ASP:OD1	3:C:382:ASP:N	2.51	0.43
16:P:20:GLY:C	16:P:21:GLU:HG3	2.44	0.43
23:X:39:DC:H2''	23:X:40:DA:C8	2.53	0.43
1:A:576:ASP:OD1	1:A:576:ASP:C	2.60	0.43
2:B:240:PHE:CE1	2:B:254:MET:SD	3.12	0.43
2:B:568:ILE:HG22	2:B:569:ASN:N	2.34	0.43
2:B:625:LEU:HD23	2:B:625:LEU:C	2.43	0.43
2:B:712:LEU:HD22	2:B:715:PRO:HB3	2.00	0.43
2:B:1018:ASP:OD1	2:B:1018:ASP:C	2.61	0.43
5:E:358:TRP:CD1	5:E:358:TRP:O	2.72	0.43
19:S:234:TRP:CD2	19:S:250:PHE:CZ	3.07	0.43
21:U:99:VAL:HG21	21:U:135:PHE:HB3	2.01	0.43
1:A:59:ARG:HB2	1:A:59:ARG:CZ	2.49	0.43
1:A:1069:ARG:O	1:A:1072:GLU:HG2	2.19	0.43
2:B:567:TYR:OH	5:E:250:MET:HB3	2.18	0.43
2:B:1113:LEU:HG	2:B:1117:LEU:CD2	2.49	0.43
25:Z:340:TYR:HA	25:Z:341:PRO:C	2.44	0.43
1:A:168:LYS:H	1:A:168:LYS:CD	2.31	0.43
1:A:328:ILE:HD12	1:A:328:ILE:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1188:VAL:HG22	1:A:1191:PHE:HD2	1.84	0.43
2:B:379:LYS:O	2:B:383:GLU:HG3	2.19	0.43
2:B:407:ARG:HA	2:B:407:ARG:NE	2.33	0.43
2:B:599:VAL:HG21	2:B:650:ILE:HD11	1.99	0.43
3:C:362:CYS:SG	3:C:394:MET:HE3	2.58	0.43
3:C:408:GLU:CD	3:C:408:GLU:O	2.62	0.43
4:D:327:GLY:O	5:E:15:VAL:N	2.52	0.43
19:S:358:LEU:HB3	19:S:359:PRO:HD2	2.00	0.43
21:U:84:GLY:HA2	25:Z:109:LEU:HD13	2.00	0.43
23:X:52:DT:H2''	23:X:53:DT:C7	2.48	0.43
25:Z:82:GLU:O	25:Z:86:VAL:HG23	2.19	0.43
1:A:748:LEU:O	1:A:752:ILE:HG12	2.19	0.43
2:B:88:GLU:OE2	2:B:88:GLU:HA	2.18	0.43
2:B:755:LEU:HD12	2:B:755:LEU:C	2.44	0.43
2:B:946:LEU:HD11	2:B:1005:GLY:CA	2.49	0.43
3:C:139:MET:HA	3:C:139:MET:HE2	2.01	0.43
5:E:412:HIS:O	5:E:412:HIS:ND1	2.48	0.43
6:F:198:SER:O	6:F:200:GLN:NE2	2.43	0.43
6:F:309:TYR:CE1	7:G:38:PHE:HB3	2.54	0.43
20:T:295:ARG:NH1	23:X:36:DC:O4'	2.51	0.43
24:Y:-20:DG:H2''	24:Y:-19:DT:C6	2.54	0.43
25:Z:155:PHE:CE2	25:Z:159:MET:HE2	2.54	0.43
2:B:541:LEU:HD23	2:B:546:LEU:HD11	2.00	0.43
2:B:580:ASP:C	2:B:581:ARG:HD3	2.44	0.43
2:B:673:PRO:HG3	2:B:945:GLU:OE1	2.19	0.43
2:B:863:ASP:OD1	2:B:863:ASP:C	2.62	0.43
2:B:911:VAL:HG13	2:B:911:VAL:O	2.19	0.43
6:F:21:ARG:NH1	6:F:24:GLU:OE1	2.41	0.43
6:F:310:MET:HB2	28:F:401:SF4:S1	2.59	0.43
13:M:34:ASP:C	13:M:34:ASP:OD1	2.61	0.43
21:U:105:ASP:HB3	25:Z:54:ARG:HE	1.84	0.43
1:A:174:ILE:HD12	1:A:175:ILE:H	1.84	0.42
1:A:394:GLU:CD	1:A:395:LYS:N	2.77	0.42
1:A:414:VAL:HG12	1:A:416:PRO:HD2	2.01	0.42
1:A:650:MET:SD	1:A:654:THR:HG21	2.59	0.42
1:A:953:MET:SD	1:A:954:LYS:N	2.92	0.42
1:A:1033:VAL:HG12	1:A:1289:LEU:CD2	2.49	0.42
2:B:541:LEU:HD12	2:B:541:LEU:C	2.44	0.42
2:B:751:ILE:HD13	2:B:751:ILE:HA	1.95	0.42
3:C:287:PRO:HB2	3:C:333:MET:SD	2.59	0.42
11:K:330:MET:HE1	12:L:108:GLN:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:24:LYS:C	12:L:24:LYS:HD2	2.44	0.42
12:L:124:GLN:HB3	12:L:128:ARG:HD3	2.00	0.42
20:T:372:GLN:CD	20:T:372:GLN:N	2.77	0.42
23:X:16:DT:H2''	23:X:17:DG:N7	2.34	0.42
1:A:780:MET:SD	2:B:935:PRO:HG3	2.59	0.42
1:A:1048:MET:SD	1:A:1066:GLY:HA2	2.59	0.42
1:A:1050:LEU:H	1:A:1278:HIS:CD2	2.37	0.42
1:A:1069:ARG:HA	1:A:1072:GLU:HG2	2.01	0.42
2:B:423:ASN:OD1	2:B:423:ASN:O	2.36	0.42
6:F:144:ALA:C	6:F:145:SER:HG	2.27	0.42
9:I:91:PRO:HD2	9:I:91:PRO:O	2.19	0.42
13:M:127:LEU:O	13:M:128:GLU:C	2.62	0.42
15:O:40:ILE:HG23	15:O:40:ILE:O	2.18	0.42
19:S:26:LEU:N	19:S:34:VAL:HG13	2.34	0.42
23:X:24:DC:H2'	23:X:25:DT:C6	2.54	0.42
1:A:308:GLU:O	1:A:312:PHE:CD1	2.72	0.42
1:A:394:GLU:OE1	1:A:395:LYS:N	2.52	0.42
2:B:226:ARG:C	2:B:226:ARG:HD2	2.44	0.42
2:B:234:ILE:HD12	2:B:235:PRO:HD2	2.01	0.42
2:B:1046:ARG:HG3	2:B:1047:LEU:N	2.33	0.42
9:I:42:LEU:HA	9:I:45:ILE:HG22	2.01	0.42
13:M:10:LEU:HA	13:M:13:ILE:HG22	2.01	0.42
2:B:206:SER:HA	2:B:210:LYS:O	2.19	0.42
2:B:404:LYS:HE3	19:S:141:LEU:HD23	2.01	0.42
2:B:511:ILE:HD12	2:B:572:VAL:HG11	2.00	0.42
4:D:373:MET:SD	4:D:373:MET:C	3.02	0.42
9:I:45:ILE:HG23	9:I:46:THR:N	2.34	0.42
11:K:51:VAL:HG13	12:L:117:SER:OG	2.19	0.42
11:K:197:ILE:HD13	17:Q:16:ASN:HB3	2.01	0.42
19:S:17:GLU:OE1	19:S:25:GLN:N	2.51	0.42
25:Z:192:PHE:O	25:Z:193:HIS:CG	2.73	0.42
2:B:80:ILE:HD12	2:B:114:THR:O	2.19	0.42
2:B:243:MET:SD	2:B:313:LEU:HD21	2.59	0.42
2:B:508:ASP:OD1	2:B:508:ASP:C	2.62	0.42
2:B:719:MET:HE2	2:B:738:ASN:ND2	2.34	0.42
2:B:1021:HIS:ND1	2:B:1021:HIS:C	2.78	0.42
2:B:1023:ARG:CZ	2:B:1026:GLY:H	2.32	0.42
3:C:110:LEU:HD13	3:C:237:ALA:N	2.35	0.42
3:C:117:THR:O	3:C:121:VAL:HG12	2.20	0.42
11:K:118:ASP:OD1	11:K:119:PRO:N	2.52	0.42
1:A:13:LYS:HB3	2:B:1128:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:GLU:OE2	2:B:1060:ALA:HB1	2.19	0.42
1:A:519:ALA:O	1:A:523:MET:HB2	2.19	0.42
1:A:629:GLU:O	1:A:630:ASP:HB2	2.20	0.42
1:A:996:GLU:O	1:A:998:ARG:N	2.53	0.42
1:A:1234:ALA:O	1:A:1237:ALA:HB3	2.19	0.42
2:B:357:TYR:CE2	2:B:479:LEU:HD11	2.54	0.42
2:B:380:PHE:CD1	2:B:383:GLU:OE2	2.72	0.42
2:B:993:ILE:N	2:B:993:ILE:HD13	2.34	0.42
5:E:366:VAL:O	5:E:366:VAL:CG1	2.67	0.42
6:F:175:GLU:O	6:F:178:GLU:HG2	2.20	0.42
11:K:142:LEU:HD23	11:K:142:LEU:C	2.44	0.42
12:L:129:ASN:C	12:L:129:ASN:ND2	2.78	0.42
17:Q:55:LEU:O	17:Q:59:LEU:HD22	2.19	0.42
18:R:197:PHE:CE2	18:R:199:ALA:HB3	2.55	0.42
21:U:36:MET:HE2	21:U:38:PHE:CD2	2.54	0.42
21:U:100:ALA:HA	21:U:138:THR:O	2.20	0.42
23:X:58:DT:H2'	23:X:59:DT:C7	2.49	0.42
25:Z:125:THR:HG21	25:Z:130:LEU:HD12	2.01	0.42
1:A:1149:VAL:HG23	1:A:1150:ARG:N	2.35	0.42
2:B:392:ILE:CG2	2:B:393:PRO:HD3	2.49	0.42
2:B:523:VAL:HG13	2:B:547:GLY:HA2	2.01	0.42
3:C:259:MET:HE3	3:C:263:SER:HB3	2.01	0.42
11:K:190:ILE:HD12	11:K:190:ILE:H	1.84	0.42
13:M:166:ARG:O	13:M:168:ASN:N	2.52	0.42
18:R:252:ASP:OD1	18:R:252:ASP:O	2.38	0.42
24:Y:7:DC:C2'	24:Y:8:DT:H71	2.49	0.42
25:Z:62:SER:OG	25:Z:64:ARG:NE	2.53	0.42
1:A:550:TYR:OH	1:A:782:LEU:HD22	2.20	0.42
1:A:1317:MET:SD	1:A:1318:LEU:HG	2.59	0.42
2:B:119:TYR:CE2	2:B:126:ILE:HG21	2.55	0.42
2:B:423:ASN:OD1	2:B:423:ASN:C	2.63	0.42
2:B:873:SER:CB	16:P:34:ILE:HD11	2.50	0.42
2:B:892:GLU:O	2:B:895:ASP:OD1	2.37	0.42
11:K:115:ILE:HG22	11:K:117:ALA:H	1.84	0.42
11:K:210:LEU:C	11:K:210:LEU:HD12	2.45	0.42
18:R:197:PHE:CD1	23:X:25:DT:H2''	2.55	0.42
22:W:194:LYS:O	22:W:197:VAL:HG22	2.20	0.42
22:W:334:LEU:HD12	22:W:337:PHE:HD2	1.84	0.42
24:Y:-17:DA:H2''	24:Y:-16:DC:O4'	2.20	0.42
1:A:121:GLU:O	1:A:125:PHE:CD1	2.72	0.42
1:A:367:THR:CG2	1:A:368:VAL:H	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:694:ARG:O	2:B:999:GLU:HB3	2.20	0.42
1:A:1020:ASP:OD1	1:A:1020:ASP:C	2.62	0.42
2:B:74:TYR:O	2:B:75:LEU:HD23	2.19	0.42
2:B:93:VAL:HG22	2:B:94:THR:H	1.84	0.42
2:B:140:LEU:O	2:B:141:ARG:HB2	2.20	0.42
2:B:758:ASN:O	2:B:762:LEU:CD2	2.68	0.42
3:C:133:MET:SD	3:C:133:MET:N	2.93	0.42
4:D:119:LYS:HG2	4:D:123:TRP:CD1	2.54	0.42
5:E:103:CYS:SG	5:E:104:SER:N	2.90	0.42
13:M:21:CYS:HB3	13:M:61:LEU:HD12	2.02	0.42
13:M:57:ASP:C	13:M:58:LEU:HD22	2.45	0.42
13:M:89:VAL:O	13:M:92:GLN:HG3	2.19	0.42
13:M:102:ALA:O	13:M:127:LEU:HA	2.20	0.42
13:M:127:LEU:HD12	13:M:127:LEU:N	2.35	0.42
13:M:181:ARG:HH11	13:M:181:ARG:HG2	1.84	0.42
18:R:233:ALA:O	18:R:237:TYR:CD2	2.72	0.42
19:S:26:LEU:O	19:S:34:VAL:C	2.63	0.42
19:S:31:CYS:C	19:S:33:CYS:N	2.78	0.42
19:S:309:ARG:HA	19:S:312:PHE:CE2	2.54	0.42
23:X:38:DT:H2"	23:X:39:DC:C6	2.55	0.42
1:A:816:ARG:NH2	2:B:641:CYS:O	2.48	0.42
1:A:1213:HIS:O	1:A:1224:LYS:N	2.45	0.42
2:B:392:ILE:HG22	2:B:393:PRO:HD3	2.00	0.42
3:C:270:MET:HG2	3:C:288:LEU:HD13	2.02	0.42
3:C:288:LEU:HD12	3:C:288:LEU:H	1.84	0.42
5:E:258:LYS:HE2	5:E:258:LYS:HA	2.02	0.42
14:N:83:LEU:HD12	14:N:83:LEU:C	2.45	0.42
14:N:83:LEU:HD12	14:N:85:GLY:N	2.34	0.42
16:P:27:GLU:O	16:P:27:GLU:HG3	2.20	0.42
21:U:127:ARG:NH2	25:Z:89:ASP:OD2	2.50	0.42
25:Z:132:VAL:HG12	25:Z:136:PHE:CZ	2.54	0.42
2:B:750:ASP:OD1	2:B:750:ASP:N	2.53	0.41
3:C:61:ASN:O	3:C:61:ASN:ND2	2.52	0.41
5:E:289:VAL:HG11	5:E:292:MET:HE2	2.02	0.41
5:E:308:VAL:HG13	5:E:309:ALA:N	2.35	0.41
5:E:351:ARG:HG2	5:E:430:LEU:HD11	2.01	0.41
6:F:303:SER:O	6:F:307:CYS:N	2.46	0.41
8:H:7:MET:HB2	8:H:72:PHE:CZ	2.54	0.41
13:M:18:MET:HE3	13:M:33:LEU:HD23	2.02	0.41
15:O:123:MET:SD	15:O:123:MET:C	3.03	0.41
19:S:117:LEU:HA	19:S:120:CYS:SG	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:THR:CG2	1:A:368:VAL:N	2.82	0.41
1:A:1314:SER:HB3	1:A:1345:GLU:OE2	2.20	0.41
2:B:93:VAL:HG22	2:B:94:THR:N	2.36	0.41
2:B:672:ILE:HG12	2:B:686:GLN:HG2	2.02	0.41
2:B:1026:GLY:HA2	19:S:23:GLN:HA	2.03	0.41
4:D:349:THR:O	4:D:384:VAL:N	2.43	0.41
1:A:18:ILE:O	1:A:1338:ASP:N	2.53	0.41
1:A:945:LEU:C	1:A:945:LEU:HD23	2.44	0.41
2:B:63:GLU:OE1	2:B:63:GLU:N	2.53	0.41
2:B:600:LYS:HE3	2:B:600:LYS:HA	2.02	0.41
2:B:661:PRO:O	2:B:664:LEU:HD13	2.19	0.41
2:B:699:TYR:HA	17:Q:59:LEU:CD1	2.50	0.41
2:B:1018:ASP:OD1	2:B:1018:ASP:O	2.38	0.41
3:C:110:LEU:HD11	3:C:157:VAL:CG2	2.50	0.41
3:C:448:GLU:C	3:C:448:GLU:CD	2.87	0.41
4:D:269:LEU:CD1	4:D:271:LEU:HD11	2.48	0.41
9:I:102:GLU:HG3	9:I:103:GLU:OE1	2.21	0.41
11:K:207:GLU:CD	11:K:207:GLU:C	2.88	0.41
11:K:210:LEU:HD12	11:K:210:LEU:O	2.20	0.41
13:M:108:GLN:O	13:M:108:GLN:CG	2.68	0.41
23:X:35:DC:H2'	23:X:36:DC:C6	2.56	0.41
1:A:234:ASP:HA	1:A:237:LEU:CD1	2.50	0.41
1:A:1230:ASP:O	1:A:1230:ASP:CG	2.63	0.41
1:A:1314:SER:O	1:A:1318:LEU:HG	2.20	0.41
2:B:248:ASP:OD2	10:J:11:GLY:N	2.46	0.41
2:B:616:GLN:HA	2:B:616:GLN:OE1	2.21	0.41
13:M:108:GLN:O	13:M:108:GLN:CD	2.63	0.41
18:R:231:ARG:NH1	19:S:381:ASP:OD1	2.51	0.41
19:S:301:LEU:C	19:S:301:LEU:HD12	2.45	0.41
22:W:232:GLU:O	22:W:236:ARG:HG2	2.20	0.41
1:A:361:VAL:HG22	1:A:362:ASP:N	2.34	0.41
4:D:346:LEU:HD21	4:D:385:CYS:HB3	2.01	0.41
5:E:268:LEU:HD22	5:E:268:LEU:H	1.85	0.41
19:S:135:MET:HA	19:S:138:ILE:HD12	2.03	0.41
21:U:17:ARG:HD2	21:U:32:LEU:HD22	2.02	0.41
22:W:374:ARG:O	25:Z:409:THR:HG23	2.21	0.41
1:A:719:ALA:O	1:A:722:LYS:HG2	2.21	0.41
1:A:1348:ILE:HD13	1:A:1348:ILE:HA	1.94	0.41
2:B:634:ASP:OD1	2:B:635:VAL:N	2.54	0.41
2:B:719:MET:HG2	2:B:953:VAL:HG23	2.02	0.41
2:B:781:ARG:NH1	19:S:129:HIS:NE2	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:246:PHE:HB2	3:C:521:PHE:CZ	2.55	0.41
3:C:453:GLU:O	3:C:457:ASN:ND2	2.39	0.41
6:F:195:ALA:O	6:F:205:GLN:NE2	2.51	0.41
13:M:30:GLN:HA	13:M:33:LEU:HD12	2.02	0.41
15:O:95:LYS:HE3	15:O:140:ARG:CZ	2.51	0.41
18:R:257:ASN:HB2	24:Y:-27:DA:O4'	2.21	0.41
20:T:333:ALA:HB3	20:T:336:GLU:OE1	2.21	0.41
20:T:336:GLU:OE1	20:T:336:GLU:N	2.48	0.41
21:U:63:TRP:CH2	21:U:99:VAL:HG22	2.56	0.41
21:U:70:TYR:HB3	21:U:74:ILE:HG23	2.03	0.41
1:A:144:LYS:HG2	1:A:145:LYS:N	2.36	0.41
4:D:376:LEU:N	4:D:376:LEU:HD22	2.35	0.41
8:H:130:GLU:HA	8:H:137:ALA:HA	2.02	0.41
17:Q:24:LEU:HD12	17:Q:29:TYR:CE2	2.56	0.41
18:R:214:PHE:CE2	24:Y:-24:DA:H1'	2.56	0.41
19:S:313:ARG:N	19:S:355:ALA:O	2.46	0.41
23:X:22:DA:C2	24:Y:-20:DG:N2	2.89	0.41
1:A:737:GLN:O	1:A:737:GLN:HG2	2.20	0.41
1:A:1316:LEU:HB2	1:A:1345:GLU:OE1	2.20	0.41
2:B:75:LEU:HD23	2:B:75:LEU:N	2.36	0.41
3:C:325:LYS:HD2	3:C:334:TYR:CE1	2.56	0.41
3:C:350:LEU:O	3:C:353:VAL:HG12	2.21	0.41
3:C:394:MET:SD	3:C:397:LYS:HE3	2.61	0.41
4:D:140:ILE:N	4:D:140:ILE:HD12	2.35	0.41
11:K:97:ASN:O	16:P:48:ARG:CZ	2.69	0.41
14:N:119:GLY:O	14:N:122:GLU:N	2.44	0.41
18:R:295:MET:HE3	18:R:302:LEU:CD1	2.51	0.41
19:S:8:PRO:HG3	19:S:36:THR:HG21	2.03	0.41
22:W:284:TRP:HA	22:W:288:GLU:HB3	2.02	0.41
25:Z:75:GLN:OE1	25:Z:101:ARG:NH1	2.52	0.41
1:A:355:ASN:OD1	2:B:1034:GLN:HG3	2.20	0.41
1:A:496:TYR:O	1:A:497:ASN:HB2	2.21	0.41
1:A:795:MET:HE3	1:A:795:MET:HB2	2.01	0.41
1:A:926:ASP:OD1	1:A:926:ASP:N	2.54	0.41
2:B:172:LYS:HD2	2:B:172:LYS:H	1.85	0.41
2:B:229:THR:O	2:B:229:THR:HG22	2.21	0.41
2:B:719:MET:HE1	17:Q:51:ALA:HB2	2.02	0.41
2:B:719:MET:HE3	2:B:953:VAL:CG2	2.51	0.41
2:B:785:GLN:O	2:B:786:THR:OG1	2.29	0.41
3:C:357:ARG:HD2	6:F:289:LEU:HD13	2.03	0.41
3:C:384:ALA:O	3:C:385:MET:SD	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:460:LEU:HD12	3:C:460:LEU:N	2.36	0.41
4:D:318:LEU:HD23	4:D:318:LEU:C	2.46	0.41
7:G:34:PRO:HA	7:G:35:PRO:HD3	1.92	0.41
7:G:71:MET:SD	7:G:72:PRO:HD2	2.61	0.41
7:G:101:PRO:HG2	7:G:110:MET:HE1	2.02	0.41
8:H:128:VAL:O	8:H:128:VAL:HG23	2.20	0.41
11:K:44:ARG:C	11:K:44:ARG:CD	2.94	0.41
11:K:236:LEU:HD22	11:K:305:HIS:CE1	2.56	0.41
12:L:73:THR:HG23	12:L:74:HIS:N	2.35	0.41
13:M:63:ALA:N	13:M:70:ASP:O	2.48	0.41
13:M:106:VAL:HG21	13:M:109:GLY:O	2.20	0.41
13:M:121:MET:CG	13:M:122:ALA:N	2.83	0.41
13:M:163:TYR:HB2	13:M:165:LEU:HD13	2.02	0.41
15:O:5:LEU:HD21	15:O:62:SER:OG	2.20	0.41
18:R:258:MET:HE3	18:R:317:VAL:C	2.46	0.41
19:S:8:PRO:HD3	19:S:36:THR:HG21	2.03	0.41
19:S:33:CYS:SG	19:S:36:THR:HG23	2.61	0.41
21:U:107:VAL:HG12	21:U:126:PHE:CZ	2.55	0.41
21:U:127:ARG:NE	25:Z:89:ASP:OD2	2.47	0.41
22:W:197:VAL:HG11	22:W:250:GLU:CG	2.51	0.41
22:W:380:GLU:HA	25:Z:360:TYR:CE1	2.56	0.41
24:Y:-29:DA:C6	24:Y:-28:DA:N6	2.88	0.41
24:Y:-24:DA:H2'	24:Y:-23:DG:C8	2.55	0.41
2:B:646:TYR:O	2:B:647:GLU:C	2.64	0.41
2:B:823:ASN:OD1	2:B:824:LYS:HG2	2.21	0.41
2:B:1079:VAL:O	2:B:1101:VAL:HA	2.20	0.41
3:C:439:CYS:CB	3:C:520:ILE:HD11	2.51	0.41
3:C:492:THR:HA	3:C:495:GLU:HB3	2.03	0.41
5:E:30:TYR:HB2	5:E:33:ARG:HB3	2.03	0.41
5:E:285:LEU:C	5:E:286:MET:HE2	2.46	0.41
6:F:145:SER:OG	6:F:146:LYS:N	2.52	0.41
8:H:87:GLY:O	8:H:148:ILE:N	2.52	0.41
10:J:21:HIS:O	10:J:34:ILE:HG12	2.21	0.41
12:L:67:PHE:CD1	12:L:67:PHE:C	2.99	0.41
13:M:31:ASP:N	13:M:31:ASP:OD1	2.54	0.41
13:M:129:GLN:C	13:M:129:GLN:CD	2.88	0.41
19:S:74:ARG:HG2	19:S:77:ARG:HH12	1.85	0.41
19:S:88:THR:O	19:S:92:THR:HG22	2.20	0.41
21:U:1:MET:SD	21:U:1:MET:C	3.04	0.41
22:W:383:ASP:HB3	25:Z:359:MET:O	2.21	0.41
1:A:234:ASP:HA	1:A:237:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:ILE:HG21	1:A:505:MET:CG	2.50	0.40
1:A:967:GLN:OE1	1:A:971:LYS:HG3	2.21	0.40
1:A:1237:ALA:HB2	13:M:133:GLN:HE21	1.86	0.40
2:B:66:THR:HG22	2:B:67:SER:N	2.36	0.40
8:H:11:VAL:HG12	8:H:12:ARG:N	2.36	0.40
9:I:92:VAL:HG13	9:I:93:THR:CG2	2.49	0.40
12:L:98:ARG:HA	12:L:98:ARG:NE	2.36	0.40
19:S:6:ARG:NE	19:S:12:SER:O	2.52	0.40
19:S:83:LEU:HB2	19:S:85:LEU:HD22	2.03	0.40
19:S:94:VAL:O	19:S:98:GLN:OE1	2.38	0.40
19:S:94:VAL:O	19:S:98:GLN:HG2	2.21	0.40
19:S:204:THR:O	19:S:208:VAL:HG13	2.21	0.40
22:W:352:GLU:OE1	22:W:352:GLU:N	2.53	0.40
23:X:32:DA:C2'	23:X:33:DG:O5'	2.69	0.40
24:Y:-51:DA:H4'	24:Y:-50:DG:OP1	2.20	0.40
1:A:59:ARG:O	1:A:71:THR:OG1	2.32	0.40
2:B:594:ARG:NH2	2:B:658:GLU:OE2	2.52	0.40
3:C:111:LEU:HD12	3:C:111:LEU:N	2.35	0.40
3:C:259:MET:HE1	3:C:262:THR:OG1	2.21	0.40
3:C:312:LEU:HB3	3:C:334:TYR:CZ	2.57	0.40
3:C:439:CYS:HB3	3:C:520:ILE:HD11	2.03	0.40
5:E:105:SER:O	5:E:133:LEU:HD13	2.20	0.40
6:F:56:ARG:NE	6:F:56:ARG:HA	2.37	0.40
8:H:185:THR:C	8:H:186:LEU:HD13	2.47	0.40
12:L:129:ASN:ND2	12:L:129:ASN:O	2.45	0.40
13:M:120:ASP:OD1	13:M:120:ASP:C	2.63	0.40
19:S:16:VAL:CG1	19:S:17:GLU:N	2.85	0.40
19:S:16:VAL:HG12	19:S:17:GLU:N	2.36	0.40
1:A:238:LEU:HD22	1:A:238:LEU:N	2.36	0.40
2:B:786:THR:HG22	2:B:787:PHE:N	2.36	0.40
5:E:413:PRO:O	5:E:416:VAL:HG12	2.21	0.40
7:G:68:MET:C	7:G:68:MET:SD	3.05	0.40
11:K:3:ALA:O	11:K:7:VAL:HG23	2.21	0.40
11:K:24:VAL:HG23	11:K:25:HIS:N	2.36	0.40
11:K:69:ASP:OD1	11:K:70:ALA:N	2.45	0.40
11:K:188:GLY:O	11:K:191:ARG:NE	2.54	0.40
13:M:82:VAL:HG23	13:M:106:VAL:HG23	2.03	0.40
14:N:114:SER:OG	14:N:115:TYR:N	2.54	0.40
19:S:110:ARG:HH22	24:Y:-20:DG:H21	1.68	0.40
21:U:29:PHE:CD1	21:U:80:TYR:HB3	2.56	0.40
21:U:83:TYR:CD2	25:Z:109:LEU:HD11	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:219:ILE:HG22	25:Z:221:CYS:H	1.87	0.40
1:A:902:TYR:CD1	1:A:903:GLY:N	2.90	0.40
1:A:924:VAL:O	1:A:928:ILE:HG22	2.21	0.40
1:A:973:ILE:HA	1:A:976:VAL:CG1	2.51	0.40
1:A:1304:THR:O	1:A:1308:LEU:HD23	2.22	0.40
2:B:934:PHE:N	2:B:935:PRO:HD2	2.37	0.40
4:D:341:LEU:HG	5:E:238:LEU:HD23	2.02	0.40
6:F:307:CYS:O	6:F:310:MET:HB3	2.21	0.40
11:K:44:ARG:HD2	11:K:44:ARG:O	2.22	0.40
11:K:190:ILE:HD12	11:K:190:ILE:N	2.35	0.40
15:O:137:VAL:O	15:O:138:ASP:CG	2.65	0.40
17:Q:56:ILE:HG13	17:Q:57:GLU:N	2.35	0.40
19:S:190:PRO:HG2	22:W:155:THR:HG23	2.02	0.40
1:A:262:ILE:HD13	2:B:1112:LEU:CD1	2.52	0.40
1:A:283:LEU:HD23	1:A:283:LEU:C	2.44	0.40
1:A:1194:GLU:C	1:A:1194:GLU:CD	2.89	0.40
2:B:385:LYS:HA	2:B:385:LYS:HE2	2.02	0.40
3:C:123:LYS:O	3:C:127:ASP:OD1	2.40	0.40
3:C:516:VAL:HG13	3:C:517:ASP:N	2.37	0.40
7:G:42:ASP:OD1	7:G:42:ASP:N	2.55	0.40
7:G:68:MET:HE2	7:G:68:MET:O	2.21	0.40
9:I:11:LEU:CD1	9:I:16:VAL:HG13	2.51	0.40
9:I:102:GLU:C	9:I:103:GLU:OE1	2.65	0.40
13:M:13:ILE:O	13:M:17:ILE:HG22	2.22	0.40
22:W:185:LYS:NZ	22:W:188:GLU:OE2	2.48	0.40
25:Z:287:LYS:HD2	25:Z:287:LYS:C	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1377/1390 (99%)	1300 (94%)	76 (6%)	1 (0%)	48	81
2	B	1091/1133 (96%)	1030 (94%)	60 (6%)	1 (0%)	48	81
3	C	508/534 (95%)	481 (95%)	27 (5%)	0	100	100
4	D	168/398 (42%)	152 (90%)	16 (10%)	0	100	100
5	E	396/708 (56%)	375 (95%)	21 (5%)	0	100	100
6	F	301/316 (95%)	290 (96%)	11 (4%)	0	100	100
7	G	80/223 (36%)	71 (89%)	9 (11%)	0	100	100
8	H	185/204 (91%)	174 (94%)	11 (6%)	0	100	100
9	I	122/148 (82%)	117 (96%)	5 (4%)	0	100	100
10	J	54/108 (50%)	50 (93%)	4 (7%)	0	100	100
11	K	341/346 (99%)	326 (96%)	15 (4%)	0	100	100
12	L	105/133 (79%)	98 (93%)	7 (7%)	0	100	100
13	M	207/210 (99%)	193 (93%)	14 (7%)	0	100	100
14	N	76/127 (60%)	73 (96%)	3 (4%)	0	100	100
15	O	146/150 (97%)	137 (94%)	9 (6%)	0	100	100
16	P	44/58 (76%)	37 (84%)	7 (16%)	0	100	100
17	Q	64/67 (96%)	62 (97%)	1 (2%)	1 (2%)	7	37
18	R	176/200 (88%)	173 (98%)	3 (2%)	0	100	100
19	S	353/419 (84%)	323 (92%)	26 (7%)	4 (1%)	11	44
20	T	95/484 (20%)	94 (99%)	1 (1%)	0	100	100
21	U	139/368 (38%)	138 (99%)	1 (1%)	0	100	100
22	W	240/1519 (16%)	235 (98%)	5 (2%)	0	100	100
25	Z	383/411 (93%)	370 (97%)	13 (3%)	0	100	100
All	All	6651/9654 (69%)	6299 (95%)	345 (5%)	7 (0%)	49	81

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	S	65	VAL
1	A	185	VAL
17	Q	10	CYS
19	S	45	SER
2	B	40	VAL
19	S	365	SER
19	S	35	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1204/1212 (99%)	1190 (99%)	14 (1%)	63	73
2	B	959/988 (97%)	952 (99%)	7 (1%)	76	79
3	C	458/476 (96%)	456 (100%)	2 (0%)	84	83
4	D	155/347 (45%)	154 (99%)	1 (1%)	78	80
5	E	358/622 (58%)	357 (100%)	1 (0%)	86	84
6	F	269/280 (96%)	267 (99%)	2 (1%)	76	79
7	G	79/195 (40%)	79 (100%)	0	100	100
8	H	168/181 (93%)	166 (99%)	2 (1%)	63	73
9	I	116/136 (85%)	116 (100%)	0	100	100
10	J	49/94 (52%)	49 (100%)	0	100	100
11	K	299/302 (99%)	299 (100%)	0	100	100
12	L	96/119 (81%)	95 (99%)	1 (1%)	68	76
13	M	191/192 (100%)	190 (100%)	1 (0%)	81	81
14	N	68/111 (61%)	67 (98%)	1 (2%)	57	70
15	O	129/131 (98%)	129 (100%)	0	100	100
16	P	43/55 (78%)	42 (98%)	1 (2%)	44	63
17	Q	55/56 (98%)	55 (100%)	0	100	100
18	R	152/172 (88%)	151 (99%)	1 (1%)	76	79
19	S	318/365 (87%)	318 (100%)	0	100	100
20	T	88/440 (20%)	88 (100%)	0	100	100
21	U	124/334 (37%)	124 (100%)	0	100	100
22	W	215/1250 (17%)	215 (100%)	0	100	100
25	Z	340/356 (96%)	338 (99%)	2 (1%)	78	80
All	All	5933/8414 (70%)	5897 (99%)	36 (1%)	76	80

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	137	LEU
1	A	290	ASN
1	A	450	VAL
1	A	514	GLU
1	A	536	GLU
1	A	761	ASP
1	A	790	ILE
1	A	831	LYS
1	A	1061	MET
1	A	1109	LEU
1	A	1189	LEU
1	A	1268	ILE
1	A	1277	ASN
2	B	28	ARG
2	B	320	HIS
2	B	618	TYR
2	B	796	ASP
2	B	866	ILE
2	B	1055	LEU
2	B	1117	LEU
3	C	153	ASP
3	C	288	LEU
4	D	137	ILE
5	E	422	LEU
6	F	42	MET
6	F	309	TYR
8	H	80	PHE
8	H	149	ARG
12	L	129	ASN
13	M	143	GLU
14	N	88	ASP
16	P	52	LEU
18	R	258	MET
25	Z	151	ARG
25	Z	287	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	599	GLN
1	A	824	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1168	HIS
1	A	1239	HIS
1	A	1382	ASN
2	B	208	HIS
2	B	253	GLN
2	B	260	HIS
2	B	395	GLN
2	B	405	HIS
2	B	413	ASN
2	B	458	GLN
2	B	626	HIS
2	B	636	ASN
2	B	979	HIS
2	B	982	ASN
2	B	1014	HIS
2	B	1100	HIS
2	B	1121	ASN
3	C	113	ASN
3	C	245	HIS
3	C	257	ASN
4	D	122	ASN
4	D	270	GLN
4	D	381	HIS
5	E	29	GLN
5	E	76	GLN
6	F	27	HIS
6	F	90	ASN
6	F	240	ASN
9	I	61	GLN
10	J	26	ASN
11	K	96	ASN
11	K	108	HIS
12	L	38	HIS
12	L	105	ASN
13	M	22	HIS
17	Q	26	GLN
18	R	164	GLN
18	R	166	GLN
19	S	303	HIS
25	Z	139	HIS
25	Z	170	ASN
25	Z	195	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	Z	331	HIS
25	Z	368	ASN
25	Z	411	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 11 ligands modelled in this entry, 10 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	$\# Z > 2$
28	SF4	F	401	3,6	0,12,12	-	-	-		

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
28	SF4	F	401	3,6	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

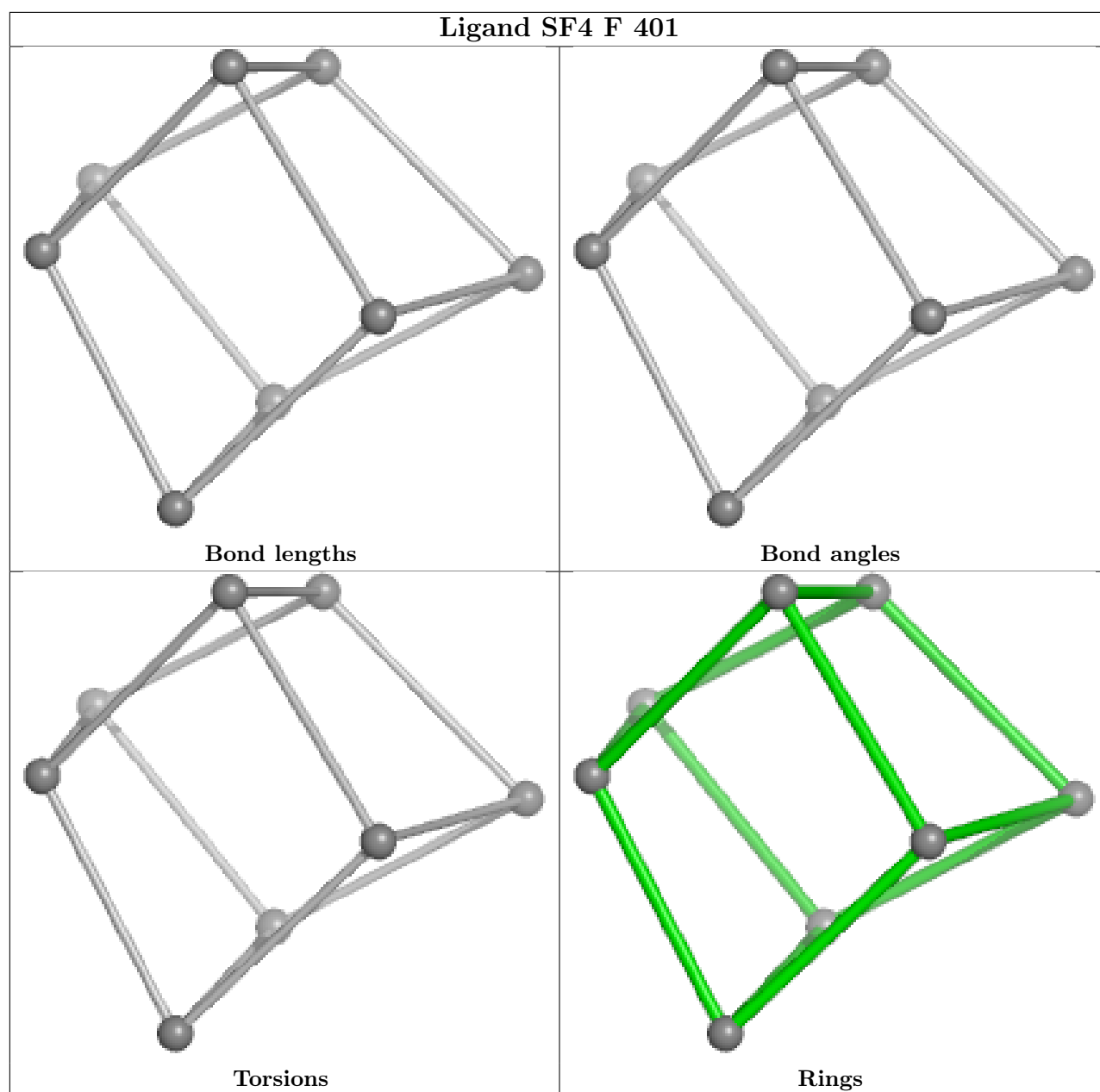
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	F	401	SF4	7	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.

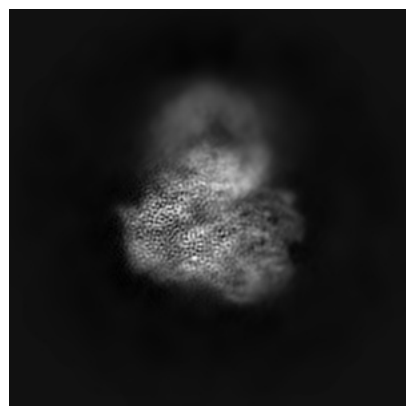
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50734. These allow visual inspection of the internal detail of the map and identification of artifacts.

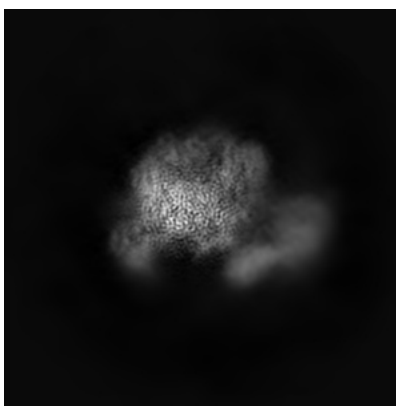
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

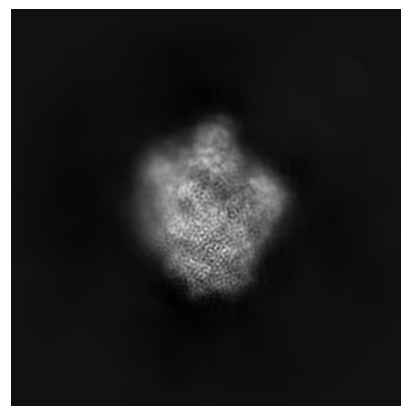
6.1.1 Primary map



X

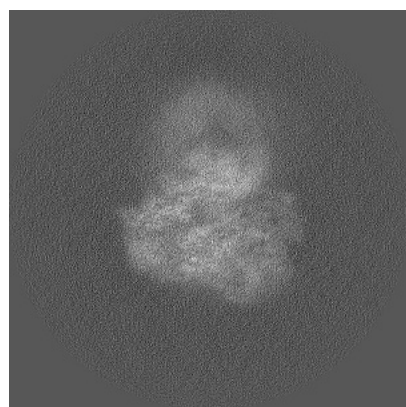


Y

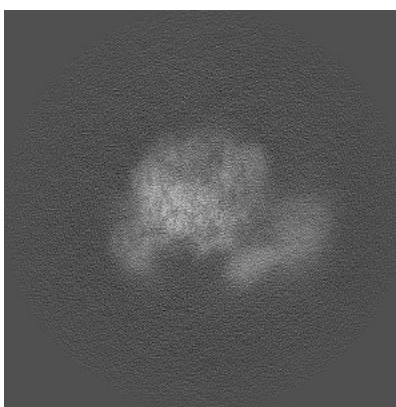


Z

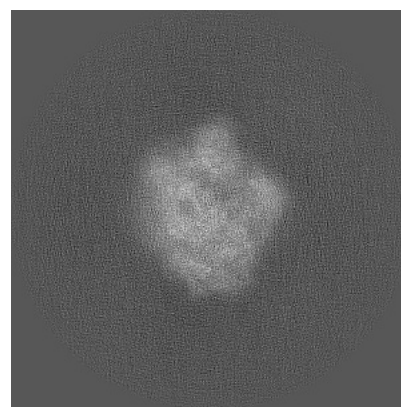
6.1.2 Raw map



X



Y

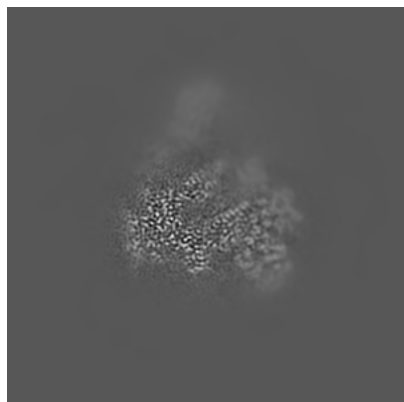


Z

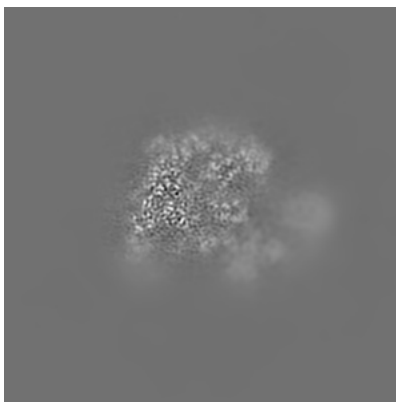
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

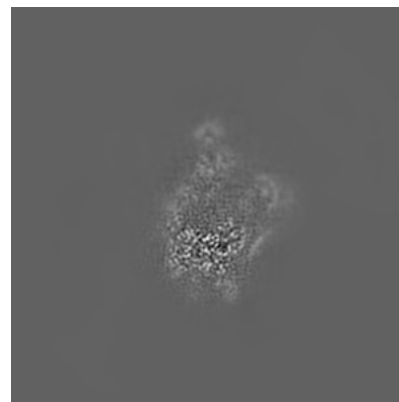
6.2.1 Primary map



X Index: 210

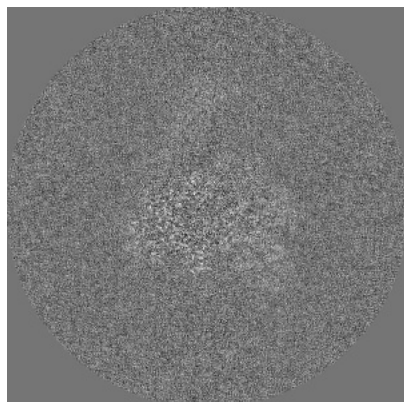


Y Index: 210

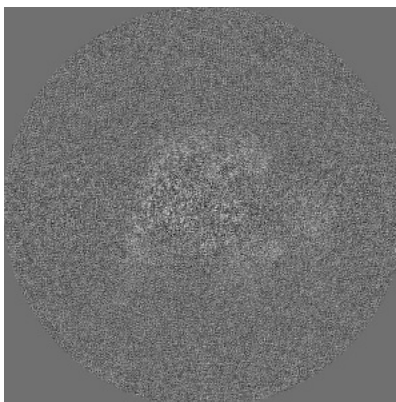


Z Index: 210

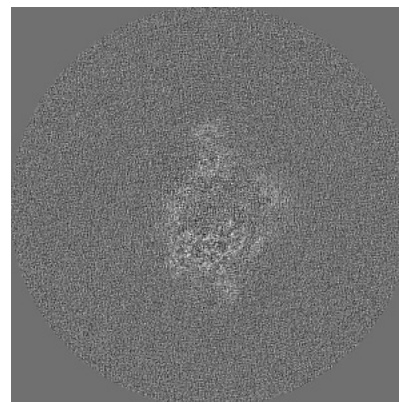
6.2.2 Raw map



X Index: 210



Y Index: 210

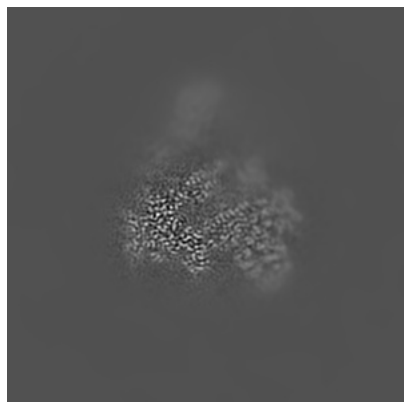


Z Index: 210

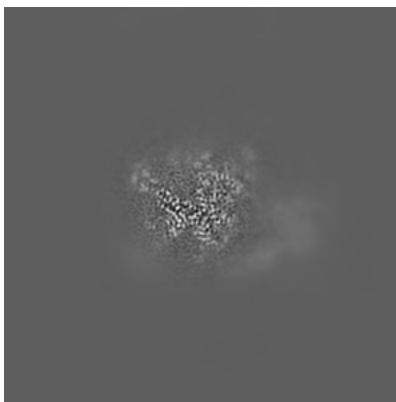
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

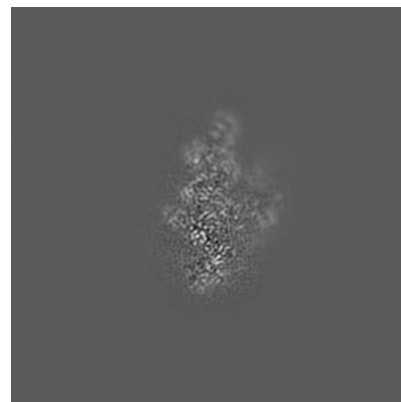
6.3.1 Primary map



X Index: 211

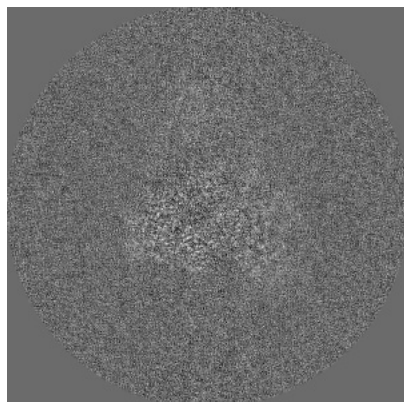


Y Index: 178

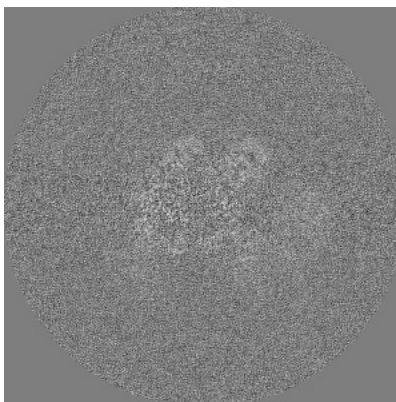


Z Index: 184

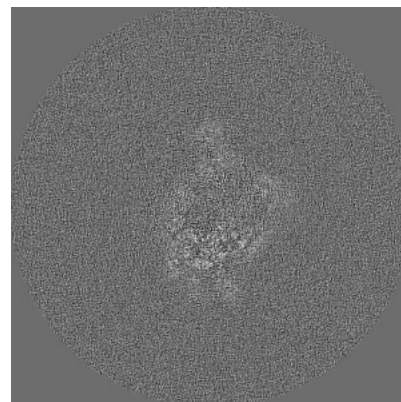
6.3.2 Raw map



X Index: 211



Y Index: 202

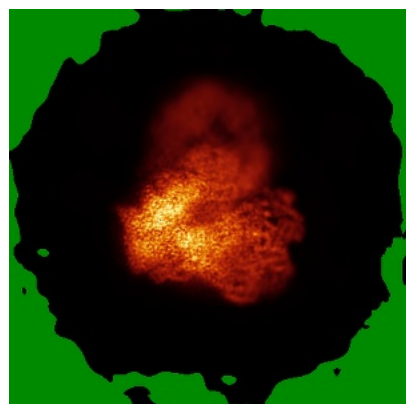


Z Index: 209

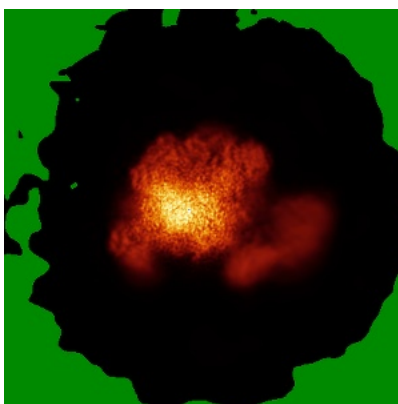
The images above show the largest variance slices of the map in three orthogonal directions.

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

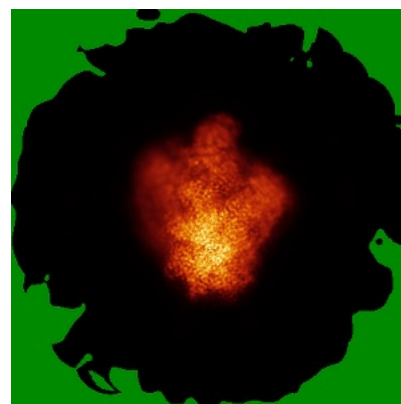
6.4.1 Primary map



X

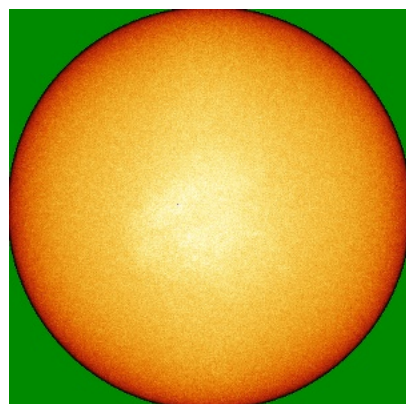


Y

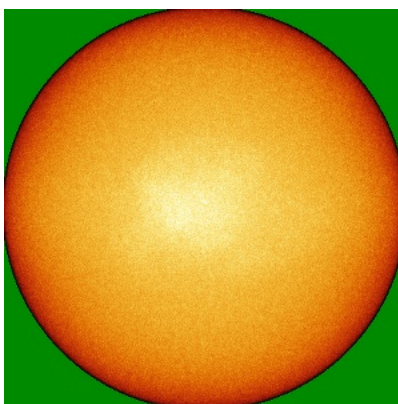


Z

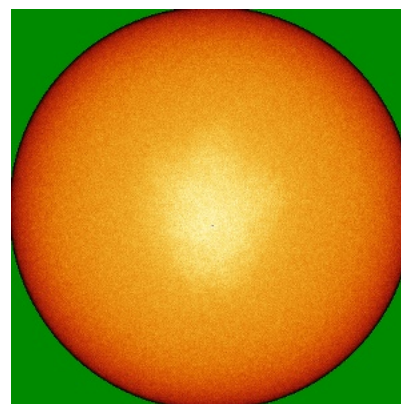
6.4.2 Raw map



X



Y

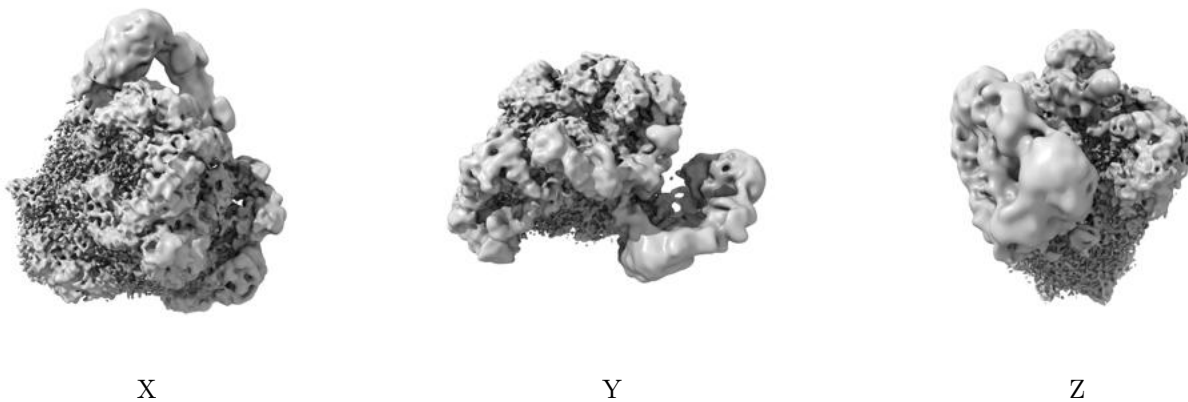


Z

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.

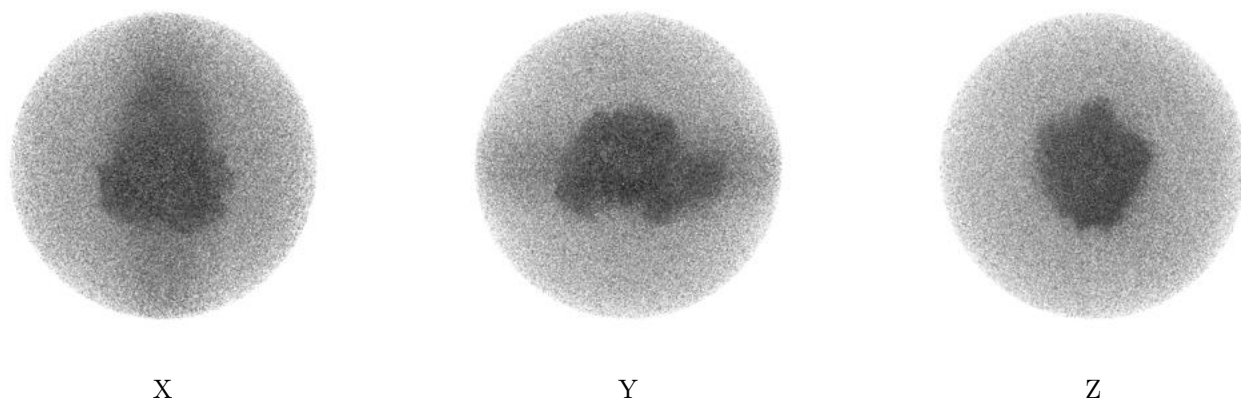
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.004. 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.

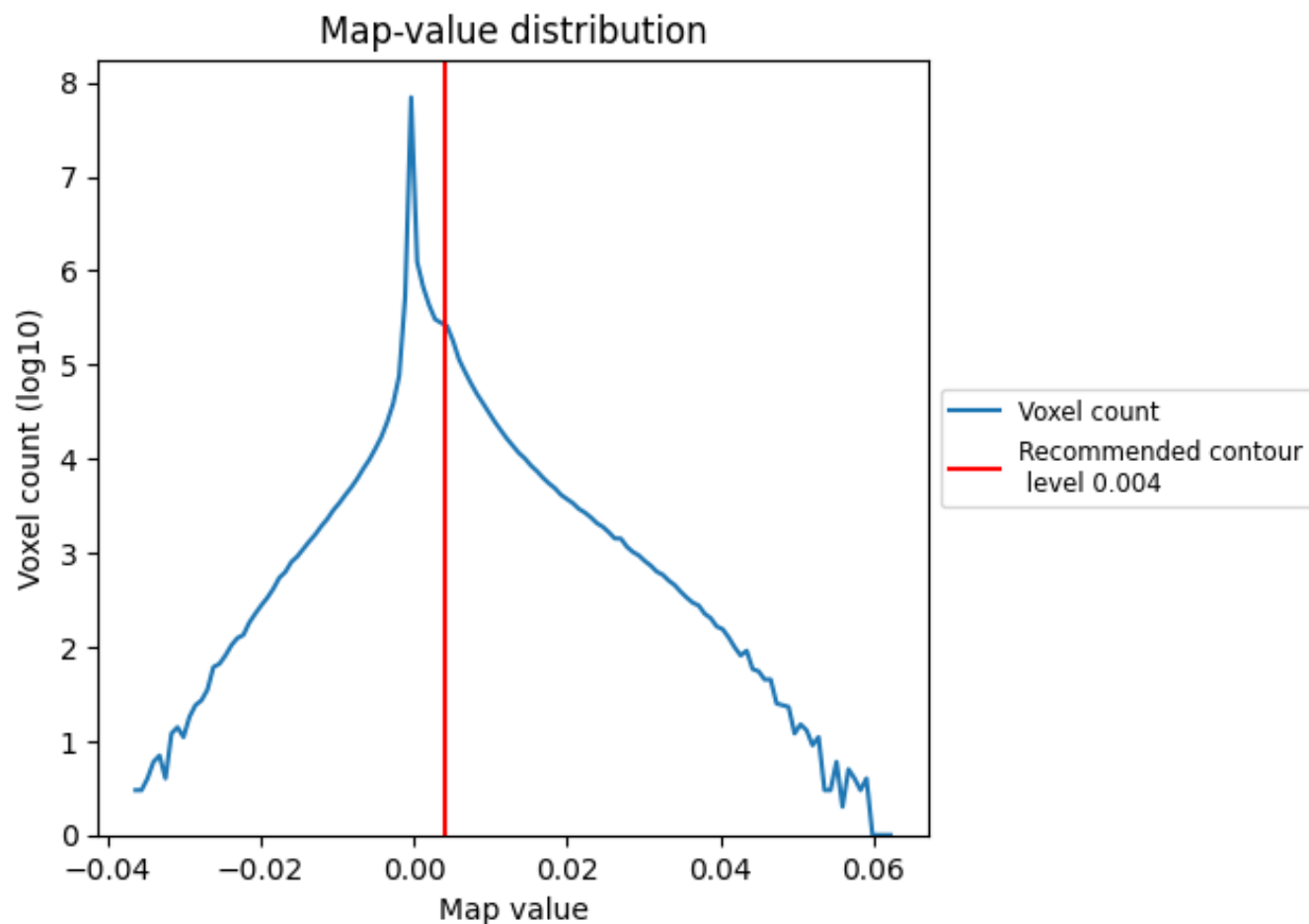
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

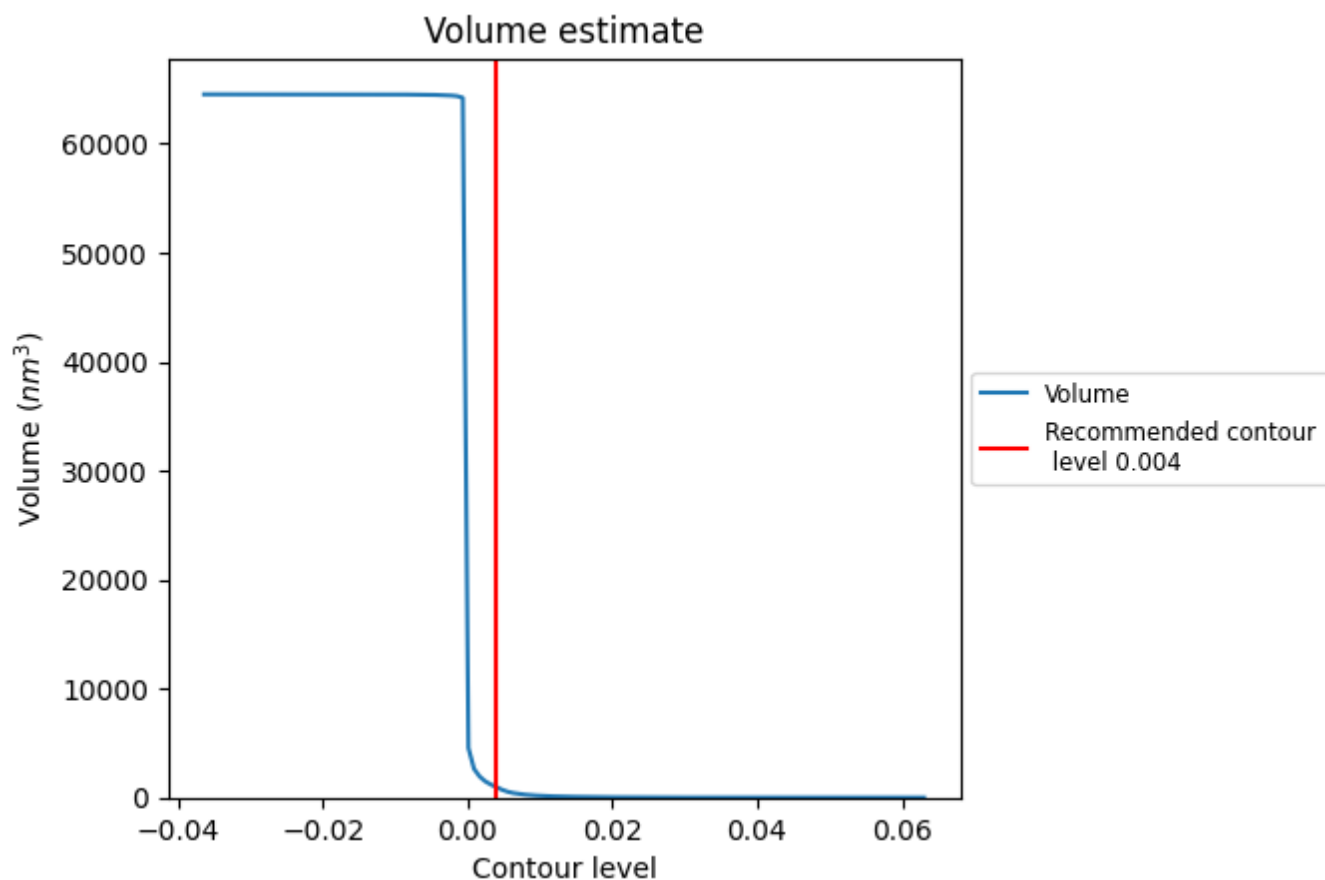
This section contains the results of statistical analysis of the map.

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.

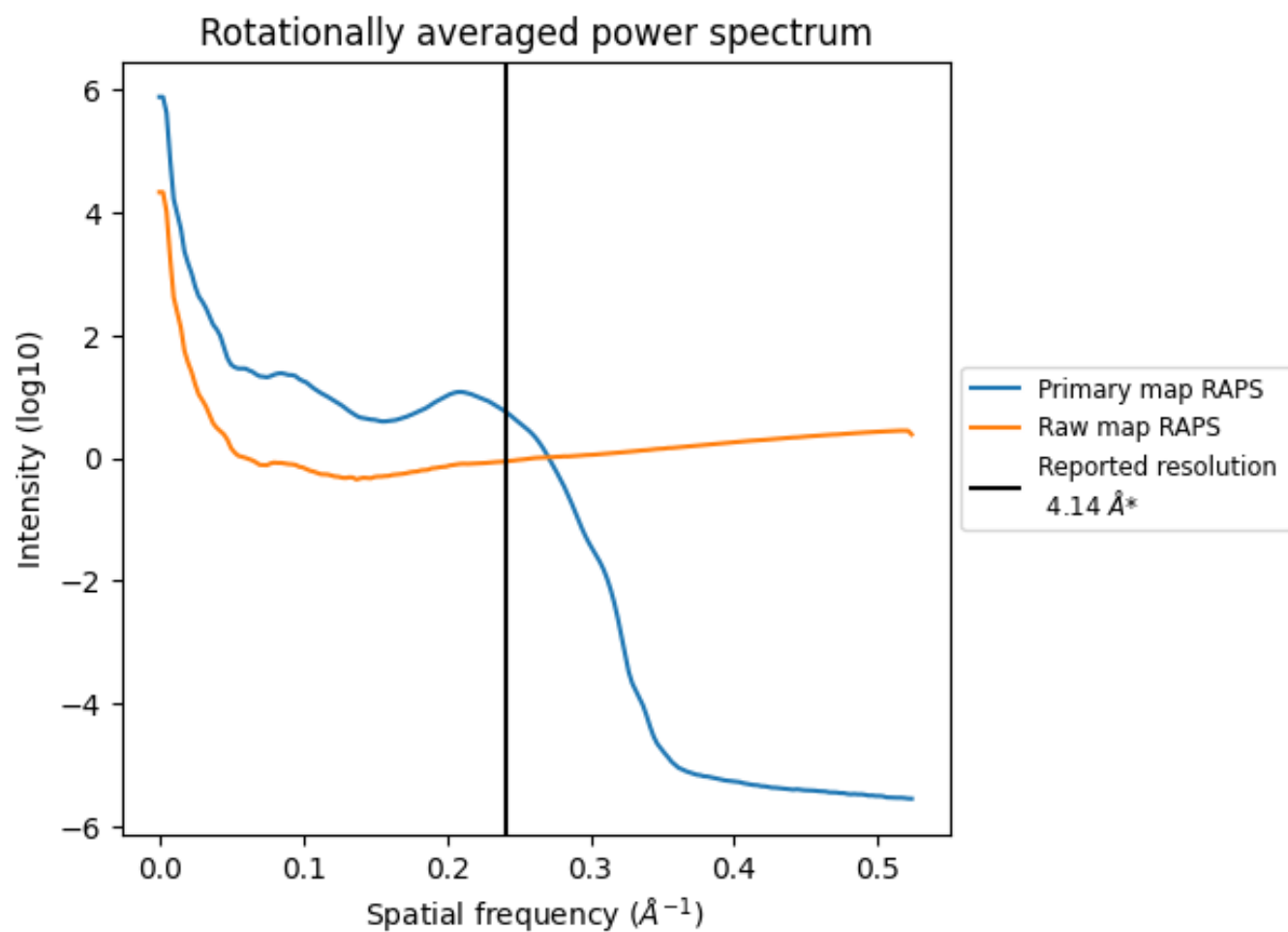
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 952 nm³; this corresponds to an approximate mass of 860 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 ⓘ

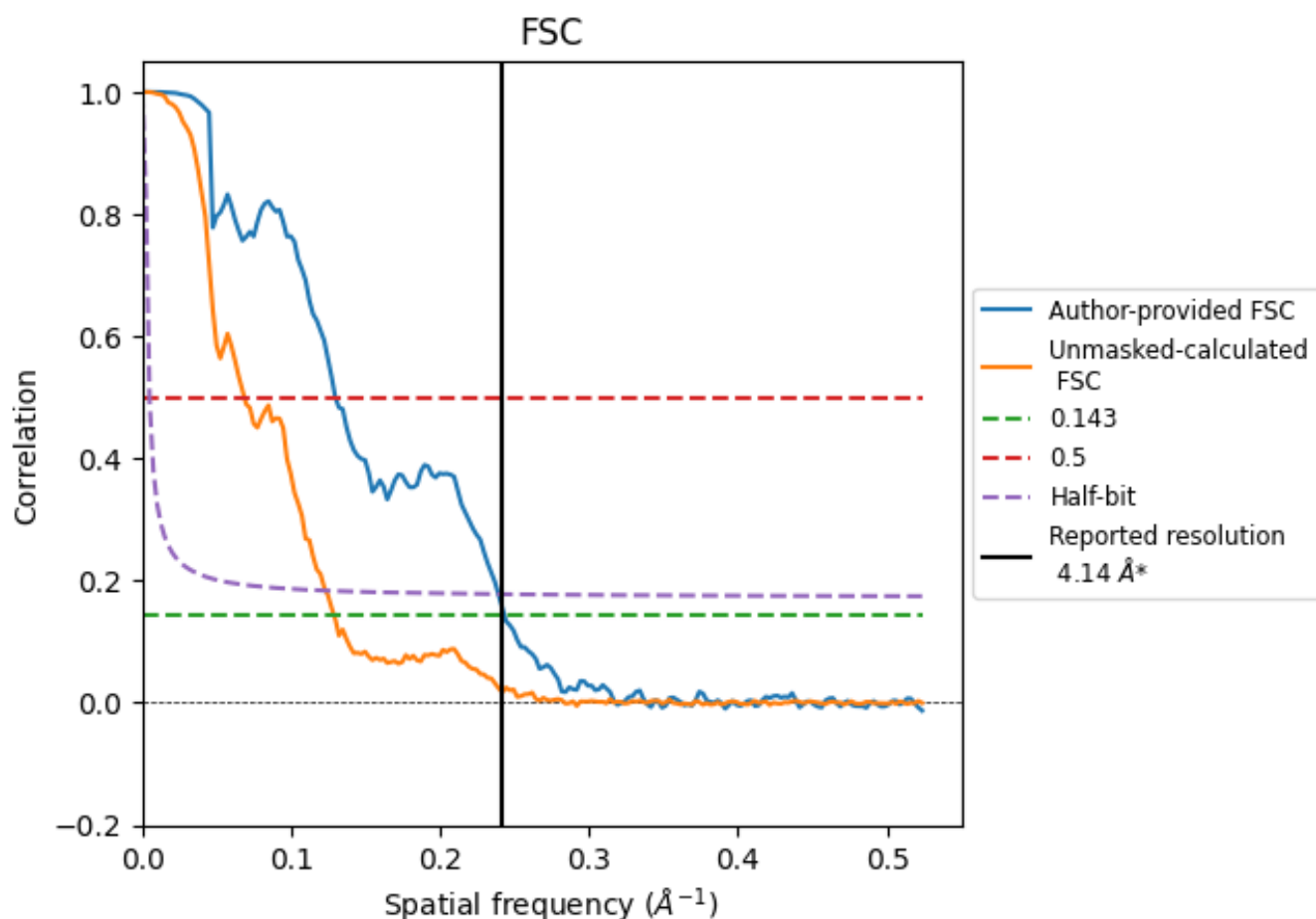


*Reported resolution corresponds to spatial frequency of 0.242 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.242 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

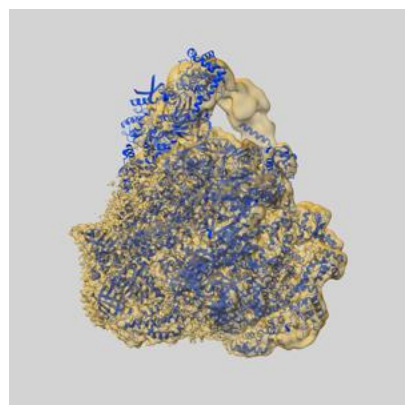
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.14	-	-
Author-provided FSC curve	4.11	7.71	4.18
Unmasked-calculated*	7.76	14.58	8.12

*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 7.76 differs from the reported value 4.14 by more than 10 %

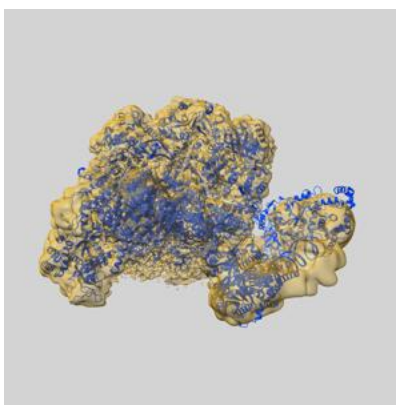
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50734 and PDB model 9FSS. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

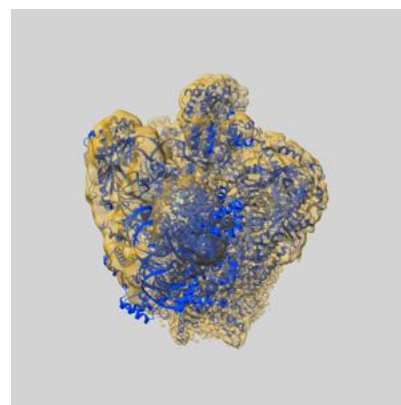
9.1 Map-model overlay [i](#)



X



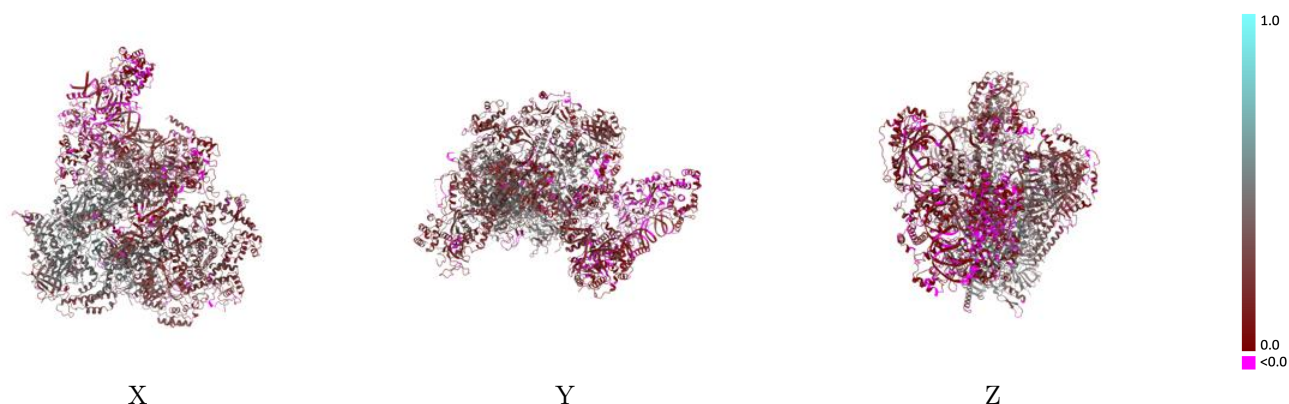
Y



Z

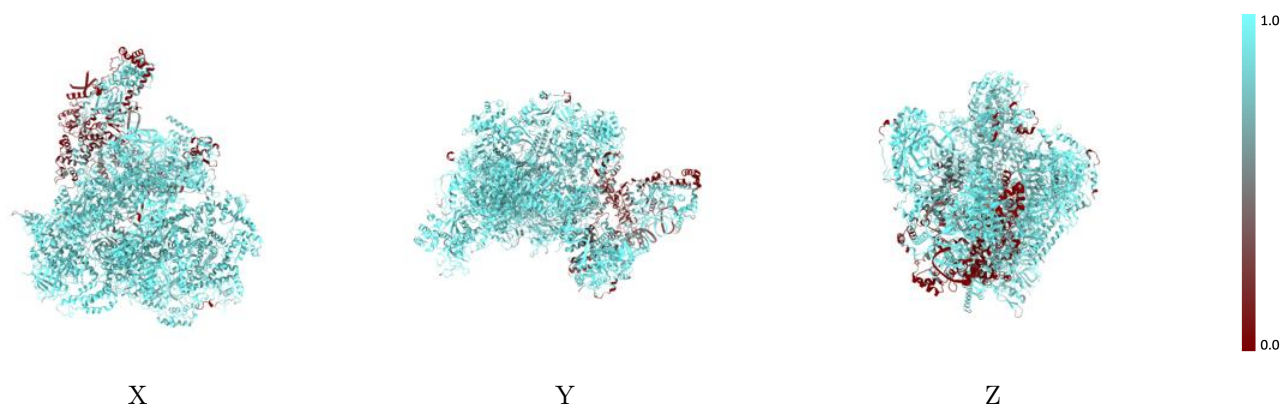
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



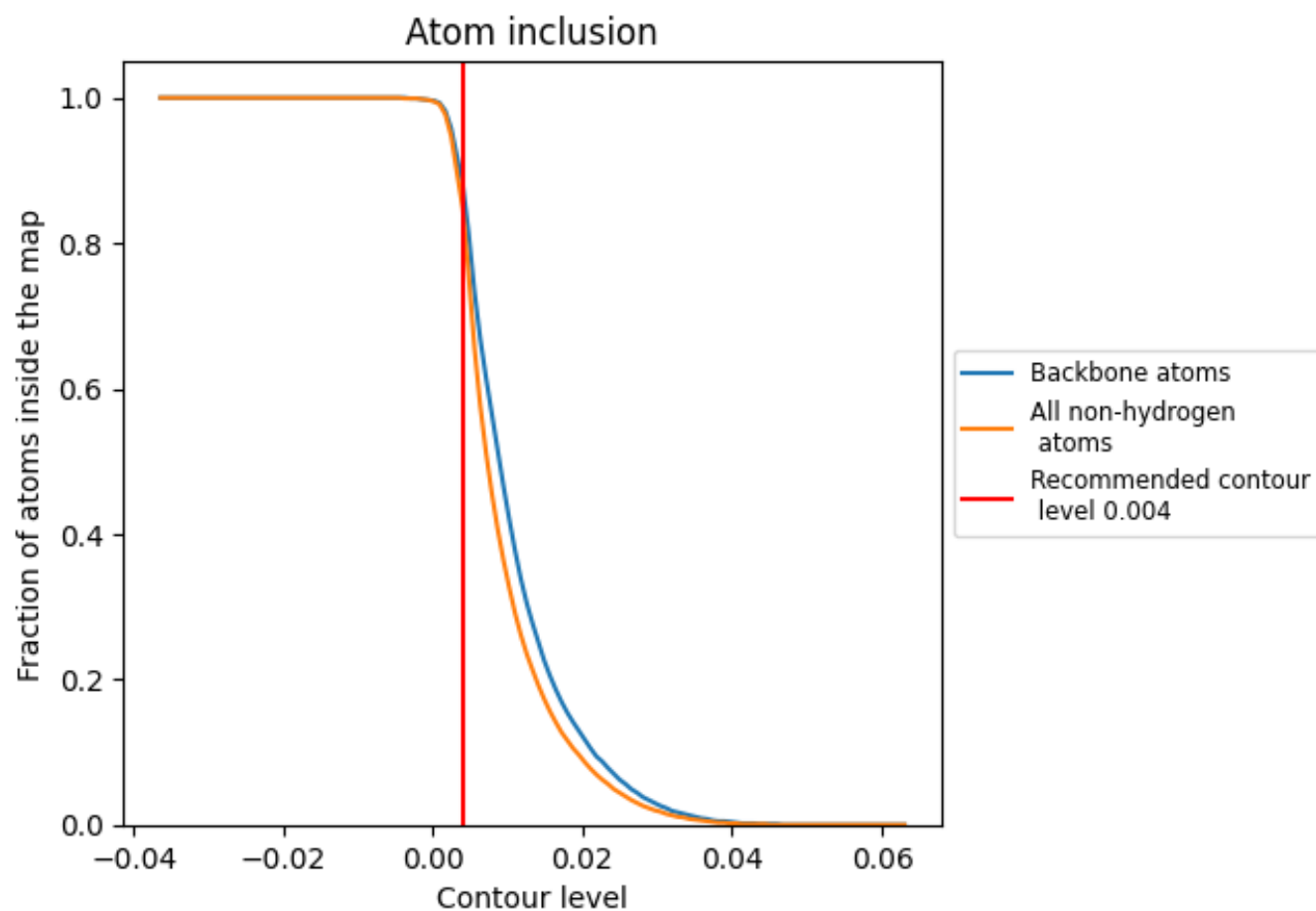
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.004).

9.4 Atom inclusion ⓘ



At the recommended contour level, 88% of all backbone atoms, 85% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8480	 0.2640
A	 0.9400	 0.3760
B	 0.9410	 0.4050
C	 0.8950	 0.2400
D	 0.8530	 0.1880
E	 0.6640	 0.1830
F	 0.7960	 0.1590
G	 0.9520	 0.2460
H	 0.9450	 0.2630
I	 0.9610	 0.2110
J	 0.9390	 0.2150
K	 0.9440	 0.4070
L	 0.9420	 0.3830
M	 0.9610	 0.2680
N	 0.9520	 0.4320
O	 0.9500	 0.3450
P	 0.9680	 0.3790
Q	 0.9530	 0.4660
R	 0.9470	 0.1050
S	 0.7220	 0.1400
T	 0.8970	 0.0800
U	 0.8740	 0.0530
W	 0.2970	 0.0490
X	 0.7810	 0.1410
Y	 0.8500	 0.1120
Z	 0.4760	 0.0420

