



## Full wwPDB EM Validation Report ⓘ

Jun 20, 2026 – 06:15 pm BST

PDB ID : 28ZV / pdb\_000028zv  
EMDB ID : EMD-57005  
Title : human 48S PIC with mRNA (non-Kozak)  
Authors : von Loeffelholz, O.; Barchet, C.; Klaholz, B.  
Deposited on : 2026-03-03  
Resolution : 2.90 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

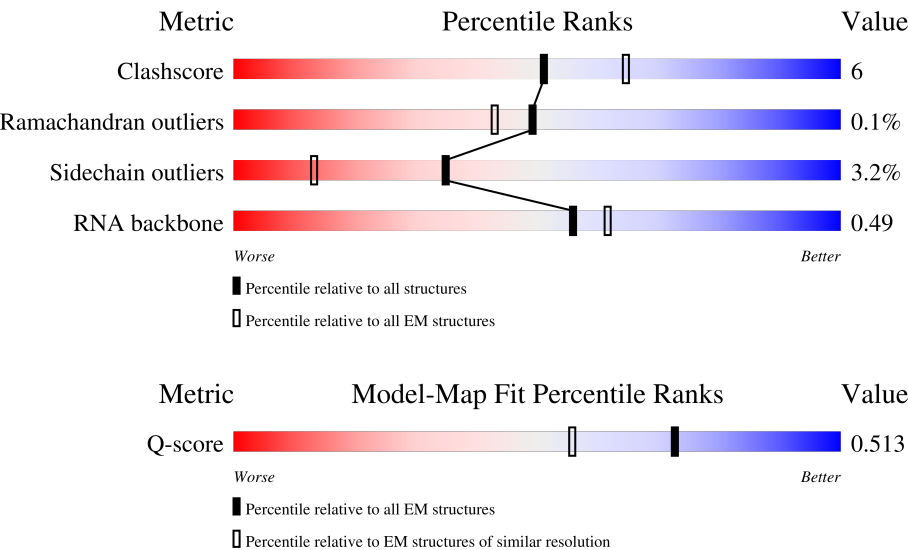
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.90 Å.

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









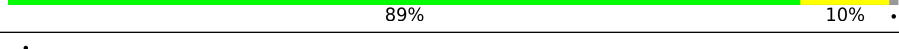
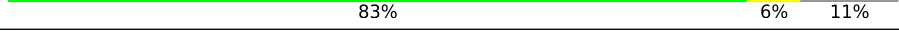
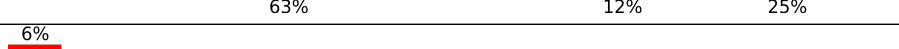
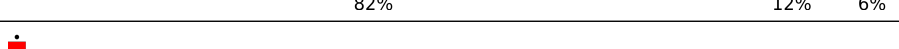
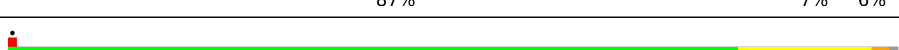

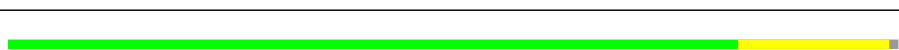

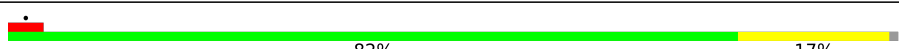





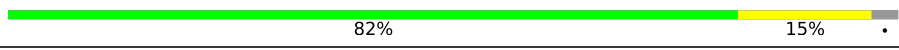
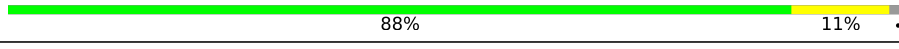



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 ( 2.40 - 3.40 )

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

Mol	Chain	Length	Quality of chain
1	S2	1869	
2	Ln	25	
3	SE	263	

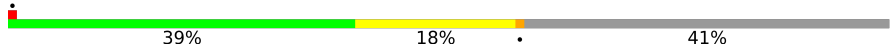




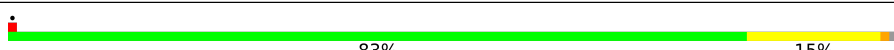
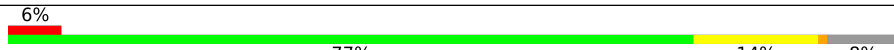
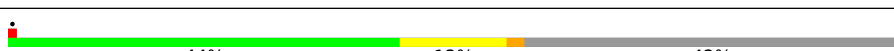
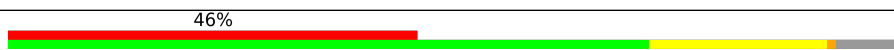
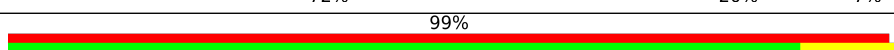
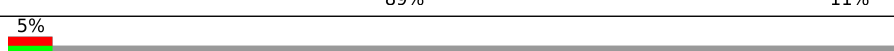
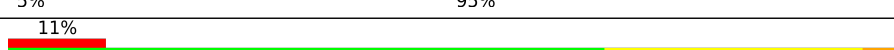
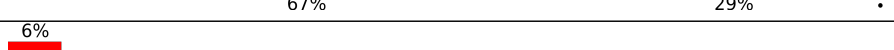
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Mol	Chain	Length	Quality of chain
4	SA	295	
5	SB	264	
6	SH	194	
7	SI	208	
8	SL	158	
9	SV	83	
10	SX	143	
11	Sa	115	
12	SC	293	
13	SG	249	
14	SJ	194	
15	SN	151	
16	SO	151	
17	SW	130	
18	SY	133	
19	Sb	84	
20	Se	133	
21	B	50	
22	SD	243	
23	SF	204	
24	Sf	156	
25	SR	135	
26	Sd	56	
27	Sg	317	
28	Sc	69	

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Mol	Chain	Length	Quality of chain
29	SK	165	
30	SM	132	
31	SU	119	
32	SQ	146	
33	SS	152	
34	ST	145	
35	SP	145	
36	SZ	125	
37	D	315	
38	E	472	
39	F	333	
40	G	75	
41	H	144	

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
1	OMU	S2	116	-	-	X	-

## 2 Entry composition

There are 47 unique types of molecules in this entry. The entry contains 85772 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 RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	S2	1740	Total	C	N	O	P	0	0
			36955	16511	6600	12105	1739		

- Molecule 2 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ln	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 3 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	SE	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 4 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SA	219	Total	C	N	O	S	0	0
			1727	1096	302	320	9		

- Molecule 5 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SB	214	Total	C	N	O	S	0	0
			1738	1103	310	311	14		

- Molecule 6 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SH	189	Total	C	N	O	S	0	0
			1523	972	280	270	1		

- Molecule 7 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SI	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

- Molecule 8 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SL	150	Total	C	N	O	S	0	0
			1220	776	228	210	6		

- Molecule 9 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SV	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 10 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SX	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 11 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Sa	102	Total	C	N	O	S	0	0
			821	512	171	133	5		

- Molecule 12 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SC	220	Total	C	N	O	S	0	0
			1709	1106	294	299	10		

- Molecule 13 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SG	234	Total	C	N	O	S	0	0
			1903	1188	384	324	7		

- Molecule 14 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	SJ	182	Total	C	N	O	S	0	0
			1512	962	303	245	2		

- Molecule 15 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	SN	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 16 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	SO	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SO	138	IAS	ASP	conflict	UNP P62263

- Molecule 17 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	SW	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 18 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SY	124	Total	C	N	O	S	0	0
			1014	641	198	170	5		

- Molecule 19 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Sb	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 20 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Se	59	Total	C	N	O	S	0	0
			468	290	102	75	1		

- Molecule 21 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	B	28	Total	C	N	O	P	0	0
			587	264	98	197	28		

- Molecule 22 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	SD	227	Total	C	N	O	S	0	0
			1765	1125	317	315	8		

- Molecule 23 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	SF	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 24 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Sf	63	Total	C	N	O	S	0	0
			515	324	98	86	7		

- Molecule 25 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	SR	131	Total	C	N	O	S	0	0
			1064	668	198	194	4		

- Molecule 26 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Sd	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 27 is a protein called Receptor of activated protein C kinase 1.



Mol	Chain	Residues	Atoms					AltConf	Trace
27	Sg	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 28 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Sc	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 29 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	SK	97	Total	C	N	O	S	0	0
			816	533	144	133	6		

- Molecule 30 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	SM	118	Total	C	N	O	S	0	0
			906	568	158	172	8		

- Molecule 31 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	SU	102	Total	C	N	O	S	0	0
			811	508	154	145	4		

- Molecule 32 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	SQ	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 33 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	SS	145	Total	C	N	O	S	0	0
			1198	751	242	203	2		

- Molecule 34 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	ST	143	Total	C	N	O	S	0	0
			1113	698	214	198	3		

- Molecule 35 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	SP	134	Total	C	N	O	S	0	0
			1103	703	208	185	7		

- Molecule 36 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	SZ	73	Total	C	N	O	S	0	0
			585	374	108	102	1		

- Molecule 37 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	D	292	Total	C	N	O	S	0	0
			2352	1477	411	451	13		

- Molecule 38 is a protein called Eukaryotic translation initiation factor 2 subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	E	472	Total	C	N	O	S	0	0
			3585	2272	628	667	18		

- Molecule 39 is a protein called Eukaryotic translation initiation factor 2 subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	F	16	Total	C	N	O	S	0	0
			143	91	25	26	1		

- Molecule 40 is a RNA chain called initiator tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	G	75	Total	C	N	O	P	1	0
			1623	728	299	521	75		

- Molecule 41 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	H	111	Total	C	N	O	S	0	0
			895	556	170	164	5		

- Molecule 42 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
42	S2	13	Total	K	0
			13	13	
42	SX	1	Total	K	0
			1	1	
42	Sd	1	Total	K	0
			1	1	

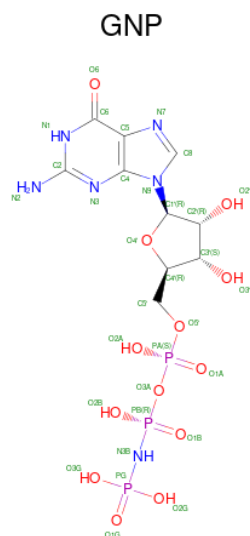
- Molecule 43 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
43	S2	70	Total	Mg	0
			70	70	

- Molecule 44 is ZINC ION (CCD ID: ZN) (formula: Zn).

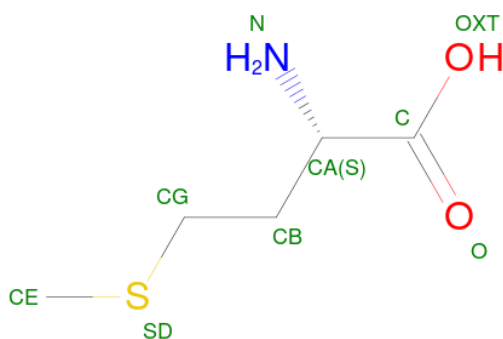
Mol	Chain	Residues	Atoms		AltConf
44	Sa	1	Total	Zn	0
			1	1	
44	Sf	1	Total	Zn	0
			1	1	
44	Sd	1	Total	Zn	0
			1	1	

- Molecule 45 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					AltConf
45	E	1	Total	C	N	O	P	0
			32	10	6	13	3	

- Molecule 46 is METHIONINE (CCD ID: MET) (formula:  $\text{C}_5\text{H}_{11}\text{NO}_2\text{S}$ ).



Mol	Chain	Residues	Atoms					AltConf
46	E	1	Total	C	N	O	S	0
			8	5	1	1	1	

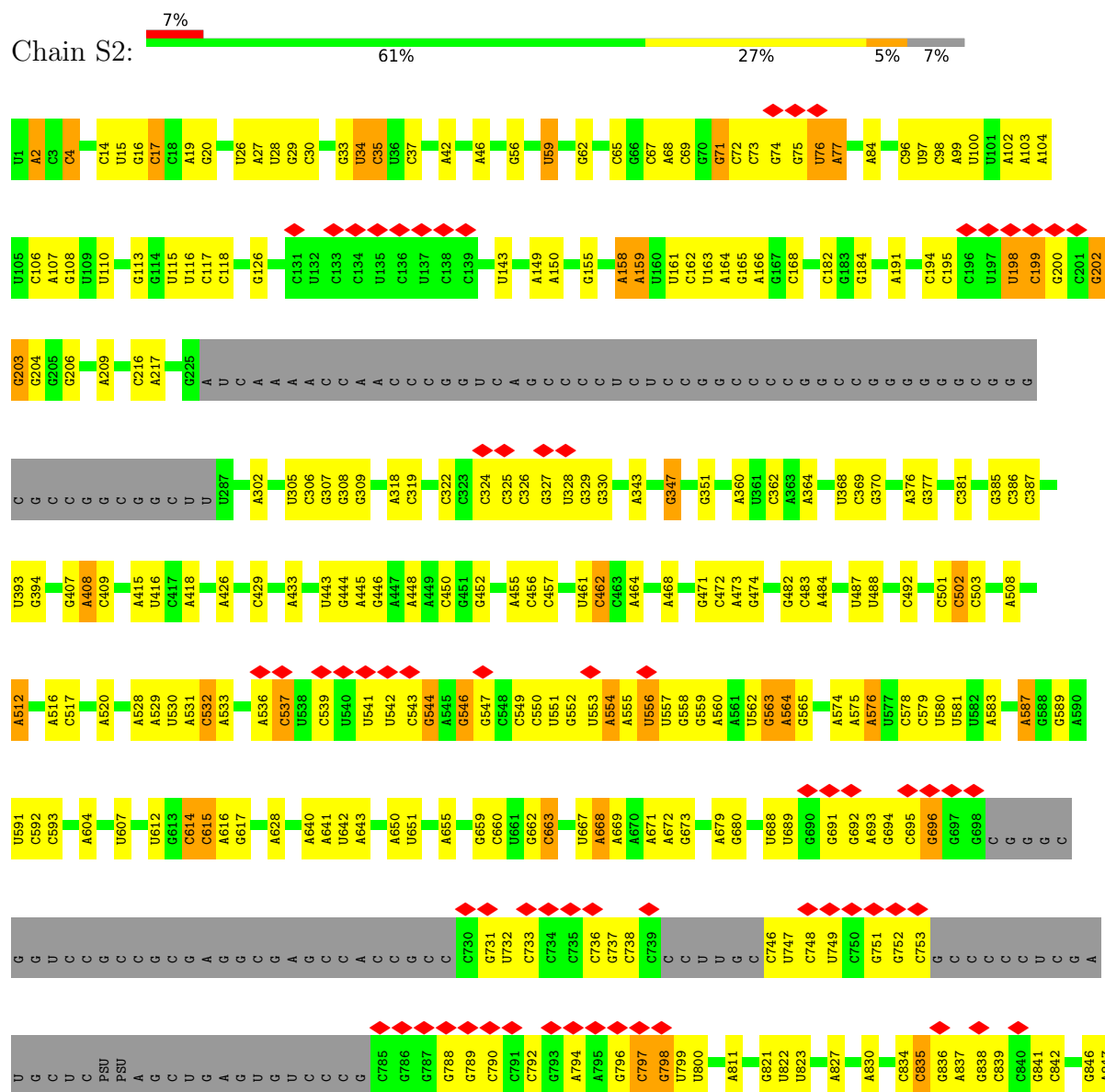
- Molecule 47 is water.

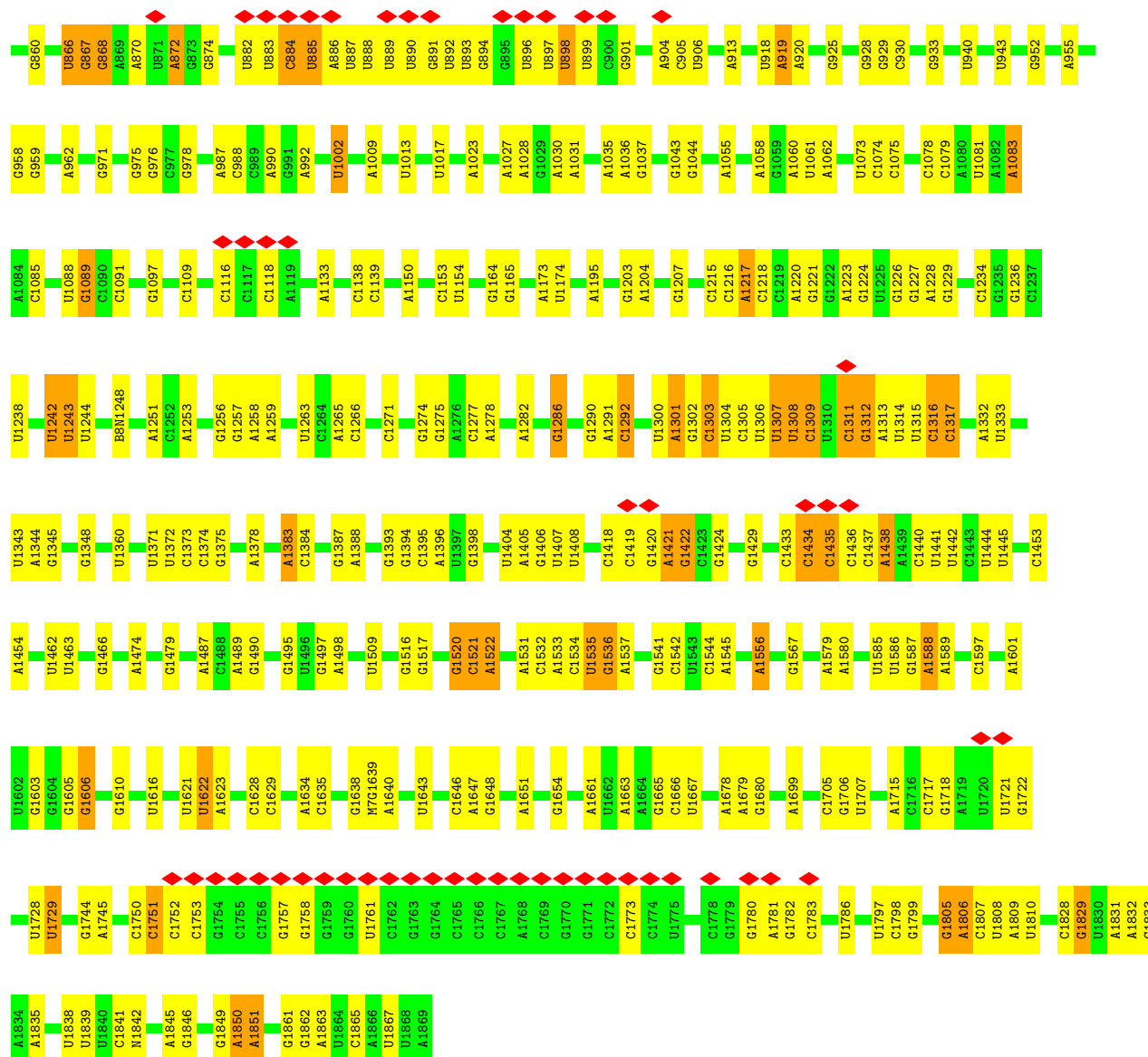
Mol	Chain	Residues	Atoms		AltConf
47	S2	327	Total 327	O 327	0
47	SE	4	Total 4	O 4	0
47	SL	1	Total 1	O 1	0
47	Sa	1	Total 1	O 1	0
47	SO	2	Total 2	O 2	0
47	B	2	Total 2	O 2	0
47	SQ	1	Total 1	O 1	0

### 3 Residue-property plots [i](#)

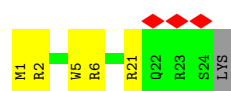
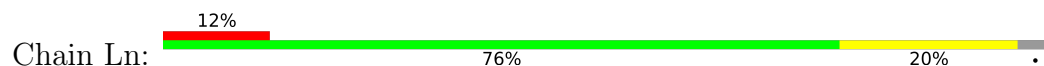
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 18S ribosomal RNA





• Molecule 2: 60S ribosomal protein L41

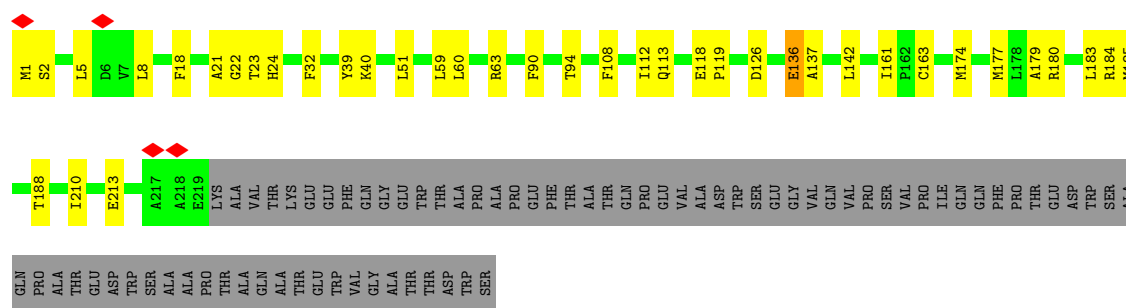


• Molecule 3: Small ribosomal subunit protein eS4, X isoform



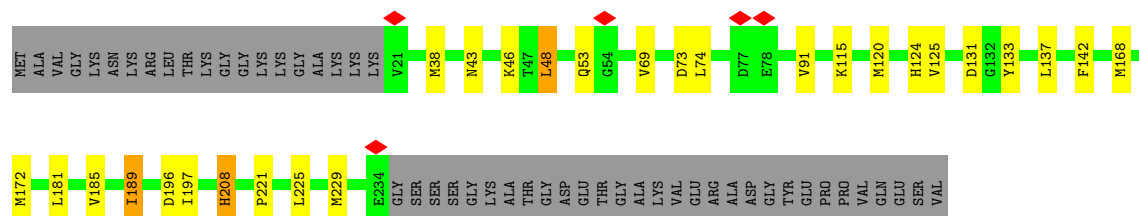
• Molecule 4: 40S ribosomal protein SA

Chain SA: 




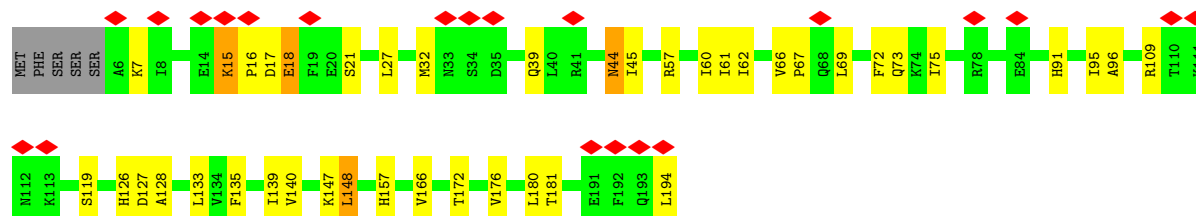
- Molecule 5: 40S ribosomal protein S3a

Chain SB: 




- Molecule 6: 40S ribosomal protein S7

Chain SH: 




- Molecule 7: 40S ribosomal protein S8

Chain SI: 

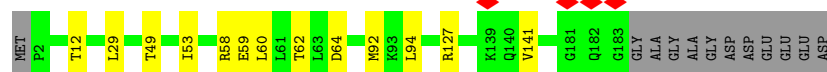
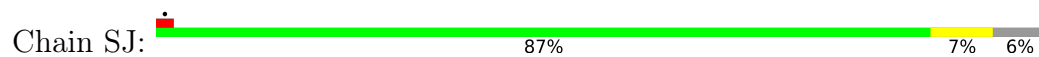


- Molecule 8: Small ribosomal subunit protein uS17

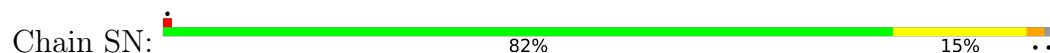
Chain SL: 



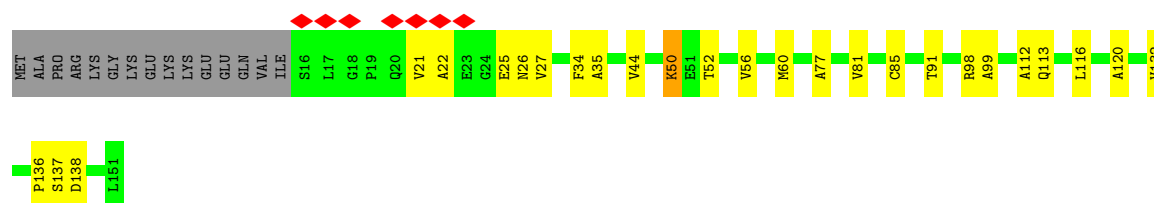




- Molecule 15: 40S ribosomal protein S13



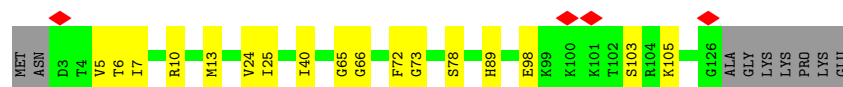
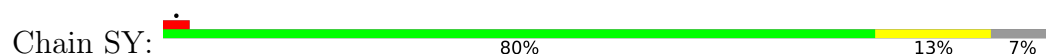
- Molecule 16: 40S ribosomal protein S14



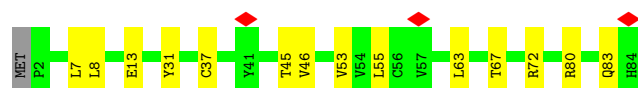
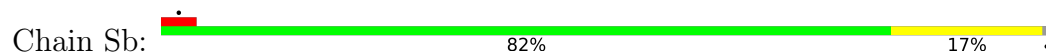
- Molecule 17: 40S ribosomal protein S15a



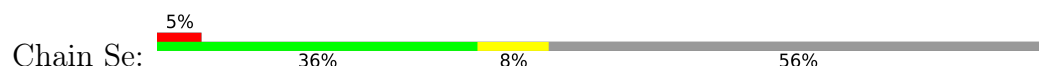
- Molecule 18: 40S ribosomal protein S24

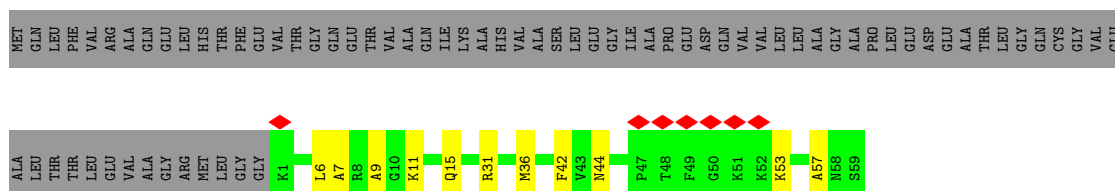


- Molecule 19: 40S ribosomal protein S27

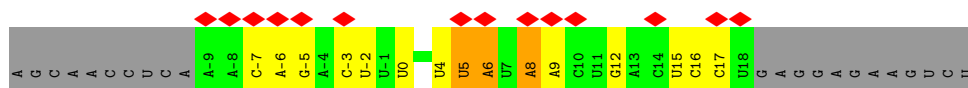
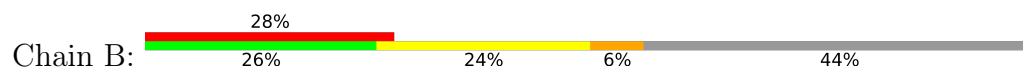


- Molecule 20: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein

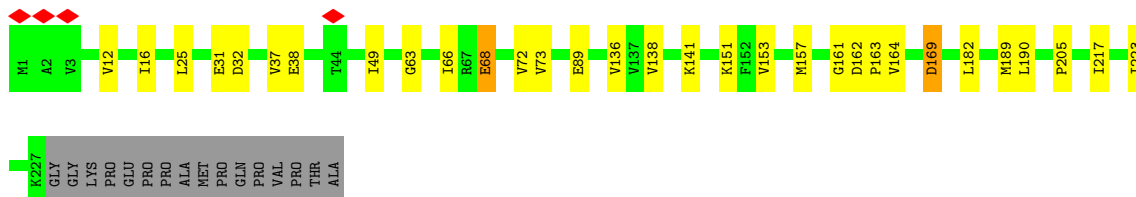
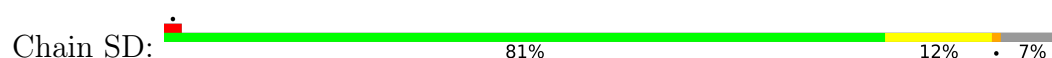




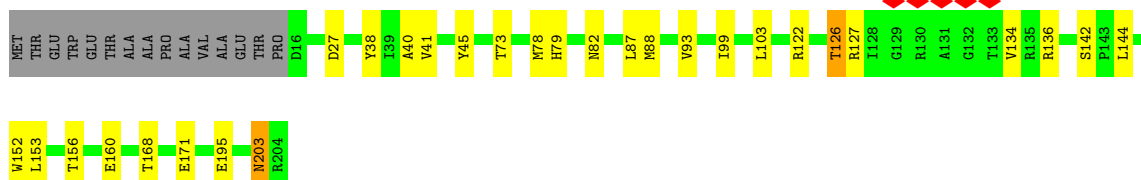
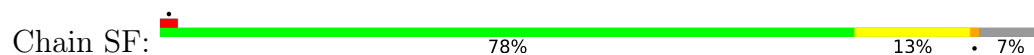
- Molecule 21: mRNA



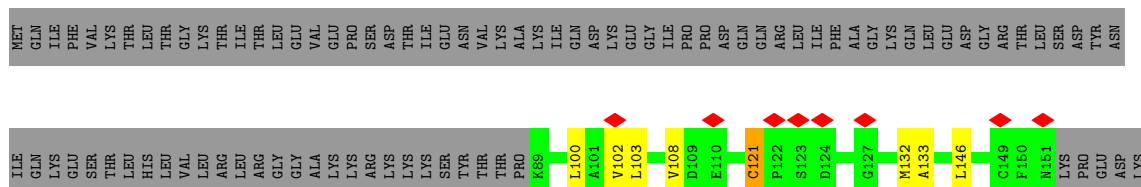
- Molecule 22: 40S ribosomal protein S3



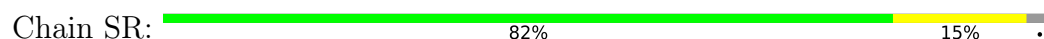
- Molecule 23: 40S ribosomal protein S5



- Molecule 24: Ubiquitin



- Molecule 25: 40S ribosomal protein S17





- Molecule 26: 40S ribosomal protein S29

Chain Sd: 88% 11%



- Molecule 27: Receptor of activated protein C kinase 1

Chain Sg: 78% 20%



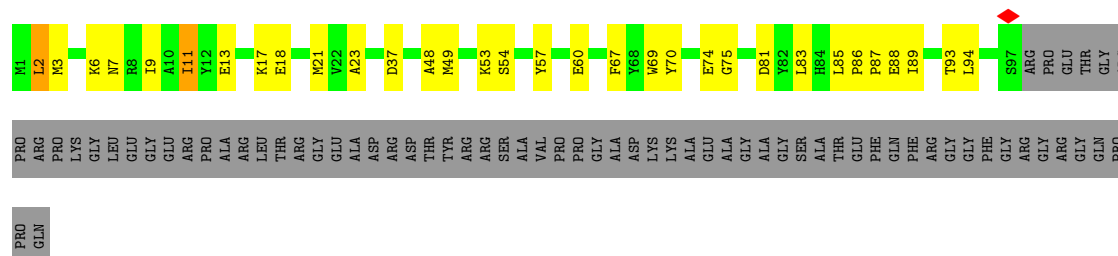
- Molecule 28: 40S ribosomal protein S28

Chain Sc: 68% 23% 7%



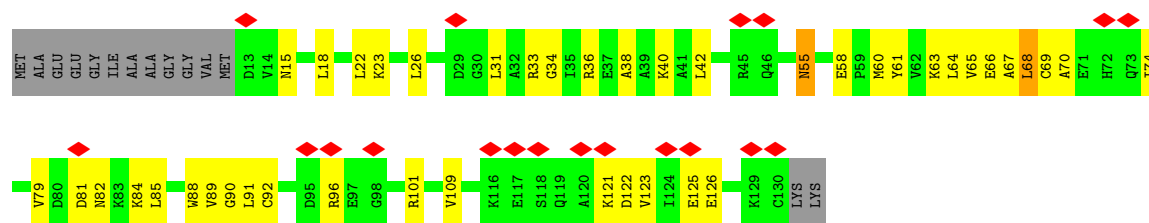
- Molecule 29: 40S ribosomal protein S10

Chain SK: 39% 18% 41%

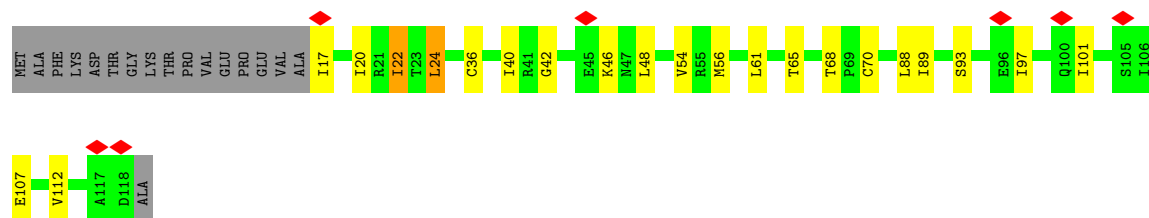


- Molecule 30: 40S ribosomal protein S12

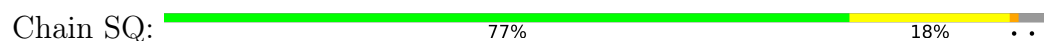
Chain SM: 14% 57% 31% 11%



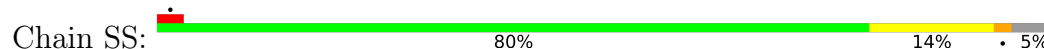
- Molecule 31: 40S ribosomal protein S20



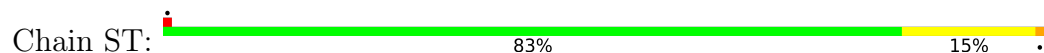
- Molecule 32: 40S ribosomal protein S16



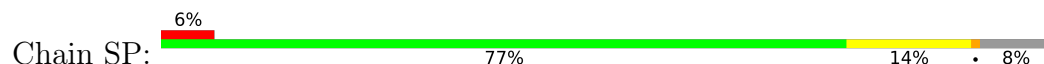
- Molecule 33: 40S ribosomal protein S18



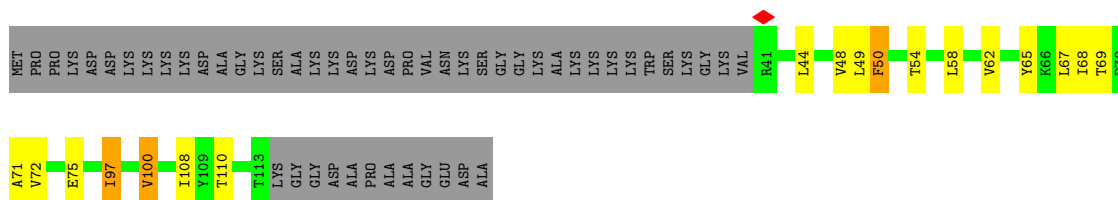
- Molecule 34: Small ribosomal subunit protein eS19

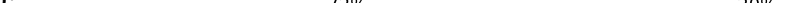


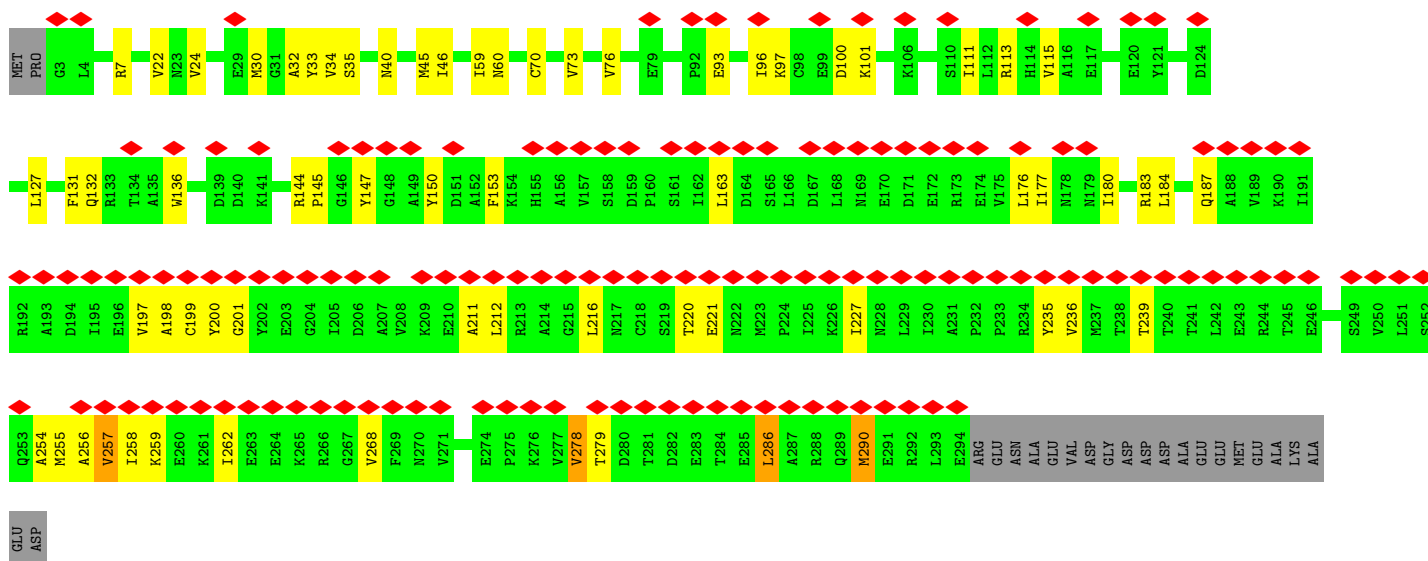
- Molecule 35: 40S ribosomal protein S15

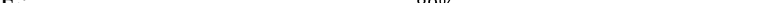


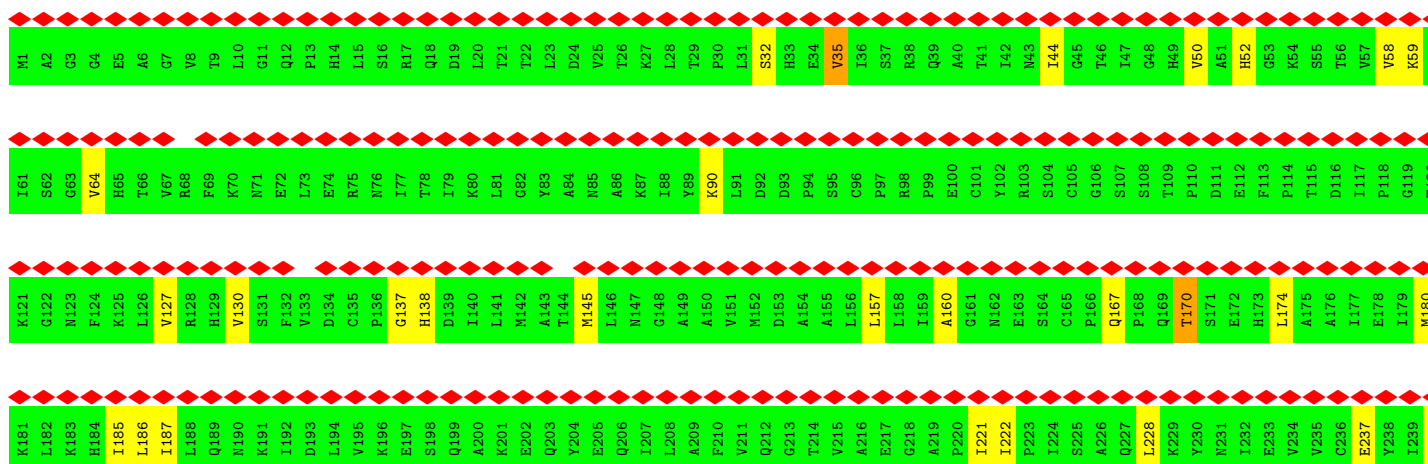
- Molecule 36: Small ribosomal subunit protein eS25

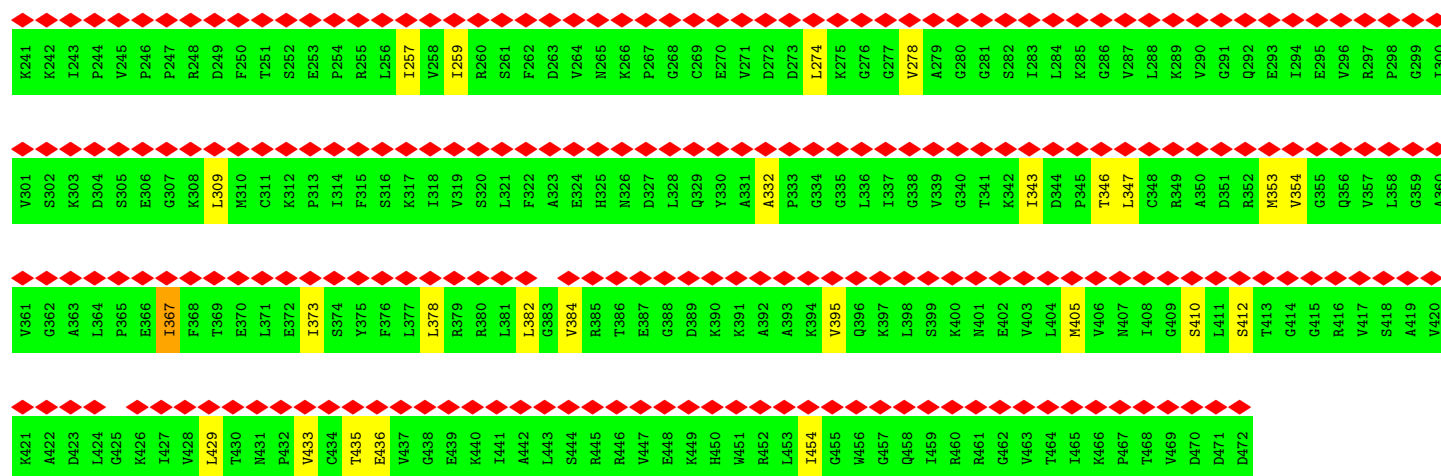


- Chain D:  46% 72% 20% 7%

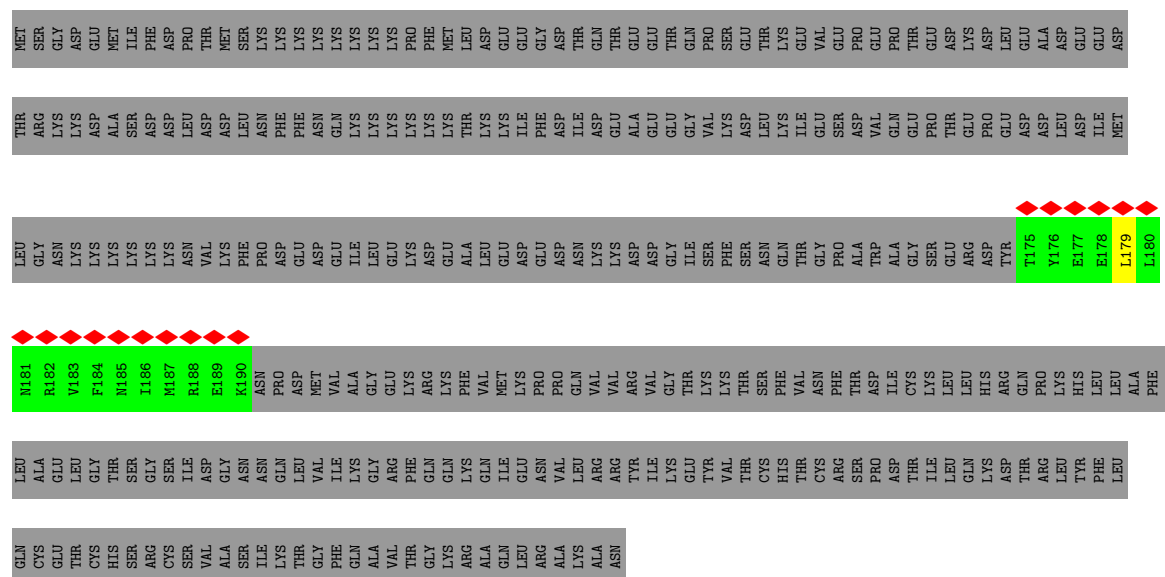


- Chain E:  99% 89% 11%

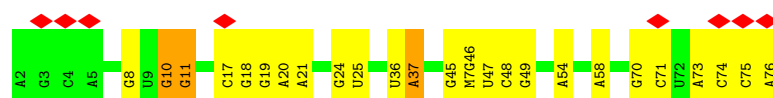




• Molecule 39: Eukaryotic translation initiation factor 2 subunit 2



• Molecule 40: initiator tRNA



• Molecule 41: Eukaryotic translation initiation factor 1A, X-chromosomal



ILE  
GLN  
PHE  
ASP  
ASP  
ILE  
GLY  
ASP  
ASP  
ASP  
GLU  
ASP  
ILE  
ASP  
ASP  
ILE



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39810	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	50.738	Depositor
Minimum map value	-19.475	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.445	Depositor
Recommended contour level	4.71	Depositor
Map size (Å)	374.40002, 374.40002, 374.40002	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.72, 0.72, 0.72	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UY1, IAS, PSU, K, 2MG, ZN, T6A, 1MA, NMM, B8N, OMC, OMU, MG, A2M, OMG, GNP, H2U, MA6, 6MZ, M7G, 5MC, 4AC, 1MG

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	S2	0.23	0/39125	0.28	0/60957
2	Ln	0.18	0/231	0.30	0/294
3	SE	0.17	0/2118	0.36	0/2849
4	SA	0.20	0/1764	0.35	0/2396
5	SB	0.18	0/1765	0.36	0/2362
6	SH	0.17	0/1546	0.38	0/2071
7	SI	0.17	0/1715	0.35	0/2287
8	SL	0.19	0/1241	0.37	0/1662
9	SV	0.19	0/643	0.31	0/860
10	SX	0.19	0/1116	0.33	0/1490
11	Sa	0.20	0/836	0.33	0/1121
12	SC	0.20	0/1746	0.34	0/2358
13	SG	0.17	0/1926	0.34	0/2563
14	SJ	0.17	0/1537	0.34	0/2052
15	SN	0.18	0/1232	0.34	0/1656
16	SO	0.34	1/1020 (0.1%)	0.44	0/1366
17	SW	0.22	0/1051	0.37	0/1406
18	SY	0.18	0/1031	0.36	0/1370
19	Sb	0.18	0/665	0.38	0/891
20	Se	0.18	0/474	0.35	0/623
21	B	0.14	0/654	0.29	0/1014
22	SD	0.21	0/1793	0.34	0/2414
23	SF	0.22	0/1516	0.37	0/2037
24	Sf	0.15	0/525	0.42	0/695
25	SR	0.20	0/1078	0.38	0/1447
26	Sd	0.23	0/470	0.35	0/623
27	Sg	0.20	0/2493	0.39	0/3394
28	Sc	0.20	0/508	0.37	0/680
29	SK	0.22	0/840	0.42	0/1133
30	SM	0.18	0/916	0.48	0/1233
31	SU	0.20	0/821	0.35	0/1103

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	SQ	0.23	0/1142	0.43	0/1528
33	SS	0.21	0/1216	0.37	0/1628
34	ST	0.21	0/1119	0.37	0/1498
35	SP	0.20	0/1126	0.40	0/1505
36	SZ	0.19	0/591	0.41	0/794
37	D	0.14	0/2384	0.34	0/3213
38	E	0.13	0/3643	0.33	0/4929
39	F	0.11	0/144	0.25	0/191
40	G	0.19	0/1600	0.23	0/2492
41	H	0.15	0/905	0.35	0/1202
All	All	0.21	1/88266 (0.0%)	0.32	0/127387

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	SO	136	PRO	C-N	8.65	1.45	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	S2	36955	0	18671	261	0
2	Ln	230	0	276	5	0
3	SE	2076	0	2177	14	0
4	SA	1727	0	1729	38	0
5	SB	1738	0	1809	19	0
6	SH	1523	0	1622	35	0
7	SI	1686	0	1772	21	0
8	SL	1220	0	1289	8	0
9	SV	636	0	637	23	0
10	SX	1098	0	1167	8	0
11	Sa	821	0	870	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	SC	1709	0	1797	20	0
13	SG	1903	0	2068	21	0
14	SJ	1512	0	1629	9	0
15	SN	1208	0	1294	18	0
16	SO	1016	0	1038	18	0
17	SW	1034	0	1080	15	0
18	SY	1014	0	1082	9	0
19	Sb	651	0	672	10	0
20	Se	468	0	519	7	0
21	B	587	0	299	2	0
22	SD	1765	0	1865	20	0
23	SF	1495	0	1549	25	0
24	Sf	515	0	523	11	0
25	SR	1064	0	1118	16	0
26	Sd	459	0	448	6	0
27	Sg	2436	0	2391	40	0
28	Sc	506	0	536	11	0
29	SK	816	0	841	25	0
30	SM	906	0	921	37	0
31	SU	811	0	877	14	0
32	SQ	1124	0	1193	23	0
33	SS	1198	0	1261	18	0
34	ST	1113	0	1145	16	0
35	SP	1103	0	1156	16	0
36	SZ	585	0	640	11	0
37	D	2352	0	2392	44	0
38	E	3585	0	3736	34	0
39	F	143	0	144	1	0
40	G	1623	0	829	7	0
41	H	895	0	924	11	0
42	S2	13	0	0	0	0
42	SX	1	0	0	0	0
42	Sd	1	0	0	0	0
43	S2	70	0	0	0	0
44	Sa	1	0	0	0	0
44	Sd	1	0	0	0	0
44	Sf	1	0	0	0	0
45	E	32	0	13	0	0
46	E	8	0	8	2	0
47	B	2	0	0	0	0
47	S2	327	0	0	0	0
47	SE	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	SL	1	0	0	0	0
47	SO	2	0	0	0	0
47	SQ	1	0	0	0	0
47	Sa	1	0	0	0	0
All	All	85772	0	68007	848	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 6.

All (848) 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)
38:E:157:LEU:HD22	38:E:187:ILE:HG23	1.52	0.90
23:SF:203:ASN:O	23:SF:203:ASN:ND2	2.08	0.87
3:SE:182:MET:HE3	3:SE:192:ILE:HD11	1.64	0.79
12:SC:66:LEU:HD11	12:SC:81:ILE:HD12	1.63	0.78
34:ST:62:ARG:HH12	34:ST:66:LEU:HD11	1.48	0.78
25:SR:109:LEU:O	25:SR:109:LEU:HD23	1.83	0.77
1:S2:164:A:H3'	1:S2:165:G:H21	1.52	0.73
1:S2:72:C:H42	1:S2:74:G:H22	1.37	0.73
13:SG:105:ASN:HD22	13:SG:105:ASN:C	1.97	0.72
4:SA:1:MET:HE1	9:SV:78:ILE:HG23	1.70	0.72
1:S2:1850:MA6:H103	1:S2:1851:MA6:H102	1.72	0.71
27:Sg:134:THR:HG23	27:Sg:135:LEU:HD12	1.72	0.71
25:SR:72:LYS:HE3	25:SR:72:LYS:HA	1.73	0.71
6:SH:176:VAL:O	6:SH:180:LEU:HD12	1.91	0.70
16:SO:56:VAL:HG23	16:SO:77:ALA:HB1	1.74	0.69
29:SK:7:ASN:O	29:SK:11:ILE:HG23	1.93	0.68
38:E:180:MET:HA	38:E:180:MET:HE3	1.74	0.67
27:Sg:218:LEU:HD22	27:Sg:228:TYR:CE1	2.29	0.67
27:Sg:218:LEU:HD22	27:Sg:228:TYR:HE1	1.58	0.67
16:SO:35:ALA:HB2	16:SO:112:ALA:HB2	1.76	0.66
27:Sg:42:MET:HE2	27:Sg:92:LEU:CD1	2.26	0.66
8:SL:113:LEU:HD21	8:SL:120:VAL:HG21	1.78	0.66
13:SG:105:ASN:C	13:SG:105:ASN:ND2	2.54	0.65
33:SS:15:VAL:HG23	33:SS:68:ILE:HD11	1.79	0.65
1:S2:512:A2M:H4'	1:S2:576:A2M:H2	1.78	0.65
15:SN:66:VAL:HG13	15:SN:67:THR:HG23	1.79	0.65
6:SH:95:ILE:HD11	6:SH:133:LEU:HD12	1.77	0.64
1:S2:98:C:H1'	1:S2:99:A2M:H2	1.78	0.64
1:S2:483:C:O2'	1:S2:484:A2M:H5'	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:SA:1:MET:HE3	4:SA:60:LEU:HD13	1.78	0.64
4:SA:18:PHE:CZ	4:SA:177:MET:HE1	2.32	0.64
1:S2:116:OMU:H5	1:S2:347:G:O6	1.97	0.64
27:Sg:42:MET:HE2	27:Sg:92:LEU:HD12	1.80	0.63
34:ST:62:ARG:NH1	34:ST:66:LEU:HD11	2.13	0.63
37:D:73:VAL:HG11	37:D:76:VAL:HG12	1.79	0.63
4:SA:210:ILE:HD13	25:SR:81:ARG:HD3	1.81	0.63
29:SK:89:ILE:O	29:SK:89:ILE:HD12	1.98	0.63
41:H:61:ILE:HA	41:H:91:VAL:HG22	1.81	0.63
30:SM:121:LYS:O	30:SM:125:GLU:OE1	2.17	0.63
30:SM:61:TYR:HA	30:SM:64:LEU:HD11	1.81	0.63
1:S2:575:A:H3'	1:S2:576:A2M:H5''	1.80	0.63
22:SD:25:LEU:HD12	22:SD:37:VAL:HG21	1.79	0.62
23:SF:134:VAL:HG12	23:SF:134:VAL:O	1.98	0.62
23:SF:142:SER:HB2	28:Sc:50:VAL:HG22	1.82	0.62
7:SI:140:LYS:HG3	7:SI:145:ILE:HD11	1.81	0.62
1:S2:1622:U:H3	35:SP:122:THR:HG22	1.64	0.62
28:Sc:46:VAL:HG21	28:Sc:50:VAL:HG21	1.82	0.61
30:SM:79:VAL:HG11	30:SM:85:LEU:HD22	1.83	0.60
5:SB:46:LYS:HE3	16:SO:21:VAL:HG11	1.84	0.60
1:S2:99:A2M:H2'	1:S2:100:PSU:O4'	2.02	0.60
29:SK:3:MET:HE1	29:SK:48:ALA:HB2	1.83	0.60
1:S2:1315:U:H4'	29:SK:2:LEU:HD22	1.82	0.60
27:Sg:91:ASP:OD2	27:Sg:94:THR:HG22	2.02	0.60
16:SO:56:VAL:HG22	16:SO:81:VAL:HG13	1.83	0.60
12:SC:75:ILE:HG21	12:SC:81:ILE:HD11	1.83	0.59
27:Sg:236:ILE:HG12	27:Sg:252:THR:HG22	1.84	0.59
15:SN:102:LEU:HD21	15:SN:111:ALA:HB3	1.84	0.59
1:S2:1404:U:C5	31:SU:88:LEU:HD21	2.37	0.59
13:SG:105:ASN:ND2	13:SG:105:ASN:O	2.24	0.59
1:S2:4:C:H4'	12:SC:207:ALA:HB2	1.85	0.59
6:SH:133:LEU:HD11	6:SH:176:VAL:CG1	2.32	0.59
1:S2:537:C:H41	1:S2:546:G:H21	1.49	0.58
28:Sc:46:VAL:CG2	28:Sc:50:VAL:HG21	2.33	0.58
30:SM:64:LEU:HD12	30:SM:64:LEU:H	1.68	0.58
4:SA:1:MET:HE1	9:SV:78:ILE:CG2	2.32	0.58
25:SR:109:LEU:HD22	25:SR:111:PHE:HD2	1.69	0.58
27:Sg:171:ASP:OD1	27:Sg:173:LEU:HD13	2.03	0.58
9:SV:16:LYS:H	12:SC:259:THR:HG21	1.68	0.58
8:SL:16:ILE:HD13	8:SL:36:TYR:HB2	1.85	0.58
35:SP:21:ASP:OD1	35:SP:24:GLN:NE2	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:SF:40:ALA:HB1	23:SF:45:TYR:CD2	2.39	0.58
8:SL:80:MET:HE1	8:SL:120:VAL:HG23	1.86	0.57
4:SA:137:ALA:HB1	4:SA:142:LEU:HB3	1.86	0.57
22:SD:12:VAL:HG11	26:Sd:36:LEU:HD22	1.86	0.57
1:S2:1030:A:H2'	1:S2:1031:A2M:H8	1.87	0.57
27:Sg:168:CYS:SG	27:Sg:198:VAL:HB	2.45	0.57
36:SZ:44:LEU:HD12	36:SZ:44:LEU:O	2.04	0.57
17:SW:23:ARG:HE	17:SW:23:ARG:HA	1.70	0.56
23:SF:195:GLU:HG3	37:D:45:MET:HE3	1.87	0.56
1:S2:27:A2M:HM'2	1:S2:28:U:O4'	2.05	0.56
30:SM:60:MET:HE3	30:SM:60:MET:H	1.69	0.56
1:S2:1832:6MZ:H9C2	1:S2:1833:C:H41	1.70	0.56
3:SE:252:ARG:O	3:SE:256:LEU:HD13	2.05	0.56
32:SQ:100:VAL:HG23	32:SQ:101:ASP:N	2.20	0.56
36:SZ:69:THR:OG1	36:SZ:72:VAL:HG12	2.05	0.56
30:SM:58:GLU:C	30:SM:58:GLU:OE1	2.49	0.56
4:SA:112:ILE:HD12	4:SA:113:GLN:N	2.21	0.56
38:E:257:ILE:HG23	38:E:410:SER:HB3	1.88	0.56
3:SE:56:LEU:HD11	18:SY:72:PHE:CE2	2.41	0.56
15:SN:129:TYR:HB3	15:SN:135:LEU:HD12	1.88	0.55
23:SF:27:ASP:OD1	23:SF:27:ASP:C	2.48	0.55
22:SD:38:GLU:N	22:SD:38:GLU:OE1	2.39	0.55
1:S2:1091:C:HO2'	17:SW:2:VAL:N	2.05	0.55
1:S2:943:U:O2	16:SO:137:SER:OG	2.14	0.55
8:SL:22:ARG:HD2	8:SL:23:VAL:H	1.70	0.55
33:SS:16:LEU:O	33:SS:18:THR:HG23	2.06	0.55
1:S2:867:OMG:HM22	1:S2:868:G:O4'	2.07	0.55
36:SZ:68:ILE:HD13	36:SZ:97:ILE:HD12	1.88	0.55
23:SF:40:ALA:HB1	23:SF:45:TYR:HD2	1.70	0.54
32:SQ:31:LEU:HB3	32:SQ:67:ASP:OD1	2.07	0.54
1:S2:1517:G:OP1	35:SP:122:THR:HG21	2.08	0.54
27:Sg:206:LEU:HD21	27:Sg:218:LEU:HD23	1.88	0.54
29:SK:9:ILE:O	29:SK:13:GLU:HG3	2.07	0.54
3:SE:139:LEU:HD12	3:SE:139:LEU:C	2.32	0.54
4:SA:1:MET:CE	9:SV:78:ILE:HG23	2.36	0.54
41:H:16:LYS:O	41:H:17:ASN:HB2	2.07	0.54
6:SH:140:VAL:HG22	6:SH:157:HIS:O	2.08	0.54
28:Sc:15:THR:HG22	28:Sc:16:LYS:H	1.72	0.54
6:SH:133:LEU:HD11	6:SH:176:VAL:HG11	1.89	0.54
30:SM:89:VAL:HG11	30:SM:109:VAL:HG21	1.90	0.54
1:S2:532:C:H2'	1:S2:533:A:C8	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:SO:113:GLN:HA	16:SO:113:GLN:HE21	1.73	0.54
37:D:22:VAL:HB	37:D:34:VAL:CG1	2.38	0.54
32:SQ:32:ILE:HD12	32:SQ:68:ILE:HB	1.90	0.53
24:Sf:103:LEU:HD12	24:Sf:103:LEU:O	2.08	0.53
32:SQ:32:ILE:HG23	32:SQ:39:LEU:HD13	1.90	0.53
1:S2:194:C:H2'	1:S2:195:C:C1'	2.37	0.53
8:SL:66:VAL:HG11	8:SL:141:ASN:HD22	1.74	0.53
38:E:170:THR:O	38:E:174:LEU:HD13	2.08	0.53
7:SI:190:LEU:HD22	7:SI:194:GLU:OE1	2.07	0.53
10:SX:100:VAL:CG2	10:SX:122:VAL:HG13	2.39	0.53
15:SN:48:SER:O	15:SN:52:VAL:HG13	2.08	0.53
30:SM:67:ALA:O	30:SM:70:ALA:HB3	2.09	0.53
1:S2:1587:G:C5	34:ST:78:ILE:HD11	2.44	0.53
27:Sg:270:LEU:HD23	27:Sg:310:TRP:CG	2.44	0.53
1:S2:72:C:N4	1:S2:74:G:H22	2.07	0.52
4:SA:1:MET:HG3	4:SA:60:LEU:HA	1.91	0.52
30:SM:122:ASP:HA	30:SM:125:GLU:OE1	2.09	0.52
38:E:90:LYS:HB2	38:E:127:VAL:HG21	1.90	0.52
29:SK:81:ASP:OD1	29:SK:81:ASP:C	2.51	0.52
30:SM:34:GLY:O	30:SM:38:ALA:HB2	2.10	0.52
37:D:59:ILE:C	37:D:59:ILE:HD12	2.34	0.52
1:S2:191:A:OP1	7:SI:145:ILE:HD13	2.09	0.52
15:SN:95:ALA:O	15:SN:99:ARG:HG3	2.10	0.52
31:SU:22:ILE:HG23	31:SU:89:ILE:HB	1.91	0.52
37:D:33:TYR:CZ	37:D:45:MET:HE1	2.44	0.52
1:S2:575:A:C3'	1:S2:576:A2M:H5''	2.39	0.52
3:SE:20:LEU:HD21	3:SE:46:ILE:HD12	1.92	0.52
4:SA:1:MET:HE2	9:SV:79:VAL:HG12	1.92	0.52
6:SH:66:VAL:HG12	6:SH:96:ALA:HB1	1.92	0.52
30:SM:22:LEU:HD12	30:SM:23:LYS:N	2.25	0.52
6:SH:7:LYS:HZ3	6:SH:21:SER:HB3	1.73	0.52
6:SH:17:ASP:OD1	6:SH:17:ASP:C	2.52	0.52
24:Sf:121:CYS:CA	24:Sf:132:MET:HE1	2.40	0.51
36:SZ:71:ALA:O	36:SZ:75:GLU:HG2	2.10	0.51
1:S2:71:G:H22	13:SG:170:ARG:HH12	1.58	0.51
1:S2:1406:G:H2'	1:S2:1407:U:C6	2.45	0.51
32:SQ:128:GLU:OE2	32:SQ:137:ALA:HB1	2.10	0.51
12:SC:204:ILE:HD11	12:SC:219:ILE:O	2.10	0.51
29:SK:49:MET:HE2	29:SK:69:TRP:CE3	2.45	0.51
1:S2:531:A:H61	1:S2:554:A:H61	1.58	0.51
1:S2:1291:A:C2	1:S2:1308:U:O4	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Sb:37:CYS:SG	19:Sb:63:LEU:HD11	2.51	0.51
22:SD:63:GLY:O	22:SD:66:ILE:HG22	2.10	0.51
35:SP:44:ARG:HG2	35:SP:84:ILE:HD11	1.93	0.51
1:S2:1831:A:H2'	1:S2:1832:6MZ:H8	1.92	0.51
27:Sg:10:THR:HG22	27:Sg:308:ARG:HG2	1.93	0.51
27:Sg:270:LEU:HD23	27:Sg:310:TRP:CD2	2.46	0.51
27:Sg:282:GLU:N	27:Sg:282:GLU:OE2	2.43	0.51
6:SH:109:ARG:H	6:SH:109:ARG:CD	2.24	0.51
16:SO:21:VAL:HG23	16:SO:22:ALA:N	2.26	0.51
17:SW:28:ARG:HB3	17:SW:29:PRO:HD3	1.93	0.51
25:SR:34:VAL:O	25:SR:38:ILE:HG13	2.11	0.51
27:Sg:87:LEU:HG	27:Sg:101:PHE:HB2	1.93	0.51
37:D:198:ALA:HB3	37:D:268:VAL:HB	1.93	0.51
37:D:201:GLY:HA3	38:E:343:ILE:HD12	1.93	0.51
40:G:10:1MG:C5'	40:G:46:M7G:H81	2.41	0.51
6:SH:27:LEU:HD11	6:SH:45:ILE:CD1	2.41	0.51
22:SD:68:GLU:OE2	29:SK:70:TYR:HB3	2.10	0.51
34:ST:39:LEU:HD21	34:ST:47:PRO:HG3	1.92	0.51
31:SU:46:LYS:HG3	31:SU:48:LEU:HD13	1.93	0.51
38:E:395:VAL:HG11	38:E:454:ILE:HG12	1.91	0.51
14:SJ:141:VAL:HG22	18:SY:65:GLY:HA3	1.92	0.51
30:SM:26:LEU:HD22	30:SM:89:VAL:O	2.11	0.51
37:D:59:ILE:HD12	37:D:60:ASN:N	2.26	0.51
12:SC:172:ASN:OD1	12:SC:172:ASN:C	2.54	0.51
29:SK:83:LEU:HB2	29:SK:85:LEU:HD11	1.93	0.51
4:SA:90:PHE:CE1	4:SA:94:THR:HG21	2.46	0.50
7:SI:107:THR:O	7:SI:111:GLN:HG3	2.10	0.50
34:ST:87:VAL:O	34:ST:88:MET:HG2	2.12	0.50
1:S2:98:C:C1'	1:S2:99:A2M:H2	2.41	0.50
1:S2:1405:A:H2'	1:S2:1406:G:O4'	2.12	0.50
37:D:32:ALA:O	37:D:34:VAL:HG23	2.11	0.50
1:S2:116:OMU:H5	1:S2:347:G:C6	2.45	0.50
12:SC:212:LYS:O	12:SC:216:MET:HG3	2.11	0.50
1:S2:549:C:H2'	1:S2:550:C:C6	2.46	0.50
13:SG:77:LEU:HD23	13:SG:84:TYR:HB2	1.93	0.50
37:D:76:VAL:HG23	37:D:76:VAL:O	2.11	0.50
5:SB:69:VAL:HG13	5:SB:74:LEU:HD11	1.93	0.50
7:SI:150:ASP:HA	7:SI:153:LYS:HG2	1.94	0.50
18:SY:98:GLU:C	18:SY:98:GLU:OE1	2.54	0.50
32:SQ:110:ASP:O	32:SQ:114:GLN:HG2	2.11	0.50
38:E:157:LEU:HD12	38:E:174:LEU:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Sb:83:GLN:N	19:Sb:83:GLN:OE1	2.45	0.50
35:SP:22:LEU:O	35:SP:26:LEU:HD23	2.11	0.50
4:SA:24:HIS:HB3	4:SA:51:LEU:HD21	1.94	0.50
5:SB:133:TYR:HD2	5:SB:181:LEU:HB2	1.77	0.50
18:SY:7:ILE:HD11	18:SY:40:ILE:CD1	2.41	0.50
1:S2:14:C:O2	1:S2:668:A2M:H2	2.12	0.50
1:S2:1750:C:H2'	1:S2:1751:C:C1'	2.41	0.50
1:S2:1832:6MZ:H9C2	1:S2:1833:C:N4	2.27	0.50
36:SZ:50:PHE:CE2	36:SZ:58:LEU:HD22	2.47	0.50
37:D:286:LEU:O	37:D:290:MET:SD	2.69	0.50
1:S2:116:OMU:H2'	1:S2:117:C:O4'	2.12	0.49
6:SH:127:ASP:OD1	6:SH:128:ALA:N	2.45	0.49
12:SC:65:LYS:HG2	12:SC:273:LEU:HD13	1.94	0.49
27:Sg:126:ASP:OD1	27:Sg:128:THR:HG22	2.12	0.49
38:E:228:LEU:HD23	38:E:228:LEU:H	1.77	0.49
1:S2:1395:C:O2'	1:S2:1396:A:H5'	2.12	0.49
9:SV:55:ILE:HD13	9:SV:69:ILE:HD11	1.93	0.49
32:SQ:31:LEU:C	32:SQ:31:LEU:HD23	2.37	0.49
37:D:153:PHE:O	37:D:180:ILE:HD11	2.12	0.49
37:D:254:ALA:O	37:D:257:VAL:HG12	2.12	0.49
1:S2:116:OMU:H5	1:S2:347:G:H1	1.77	0.49
1:S2:118:C:H1'	1:S2:445:A:C5	2.46	0.49
1:S2:158:A:H2'	1:S2:159:A2M:O4'	2.13	0.49
6:SH:172:THR:O	6:SH:176:VAL:HG12	2.12	0.49
37:D:255:MET:O	37:D:259:LYS:HG3	2.12	0.49
38:E:44:ILE:HG13	38:E:130:VAL:HG13	1.94	0.49
1:S2:501:C:H2'	1:S2:501:C:O2	2.12	0.49
15:SN:78:LYS:HG2	15:SN:80:LEU:HD11	1.93	0.49
12:SC:59:GLU:OE2	12:SC:59:GLU:HA	2.13	0.49
38:E:90:LYS:HG2	38:E:127:VAL:HG21	1.94	0.49
1:S2:16:G:H2'	1:S2:17:C:C6	2.48	0.49
4:SA:112:ILE:HD12	4:SA:112:ILE:C	2.37	0.49
25:SR:99:ASP:OD1	25:SR:100:PRO:HD2	2.13	0.49
30:SM:122:ASP:O	30:SM:123:VAL:HB	2.12	0.49
41:H:50:MET:HE3	41:H:51:CYS:O	2.13	0.49
1:S2:659:G:H21	10:SX:17:ARG:NH2	2.11	0.49
24:Sf:103:LEU:HD22	30:SM:36:ARG:HD3	1.95	0.49
6:SH:176:VAL:HG22	6:SH:180:LEU:CD1	2.43	0.49
12:SC:254:ASP:OD1	12:SC:254:ASP:C	2.55	0.49
29:SK:89:ILE:HD12	29:SK:89:ILE:C	2.38	0.49
30:SM:42:LEU:HD11	30:SM:65:VAL:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:550:C:H2'	1:S2:551:U:C6	2.48	0.49
8:SL:49:GLU:C	8:SL:49:GLU:OE1	2.56	0.49
24:Sf:108:VAL:HG11	30:SM:63:LYS:HD2	1.95	0.49
27:Sg:68:ASP:HB3	27:Sg:111:VAL:HG12	1.95	0.49
1:S2:1227:G:C2	1:S2:1228:A:C8	3.01	0.48
3:SE:139:LEU:HD22	3:SE:154:ILE:HG21	1.95	0.48
7:SI:78:ILE:HG23	7:SI:102:VAL:HG21	1.94	0.48
40:G:10:1MG:H5''	40:G:46:M7G:H81	1.95	0.48
1:S2:1031:A2M:HM'3	1:S2:1031:A2M:H1'	1.68	0.48
3:SE:251:GLU:OE2	3:SE:251:GLU:C	2.56	0.48
13:SG:20:ASP:OD1	13:SG:20:ASP:C	2.57	0.48
30:SM:64:LEU:O	30:SM:68:LEU:HD12	2.12	0.48
1:S2:1164:G:O2'	1:S2:1165:G:H5'	2.14	0.48
22:SD:161:GLY:O	22:SD:164:VAL:HG12	2.14	0.48
30:SM:92:CYS:HB2	30:SM:101:ARG:CB	2.43	0.48
23:SF:73:THR:HG22	23:SF:93:VAL:HG11	1.96	0.48
31:SU:36:CYS:O	31:SU:40:ILE:HD12	2.12	0.48
6:SH:69:LEU:O	6:SH:73:GLN:HG3	2.13	0.48
6:SH:126:HIS:CE1	6:SH:181:THR:HG22	2.49	0.48
15:SN:60:VAL:O	15:SN:60:VAL:HG23	2.13	0.48
1:S2:2:A:O4'	1:S2:418:A:C8	2.66	0.48
1:S2:1388:A:H61	22:SD:161:GLY:HA3	1.79	0.48
1:S2:1479:G:H4'	32:SQ:128:GLU:OE1	2.14	0.48
4:SA:179:ALA:O	4:SA:183:LEU:HD23	2.14	0.48
5:SB:48:LEU:O	5:SB:48:LEU:HD12	2.14	0.48
9:SV:71:ARG:HB3	9:SV:71:ARG:NH1	2.29	0.48
13:SG:63:MET:HG3	13:SG:99:GLY:O	2.14	0.48
14:SJ:49:THR:O	14:SJ:53:ILE:HG23	2.13	0.48
18:SY:25:ILE:HD11	18:SY:73:GLY:HA3	1.96	0.48
31:SU:68:THR:HG23	31:SU:70:CYS:O	2.14	0.48
24:Sf:146:LEU:C	24:Sf:146:LEU:HD12	2.39	0.48
27:Sg:153:CYS:SG	27:Sg:168:CYS:O	2.71	0.48
23:SF:168:THR:HG22	23:SF:171:GLU:OE2	2.13	0.48
32:SQ:61:GLU:CD	32:SQ:61:GLU:H	2.22	0.48
1:S2:1678:A2M:HM'3	1:S2:1678:A2M:H1'	1.67	0.47
24:Sf:121:CYS:HA	24:Sf:132:MET:HE1	1.96	0.47
30:SM:64:LEU:HD12	30:SM:64:LEU:N	2.28	0.47
33:SS:16:LEU:O	33:SS:17:ASN:OD1	2.32	0.47
1:S2:512:A2M:H5'	1:S2:576:A2M:N1	2.29	0.47
12:SC:211:LYS:O	12:SC:215:MET:HG3	2.14	0.47
27:Sg:304:ASP:OD1	27:Sg:304:ASP:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:SK:53:LYS:HD2	29:SK:60:GLU:HB2	1.95	0.47
6:SH:166:VAL:HG12	6:SH:166:VAL:O	2.14	0.47
1:S2:1373:C:OP1	25:SR:7:LYS:HB2	2.15	0.47
14:SJ:59:GLU:C	14:SJ:59:GLU:OE2	2.57	0.47
22:SD:223:ILE:HD12	22:SD:223:ILE:C	2.40	0.47
1:S2:659:G:H21	10:SX:17:ARG:CZ	2.27	0.47
1:S2:1271:C:O3'	1:S2:1303:C:H5'	2.13	0.47
27:Sg:133:ASN:HA	27:Sg:139:LYS:HZ2	1.78	0.47
35:SP:86:LEU:HB3	35:SP:88:GLU:OE2	2.14	0.47
1:S2:455:A:H2'	1:S2:456:C:H6	1.80	0.47
1:S2:461:U:O2'	1:S2:462:OMC:P	2.73	0.47
1:S2:563:G:C2	1:S2:564:A:C8	3.02	0.47
1:S2:1610:G:O3'	33:SS:110:ASP:OD2	2.32	0.47
9:SV:15:ARG:NH1	9:SV:24:ILE:HG21	2.30	0.47
19:Sb:7:LEU:HD12	19:Sb:7:LEU:H	1.80	0.47
33:SS:50:ILE:O	33:SS:50:ILE:HG22	2.15	0.47
35:SP:142:ILE:N	35:SP:143:PRO:HD3	2.30	0.47
37:D:100:ASP:OD1	37:D:101:LYS:N	2.48	0.47
38:E:32:SER:HB2	38:E:35:VAL:HG12	1.96	0.47
1:S2:15:U:H2'	1:S2:16:G:O4'	2.15	0.47
22:SD:169:ASP:HB2	22:SD:190:LEU:HD21	1.97	0.47
31:SU:24:LEU:HD12	31:SU:112:VAL:HG22	1.96	0.47
38:E:90:LYS:CG	38:E:127:VAL:HG21	2.45	0.47
38:E:157:LEU:CD2	38:E:187:ILE:HG23	2.34	0.47
1:S2:446:G:P	7:SI:47:ARG:HH12	2.38	0.47
23:SF:156:THR:O	23:SF:160:GLU:OE1	2.33	0.47
34:ST:51:ASN:O	34:ST:55:THR:HG23	2.13	0.47
38:E:278:VAL:HG11	46:E:502:MET:HE3	1.97	0.47
1:S2:866:PSU:O2'	1:S2:867:OMG:P	2.73	0.47
12:SC:70:VAL:HG21	12:SC:93:ILE:HG23	1.97	0.47
1:S2:84:A:N3	1:S2:150:A:O2'	2.45	0.46
1:S2:796:G:H3'	1:S2:797:C:H5''	1.97	0.46
8:SL:81:LYS:O	8:SL:81:LYS:HG3	2.15	0.46
21:B:8:A:OP1	21:B:8:A:C8	2.68	0.46
25:SR:72:LYS:O	25:SR:76:GLU:HG2	2.15	0.46
36:SZ:100:VAL:HG13	36:SZ:108:ILE:HB	1.97	0.46
41:H:61:ILE:HD11	41:H:66:ARG:HE	1.80	0.46
1:S2:1228:A:H2'	1:S2:1229:G:C8	2.50	0.46
6:SH:147:LYS:O	17:SW:42:MET:HE1	2.15	0.46
23:SF:99:ILE:HD13	23:SF:171:GLU:HG3	1.98	0.46
34:ST:18:LEU:HA	34:ST:134:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:E:222:ILE:HA	39:F:179:LEU:HD21	1.97	0.46
1:S2:562:U:H2'	1:S2:563:G:C8	2.51	0.46
1:S2:925:G:H5''	15:SN:91:LEU:HD21	1.98	0.46
1:S2:1387:G:H21	25:SR:8:THR:HG21	1.80	0.46
1:S2:1850:MA6:H103	1:S2:1851:MA6:C10	2.43	0.46
4:SA:1:MET:SD	9:SV:78:ILE:HG12	2.55	0.46
13:SG:57:ASP:HA	13:SG:106:LEU:HD23	1.97	0.46
14:SJ:60:LEU:HB2	14:SJ:94:LEU:HD21	1.98	0.46
27:Sg:35:SER:O	27:Sg:66:VAL:HG12	2.15	0.46
34:ST:126:GLN:O	34:ST:130:ASP:OD1	2.33	0.46
1:S2:537:C:H41	1:S2:546:G:N2	2.12	0.46
1:S2:1567:G:C6	33:SS:82:TRP:CG	3.03	0.46
4:SA:213:GLU:H	4:SA:213:GLU:CD	2.22	0.46
28:Sc:62:GLU:OE2	28:Sc:62:GLU:O	2.33	0.46
35:SP:75:VAL:HG21	35:SP:104:GLN:NE2	2.31	0.46
1:S2:1097:G:H4'	4:SA:32:PHE:CD1	2.50	0.46
1:S2:1301:A:H4'	26:Sd:3:HIS:HE1	1.80	0.46
1:S2:1406:G:H2'	1:S2:1407:U:H6	1.81	0.46
29:SK:21:MET:HE3	29:SK:49:MET:SD	2.56	0.46
41:H:16:LYS:O	41:H:17:ASN:CB	2.64	0.46
1:S2:29:G:H2'	1:S2:30:C:C6	2.51	0.46
1:S2:614:C:H5''	1:S2:615:C:C6	2.50	0.46
1:S2:918:PSU:O2'	1:S2:919:A:O5'	2.34	0.46
1:S2:1203:G:H2'	1:S2:1204:A:C8	2.51	0.46
1:S2:1588:A:H2'	1:S2:1589:A:C8	2.50	0.46
9:SV:24:ILE:O	9:SV:24:ILE:HG22	2.16	0.46
13:SG:228:ILE:HD12	13:SG:229:ALA:N	2.31	0.46
20:Se:6:LEU:O	20:Se:7:ALA:HB3	2.16	0.46
1:S2:1531:A:H2'	1:S2:1532:C:C6	2.51	0.46
1:S2:1661:A:C8	26:Sd:14:PHE:CD1	3.04	0.46
1:S2:1798:C:H2'	1:S2:1799:G:O4'	2.15	0.46
1:S2:1850:MA6:H2'	1:S2:1851:MA6:O4'	2.15	0.46
7:SI:119:LEU:HD13	7:SI:120:PRO:HD2	1.97	0.46
32:SQ:22:VAL:HG11	32:SQ:71:ARG:NH2	2.31	0.46
34:ST:18:LEU:HD13	34:ST:134:ILE:HD12	1.96	0.46
23:SF:152:TRP:O	23:SF:156:THR:HG22	2.15	0.46
30:SM:18:LEU:O	30:SM:22:LEU:HG	2.16	0.46
30:SM:31:LEU:HD21	30:SM:89:VAL:HB	1.97	0.46
30:SM:69:CYS:HB3	30:SM:74:ILE:HD11	1.97	0.46
37:D:34:VAL:HG21	37:D:46:ILE:HG13	1.98	0.46
37:D:111:ILE:O	37:D:115:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:102:A:H4'	1:S2:104:A:C8	2.51	0.46
1:S2:531:A:HO2'	1:S2:532:C:H6	1.55	0.46
1:S2:581:U:H4'	18:SY:66:GLY:HA2	1.99	0.46
1:S2:1238:PSU:O4	1:S2:1242:U:H5	1.99	0.46
12:SC:60:TRP:NE1	12:SC:92:GLU:OE1	2.49	0.46
4:SA:1:MET:CG	4:SA:60:LEU:HA	2.46	0.45
29:SK:13:GLU:O	29:SK:17:LYS:HG3	2.16	0.45
34:ST:65:TYR:CD1	34:ST:65:TYR:C	2.95	0.45
7:SI:34:ALA:HB2	7:SI:56:ARG:CD	2.47	0.45
31:SU:42:GLY:C	31:SU:101:ILE:HD11	2.42	0.45
31:SU:56:MET:HE3	31:SU:88:LEU:HD22	1.97	0.45
1:S2:482:G:N2	1:S2:484:A2M:H3'	2.32	0.45
1:S2:955:A:H4'	16:SO:60:MET:SD	2.56	0.45
1:S2:1453:C:H4'	25:SR:49:LYS:HA	1.99	0.45
14:SJ:127:ARG:HD2	20:Se:31:ARG:HD3	1.98	0.45
15:SN:106:ARG:CZ	15:SN:106:ARG:HB2	2.46	0.45
29:SK:74:GLU:OE2	29:SK:74:GLU:C	2.59	0.45
1:S2:443:U:H2'	1:S2:444:G:O4'	2.17	0.45
1:S2:943:U:C2	16:SO:137:SER:OG	2.65	0.45
1:S2:1374:C:H2'	1:S2:1375:G:O4'	2.17	0.45
5:SB:229:MET:HE3	5:SB:229:MET:HA	1.97	0.45
7:SI:80:ASP:OD1	7:SI:81:VAL:N	2.50	0.45
12:SC:94:ILE:HD12	12:SC:159:LYS:O	2.17	0.45
24:Sf:102:VAL:O	24:Sf:103:LEU:HG	2.17	0.45
1:S2:1316:C:O2'	1:S2:1317:C:P	2.74	0.45
1:S2:1634:A:H2'	1:S2:1635:C:O4'	2.17	0.45
6:SH:73:GLN:HB3	6:SH:135:PHE:CE2	2.51	0.45
10:SX:50:ILE:HG13	10:SX:50:ILE:O	2.16	0.45
27:Sg:79:LEU:HG	27:Sg:111:VAL:HG21	1.98	0.45
27:Sg:240:CYS:O	27:Sg:248:LEU:HD22	2.17	0.45
28:Sc:18:LEU:HD11	28:Sc:43:ILE:HD12	1.98	0.45
1:S2:76:U:H3'	1:S2:77:A:C5'	2.46	0.45
1:S2:116:OMU:HM22	1:S2:117:C:O4'	2.17	0.45
4:SA:23:THR:HG22	4:SA:23:THR:O	2.17	0.45
6:SH:45:ILE:HD13	6:SH:62:ILE:HG23	1.98	0.45
9:SV:40:ASP:OD1	9:SV:41:LYS:N	2.50	0.45
16:SO:56:VAL:CG2	16:SO:81:VAL:HG13	2.47	0.45
27:Sg:273:GLU:N	27:Sg:273:GLU:OE1	2.49	0.45
32:SQ:102:GLU:HA	32:SQ:105:LYS:HB3	1.98	0.45
1:S2:69:C:H5''	13:SG:167:LYS:HZ2	1.82	0.45
4:SA:1:MET:HB2	4:SA:59:LEU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:SJ:58:ARG:O	14:SJ:62:THR:HG23	2.16	0.45
27:Sg:42:MET:HE2	27:Sg:92:LEU:HD13	1.97	0.45
30:SM:66:GLU:HA	30:SM:69:CYS:SG	2.57	0.45
38:E:347:LEU:O	38:E:353:MET:HE2	2.17	0.45
6:SH:91:HIS:CD2	6:SH:172:THR:HG21	2.52	0.45
30:SM:33:ARG:HD2	30:SM:91:LEU:HD21	1.98	0.45
33:SS:109:GLU:C	33:SS:109:GLU:OE2	2.60	0.45
1:S2:34:PSU:HO2'	1:S2:35:C:H6	1.64	0.45
1:S2:484:A2M:O5'	1:S2:484:A2M:H8	2.16	0.45
1:S2:846:G:C5	3:SE:19:MET:SD	3.10	0.45
1:S2:928:G:H2'	1:S2:929:G:C8	2.52	0.45
4:SA:163:CYS:HB3	4:SA:174:MET:HE2	1.97	0.45
9:SV:54:ALA:C	9:SV:55:ILE:HD12	2.42	0.45
12:SC:275:LYS:HD2	12:SC:275:LYS:C	2.42	0.45
13:SG:37:ALA:HB1	13:SG:39:ASP:OD1	2.17	0.45
19:Sb:53:VAL:HG23	19:Sb:53:VAL:O	2.16	0.45
32:SQ:104:SER:HA	32:SQ:107:GLU:HG2	1.98	0.45
1:S2:1036:A:C4	1:S2:1037:G:C8	3.05	0.45
1:S2:1516:G:H4'	35:SP:122:THR:OG1	2.17	0.45
1:S2:1851:MA6:H5''	2:Ln:1:MET:HE3	1.98	0.45
4:SA:21:ALA:O	4:SA:22:GLY:C	2.60	0.45
6:SH:140:VAL:HG22	6:SH:157:HIS:C	2.42	0.45
7:SI:34:ALA:HB2	7:SI:56:ARG:HD2	1.99	0.45
13:SG:218:LYS:O	13:SG:222:GLU:HG2	2.17	0.45
25:SR:6:THR:HG22	25:SR:7:LYS:N	2.32	0.45
27:Sg:197:THR:HG23	27:Sg:239:LEU:HD22	1.99	0.45
33:SS:30:ILE:HD11	33:SS:45:LEU:CD2	2.47	0.45
37:D:183:ARG:C	37:D:184:LEU:HD12	2.41	0.45
1:S2:376:A:H2'	1:S2:377:G:O4'	2.17	0.44
1:S2:429:C:H4'	3:SE:12:VAL:HG23	1.98	0.44
4:SA:63:ARG:NH1	9:SV:39:VAL:HG22	2.32	0.44
23:SF:87:LEU:HD22	32:SQ:47:LEU:HD13	2.00	0.44
31:SU:46:LYS:CG	31:SU:48:LEU:HD13	2.47	0.44
31:SU:46:LYS:HD3	31:SU:101:ILE:HD12	1.98	0.44
37:D:220:THR:HG22	37:D:221:GLU:N	2.33	0.44
38:E:259:ILE:O	38:E:354:VAL:HG13	2.16	0.44
40:G:46:M7G:H4'	40:G:47:H2U:P	2.57	0.44
1:S2:918:PSU:O2'	1:S2:919:A:C8	2.64	0.44
20:Se:11:LYS:O	20:Se:15:GLN:OE1	2.35	0.44
29:SK:88:GLU:N	29:SK:88:GLU:OE1	2.48	0.44
31:SU:46:LYS:HZ1	31:SU:97:ILE:HG12	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:D:113:ARG:HG3	37:D:127:LEU:HD21	1.99	0.44
38:E:347:LEU:HG	38:E:353:MET:HE1	1.99	0.44
41:H:58:LEU:N	41:H:58:LEU:HD22	2.32	0.44
1:S2:1421:A:H2'	1:S2:1422:G:O4'	2.16	0.44
1:S2:1466:G:OP1	25:SR:5:ARG:HG2	2.17	0.44
1:S2:1666:C:H2'	1:S2:1667:U:O4'	2.17	0.44
1:S2:563:G:HO2'	1:S2:564:A:P	2.40	0.44
4:SA:108:PHE:HB2	4:SA:136:GLU:HG2	1.99	0.44
5:SB:196:ASP:OD1	5:SB:197:ILE:N	2.50	0.44
6:SH:27:LEU:HD11	6:SH:45:ILE:HD12	1.99	0.44
9:SV:38:GLU:OE2	9:SV:78:ILE:HD12	2.18	0.44
28:Sc:63:ARG:O	28:Sc:64:GLU:C	2.60	0.44
35:SP:65:LYS:HD3	35:SP:65:LYS:N	2.31	0.44
1:S2:1220:A:H2'	1:S2:1221:G:O4'	2.18	0.44
1:S2:1304:U:O2	1:S2:1304:U:O5'	2.34	0.44
1:S2:1536:G:H2'	1:S2:1537:A:C8	2.53	0.44
1:S2:1638:G:O3'	1:S2:1639:M7G:PA	2.74	0.44
1:S2:1828:C:C4	1:S2:1829:G:N7	2.86	0.44
30:SM:79:VAL:CG1	30:SM:85:LEU:HD22	2.47	0.44
30:SM:82:ASN:HA	30:SM:85:LEU:CD2	2.48	0.44
33:SS:95:TYR:CD1	33:SS:95:TYR:N	2.86	0.44
37:D:150:TYR:CD1	37:D:150:TYR:C	2.96	0.44
1:S2:579:C:C4	1:S2:580:U:C5	3.06	0.44
1:S2:928:G:H1	1:S2:1013:U:H3	1.65	0.44
1:S2:1223:A:O2'	1:S2:1651:A:H4'	2.17	0.44
6:SH:57:ARG:HH11	6:SH:57:ARG:HG2	1.83	0.44
6:SH:109:ARG:H	6:SH:109:ARG:HD2	1.82	0.44
28:Sc:15:THR:O	28:Sc:16:LYS:C	2.59	0.44
32:SQ:34:VAL:HG13	32:SQ:39:LEU:HD12	1.98	0.44
32:SQ:100:VAL:CG2	32:SQ:101:ASP:N	2.80	0.44
1:S2:520:A:H5''	14:SJ:12:THR:HG23	2.00	0.44
4:SA:1:MET:O	4:SA:2:SER:C	2.61	0.44
16:SO:98:ARG:HG3	16:SO:99:ALA:O	2.18	0.44
37:D:93:GLU:O	37:D:96:ILE:HG13	2.17	0.44
1:S2:640:A:H2'	1:S2:641:A:C8	2.52	0.44
13:SG:32:MET:HE2	13:SG:65:GLN:HG2	2.00	0.44
15:SN:59:GLY:HA3	19:Sb:45:THR:HG21	1.99	0.44
16:SO:44:VAL:HG11	16:SO:85:CYS:SG	2.58	0.44
17:SW:23:ARG:HA	17:SW:23:ARG:NE	2.32	0.44
25:SR:6:THR:CG2	25:SR:7:LYS:N	2.81	0.44
28:Sc:36:ASP:OD1	28:Sc:37:ASP:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1344:A:H4'	1:S2:1345:G:OP1	2.18	0.44
1:S2:1556:A:H2'	1:S2:1556:A:N3	2.33	0.44
3:SE:139:LEU:HD12	3:SE:139:LEU:O	2.18	0.44
4:SA:119:PRO:HG2	4:SA:142:LEU:HD21	1.99	0.44
5:SB:53:GLN:N	5:SB:53:GLN:OE1	2.51	0.44
22:SD:217:ILE:HD12	22:SD:217:ILE:N	2.32	0.44
34:ST:50:GLU:HA	34:ST:50:GLU:OE1	2.18	0.44
1:S2:96:C:H2'	1:S2:97:U:C6	2.53	0.43
1:S2:216:C:C2	1:S2:217:A:C8	3.06	0.43
1:S2:746:C:H2'	1:S2:747:U:O4'	2.18	0.43
1:S2:958:G:H2'	1:S2:959:G:O4'	2.17	0.43
1:S2:1434:C:H3'	1:S2:1435:C:H4'	2.00	0.43
1:S2:1535:U:H1'	23:SF:88:MET:HE3	1.99	0.43
1:S2:1808:U:H2'	1:S2:1809:A:C8	2.53	0.43
15:SN:66:VAL:CG1	15:SN:67:THR:HG23	2.48	0.43
22:SD:138:VAL:CG1	22:SD:182:LEU:HD21	2.48	0.43
38:E:367:ILE:HD12	38:E:367:ILE:O	2.18	0.43
1:S2:1286:G:O6	30:SM:36:ARG:HB2	2.18	0.43
1:S2:1383:A2M:HM'2	1:S2:1384:C:O4'	2.18	0.43
1:S2:1396:A:O2'	1:S2:1398:G:N7	2.46	0.43
4:SA:5:LEU:HD21	9:SV:41:LYS:HA	2.00	0.43
34:ST:70:ALA:HB1	34:ST:74:SER:OG	2.18	0.43
1:S2:198:U:H2'	1:S2:199:C:H2'	2.00	0.43
8:SL:136:LYS:HG2	8:SL:137:THR:HG23	2.00	0.43
27:Sg:56:GLN:C	32:SQ:102:GLU:OE1	2.61	0.43
37:D:97:LYS:O	37:D:100:ASP:OD1	2.36	0.43
37:D:197:VAL:HG13	37:D:262:ILE:HD11	1.98	0.43
37:D:211:ALA:HB1	37:D:258:ILE:HD11	2.00	0.43
38:E:405:MET:HE1	38:E:412:SER:OG	2.17	0.43
1:S2:107:A:H2'	1:S2:108:G:C8	2.53	0.43
1:S2:468:A2M:H1'	1:S2:468:A2M:HM'3	1.62	0.43
1:S2:695:C:H5''	1:S2:696:G:H5'	2.00	0.43
1:S2:1037:G:H4'	1:S2:1845:A:H4'	1.99	0.43
1:S2:1217:A:H2'	1:S2:1218:C:C6	2.53	0.43
1:S2:1277:C:H2'	1:S2:1278:A:H8	1.84	0.43
25:SR:95:ILE:HD11	25:SR:118:GLN:HB2	2.01	0.43
34:ST:21:PHE:O	34:ST:24:LYS:HG3	2.19	0.43
1:S2:1535:U:O2'	23:SF:82:ASN:OD1	2.34	0.43
7:SI:130:THR:HG22	7:SI:133:GLU:HG3	2.00	0.43
9:SV:66:ASP:OD1	9:SV:66:ASP:C	2.61	0.43
11:Sa:40:VAL:CG1	11:Sa:69:VAL:HG13	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:SO:98:ARG:HB2	16:SO:132:VAL:HG23	1.99	0.43
27:Sg:101:PHE:CD1	27:Sg:101:PHE:N	2.86	0.43
38:E:185:ILE:O	38:E:186:LEU:HD12	2.19	0.43
1:S2:455:A:H2'	1:S2:456:C:C6	2.53	0.43
1:S2:544:G:N3	1:S2:544:G:H2'	2.32	0.43
1:S2:1316:C:HO2'	1:S2:1317:C:P	2.42	0.43
9:SV:1:MET:HG2	9:SV:2:GLN:N	2.33	0.43
37:D:115:VAL:HG21	37:D:176:LEU:HD23	2.01	0.43
1:S2:116:OMU:O5'	1:S2:116:OMU:O2	2.36	0.43
1:S2:1035:A:C4	1:S2:1036:A:C8	3.07	0.43
1:S2:1173:A:H2'	1:S2:1174:PSU:O4'	2.19	0.43
1:S2:1234:C:N4	33:SS:137:LYS:HE3	2.33	0.43
4:SA:18:PHE:HD1	4:SA:23:THR:HG21	1.84	0.43
4:SA:161:ILE:HG22	4:SA:174:MET:HE1	2.01	0.43
5:SB:124:HIS:HA	5:SB:137:LEU:O	2.19	0.43
6:SH:61:ILE:HG23	6:SH:95:ILE:HD13	2.01	0.43
6:SH:139:ILE:O	6:SH:139:ILE:HG22	2.19	0.43
11:Sa:18:VAL:HG21	11:Sa:33:ASP:OD2	2.19	0.43
12:SC:127:PHE:CD2	12:SC:141:VAL:HG22	2.54	0.43
17:SW:30:CYS:SG	17:SW:61:ILE:HD11	2.59	0.43
30:SM:90:GLY:O	30:SM:91:LEU:HD23	2.18	0.43
38:E:52:HIS:HB2	38:E:160:ALA:HB2	1.99	0.43
1:S2:116:OMU:H5	1:S2:347:G:N1	2.33	0.43
1:S2:612:U:H4'	20:Se:15:GLN:NE2	2.34	0.43
7:SI:142:SER:O	7:SI:146:GLN:HB2	2.19	0.43
9:SV:18:SER:HB3	9:SV:72:LEU:HD21	2.00	0.43
9:SV:37:ALA:HB1	9:SV:46:PHE:CD1	2.53	0.43
1:S2:1388:A:C2	22:SD:205:PRO:HG2	2.54	0.43
33:SS:5:ILE:HG23	36:SZ:49:LEU:O	2.18	0.43
37:D:256:ALA:HA	37:D:259:LYS:HG3	2.00	0.43
40:G:11[1]:2MG:HN2	40:G:45:G:H21	1.66	0.43
1:S2:415:A:H2'	1:S2:416:U:O4'	2.19	0.43
1:S2:929:G:H2'	1:S2:930:C:O4'	2.18	0.43
1:S2:976:G:H21	16:SO:50:LYS:NZ	2.17	0.43
1:S2:1444:U:H2'	1:S2:1445:PSU:O4'	2.18	0.43
4:SA:18:PHE:CD1	4:SA:23:THR:HG21	2.53	0.43
6:SH:148:LEU:HA	17:SW:42:MET:HE3	2.00	0.43
9:SV:16:LYS:N	12:SC:259:THR:HG21	2.34	0.43
10:SX:100:VAL:HG23	10:SX:124:LYS:O	2.17	0.43
12:SC:253:PRO:HG2	17:SW:99:PHE:HB2	2.00	0.43
13:SG:129:VAL:HG23	13:SG:129:VAL:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:SW:111:MET:HE2	17:SW:115:GLU:HG3	2.01	0.43
22:SD:157:MET:HA	22:SD:157:MET:HE2	2.01	0.43
23:SF:127:ARG:HH11	23:SF:127:ARG:HG2	1.83	0.43
35:SP:82:ASP:OD1	35:SP:82:ASP:C	2.61	0.43
1:S2:614:C:H4'	1:S2:615:C:O5'	2.18	0.42
1:S2:798:G:H3'	1:S2:800:U:OP2	2.18	0.42
1:S2:1263:U:H4'	26:Sd:27:ARG:HD3	2.01	0.42
1:S2:1300:U:H4'	1:S2:1301:A:O5'	2.19	0.42
7:SI:113:TYR:CD1	7:SI:121:LEU:HD22	2.54	0.42
13:SG:23:LYS:O	13:SG:24:LEU:HB2	2.18	0.42
15:SN:45:LEU:HD21	15:SN:53:ILE:HD12	2.01	0.42
30:SM:36:ARG:HH12	30:SM:40:LYS:HE3	1.84	0.42
37:D:212:LEU:O	37:D:216:LEU:HG	2.19	0.42
41:H:4:ASN:HD22	41:H:70:TRP:CD1	2.37	0.42
1:S2:679:A:C5	1:S2:680:G:C8	3.07	0.42
1:S2:1088:U:H4'	1:S2:1089:G:OP2	2.19	0.42
1:S2:1520:G:O2'	1:S2:1521:C:OP1	2.28	0.42
24:Sf:100:LEU:O	24:Sf:100:LEU:HD23	2.19	0.42
31:SU:54:VAL:HB	31:SU:88:LEU:HB2	2.01	0.42
38:E:59:LYS:HD2	38:E:64:VAL:O	2.19	0.42
1:S2:1043:G:H2'	1:S2:1044:G:O4'	2.18	0.42
4:SA:63:ARG:CZ	9:SV:39:VAL:HG22	2.49	0.42
5:SB:120:MET:HG3	5:SB:142:PHE:CE2	2.54	0.42
9:SV:40:ASP:OD2	9:SV:43:THR:HG22	2.19	0.42
30:SM:26:LEU:HB2	30:SM:31:LEU:HD22	2.00	0.42
1:S2:59:U:H5''	1:S2:503:C:N4	2.35	0.42
1:S2:564:A:H2'	1:S2:565:G:O4'	2.20	0.42
1:S2:1009:A:O2'	15:SN:114:ARG:HG2	2.19	0.42
1:S2:1236:G:O6	33:SS:137:LYS:NZ	2.52	0.42
1:S2:1616:U:O2	1:S2:1661:A:H2	2.02	0.42
1:S2:1717:C:H2'	1:S2:1718:G:O4'	2.20	0.42
1:S2:1797:U:H2'	1:S2:1798:C:C6	2.54	0.42
3:SE:87:MET:HE1	3:SE:236:ILE:HD13	2.00	0.42
6:SH:95:ILE:HG22	6:SH:96:ALA:O	2.20	0.42
7:SI:80:ASP:OD1	7:SI:80:ASP:C	2.61	0.42
15:SN:60:VAL:O	15:SN:60:VAL:CG2	2.67	0.42
20:Se:53:LYS:HG2	20:Se:57:ALA:HB2	2.00	0.42
27:Sg:250:ALA:HB3	27:Sg:259:TRP:HZ3	1.85	0.42
33:SS:95:TYR:N	33:SS:95:TYR:HD1	2.17	0.42
37:D:239:THR:O	37:D:239:THR:HG23	2.19	0.42
38:E:187:ILE:HB	38:E:221:ILE:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1442:OMU:O5'	1:S2:1442:OMU:H6	2.19	0.42
6:SH:39:GLN:HG3	6:SH:75:ILE:HG21	2.01	0.42
22:SD:49:ILE:HG23	22:SD:89:GLU:HG2	2.02	0.42
23:SF:203:ASN:HD22	23:SF:203:ASN:C	2.10	0.42
38:E:137:GLY:HA2	38:E:145:MET:HE1	2.02	0.42
1:S2:574:A:H4'	18:SY:89:HIS:CB	2.49	0.42
1:S2:616:A:O3'	20:Se:9:ALA:O	2.38	0.42
1:S2:952:G:C6	1:S2:975:G:C6	3.07	0.42
1:S2:1073:U:C2	1:S2:1074:C:C5	3.08	0.42
1:S2:1165:G:H2'	10:SX:23:HIS:O	2.20	0.42
5:SB:69:VAL:HG22	5:SB:73:ASP:HB2	2.01	0.42
7:SI:64:ASN:O	7:SI:186:ASP:HB2	2.20	0.42
23:SF:153:LEU:HA	23:SF:156:THR:HG22	2.02	0.42
29:SK:11:ILE:HD11	29:SK:48:ALA:CB	2.49	0.42
29:SK:18:GLU:O	29:SK:93:THR:HG23	2.19	0.42
30:SM:15:ASN:OD1	30:SM:15:ASN:C	2.62	0.42
33:SS:15:VAL:HG11	33:SS:20:ILE:HD12	2.01	0.42
37:D:177:ILE:HA	37:D:180:ILE:HG22	2.02	0.42
1:S2:76:U:H3'	1:S2:77:A:H5''	2.02	0.42
1:S2:1265:A:H5'	1:S2:1266:C:OP2	2.19	0.42
1:S2:1545:A:H4'	32:SQ:74:GLY:HA2	2.01	0.42
4:SA:126:ASP:C	4:SA:126:ASP:OD1	2.61	0.42
7:SI:64:ASN:HA	7:SI:75:LYS:HA	2.02	0.42
14:SJ:29:LEU:HD23	20:Se:42:PHE:HE2	1.85	0.42
24:Sf:108:VAL:O	24:Sf:108:VAL:HG13	2.19	0.42
27:Sg:262:GLU:OE2	27:Sg:262:GLU:HA	2.20	0.42
34:ST:5:THR:HG22	34:ST:6:VAL:N	2.34	0.42
41:H:18:GLU:O	41:H:21:SER:N	2.53	0.42
1:S2:343:A:O2'	3:SE:140:VAL:HG11	2.19	0.42
1:S2:1226:G:C2	1:S2:1639:M7G:HM71	2.55	0.42
1:S2:1605:G:H2'	1:S2:1606:G:O4'	2.19	0.42
1:S2:1705:C:H2'	1:S2:1706:G:C8	2.55	0.42
3:SE:139:LEU:HD23	3:SE:150:PRO:HB3	2.00	0.42
4:SA:39:TYR:O	4:SA:40:LYS:HB3	2.19	0.42
4:SA:63:ARG:HG2	4:SA:185:MET:SD	2.59	0.42
6:SH:44:ASN:OD1	6:SH:44:ASN:N	2.52	0.42
17:SW:7:LEU:O	17:SW:11:LEU:HD23	2.19	0.42
19:Sb:67:THR:CG2	19:Sb:72:ARG:HD2	2.50	0.42
22:SD:16:ILE:HD11	26:Sd:36:LEU:HD13	2.02	0.42
29:SK:67:PHE:HB2	29:SK:69:TRP:CH2	2.55	0.42
34:ST:62:ARG:O	34:ST:66:LEU:HG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:E:35:VAL:HG21	38:E:332:ALA:HB2	2.00	0.42
1:S2:987:A:C6	5:SB:120:MET:HE1	2.55	0.42
1:S2:1290:G:H2'	1:S2:1291:A:O4'	2.19	0.42
1:S2:1521:C:H5'	35:SP:126:VAL:HG22	2.01	0.42
2:Ln:21:ARG:HG3	2:Ln:21:ARG:HH11	1.85	0.42
3:SE:154:ILE:HD11	3:SE:172:PHE:CG	2.55	0.42
13:SG:157:VAL:CG1	13:SG:176:ILE:HD11	2.50	0.42
17:SW:53:ILE:HD11	19:Sb:8:LEU:HD23	2.02	0.42
22:SD:32:ASP:OD1	22:SD:32:ASP:N	2.52	0.42
29:SK:89:ILE:C	29:SK:89:ILE:CD1	2.93	0.42
32:SQ:52:LEU:O	32:SQ:53:GLU:C	2.62	0.42
35:SP:141:PHE:O	35:SP:142:ILE:HG23	2.20	0.42
38:E:90:LYS:CB	38:E:127:VAL:HG21	2.49	0.42
1:S2:19:A:H2'	1:S2:20:G:O4'	2.20	0.42
1:S2:834:C:H2'	1:S2:835:C:O4'	2.20	0.42
1:S2:1311:C:O5'	1:S2:1312:G:O5'	2.38	0.42
1:S2:1728:U:H3'	1:S2:1729:U:H5''	2.01	0.42
17:SW:76:SER:HB3	17:SW:77:PRO:HD3	2.01	0.42
23:SF:103:LEU:HD21	36:SZ:67:LEU:HD22	2.00	0.42
23:SF:195:GLU:OE2	37:D:30:MET:SD	2.78	0.42
27:Sg:226:HIS:CE1	27:Sg:227:LEU:O	2.72	0.42
29:SK:23:ALA:HB3	29:SK:69:TRP:CZ3	2.55	0.42
35:SP:70:MET:HE3	35:SP:70:MET:O	2.20	0.42
1:S2:98:C:H2'	1:S2:426:A:H4'	2.02	0.41
1:S2:433:A:H5''	7:SI:22:HIS:HB3	2.02	0.41
1:S2:659:G:C1'	1:S2:662:G:H21	2.33	0.41
1:S2:1597:C:H4'	1:S2:1603:G:O6	2.20	0.41
1:S2:1805:G:H3'	1:S2:1806:A:H5''	2.02	0.41
2:Ln:21:ARG:HD2	2:Ln:21:ARG:O	2.19	0.41
5:SB:125:VAL:HG22	5:SB:172:MET:HE3	2.02	0.41
14:SJ:64:ASP:OD1	14:SJ:64:ASP:N	2.53	0.41
23:SF:122:ARG:HD2	28:Sc:57:THR:HG21	2.02	0.41
23:SF:126:THR:O	23:SF:136:ARG:HB2	2.19	0.41
27:Sg:78:ALA:HB2	27:Sg:92:LEU:HD21	2.01	0.41
37:D:144:ARG:HE	37:D:147:TYR:CB	2.33	0.41
37:D:199:CYS:O	37:D:200:TYR:C	2.63	0.41
37:D:278:VAL:HG12	37:D:279:THR:H	1.85	0.41
1:S2:202:G:N3	1:S2:202:G:H3'	2.35	0.41
1:S2:393:U:H4'	1:S2:394:G:O5'	2.20	0.41
1:S2:867:OMG:HM23	1:S2:867:OMG:H1'	1.83	0.41
1:S2:1271:C:O2	26:Sd:2:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1440:C:O2'	1:S2:1441:U:H5'	2.21	0.41
4:SA:8:LEU:HD11	9:SV:39:VAL:HG21	2.02	0.41
4:SA:39:TYR:CD2	4:SA:40:LYS:HD2	2.54	0.41
10:SX:107:ARG:HB3	10:SX:110:HIS:HB3	2.01	0.41
19:Sb:13:GLU:OE2	19:Sb:13:GLU:N	2.52	0.41
24:Sf:108:VAL:O	24:Sf:108:VAL:CG1	2.68	0.41
30:SM:85:LEU:HA	30:SM:88:TRP:HB2	2.03	0.41
36:SZ:48:VAL:HG22	36:SZ:49:LEU:N	2.35	0.41
1:S2:159:A2M:H8	1:S2:159:A2M:OP2	2.20	0.41
7:SI:97:VAL:O	7:SI:100:CYS:HB2	2.21	0.41
27:Sg:119:GLN:O	27:Sg:120:ILE:HD13	2.21	0.41
27:Sg:150:TRP:O	27:Sg:169:GLY:HA3	2.19	0.41
29:SK:37:ASP:OD1	29:SK:37:ASP:N	2.52	0.41
33:SS:112:GLU:OE2	33:SS:112:GLU:HA	2.20	0.41
46:E:502:MET:SD	46:E:502:MET:C	3.03	0.41
1:S2:693:A:N7	1:S2:694:G:O6	2.54	0.41
1:S2:1078:C:C4	1:S2:1079:C:C5	3.08	0.41
1:S2:1706:G:H2'	1:S2:1707:U:H6	1.85	0.41
2:Ln:2:ARG:HB3	2:Ln:5:TRP:CD1	2.55	0.41
15:SN:93:LYS:O	15:SN:96:VAL:HG12	2.20	0.41
22:SD:162:ASP:N	22:SD:163:PRO:CD	2.83	0.41
27:Sg:35:SER:OG	27:Sg:36:ARG:N	2.53	0.41
35:SP:14:LYS:HD2	35:SP:15:PHE:O	2.19	0.41
1:S2:194:C:H2'	1:S2:195:C:N1	2.35	0.41
1:S2:502:C:H2'	1:S2:503:C:C5	2.55	0.41
1:S2:556:U:P	1:S2:557:U:H5''	2.61	0.41
1:S2:578:C:C4	1:S2:579:C:C5	3.08	0.41
1:S2:1307:U:O2	1:S2:1308:U:C4	2.73	0.41
1:S2:1809:A:H2'	1:S2:1810:U:C6	2.55	0.41
13:SG:7:PHE:HD1	13:SG:113:ILE:HB	1.86	0.41
15:SN:32:ASP:N	15:SN:32:ASP:OD1	2.52	0.41
22:SD:68:GLU:OE2	29:SK:70:TYR:CD1	2.73	0.41
28:Sc:66:ARG:HG3	28:Sc:66:ARG:O	2.20	0.41
30:SM:60:MET:H	30:SM:60:MET:CE	2.34	0.41
37:D:45:MET:HE2	37:D:45:MET:HB2	1.95	0.41
1:S2:456:C:C2	1:S2:457:C:C5	3.08	0.41
1:S2:940:U:H3	1:S2:1002:U:H3	1.68	0.41
1:S2:1541:G:O2'	1:S2:1542:C:H5'	2.20	0.41
1:S2:1628:C:H2'	1:S2:1629:C:C6	2.55	0.41
25:SR:76:GLU:O	25:SR:79:GLU:HG3	2.21	0.41
27:Sg:58:ALA:N	32:SQ:102:GLU:OE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:SK:57:TYR:CD1	29:SK:75:GLY:HA2	2.56	0.41
38:E:237:GLU:O	38:E:240:VAL:HG12	2.20	0.41
1:S2:166:A2M:HM'3	1:S2:166:A2M:H1'	1.62	0.41
1:S2:407:G:H3'	1:S2:408:A:C5'	2.49	0.41
1:S2:1535:U:H1'	23:SF:88:MET:CE	2.50	0.41
4:SA:180:ARG:O	4:SA:184:ARG:HG2	2.21	0.41
6:SH:66:VAL:N	6:SH:67:PRO:CD	2.84	0.41
18:SY:10:ARG:HG3	18:SY:24:VAL:CG2	2.51	0.41
30:SM:58:GLU:OE1	30:SM:58:GLU:O	2.38	0.41
33:SS:142:ARG:NE	33:SS:142:ARG:HA	2.35	0.41
37:D:34:VAL:HG12	37:D:35:SER:N	2.36	0.41
37:D:200:TYR:HA	38:E:347:LEU:HD22	2.02	0.41
38:E:58:VAL:CG2	38:E:59:LYS:HE2	2.51	0.41
38:E:435:THR:HG22	38:E:436:GLU:O	2.21	0.41
1:S2:650:A:H2'	1:S2:651:PSU:O4'	2.21	0.41
1:S2:659:G:H2'	1:S2:663:C:C6	2.55	0.41
1:S2:1074:C:C2	1:S2:1075:C:C5	3.09	0.41
6:SH:7:LYS:NZ	6:SH:21:SER:O	2.54	0.41
6:SH:69:LEU:HG	6:SH:96:ALA:HB2	2.02	0.41
12:SC:253:PRO:HA	12:SC:256:TRP:CE2	2.56	0.41
13:SG:74:ARG:O	13:SG:75:LEU:HD23	2.19	0.41
30:SM:22:LEU:HD12	30:SM:23:LYS:H	1.86	0.41
34:ST:21:PHE:CG	34:ST:134:ILE:HD11	2.56	0.41
36:SZ:68:ILE:HD13	36:SZ:97:ILE:CD1	2.51	0.41
37:D:145:PRO:O	37:D:147:TYR:N	2.53	0.41
37:D:227:ILE:HG23	37:D:236:VAL:C	2.46	0.41
1:S2:14:C:O2'	1:S2:668:A2M:N1	2.54	0.41
1:S2:106:C:H2'	1:S2:107:A:H8	1.86	0.41
1:S2:529:A:H2'	1:S2:530:U:C6	2.56	0.41
1:S2:641:A:H2'	1:S2:642:U:O4'	2.20	0.41
1:S2:884:C:H2'	1:S2:885:U:C6	2.56	0.41
1:S2:988:C:H4'	5:SB:115:LYS:O	2.21	0.41
1:S2:1139:C:O2	1:S2:1139:C:O4'	2.37	0.41
1:S2:1639:M7G:H3'	1:S2:1640:A:P	2.61	0.41
1:S2:1750:C:H2'	1:S2:1751:C:O4'	2.21	0.41
5:SB:38:MET:SD	5:SB:185:VAL:HG11	2.61	0.41
13:SG:149:LYS:C	13:SG:149:LYS:HD3	2.46	0.41
16:SO:34:PHE:CD1	16:SO:34:PHE:C	2.97	0.41
17:SW:41:MET:HG2	17:SW:129:PHE:CE2	2.56	0.41
19:Sb:53:VAL:O	19:Sb:53:VAL:CG2	2.68	0.41
21:B:5:U:H4'	21:B:6:A:OP1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:SF:78:MET:O	23:SF:79:HIS:HB2	2.21	0.41
27:Sg:31:ILE:HG13	27:Sg:43:TRP:HB2	2.03	0.41
27:Sg:196:ASN:HB2	27:Sg:211:GLY:HA2	2.03	0.41
29:SK:94:LEU:HD12	29:SK:94:LEU:N	2.36	0.41
37:D:132:GLN:O	37:D:136:TRP:CD1	2.74	0.41
37:D:227:ILE:HG22	37:D:235:TYR:HD2	1.85	0.41
38:E:429:LEU:HD21	38:E:433:VAL:HG23	2.01	0.41
40:G:46:M7G:H2'	40:G:46:M7G:N3	2.36	0.41
1:S2:1845:A:H2'	1:S2:1846:G:C8	2.56	0.41
7:SI:149:TYR:O	7:SI:153:LYS:HG2	2.20	0.41
11:Sa:53:ILE:HD13	16:SO:120:ALA:HB2	2.03	0.41
11:Sa:53:ILE:HD11	16:SO:116:LEU:CD2	2.51	0.41
15:SN:11:LEU:O	15:SN:11:LEU:HG	2.20	0.41
15:SN:29:THR:O	15:SN:32:ASP:OD1	2.39	0.41
17:SW:125:ILE:HG23	17:SW:125:ILE:O	2.21	0.41
23:SF:38:TYR:CE2	23:SF:144:LEU:HB2	2.56	0.41
37:D:163:LEU:HD11	37:D:177:ILE:HD11	2.02	0.41
41:H:77:ILE:HG22	41:H:94:LYS:HA	2.03	0.41
1:S2:456:C:N3	1:S2:457:C:C5	2.89	0.40
1:S2:860:G:N2	17:SW:107:SER:OG	2.52	0.40
1:S2:1217:A:H2'	1:S2:1218:C:H6	1.85	0.40
1:S2:1307:U:O2'	24:Sf:133:ALA:HB1	2.21	0.40
1:S2:1393:G:O2'	1:S2:1394:G:H5'	2.21	0.40
1:S2:1678:A2M:O2'	1:S2:1679:A:H5'	2.21	0.40
5:SB:133:TYR:CE1	5:SB:221:PRO:HD2	2.56	0.40
5:SB:168:MET:HG2	5:SB:197:ILE:HG21	2.03	0.40
6:SH:109:ARG:CD	6:SH:109:ARG:N	2.85	0.40
27:Sg:161:SER:O	27:Sg:162:ASN:C	2.64	0.40
31:SU:107:GLU:OE1	31:SU:107:GLU:N	2.54	0.40
33:SS:41:ALA:O	33:SS:45:LEU:HD22	2.22	0.40
1:S2:528:A:H2'	1:S2:529:A:C8	2.56	0.40
1:S2:872:A:C5	1:S2:874:G:C8	3.10	0.40
1:S2:1522:A:O2'	33:SS:145:THR:HA	2.22	0.40
1:S2:1841:C:H2'	1:S2:1842:4AC:H6	2.02	0.40
12:SC:81:ILE:HD13	12:SC:81:ILE:N	2.36	0.40
18:SY:105:LYS:HA	18:SY:105:LYS:HD3	1.95	0.40
30:SM:84:LYS:O	30:SM:88:TRP:HD1	2.03	0.40
32:SQ:85:ARG:NH2	32:SQ:119:LEU:HD11	2.37	0.40
37:D:7:ARG:HG2	37:D:40:ASN:HB2	2.03	0.40
37:D:176:LEU:O	37:D:180:ILE:HG22	2.21	0.40
1:S2:202:G:H2'	1:S2:203:G:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:587:A:H5'	1:S2:592:C:H41	1.87	0.40
1:S2:1243:U:H2'	1:S2:1244:PSU:O4'	2.21	0.40
1:S2:1407:U:H2'	1:S2:1408:U:C6	2.56	0.40
4:SA:183:LEU:HD13	4:SA:188:THR:OG1	2.22	0.40
10:SX:60:LYS:HG2	10:SX:114:ASP:O	2.21	0.40
16:SO:25:GLU:O	16:SO:26:ASN:C	2.63	0.40
19:Sb:31:TYR:CD1	19:Sb:31:TYR:N	2.90	0.40
22:SD:151:LYS:HG2	22:SD:153:VAL:HG13	2.03	0.40
31:SU:61:LEU:HD12	31:SU:61:LEU:N	2.36	0.40
32:SQ:105:LYS:O	32:SQ:105:LYS:HD2	2.22	0.40
35:SP:28:MET:HE2	35:SP:28:MET:HB3	1.99	0.40
36:SZ:58:LEU:O	36:SZ:62:VAL:HB	2.22	0.40
38:E:50:VAL:HG11	38:E:138:HIS:CE1	2.57	0.40
40:G:36:U:H2'	40:G:37:T6A:H8	1.86	0.40
1:S2:512:A2M:H1'	1:S2:512:A2M:HM'3	1.73	0.40
1:S2:962:A:N1	1:S2:1055:A:O2'	2.54	0.40
1:S2:1303:C:O2	1:S2:1303:C:O5'	2.40	0.40
1:S2:1332:A:O2'	22:SD:141:LYS:HD3	2.21	0.40
1:S2:1453:C:H5'	25:SR:48:ASN:HB2	2.02	0.40
1:S2:1851:MA6:C5'	2:Ln:1:MET:HE3	2.52	0.40
5:SB:69:VAL:CG1	5:SB:74:LEU:HD11	2.51	0.40
5:SB:142:PHE:HB2	5:SB:208:HIS:CE1	2.56	0.40
6:SH:15:LYS:H	6:SH:16:PRO:HD2	1.87	0.40
13:SG:132:ARG:O	13:SG:133:LEU:HD22	2.21	0.40
27:Sg:220:ASP:O	27:Sg:224:GLY:HA2	2.21	0.40
41:H:18:GLU:O	41:H:19:ASN:C	2.64	0.40
41:H:27:VAL:HG21	41:H:93:LEU:HD21	2.03	0.40
1:S2:65:C:C4	13:SG:133:LEU:HD13	2.57	0.40
1:S2:897:U:H3'	1:S2:898:U:O4'	2.22	0.40
1:S2:1083:A:N7	1:S2:1841:C:O2'	2.52	0.40
1:S2:1291:A:H5'	1:S2:1292:C:OP1	2.22	0.40
1:S2:1308:U:H2'	1:S2:1309:C:O4'	2.21	0.40
1:S2:1438:A:OP1	1:S2:1438:A:H4'	2.21	0.40
5:SB:185:VAL:O	5:SB:189:ILE:HD13	2.22	0.40
7:SI:29:LEU:HD12	7:SI:30:GLY:N	2.36	0.40
29:SK:86:PRO:HA	29:SK:87:PRO:HD3	1.94	0.40
30:SM:55:ASN:OD1	30:SM:81:ASP:HA	2.22	0.40
32:SQ:31:LEU:HD21	32:SQ:33:LYS:HD2	2.04	0.40
32:SQ:105:LYS:HD2	32:SQ:105:LYS:C	2.47	0.40
40:G:24:G:H2'	40:G:25:U:O4'	2.20	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	
2	Ln	22/25 (88%)	22 (100%)	0	0	100	100
3	SE	260/263 (99%)	249 (96%)	11 (4%)	0	100	100
4	SA	217/295 (74%)	207 (95%)	10 (5%)	0	100	100
5	SB	212/264 (80%)	201 (95%)	11 (5%)	0	100	100
6	SH	187/194 (96%)	168 (90%)	17 (9%)	2 (1%)	11	36
7	SI	204/208 (98%)	193 (95%)	11 (5%)	0	100	100
8	SL	148/158 (94%)	139 (94%)	8 (5%)	1 (1%)	18	48
9	SV	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
10	SX	139/143 (97%)	133 (96%)	6 (4%)	0	100	100
11	Sa	100/115 (87%)	96 (96%)	4 (4%)	0	100	100
12	SC	218/293 (74%)	212 (97%)	6 (3%)	0	100	100
13	SG	232/249 (93%)	224 (97%)	8 (3%)	0	100	100
14	SJ	180/194 (93%)	172 (96%)	8 (4%)	0	100	100
15	SN	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
16	SO	132/151 (87%)	120 (91%)	12 (9%)	0	100	100
17	SW	127/130 (98%)	119 (94%)	8 (6%)	0	100	100
18	SY	122/133 (92%)	119 (98%)	3 (2%)	0	100	100
19	Sb	81/84 (96%)	75 (93%)	6 (7%)	0	100	100
20	Se	57/133 (43%)	49 (86%)	8 (14%)	0	100	100
22	SD	225/243 (93%)	215 (96%)	10 (4%)	0	100	100
23	SF	187/204 (92%)	175 (94%)	12 (6%)	0	100	100
24	Sf	61/156 (39%)	54 (88%)	7 (12%)	0	100	100
25	SR	129/135 (96%)	126 (98%)	3 (2%)	0	100	100
26	Sd	53/56 (95%)	50 (94%)	3 (6%)	0	100	100
27	Sg	311/317 (98%)	292 (94%)	19 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	Sc	62/69 (90%)	56 (90%)	6 (10%)	0	100	100
29	SK	95/165 (58%)	88 (93%)	7 (7%)	0	100	100
30	SM	116/132 (88%)	105 (90%)	10 (9%)	1 (1%)	14	41
31	SU	100/119 (84%)	95 (95%)	5 (5%)	0	100	100
32	SQ	139/146 (95%)	132 (95%)	7 (5%)	0	100	100
33	SS	143/152 (94%)	134 (94%)	9 (6%)	0	100	100
34	ST	140/145 (97%)	135 (96%)	5 (4%)	0	100	100
35	SP	132/145 (91%)	128 (97%)	4 (3%)	0	100	100
36	SZ	71/125 (57%)	68 (96%)	3 (4%)	0	100	100
37	D	290/315 (92%)	268 (92%)	21 (7%)	1 (0%)	36	65
38	E	470/472 (100%)	446 (95%)	23 (5%)	1 (0%)	43	72
39	F	14/333 (4%)	12 (86%)	2 (14%)	0	100	100
41	H	109/144 (76%)	95 (87%)	13 (12%)	1 (1%)	14	41
All	All	5714/6839 (84%)	5394 (94%)	313 (6%)	7 (0%)	49	77

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	SH	15	LYS
41	H	17	ASN
37	D	24	VAL
38	E	274	LEU
6	SH	18	GLU
30	SM	96	ARG
8	SL	23	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	
2	Ln	23/24 (96%)	22 (96%)	1 (4%)	26	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	SE	224/225 (100%)	221 (99%)	3 (1%)	61	86
4	SA	182/243 (75%)	180 (99%)	2 (1%)	65	88
5	SB	195/231 (84%)	188 (96%)	7 (4%)	31	65
6	SH	169/174 (97%)	161 (95%)	8 (5%)	23	56
7	SI	178/180 (99%)	173 (97%)	5 (3%)	38	72
8	SL	134/142 (94%)	131 (98%)	3 (2%)	45	77
9	SV	67/67 (100%)	66 (98%)	1 (2%)	57	84
10	SX	113/115 (98%)	109 (96%)	4 (4%)	32	66
11	Sa	89/98 (91%)	87 (98%)	2 (2%)	45	77
12	SC	186/225 (83%)	178 (96%)	8 (4%)	26	60
13	SG	204/218 (94%)	202 (99%)	2 (1%)	68	89
14	SJ	161/168 (96%)	160 (99%)	1 (1%)	78	93
15	SN	130/131 (99%)	125 (96%)	5 (4%)	29	64
16	SO	105/118 (89%)	101 (96%)	4 (4%)	29	64
17	SW	112/113 (99%)	109 (97%)	3 (3%)	39	73
18	SY	108/115 (94%)	103 (95%)	5 (5%)	24	57
19	Sb	75/76 (99%)	72 (96%)	3 (4%)	28	62
20	Se	48/104 (46%)	46 (96%)	2 (4%)	26	60
22	SD	190/202 (94%)	183 (96%)	7 (4%)	30	64
23	SF	159/170 (94%)	156 (98%)	3 (2%)	50	79
24	Sf	56/140 (40%)	55 (98%)	1 (2%)	51	80
25	SR	119/122 (98%)	117 (98%)	2 (2%)	53	82
26	Sd	48/49 (98%)	47 (98%)	1 (2%)	47	77
27	Sg	272/275 (99%)	261 (96%)	11 (4%)	28	62
28	Sc	57/62 (92%)	52 (91%)	5 (9%)	9	29
29	SK	88/136 (65%)	84 (96%)	4 (4%)	24	58
30	SM	98/108 (91%)	95 (97%)	3 (3%)	35	69
31	SU	94/107 (88%)	88 (94%)	6 (6%)	16	44
32	SQ	117/121 (97%)	112 (96%)	5 (4%)	26	60
33	SS	126/132 (96%)	118 (94%)	8 (6%)	16	45
34	ST	112/114 (98%)	110 (98%)	2 (2%)	51	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	SP	120/130 (92%)	116 (97%)	4 (3%)	33	67
36	SZ	65/103 (63%)	59 (91%)	6 (9%)	8	27
37	D	262/280 (94%)	255 (97%)	7 (3%)	39	73
38	E	397/397 (100%)	387 (98%)	10 (2%)	42	74
39	F	16/304 (5%)	16 (100%)	0	100	100
41	H	94/123 (76%)	90 (96%)	4 (4%)	26	60
All	All	4993/5842 (86%)	4835 (97%)	158 (3%)	35	68

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Ln	6	ARG
3	SE	19	MET
3	SE	162	ILE
3	SE	204	SER
4	SA	118	GLU
4	SA	136	GLU
5	SB	43	ASN
5	SB	48	LEU
5	SB	91	VAL
5	SB	131	ASP
5	SB	189	ILE
5	SB	208	HIS
5	SB	225	LEU
6	SH	18	GLU
6	SH	32	MET
6	SH	44	ASN
6	SH	60	ILE
6	SH	72	PHE
6	SH	119	SER
6	SH	148	LEU
6	SH	194	LEU
7	SI	62	VAL
7	SI	89	GLU
7	SI	138	ASN
7	SI	163	GLU
7	SI	167	GLN
8	SL	54	THR
8	SL	74	SER
8	SL	132	ARG

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Mol	Chain	Res	Type
9	SV	13	VAL
10	SX	90	CYS
10	SX	102	VAL
10	SX	115	ILE
10	SX	139	GLU
11	Sa	46	GLU
11	Sa	67	LEU
12	SC	80	GLU
12	SC	190	SER
12	SC	192	LEU
12	SC	193	VAL
12	SC	221	ASP
12	SC	230	THR
12	SC	245	SER
12	SC	276	THR
13	SG	13	GLN
13	SG	105	ASN
14	SJ	92	MET
15	SN	31	ASP
15	SN	45	LEU
15	SN	80	LEU
15	SN	84	LEU
15	SN	135	LEU
16	SO	27	VAL
16	SO	50	LYS
16	SO	52	THR
16	SO	91	THR
17	SW	66	THR
17	SW	80	ASP
17	SW	90	GLN
18	SY	5	VAL
18	SY	6	THR
18	SY	13	MET
18	SY	78	SER
18	SY	103	SER
19	Sb	46	VAL
19	Sb	55	LEU
19	Sb	80	ARG
20	Se	36	MET
20	Se	44	ASN
22	SD	31	GLU
22	SD	68	GLU

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Mol	Chain	Res	Type
22	SD	72	VAL
22	SD	73	VAL
22	SD	136	VAL
22	SD	169	ASP
22	SD	189	MET
23	SF	41	VAL
23	SF	126	THR
23	SF	203	ASN
24	Sf	121	CYS
25	SR	62	GLN
25	SR	93	GLN
26	Sd	8	TRP
27	Sg	51	ASN
27	Sg	63	SER
27	Sg	98	THR
27	Sg	111	VAL
27	Sg	171	ASP
27	Sg	176	VAL
27	Sg	186	THR
27	Sg	197	THR
27	Sg	207	CYS
27	Sg	221	LEU
27	Sg	265	ILE
28	Sc	10	LYS
28	Sc	29	GLN
28	Sc	50	VAL
28	Sc	52	GLU
28	Sc	59	LEU
29	SK	2	LEU
29	SK	6	LYS
29	SK	11	ILE
29	SK	54	SER
30	SM	55	ASN
30	SM	68	LEU
30	SM	126	GLU
31	SU	17	ILE
31	SU	20	ILE
31	SU	22	ILE
31	SU	24	LEU
31	SU	65	THR
31	SU	93	SER
32	SQ	12	VAL

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Mol	Chain	Res	Type
32	SQ	32	ILE
32	SQ	34	VAL
32	SQ	37	ARG
32	SQ	97	GLN
33	SS	1	MET
33	SS	5	ILE
33	SS	36	VAL
33	SS	45	LEU
33	SS	59	LEU
33	SS	73	ASN
33	SS	95	TYR
33	SS	131	VAL
34	ST	39	LEU
34	ST	143	LYS
35	SP	120	SER
35	SP	126	VAL
35	SP	142	ILE
35	SP	144	LEU
36	SZ	50	PHE
36	SZ	54	THR
36	SZ	65	TYR
36	SZ	97	ILE
36	SZ	100	VAL
36	SZ	110	THR
37	D	70	CYS
37	D	131	PHE
37	D	187	GLN
37	D	257	VAL
37	D	278	VAL
37	D	286	LEU
37	D	290	MET
38	E	35	VAL
38	E	167	GLN
38	E	170	THR
38	E	309	LEU
38	E	346	THR
38	E	367	ILE
38	E	373	ILE
38	E	378	LEU
38	E	382	LEU
38	E	384	VAL
41	H	22	GLU

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Mol	Chain	Res	Type
41	H	26	LEU
41	H	55	VAL
41	H	91	VAL

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

Mol	Chain	Res	Type
3	SE	36	HIS
4	SA	132	GLN
4	SA	169	HIS
5	SB	75	GLN
5	SB	149	GLN
6	SH	33	ASN
6	SH	91	HIS
6	SH	97	GLN
6	SH	112	ASN
6	SH	168	HIS
7	SI	155	ASN
7	SI	181	GLN
8	SL	11	GLN
8	SL	13	GLN
9	SV	35	ASN
10	SX	73	GLN
10	SX	97	ASN
12	SC	178	HIS
13	SG	155	GLN
16	SO	103	ASN
18	SY	63	HIS
18	SY	112	ASN
19	Sb	51	GLN
22	SD	57	ASN
22	SD	145	GLN
23	SF	95	HIS
25	SR	62	GLN
26	Sd	26	ASN
26	Sd	37	ASN
27	Sg	226	HIS
29	SK	7	ASN
29	SK	32	HIS
29	SK	42	ASN
29	SK	84	HIS
30	SM	55	ASN

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Mol	Chain	Res	Type
31	SU	85	HIS
31	SU	100	GLN
32	SQ	48	GLN
32	SQ	86	GLN
33	SS	72	GLN
34	ST	83	GLN
35	SP	104	GLN
35	SP	137	HIS
37	D	126	GLN
37	D	155	HIS
37	D	179	ASN
38	E	33	HIS
38	E	199	GLN
38	E	407	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S2	1713/1869 (91%)	341 (19%)	9 (0%)
21	B	27/50 (54%)	15 (55%)	1 (3%)
40	G	72/75 (96%)	16 (22%)	0
All	All	1812/1994 (90%)	372 (20%)	10 (0%)

All (372) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S2	2	A
1	S2	4	C
1	S2	17	C
1	S2	26	U
1	S2	33	G
1	S2	35	C
1	S2	37	C
1	S2	42	A
1	S2	46	A
1	S2	56	G
1	S2	59	U
1	S2	62	G
1	S2	67	C
1	S2	68	A
1	S2	71	G

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Mol	Chain	Res	Type
1	S2	73	C
1	S2	75	G
1	S2	76	U
1	S2	77	A
1	S2	103	A
1	S2	110	U
1	S2	113	G
1	S2	115	U
1	S2	126	G
1	S2	143	U
1	S2	149	A
1	S2	155	G
1	S2	158	A
1	S2	159	A2M
1	S2	161	U
1	S2	162	C
1	S2	163	U
1	S2	168	C
1	S2	182	C
1	S2	184	G
1	S2	198	U
1	S2	199	C
1	S2	200	G
1	S2	202	G
1	S2	203	G
1	S2	204	G
1	S2	206	G
1	S2	209	A
1	S2	302	A
1	S2	305	U
1	S2	306	C
1	S2	307	G
1	S2	308	G
1	S2	309	G
1	S2	318	A
1	S2	319	C
1	S2	322	C
1	S2	324	C
1	S2	325	C
1	S2	326	C
1	S2	327	G
1	S2	328	U

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Mol	Chain	Res	Type
1	S2	329	G
1	S2	330	G
1	S2	347	G
1	S2	351	G
1	S2	360	A
1	S2	362	C
1	S2	364	A
1	S2	368	U
1	S2	369	C
1	S2	370	G
1	S2	381	C
1	S2	385	G
1	S2	386	C
1	S2	387	C
1	S2	408	A
1	S2	409	C
1	S2	448	A
1	S2	450	C
1	S2	452	G
1	S2	462	OMC
1	S2	464	A
1	S2	471	G
1	S2	472	C
1	S2	473	A
1	S2	474	G
1	S2	487	U
1	S2	488	U
1	S2	492	C
1	S2	502	C
1	S2	508	A
1	S2	516	A
1	S2	517	OMC
1	S2	532	C
1	S2	536	A
1	S2	537	C
1	S2	539	C
1	S2	541	U
1	S2	542	U
1	S2	543	C
1	S2	544	G
1	S2	546	G
1	S2	547	G

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Mol	Chain	Res	Type
1	S2	552	G
1	S2	553	U
1	S2	554	A
1	S2	555	A
1	S2	556	U
1	S2	558	G
1	S2	559	G
1	S2	560	A
1	S2	563	G
1	S2	564	A
1	S2	576	A2M
1	S2	583	A
1	S2	587	A
1	S2	589	G
1	S2	591	U
1	S2	593	C
1	S2	604	A
1	S2	607	U
1	S2	614	C
1	S2	615	C
1	S2	617	G
1	S2	628	A
1	S2	643	A
1	S2	655	A
1	S2	660	C
1	S2	663	C
1	S2	668	A2M
1	S2	669	A
1	S2	671	A
1	S2	672	A
1	S2	673	G
1	S2	688	U
1	S2	689	U
1	S2	691	G
1	S2	692	G
1	S2	696	G
1	S2	731	G
1	S2	732	U
1	S2	733	C
1	S2	736	C
1	S2	737	G
1	S2	738	C

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Mol	Chain	Res	Type
1	S2	748	C
1	S2	749	U
1	S2	751	G
1	S2	752	G
1	S2	753	C
1	S2	788	G
1	S2	789	G
1	S2	790	C
1	S2	792	C
1	S2	794	A
1	S2	797	C
1	S2	798	G
1	S2	799	U
1	S2	811	A
1	S2	821	G
1	S2	822	PSU
1	S2	823	U
1	S2	827	A
1	S2	830	A
1	S2	835	C
1	S2	836	G
1	S2	837	A
1	S2	838	G
1	S2	839	C
1	S2	841	G
1	S2	842	C
1	S2	847	A
1	S2	867	OMG
1	S2	868	G
1	S2	870	A
1	S2	872	A
1	S2	882	U
1	S2	883	U
1	S2	884	C
1	S2	885	U
1	S2	886	A
1	S2	887	U
1	S2	888	U
1	S2	889	U
1	S2	890	U
1	S2	891	G
1	S2	892	U

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Mol	Chain	Res	Type
1	S2	893	U
1	S2	894	G
1	S2	896	U
1	S2	898	U
1	S2	899	U
1	S2	901	G
1	S2	904	A
1	S2	905	C
1	S2	906	U
1	S2	913	A
1	S2	919	A
1	S2	920	A
1	S2	933	G
1	S2	971	G
1	S2	978	G
1	S2	990	A
1	S2	992	A
1	S2	1002	U
1	S2	1017	U
1	S2	1023	A
1	S2	1027	A
1	S2	1028	A
1	S2	1058	A
1	S2	1060	A
1	S2	1061	U
1	S2	1062	A
1	S2	1081	U
1	S2	1083	A
1	S2	1085	C
1	S2	1089	G
1	S2	1109	C
1	S2	1116	C
1	S2	1118	C
1	S2	1133	A
1	S2	1138	C
1	S2	1150	A
1	S2	1153	C
1	S2	1154	U
1	S2	1195	A
1	S2	1207	G
1	S2	1215	C
1	S2	1216	C

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Mol	Chain	Res	Type
1	S2	1217	A
1	S2	1224	G
1	S2	1242	U
1	S2	1243	U
1	S2	1251	A
1	S2	1253	A
1	S2	1256	G
1	S2	1257	G
1	S2	1258	A
1	S2	1259	A
1	S2	1274	G
1	S2	1275	G
1	S2	1282	A
1	S2	1286	G
1	S2	1292	C
1	S2	1301	A
1	S2	1302	G
1	S2	1303	C
1	S2	1305	C
1	S2	1306	U
1	S2	1307	U
1	S2	1308	U
1	S2	1309	C
1	S2	1311	C
1	S2	1312	G
1	S2	1313	A
1	S2	1314	U
1	S2	1317	C
1	S2	1333	U
1	S2	1343	U
1	S2	1348	G
1	S2	1371	U
1	S2	1372	U
1	S2	1378	A
1	S2	1418	C
1	S2	1419	C
1	S2	1420	G
1	S2	1421	A
1	S2	1422	G
1	S2	1424	G
1	S2	1429	G
1	S2	1433	C

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Mol	Chain	Res	Type
1	S2	1434	C
1	S2	1435	C
1	S2	1436	C
1	S2	1437	C
1	S2	1438	A
1	S2	1454	A
1	S2	1462	U
1	S2	1463	U
1	S2	1474	A
1	S2	1487	A
1	S2	1489	A
1	S2	1490	OMG
1	S2	1495	G
1	S2	1497	G
1	S2	1498	A
1	S2	1509	U
1	S2	1520	G
1	S2	1521	C
1	S2	1522	A
1	S2	1533	A
1	S2	1534	C
1	S2	1535	U
1	S2	1536	G
1	S2	1544	C
1	S2	1556	A
1	S2	1579	A
1	S2	1580	A
1	S2	1585	U
1	S2	1586	U
1	S2	1588	A
1	S2	1601	A
1	S2	1606	G
1	S2	1621	U
1	S2	1622	U
1	S2	1623	A
1	S2	1646	C
1	S2	1647	A
1	S2	1648	G
1	S2	1654	G
1	S2	1663	A
1	S2	1665	G
1	S2	1680	G

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Mol	Chain	Res	Type
1	S2	1699	A
1	S2	1715	A
1	S2	1721	U
1	S2	1722	G
1	S2	1729	U
1	S2	1744	G
1	S2	1745	A
1	S2	1751	C
1	S2	1752	C
1	S2	1753	C
1	S2	1757	G
1	S2	1758	G
1	S2	1761	U
1	S2	1773	C
1	S2	1780	G
1	S2	1781	A
1	S2	1782	G
1	S2	1783	C
1	S2	1786	U
1	S2	1805	G
1	S2	1806	A
1	S2	1807	C
1	S2	1829	G
1	S2	1835	A
1	S2	1838	U
1	S2	1839	U
1	S2	1849	G
1	S2	1861	G
1	S2	1862	G
1	S2	1863	A
1	S2	1865	C
1	S2	1867	U
21	B	-7	C
21	B	-6	A
21	B	-5	G
21	B	-3	C
21	B	-2	U
21	B	0	U
21	B	4	U
21	B	5	U
21	B	6	A
21	B	8	A

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Mol	Chain	Res	Type
21	B	9	A
21	B	12	G
21	B	15	U
21	B	16	C
21	B	17	C
40	G	8	G
40	G	11[1]	2MG
40	G	17	C
40	G	18	G
40	G	19	G
40	G	20	A
40	G	21	A
40	G	48	5MC
40	G	49	G
40	G	54	A
40	G	70	G
40	G	71	C
40	G	73	A
40	G	74	C
40	G	75	C
40	G	76	A

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	S2	34	PSU
1	S2	324	C
1	S2	563	G
1	S2	614	C
1	S2	798	G
1	S2	866	PSU
1	S2	1257	G
1	S2	1316	C
1	S2	1520	G
21	B	5	U

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

100 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	PSU	S2	34	1	18,21,22	0.55	0	22,30,33	0.42	0
1	PSU	S2	649	1	18,21,22	0.53	0	22,30,33	0.61	0
1	OMU	S2	1442	43,1	19,22,23	0.32	0	26,31,34	0.40	0
1	PSU	S2	1347	1	18,21,22	0.59	0	22,30,33	0.57	0
1	PSU	S2	815	1	18,21,22	0.50	0	22,30,33	0.57	0
34	NMM	ST	67	34	9,11,12	0.61	0	6,12,14	1.79	2 (33%)
40	1MG	G	10	40	22,26,27	0.29	0	33,39,42	0.61	1 (3%)
16	IAS	SO	138	16	6,7,8	1.05	0	6,8,10	1.66	3 (50%)
1	OMC	S2	1272	1	19,22,23	0.30	0	26,31,34	0.33	0
1	A2M	S2	668	43,1	22,25,26	0.13	0	31,36,39	0.31	0
1	A2M	S2	484	1	22,25,26	0.08	0	31,36,39	0.20	0
1	PSU	S2	966	1	18,21,22	0.54	0	22,30,33	0.56	0
1	PSU	S2	63	1	18,21,22	0.50	0	22,30,33	0.61	0
1	PSU	S2	814	1	18,21,22	0.52	0	22,30,33	0.59	0
1	A2M	S2	159	1	22,25,26	0.12	0	31,36,39	0.24	0
1	PSU	S2	1136	1	18,21,22	0.53	0	22,30,33	0.59	0
1	PSU	S2	863	1	18,21,22	0.57	0	22,30,33	0.51	0
1	PSU	S2	105	1	18,21,22	0.52	0	22,30,33	0.59	0
1	PSU	S2	109	1	18,21,22	0.55	0	22,30,33	0.56	0
1	PSU	S2	801	1	18,21,22	0.54	0	22,30,33	0.57	0
1	OMG	S2	509	43,1	23,26,27	0.34	0	33,38,41	0.46	0
1	PSU	S2	1596	1	18,21,22	0.54	0	22,30,33	0.57	0
1	PSU	S2	1643	43,1	18,21,22	0.61	1 (5%)	22,30,33	0.52	0
1	OMG	S2	1490	43,1	23,26,27	0.41	0	33,38,41	0.44	0
1	A2M	S2	99	43,1	22,25,26	0.12	0	31,36,39	0.46	0
1	PSU	S2	1692	1	18,21,22	0.52	0	22,30,33	0.59	0
1	PSU	S2	1244	1	18,21,22	0.55	0	22,30,33	0.57	0
1	PSU	S2	918	1	18,21,22	0.48	0	22,30,33	0.40	0
1	OMU	S2	354	1	19,22,23	0.32	0	26,31,34	0.62	0
1	PSU	S2	681	1	18,21,22	0.56	0	22,30,33	0.54	0
1	MA6	S2	1851	1	23,26,27	0.33	0	34,38,41	0.66	1 (2%)
1	MA6	S2	1850	1	23,26,27	0.32	0	34,38,41	0.61	1 (2%)
1	PSU	S2	609	1	18,21,22	0.54	0	22,30,33	0.55	0
1	A2M	S2	590	1	22,25,26	0.11	0	31,36,39	0.29	0
1	OMG	S2	436	1	23,26,27	0.35	0	33,38,41	0.46	0
1	4AC	S2	1337	1	21,24,25	0.36	0	29,34,37	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	OMG	S2	601	1	23,26,27	0.32	0	33,38,41	0.33	0
1	OMC	S2	1391	1	19,22,23	0.31	0	26,31,34	0.44	0
1	OMG	S2	683	1	23,26,27	0.33	0	33,38,41	0.45	0
1	PSU	S2	1360	42,1	18,21,22	0.57	0	22,30,33	0.62	1 (4%)
1	OMU	S2	1804	1	19,22,23	0.32	0	26,31,34	0.42	0
1	PSU	S2	406	1	18,21,22	0.52	0	22,30,33	0.56	0
1	PSU	S2	667	1	18,21,22	0.61	1 (5%)	22,30,33	0.52	0
1	PSU	S2	651	1	18,21,22	0.55	0	22,30,33	0.59	0
1	4AC	S2	1842	1	21,24,25	0.32	0	29,34,37	0.30	0
1	PSU	S2	1056	1	18,21,22	0.53	0	22,30,33	0.57	0
1	PSU	S2	1045	1	18,21,22	0.49	0	22,30,33	0.63	0
1	PSU	S2	866	1	18,21,22	0.47	0	22,30,33	0.71	0
1	PSU	S2	1004	1	18,21,22	0.54	0	22,30,33	0.59	0
1	OMC	S2	1703	43,1	19,22,23	0.29	0	26,31,34	0.45	0
1	PSU	S2	366	1	18,21,22	0.54	0	22,30,33	0.53	0
1	PSU	S2	1238	1	18,21,22	0.55	0	22,30,33	0.57	0
1	PSU	S2	822	1	18,21,22	0.48	0	22,30,33	0.60	0
1	PSU	S2	300	1	18,21,22	0.52	0	22,30,33	0.55	0
1	PSU	S2	1625	1	18,21,22	0.55	0	22,30,33	0.59	0
1	OMG	S2	1447	1	23,26,27	0.32	0	33,38,41	0.45	0
1	PSU	S2	36	1	18,21,22	0.49	0	22,30,33	0.38	0
1	A2M	S2	1678	1	22,25,26	0.10	0	31,36,39	0.27	0
1	PSU	S2	100	43,1	18,21,22	0.49	0	22,30,33	0.58	0
1	A2M	S2	468	1	22,25,26	0.09	0	31,36,39	0.27	0
1	UY1	S2	1326	43,1	19,22,23	0.44	0	22,31,34	0.43	0
1	A2M	S2	1383	1	22,25,26	0.12	0	31,36,39	0.54	1 (3%)
1	OMG	S2	867	1	23,26,27	0.28	0	33,38,41	0.35	0
1	OMC	S2	174	1	19,22,23	0.31	0	26,31,34	0.48	0
1	PSU	S2	1046	1	18,21,22	0.56	0	22,30,33	0.53	0
1	PSU	S2	119	1	18,21,22	0.52	0	22,30,33	0.51	0
1	PSU	S2	296	1	18,21,22	0.51	0	22,30,33	0.54	0
1	PSU	S2	1367	1	18,21,22	0.54	0	22,30,33	0.59	0
1	PSU	S2	218	1	18,21,22	0.51	0	22,30,33	0.59	0
1	PSU	S2	1003	1	18,21,22	0.54	0	22,30,33	0.56	0
1	A2M	S2	27	1	22,25,26	0.09	0	31,36,39	0.23	0
40	1MA	G	58	40	21,25,26	0.48	0	31,37,40	0.75	1 (3%)
40	5MC	G	48	40	18,22,23	0.49	0	26,32,35	0.58	0
1	OMU	S2	172	1	19,22,23	0.26	0	26,31,34	0.50	0
1	A2M	S2	166	1	22,25,26	0.08	0	31,36,39	0.32	0
40	H2U	G	47	40	18,21,22	0.31	0	21,30,33	0.45	0
1	OMU	S2	1288	1	19,22,23	0.31	0	26,31,34	0.43	0
1	OMC	S2	517	1	19,22,23	0.29	0	26,31,34	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PSU	S2	686	1	18,21,22	0.53	0	22,30,33	0.53	0
1	OMU	S2	121	1	19,22,23	0.30	0	26,31,34	0.45	0
1	PSU	S2	1445	1	18,21,22	0.57	0	22,30,33	0.60	0
1	OMU	S2	428	1	19,22,23	0.27	0	26,31,34	0.44	0
1	OMC	S2	462	1	19,22,23	0.31	0	26,31,34	0.40	0
1	PSU	S2	1232	1	18,21,22	0.54	0	22,30,33	0.55	0
1	PSU	S2	93	1	18,21,22	0.53	0	22,30,33	0.55	0
1	PSU	S2	1186	1	18,21,22	0.49	0	22,30,33	0.59	0
1	B8N	S2	1248	1	24,29,30	0.64	1 (4%)	29,42,45	0.64	0
40	2MG	G	26	40	23,26,27	0.34	0	32,38,41	0.32	0
1	6MZ	S2	1832	43,42,1	22,25,26	0.13	0	30,36,39	0.28	0
1	OMU	S2	116	1	19,22,23	0.31	0	26,31,34	0.49	0
1	OMG	S2	644	1	23,26,27	0.31	0	33,38,41	0.42	0
1	PSU	S2	572	1	18,21,22	0.55	0	22,30,33	0.54	0
1	PSU	S2	1177	1	18,21,22	0.53	0	22,30,33	0.58	0
1	OMG	S2	1328	42,1	23,26,27	0.34	0	33,38,41	0.43	0
1	A2M	S2	1031	1	22,25,26	0.09	0	31,36,39	0.24	0
1	A2M	S2	512	1	22,25,26	0.10	0	31,36,39	0.47	1 (3%)
40	T6A	G	37	40	31,34,35	0.45	0	44,49,52	0.59	1 (2%)
1	A2M	S2	576	1	22,25,26	0.09	0	31,36,39	0.29	0
1	PSU	S2	1174	1	18,21,22	0.54	0	22,30,33	0.56	0

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
1	PSU	S2	34	1	-	1/7/25/26	0/2/2/2
1	PSU	S2	649	1	-	0/7/25/26	0/2/2/2
1	OMU	S2	1442	43,1	-	0/9/27/28	0/2/2/2
1	PSU	S2	1347	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	815	1	-	0/7/25/26	0/2/2/2
34	NMM	ST	67	34	-	2/9/11/13	-
40	1MG	G	10	40	-	1/7/25/26	0/3/3/3
16	IAS	SO	138	16	-	1/7/7/8	-
1	OMC	S2	1272	1	-	0/9/27/28	0/2/2/2
1	A2M	S2	668	43,1	-	1/9/27/28	0/3/3/3
1	A2M	S2	484	1	-	0/9/27/28	0/3/3/3
1	PSU	S2	966	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	63	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	814	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	S2	159	1	-	3/9/27/28	0/3/3/3
1	PSU	S2	1136	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	863	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	105	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	109	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	801	1	-	0/7/25/26	0/2/2/2
1	OMG	S2	509	43,1	-	0/9/27/28	0/3/3/3
1	PSU	S2	1596	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1643	43,1	-	0/7/25/26	0/2/2/2
1	OMG	S2	1490	43,1	-	3/9/27/28	0/3/3/3
1	A2M	S2	99	43,1	-	2/9/27/28	0/3/3/3
1	PSU	S2	1692	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1244	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	918	1	-	1/7/25/26	0/2/2/2
1	OMU	S2	354	1	-	1/9/27/28	0/2/2/2
1	PSU	S2	681	1	-	0/7/25/26	0/2/2/2
1	MA6	S2	1851	1	-	2/11/29/30	0/3/3/3
1	MA6	S2	1850	1	-	0/11/29/30	0/3/3/3
1	PSU	S2	609	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	590	1	-	3/9/27/28	0/3/3/3
1	OMG	S2	436	1	-	0/9/27/28	0/3/3/3
1	4AC	S2	1337	1	-	0/11/29/30	0/2/2/2
1	OMG	S2	601	1	-	0/9/27/28	0/3/3/3
1	OMC	S2	1391	1	-	0/9/27/28	0/2/2/2
1	OMG	S2	683	1	-	0/9/27/28	0/3/3/3
1	PSU	S2	1360	42,1	-	0/7/25/26	0/2/2/2
1	OMU	S2	1804	1	-	1/9/27/28	0/2/2/2
1	PSU	S2	406	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	667	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	651	1	-	0/7/25/26	0/2/2/2
1	4AC	S2	1842	1	-	0/11/29/30	0/2/2/2
1	PSU	S2	1056	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1045	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	866	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1004	1	-	0/7/25/26	0/2/2/2
1	OMC	S2	1703	43,1	-	0/9/27/28	0/2/2/2
1	PSU	S2	366	1	-	2/7/25/26	0/2/2/2
1	PSU	S2	1238	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	822	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	300	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1625	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	S2	1447	1	-	2/9/27/28	0/3/3/3
1	PSU	S2	36	1	-	3/7/25/26	0/2/2/2
1	A2M	S2	1678	1	-	1/9/27/28	0/3/3/3
1	PSU	S2	100	43,1	-	0/7/25/26	0/2/2/2
1	A2M	S2	468	1	-	1/9/27/28	0/3/3/3
1	UY1	S2	1326	43,1	-	2/9/27/28	0/2/2/2
1	A2M	S2	1383	1	-	0/9/27/28	0/3/3/3
1	OMG	S2	867	1	-	1/9/27/28	0/3/3/3
1	OMC	S2	174	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	1046	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	119	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	296	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1367	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	218	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1003	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	27	1	-	0/9/27/28	0/3/3/3
40	1MA	G	58	40	-	0/7/25/26	0/3/3/3
40	5MC	G	48	40	-	3/7/25/26	0/2/2/2
1	OMU	S2	172	1	-	0/9/27/28	0/2/2/2
1	A2M	S2	166	1	-	1/9/27/28	0/3/3/3
40	H2U	G	47	40	-	4/7/38/39	0/2/2/2
1	OMU	S2	1288	1	-	0/9/27/28	0/2/2/2
1	OMC	S2	517	1	-	2/9/27/28	0/2/2/2
1	PSU	S2	686	1	-	0/7/25/26	0/2/2/2
1	OMU	S2	121	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	1445	1	-	0/7/25/26	0/2/2/2
1	OMU	S2	428	1	-	4/9/27/28	0/2/2/2
1	OMC	S2	462	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	1232	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	93	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1186	1	-	0/7/25/26	0/2/2/2
1	B8N	S2	1248	1	-	2/16/34/35	0/2/2/2
40	2MG	G	26	40	-	4/9/27/28	0/3/3/3
1	6MZ	S2	1832	43,42,1	-	2/9/27/28	0/3/3/3
1	OMU	S2	116	1	-	2/9/27/28	0/2/2/2
1	OMG	S2	644	1	-	1/9/27/28	0/3/3/3
1	PSU	S2	572	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1177	1	-	0/7/25/26	0/2/2/2
1	OMG	S2	1328	42,1	-	0/9/27/28	0/3/3/3
1	A2M	S2	1031	1	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	S2	512	1	-	1/9/27/28	0/3/3/3
40	T6A	G	37	40	-	5/23/41/42	0/3/3/3
1	A2M	S2	576	1	-	3/9/27/28	0/3/3/3
1	PSU	S2	1174	1	-	0/7/25/26	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	667	PSU	O4'-C1'	-2.04	1.41	1.43
1	S2	1248	B8N	O4'-C1'	-2.02	1.41	1.43
1	S2	1643	PSU	O4'-C1'	-2.02	1.41	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	ST	67	NMM	NE-CZ-NH2	-3.36	116.40	119.48
40	G	10	1MG	C6-C5-C4	-2.59	117.11	119.97
34	ST	67	NMM	NE-CZ-NH1	2.42	124.80	120.26
1	S2	1850	MA6	C2-N1-C6	2.38	117.38	111.75
1	S2	1851	MA6	C2-N1-C6	2.37	117.34	111.75
40	G	37	T6A	C12-N11-C10	2.36	125.86	121.94
16	SO	138	IAS	OD1-CG-CB	-2.30	118.72	125.43
16	SO	138	IAS	OXT-C-O	-2.16	119.17	124.09
40	G	58	1MA	N1-C6-N6	2.16	125.25	119.77
1	S2	1360	PSU	O4'-C1'-C2'	2.15	108.17	105.14
1	S2	1383	A2M	C2'-C3'-C4'	-2.07	97.51	101.99
16	SO	138	IAS	OXT-C-CA	2.04	120.35	113.38
1	S2	512	A2M	C2'-C3'-C4'	-2.02	97.60	101.99

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	ST	67	NMM	O-C-CA-CB
1	S2	34	PSU	O4'-C1'-C5-C6
1	S2	36	PSU	C2'-C1'-C5-C4
1	S2	99	A2M	O4'-C1'-N9-C8
1	S2	99	A2M	O4'-C1'-N9-C4
1	S2	116	OMU	O4'-C1'-N1-C2
1	S2	116	OMU	O4'-C1'-N1-C6
1	S2	159	A2M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	S2	166	A2M	C1'-C2'-O2'-CM'
1	S2	354	OMU	C1'-C2'-O2'-CM2
1	S2	366	PSU	C2'-C1'-C5-C4
1	S2	428	OMU	C2'-C1'-N1-C2
1	S2	428	OMU	C2'-C1'-N1-C6
1	S2	468	A2M	C1'-C2'-O2'-CM'
1	S2	512	A2M	C1'-C2'-O2'-CM'
1	S2	576	A2M	C1'-C2'-O2'-CM'
1	S2	1031	A2M	C1'-C2'-O2'-CM'
1	S2	1248	B8N	C31-C32-C33-C34
1	S2	1326	UY1	C2'-C1'-C5-C6
1	S2	1490	OMG	O4'-C4'-C5'-O5'
1	S2	1678	A2M	C1'-C2'-O2'-CM'
1	S2	1832	6MZ	C5-C6-N6-C9
1	S2	1832	6MZ	N1-C6-N6-C9
16	SO	138	IAS	CA-CB-CG-OD1
40	G	10	1MG	O4'-C4'-C5'-O5'
40	G	26	2MG	O4'-C1'-N9-C8
40	G	26	2MG	O4'-C1'-N9-C4
40	G	26	2MG	N1-C2-N2-CM2
40	G	26	2MG	N3-C2-N2-CM2
40	G	37	T6A	C14-C12-C13-ODB
40	G	47	H2U	O4'-C1'-N1-C6
40	G	47	H2U	C2'-C1'-N1-C2
40	G	47	H2U	C2'-C1'-N1-C6
40	G	48	5MC	O4'-C4'-C5'-O5'
1	S2	159	A2M	O4'-C4'-C5'-O5'
1	S2	517	OMC	C3'-C4'-C5'-O5'
1	S2	576	A2M	O4'-C4'-C5'-O5'
1	S2	576	A2M	C3'-C4'-C5'-O5'
1	S2	1447	OMG	C3'-C4'-C5'-O5'
1	S2	1851	MA6	O4'-C4'-C5'-O5'
40	G	48	5MC	C3'-C4'-C5'-O5'
1	S2	517	OMC	O4'-C4'-C5'-O5'
1	S2	1851	MA6	C3'-C4'-C5'-O5'
40	G	37	T6A	C14-C12-C13-ODA
40	G	37	T6A	N11-C12-C13-ODB
1	S2	1447	OMG	O4'-C4'-C5'-O5'
40	G	37	T6A	C13-C12-C14-C15
1	S2	590	A2M	C2'-C1'-N9-C4
40	G	37	T6A	N11-C12-C13-ODA
40	G	48	5MC	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
1	S2	590	A2M	C2'-C1'-N9-C8
40	G	47	H2U	O4'-C1'-N1-C2
34	ST	67	NMM	N-CA-CB-CG
1	S2	1490	OMG	C4'-C5'-O5'-P
1	S2	428	OMU	O4'-C1'-N1-C6
1	S2	644	OMG	C4'-C5'-O5'-P
1	S2	36	PSU	O4'-C1'-C5-C4
1	S2	1248	B8N	O4'-C1'-C5-C4
1	S2	428	OMU	O4'-C1'-N1-C2
1	S2	1490	OMG	C3'-C4'-C5'-O5'
1	S2	867	OMG	C1'-C2'-O2'-CM2
1	S2	590	A2M	O4'-C1'-N9-C8
1	S2	36	PSU	O4'-C1'-C5-C6
1	S2	366	PSU	O4'-C1'-C5-C6
1	S2	918	PSU	O4'-C1'-C5-C6
1	S2	1326	UY1	O4'-C1'-C5-C6
1	S2	668	A2M	O4'-C4'-C5'-O5'
1	S2	159	A2M	C4'-C5'-O5'-P
1	S2	1804	OMU	C3'-C4'-C5'-O5'

There are no ring outliers.

32 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	S2	34	PSU	1	0
1	S2	1442	OMU	1	0
40	G	10	1MG	2	0
1	S2	668	A2M	2	0
1	S2	484	A2M	3	0
1	S2	159	A2M	2	0
1	S2	99	A2M	3	0
1	S2	1244	PSU	1	0
1	S2	918	PSU	2	0
1	S2	1851	MA6	5	0
1	S2	1850	MA6	3	0
1	S2	651	PSU	1	0
1	S2	1842	4AC	1	0
1	S2	866	PSU	1	0
1	S2	1238	PSU	1	0
1	S2	1678	A2M	2	0
1	S2	100	PSU	1	0
1	S2	468	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	S2	1383	A2M	1	0
1	S2	867	OMG	3	0
1	S2	27	A2M	1	0
1	S2	166	A2M	1	0
40	G	47	H2U	1	0
1	S2	1445	PSU	1	0
1	S2	462	OMC	1	0
1	S2	1832	6MZ	3	0
1	S2	116	OMU	7	0
1	S2	1031	A2M	2	0
1	S2	512	A2M	3	0
40	G	37	T6A	1	0
1	S2	576	A2M	4	0
1	S2	1174	PSU	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 90 ligands modelled in this entry, 88 are monoatomic - leaving 2 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
45	GNP	E	501	-	33,34,34	2.24	5 (15%)	46,54,54	1.54	4 (8%)
46	MET	E	502	-	6,7,8	0.55	0	2,7,9	0.28	0

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
45	GNP	E	501	-	-	7/18/38/38	0/3/3/3
46	MET	E	502	-	-	1/5/6/8	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	E	501	GNP	PB-O3A	7.99	1.69	1.59
45	E	501	GNP	PG-N3B	6.67	1.80	1.63
45	E	501	GNP	PG-O1G	4.65	1.53	1.46
45	E	501	GNP	PB-O1B	3.14	1.51	1.46
45	E	501	GNP	PB-O2B	-2.25	1.50	1.56

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	E	501	GNP	O1G-PG-N3B	-7.53	100.69	111.77
45	E	501	GNP	O2B-PB-O1B	4.72	119.81	109.92
45	E	501	GNP	O3A-PB-N3B	-2.30	100.20	106.59
45	E	501	GNP	O2G-PG-O3G	2.26	113.66	107.64

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	E	501	GNP	PB-N3B-PG-O1G
45	E	501	GNP	PG-N3B-PB-O1B
45	E	501	GNP	PG-N3B-PB-O3A
45	E	501	GNP	PA-O3A-PB-O1B
45	E	501	GNP	PA-O3A-PB-O2B
45	E	501	GNP	O4'-C4'-C5'-O5'
45	E	501	GNP	C3'-C4'-C5'-O5'
46	E	502	MET	C-CA-CB-CG

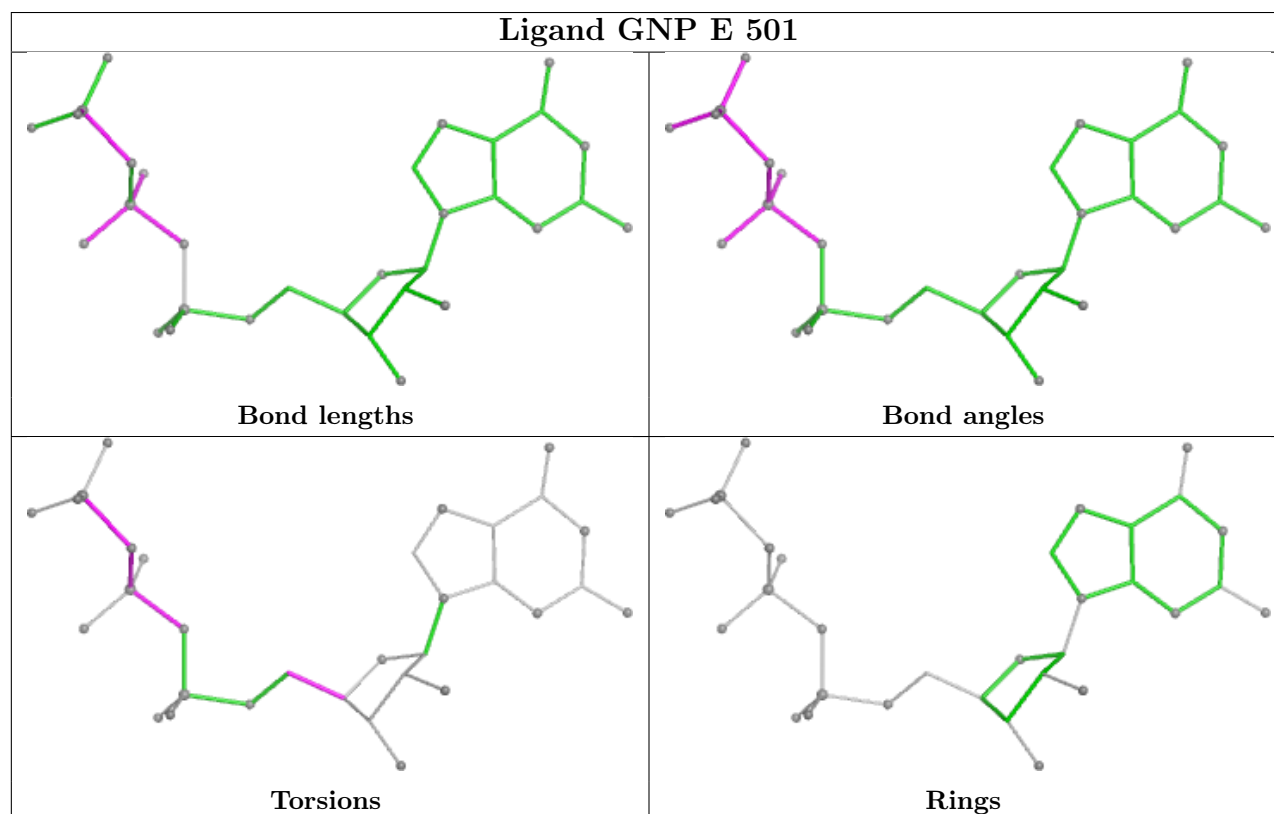
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	E	502	MET	2	0

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

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
40	G	1
1	S2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	46:M7G	O3'	47:H2U	P	3.82
1	S2	1639:M7G	O3'	1640:A	P	2.81

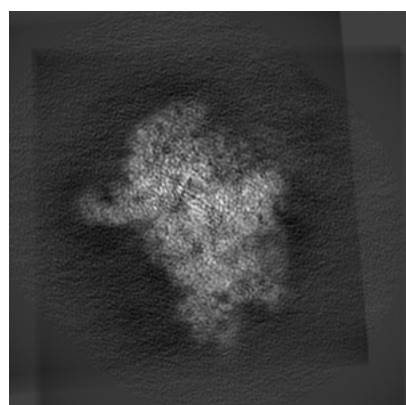
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-57005. These allow visual inspection of the internal detail of the map and identification of artifacts.

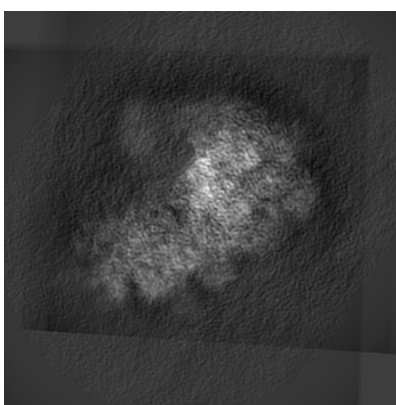
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

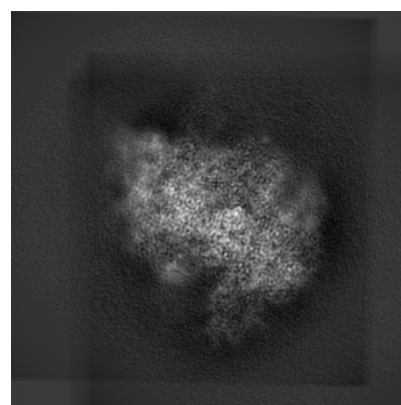
#### 6.1.1 Primary map



X



Y

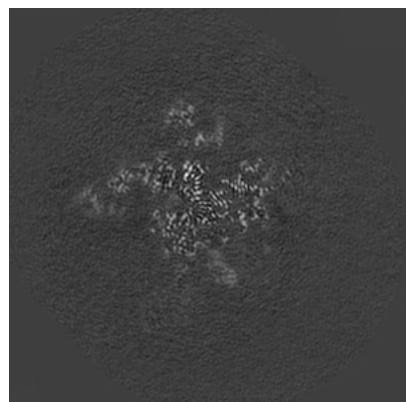


Z

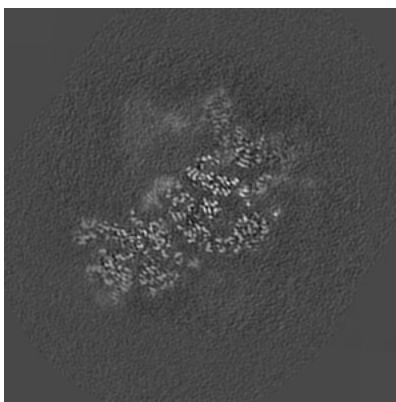
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

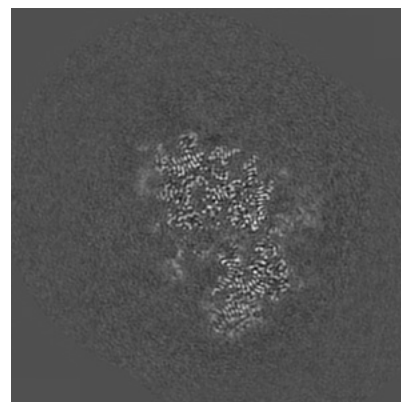
#### 6.2.1 Primary map



X Index: 260



Y Index: 260



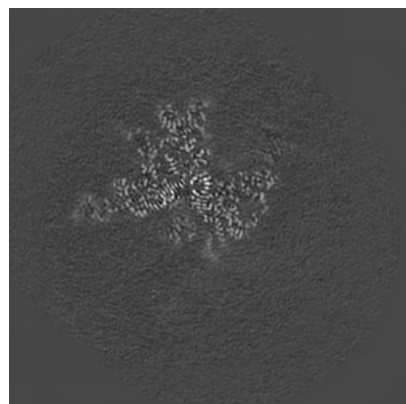
Z Index: 260



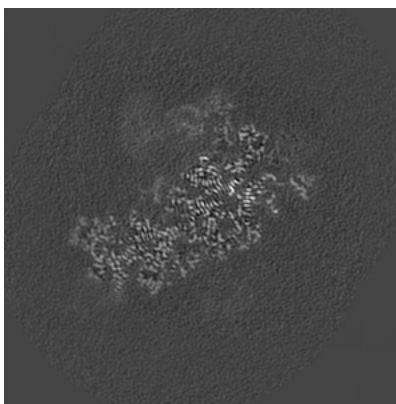
The images above show central slices of the map in three orthogonal directions.

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

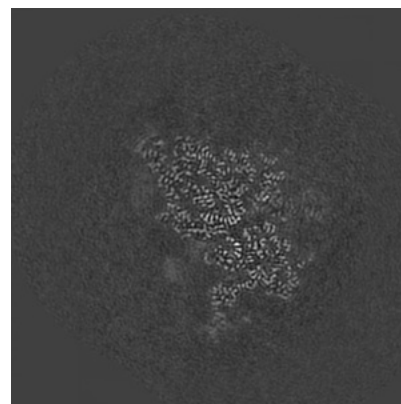
### 6.3.1 Primary map



X Index: 291



Y Index: 253

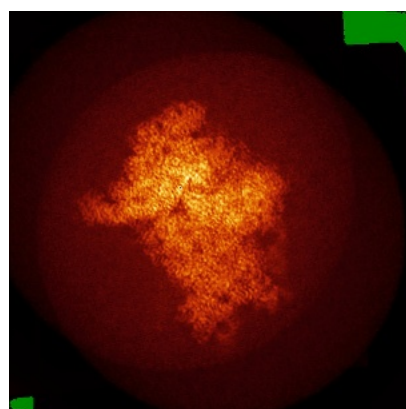


Z Index: 279

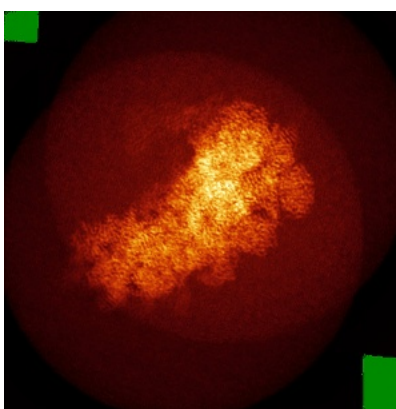
The images above show the largest variance slices of the map in three orthogonal directions.

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

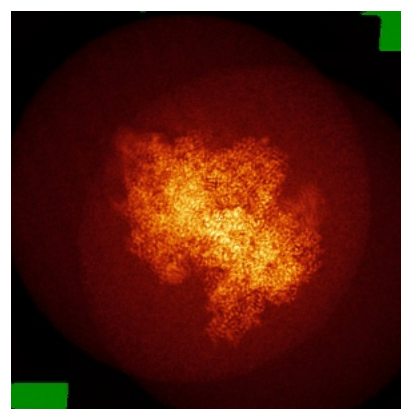
### 6.4.1 Primary map



X



Y

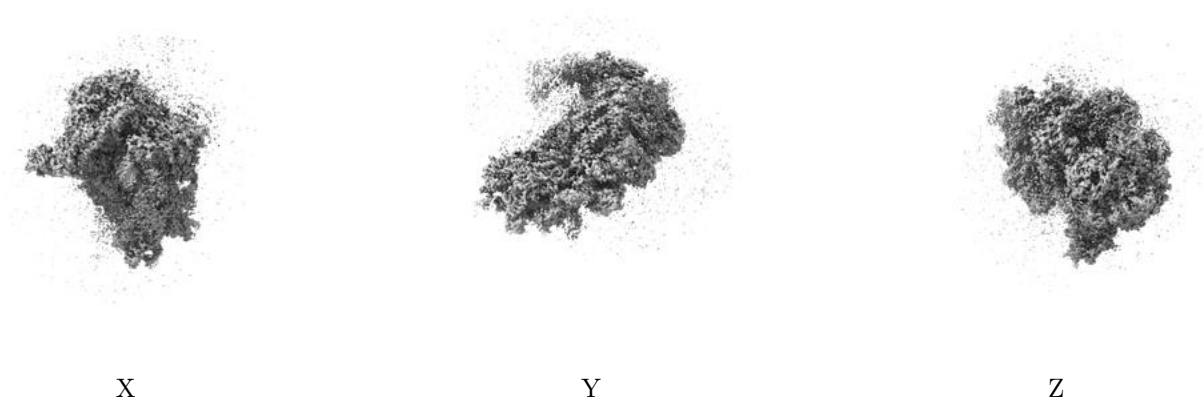


Z

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

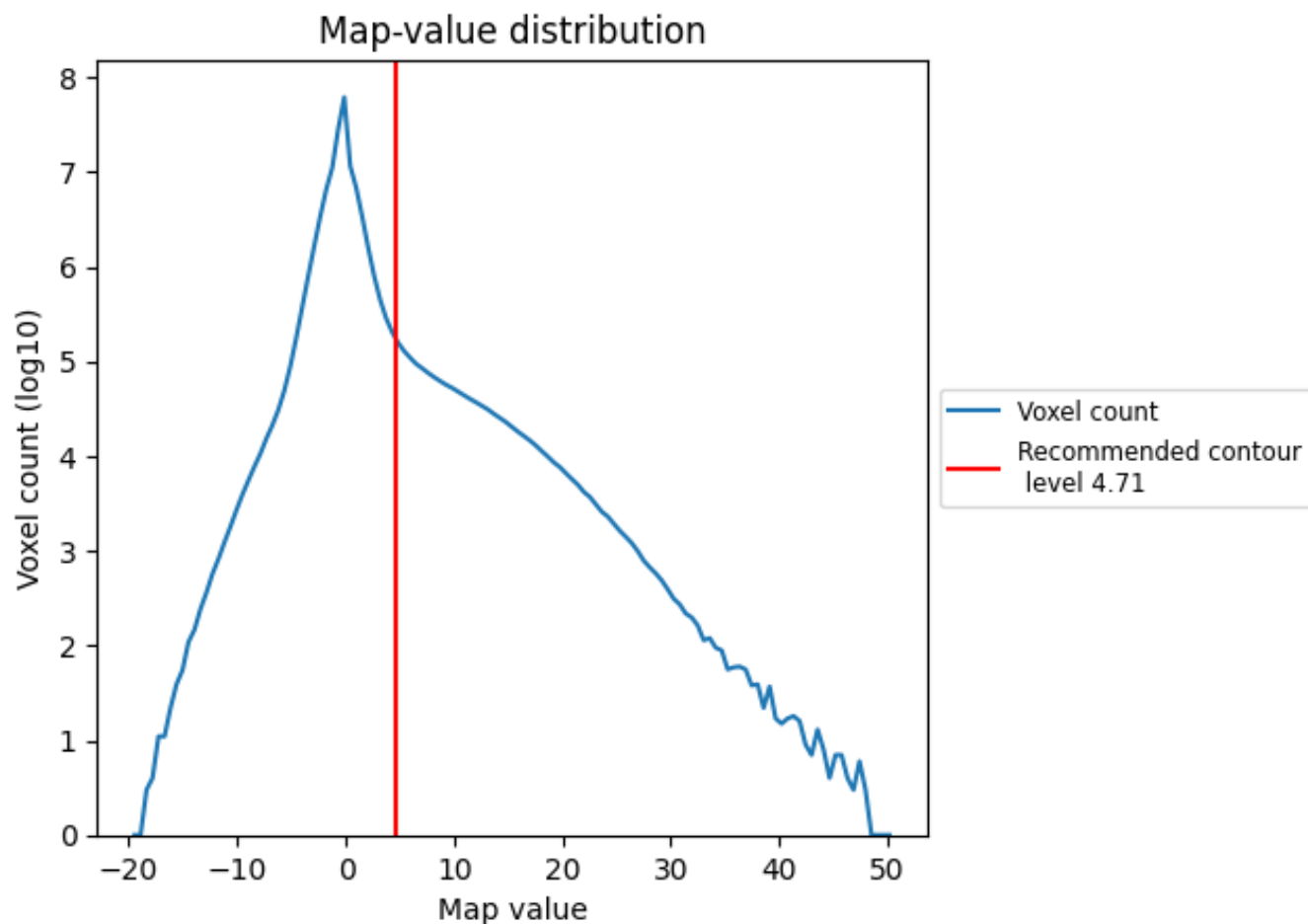
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

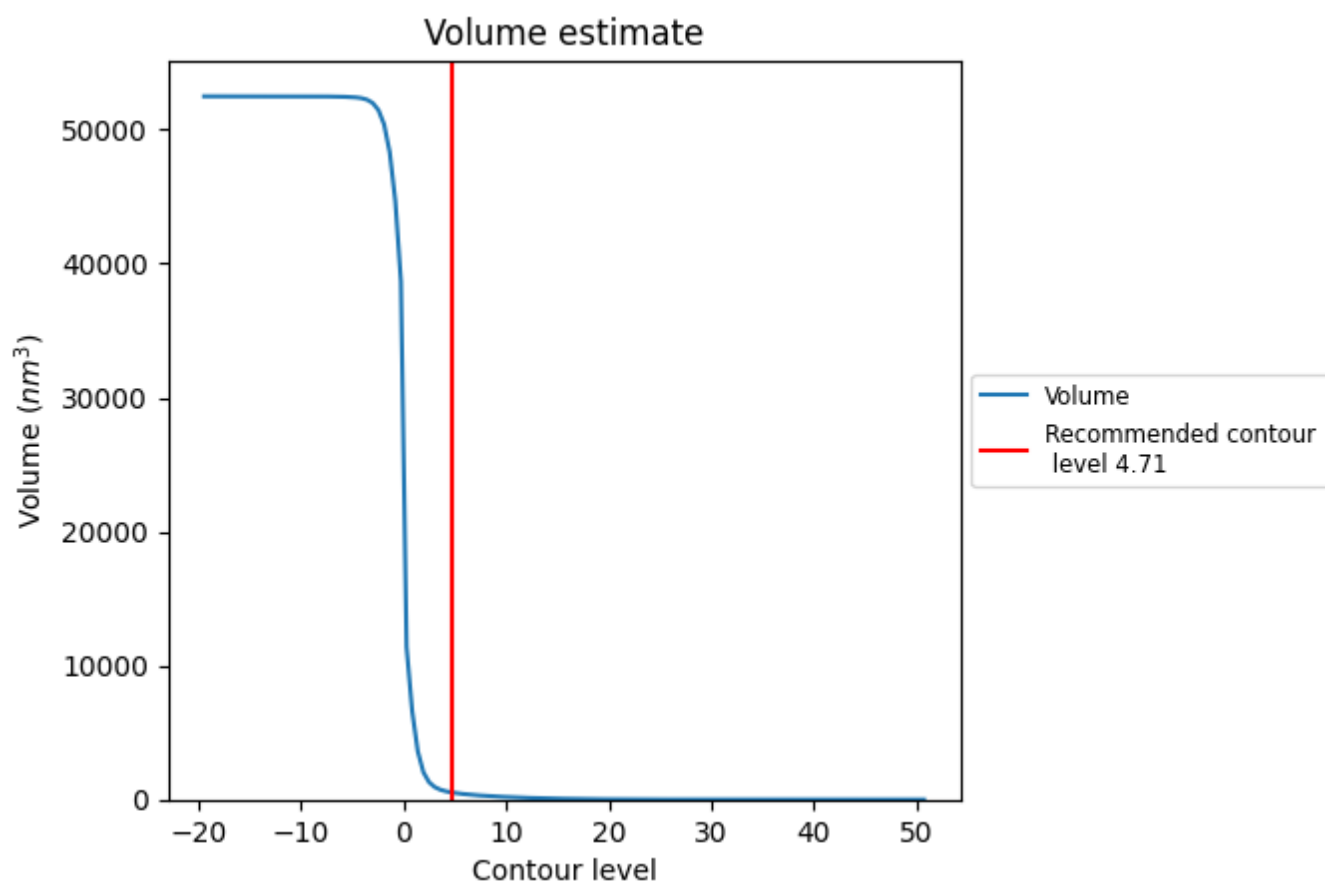
This section contains the results of statistical analysis of the map.

### 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.

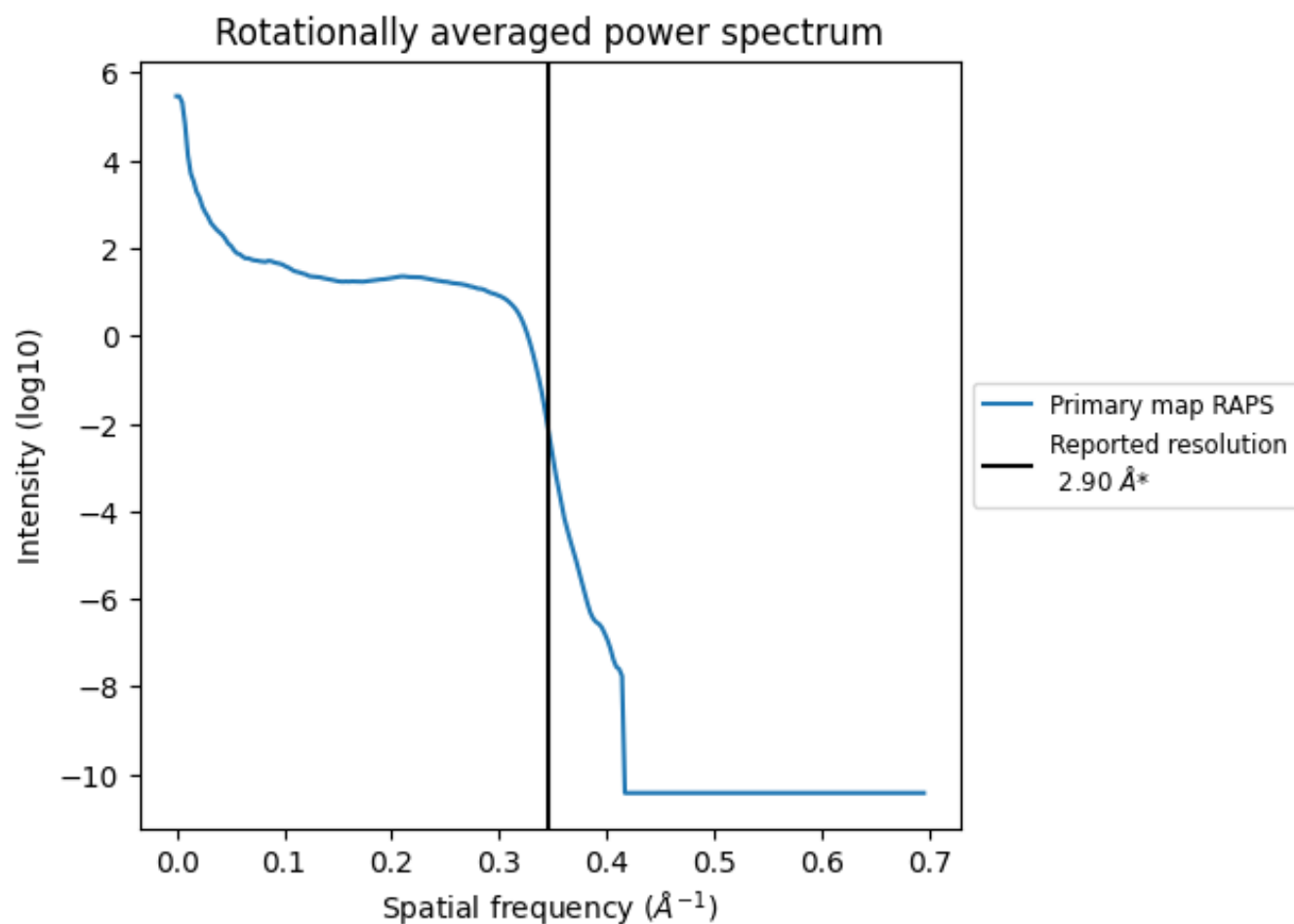
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 527  $\text{nm}^3$ ; this corresponds to an approximate mass of 476 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 0.345 Å<sup>-1</sup>

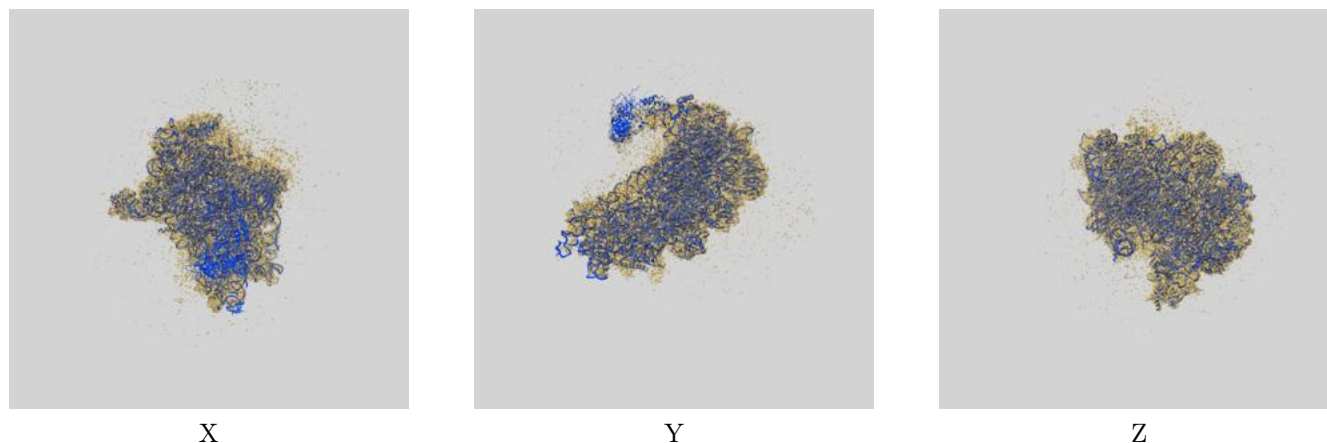
## 8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

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

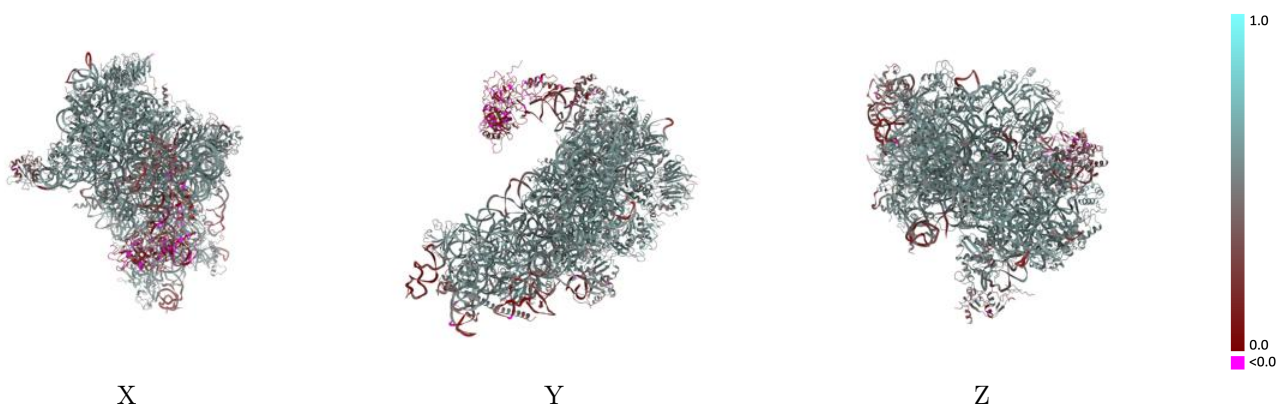
This section contains information regarding the fit between EMDB map EMD-57005 and PDB model 28ZV. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

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



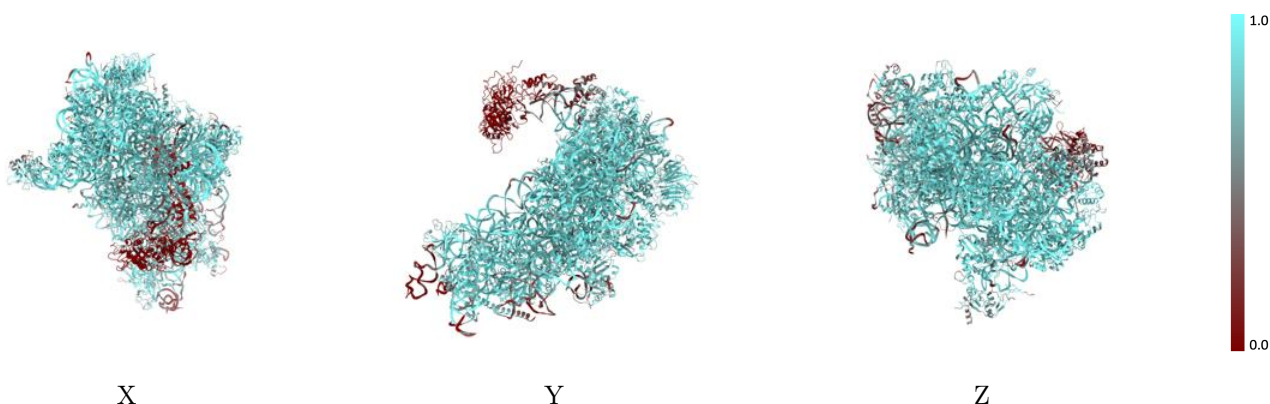
The images above show the 3D surface view of the map at the recommended contour level 4.71 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

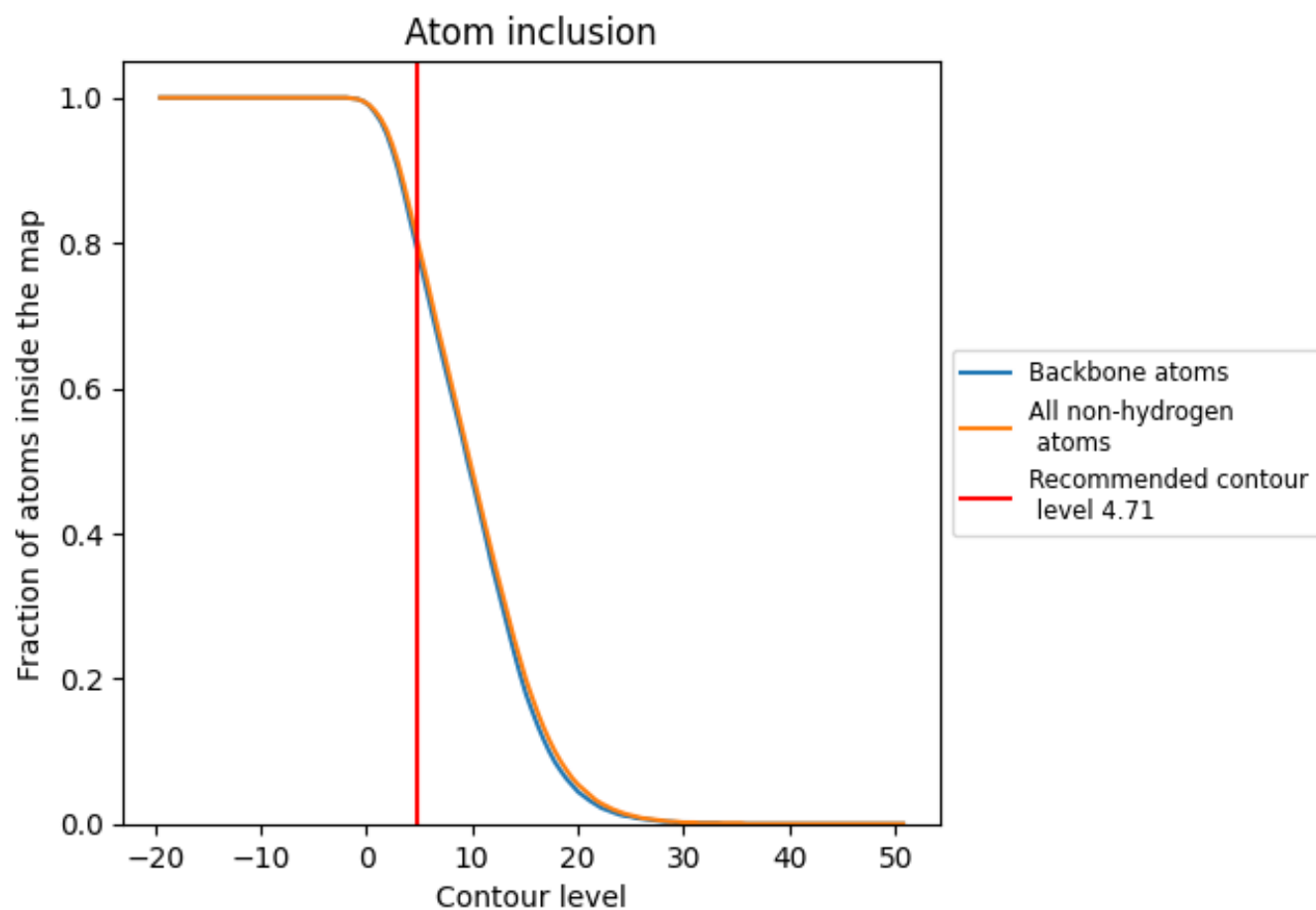
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (4.71).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 81% 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 (4.71) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8120	 0.5130
B	 0.4820	 0.3090
D	 0.4090	 0.3570
E	 0.0340	 0.1700
F	 0.0150	 0.1630
G	 0.7290	 0.3770
H	 0.7430	 0.5200
Ln	 0.7750	 0.5530
S2	 0.8920	 0.5310
SA	 0.8880	 0.5590
SB	 0.8600	 0.5570
SC	 0.9130	 0.5820
SD	 0.8710	 0.5550
SE	 0.8740	 0.5750
SF	 0.8820	 0.5630
SG	 0.7600	 0.5200
SH	 0.7160	 0.4950
SI	 0.8010	 0.5410
SJ	 0.8510	 0.5600
SK	 0.8990	 0.5520
SL	 0.8350	 0.5600
SM	 0.6600	 0.3960
SN	 0.8580	 0.5520
SO	 0.8580	 0.5510
SP	 0.8330	 0.5270
SQ	 0.9120	 0.5770
SR	 0.8710	 0.5470
SS	 0.8730	 0.5560
ST	 0.9010	 0.5660
SU	 0.8130	 0.5200
SV	 0.8920	 0.5600
SW	 0.9060	 0.5840
SX	 0.8750	 0.5730
SY	 0.8460	 0.5560
SZ	 0.8890	 0.5540



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Chain	Atom inclusion	Q-score
Sa	 0.8610	 0.5690
Sb	 0.8220	 0.5410
Sc	 0.8520	 0.5530
Sd	 0.9320	 0.5870
Se	 0.7700	 0.5090
Sf	 0.7490	 0.4440
Sg	 0.8740	 0.5390