



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 07:32 PM UTC

PDB ID : 8XP3 / pdb_00008xp3
EMDB ID : EMD-38549
Title : Cryo-EM structure of the human 40S ribosome with LARP1 and LRRC47
Authors : Huang, Z.; Ye, X.; Li, Y.; Cheng, J.
Deposited on : 2024-01-02
Resolution : 3.40 Å(reported)
Based on initial model : 6Z6M

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

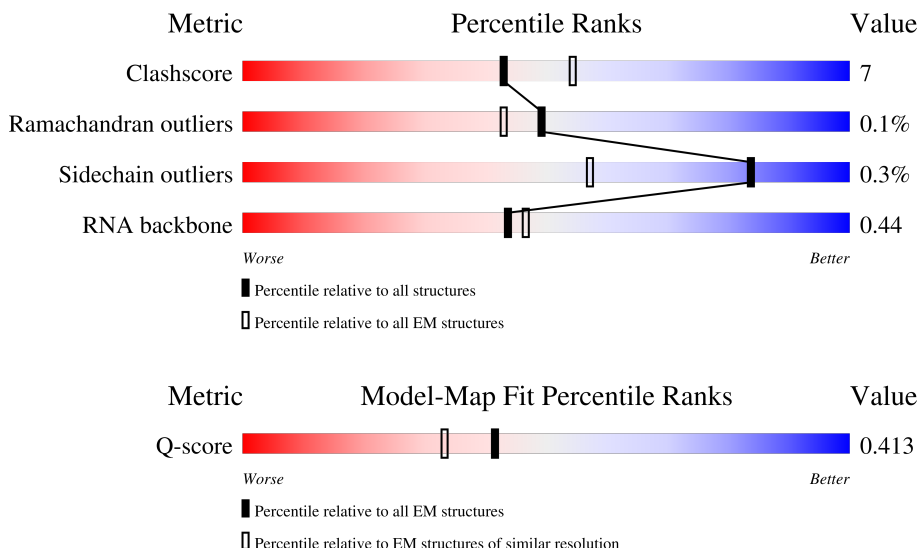
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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.



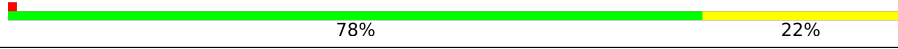
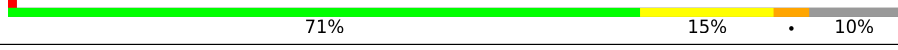
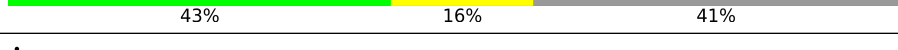
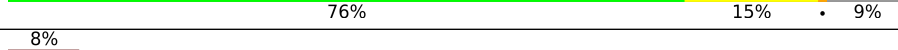
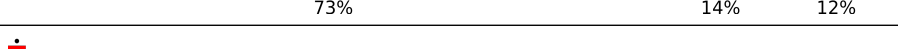
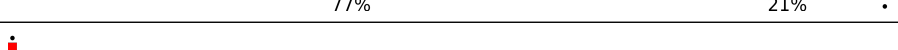
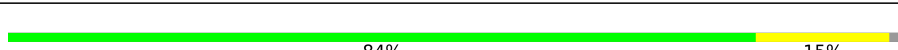
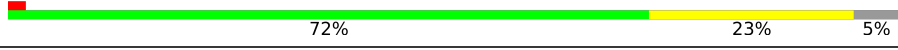
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14717 (2.90 - 3.90)

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

Mol	Chain	Length	Quality of chain
1	Ln	25	
2	S2	1869	
3	SA	295	

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Mol	Chain	Length	Quality of chain
4	SB	264	
5	SD	243	
6	SE	263	
7	SF	204	
8	SH	194	
9	SI	208	
10	SK	165	
11	SL	158	
12	SP	145	
13	SQ	146	
14	SR	135	
15	SS	152	
16	ST	145	
17	SU	119	
18	SV	83	
19	SX	143	
20	Sa	115	
21	Sc	69	
22	Sd	56	
23	Sg	317	
24	SC	293	
25	SG	249	
26	SJ	194	
27	SM	132	
28	SN	151	

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Mol	Chain	Length	Quality of chain
29	SO	151	 76%13%11%
30	SW	130	 88%12%
31	SY	133	 75%19%6%
32	SZ	125	 7%54%6%40%
33	Sb	84	 79%20%
34	Se	59	 10%85%14%
35	Sf	156	 5%37%61%
36	JD	1096	 95%
37	JC	583	 8%72%16%12%

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 80435 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60S ribosomal protein L41.

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

- Molecule 2 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S2	1740	Total	C	N	O	P	0	0
			36896	16458	6597	12102	1739		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S2	582	C	U	conflict	GB 36162
S2	583	C	A	conflict	GB 36162
S2	584	G	A	conflict	GB 36162
S2	798	A	G	conflict	GB 36162
S2	1095	U	C	conflict	GB 36162

- Molecule 3 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	SA	222	Total	C	N	O	S	0	0
			1747	1109	306	324	8		

- Molecule 4 is a protein called 40S ribosomal protein S3a.

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

- Molecule 5 is a protein called 40S ribosomal protein S3.

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

- Molecule 6 is a protein called 40S ribosomal protein S4, X isoform.

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

- Molecule 7 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SF	184	Total	C	N	O	S	0	0
			1461	914	276	264	7		

- Molecule 8 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SH	186	Total	C	N	O	S	0	0
			1497	956	274	266	1		

- Molecule 9 is a protein called 40S ribosomal protein S8.

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

- Molecule 10 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SK	98	Total	C	N	O	S	0	0
			827	539	148	134	6		

- Molecule 11 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SL	144	Total	C	N	O	S	0	0
			1182	752	224	200	6		

- Molecule 12 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SP	127	Total	C	N	O	S	0	0
			1045	663	198	177	7		

- Molecule 13 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SQ	144	Total	C	N	O	S	0	0
			1142	726	216	197	3		

- Molecule 14 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	SR	135	Total	C	N	O	S	0	0
			1090	685	202	198	5		

- Molecule 15 is a protein called 40S ribosomal protein S18.

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

- Molecule 16 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	ST	143	Total	C	N	O	S	0	0
			1112	697	214	198	3		

- Molecule 17 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	SU	104	Total	C	N	O	S	0	0
			821	514	155	148	4		

- Molecule 18 is a protein called 40S ribosomal protein S21.

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

- Molecule 19 is a protein called 40S ribosomal protein S23.

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

- Molecule 20 is a protein called 40S ribosomal protein S26.

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

- Molecule 21 is a protein called 40S ribosomal protein S28.

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

- Molecule 22 is a protein called 40S ribosomal protein S29.

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

- Molecule 23 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 24 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	SC	222	Total	C	N	O	S	0	0
			1725	1115	298	302	10		

- Molecule 25 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	SG	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 26 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	SJ	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 27 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	SM	122	Total	C	N	O	S	0	0
			940	590	164	177	9		

- Molecule 28 is a protein called 40S ribosomal protein S13.

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

- Molecule 29 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	SO	135	Total	C	N	O	S	0	0
			1010	618	198	188	6		

- Molecule 30 is a protein called 40S ribosomal protein S15a.

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

- Molecule 31 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	SY	125	Total	C	N	O	S	0	0
			1022	645	200	172	5		

- Molecule 32 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	SZ	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 33 is a protein called 40S ribosomal protein S27.

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

- Molecule 34 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Se	58	Total	C	N	O	S	0	0
			459	284	100	74	1		

- Molecule 35 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Sf	61	Total	C	N	O	S	0	0
			497	312	94	84	7		

- Molecule 36 is a protein called La-related protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	JD	52	Total	C	N	O	S	0	0
			429	269	75	83	2		

- Molecule 37 is a protein called Leucine-rich repeat-containing protein 47.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	JC	512	Total	C	N	O	S	0	0
			3941	2479	713	734	15		

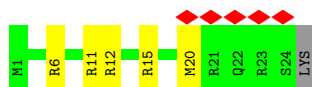
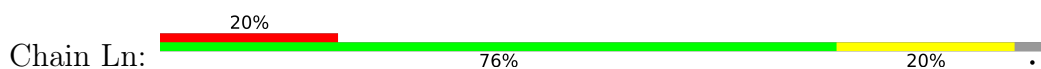
- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

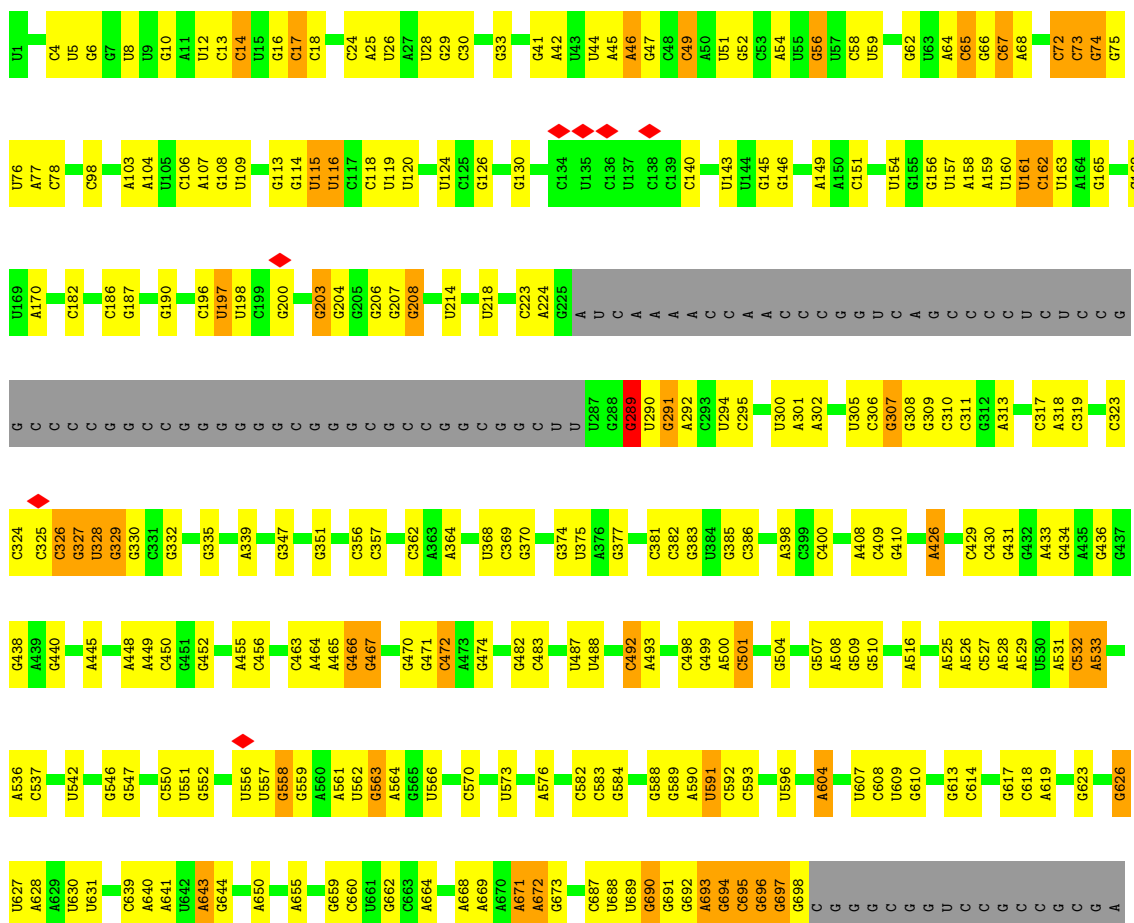
3 Residue-property plots

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

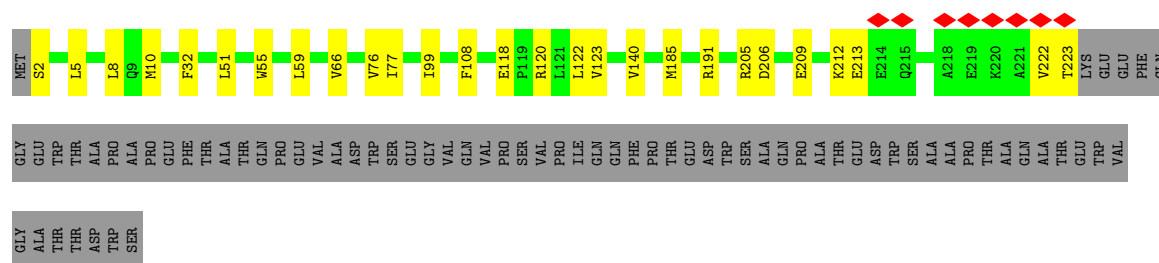
- Molecule 1: 60S ribosomal protein L41



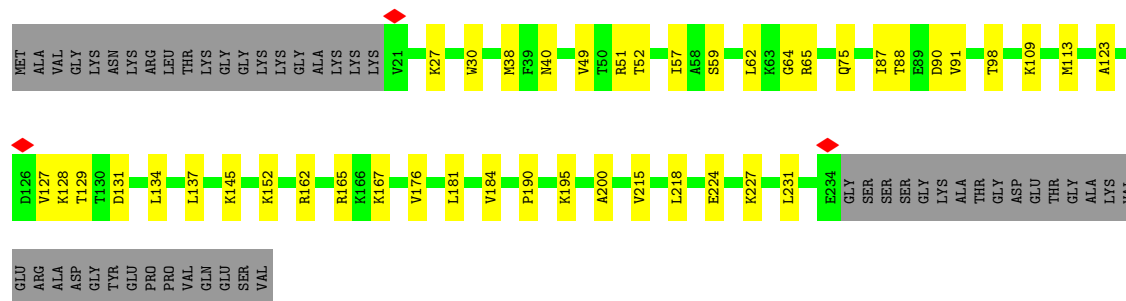
- Molecule 2: 18S rRNA



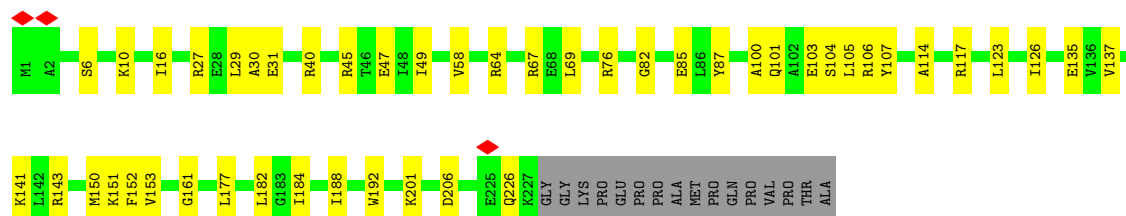
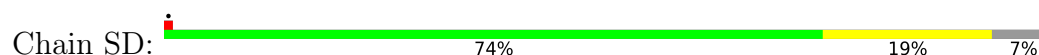




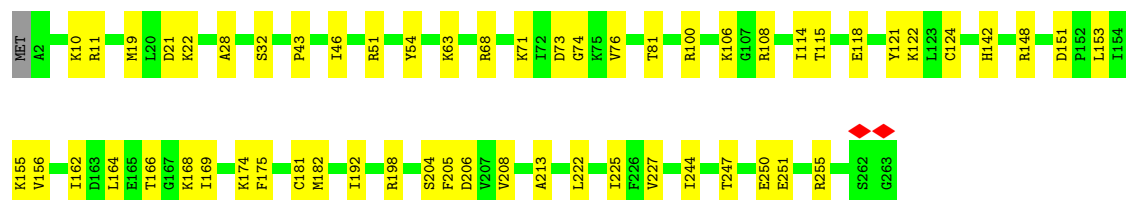
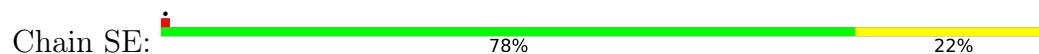
• Molecule 4: 40S ribosomal protein S3a



• Molecule 5: 40S ribosomal protein S3

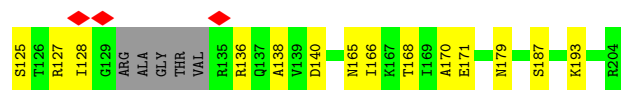


• Molecule 6: 40S ribosomal protein S4, X isoform

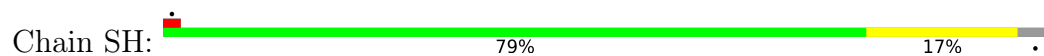


• Molecule 7: 40S ribosomal protein S5

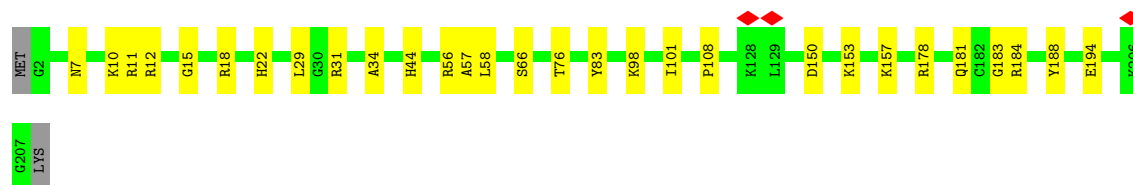
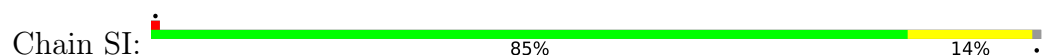




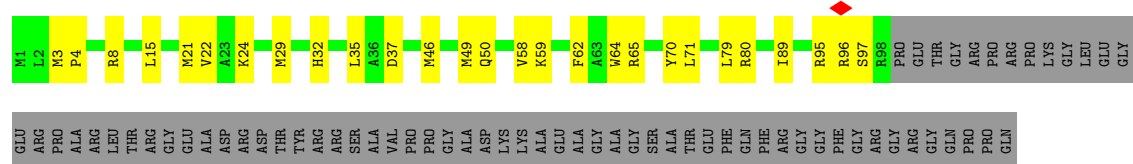
- Molecule 8: 40S ribosomal protein S7



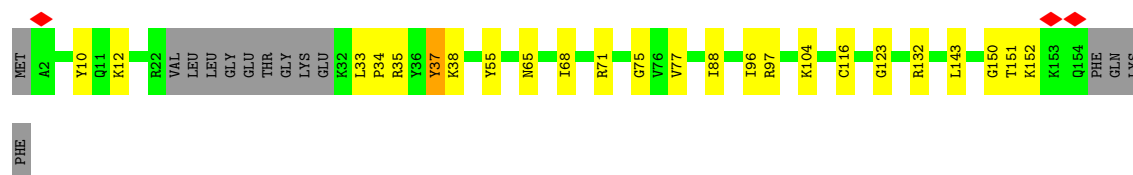
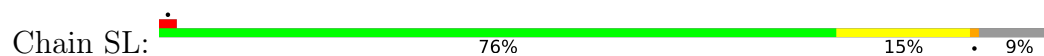
- Molecule 9: 40S ribosomal protein S8



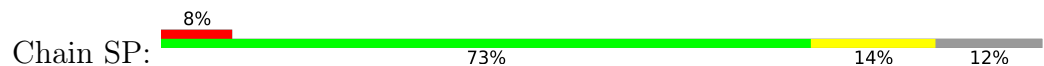
- Molecule 10: 40S ribosomal protein S10

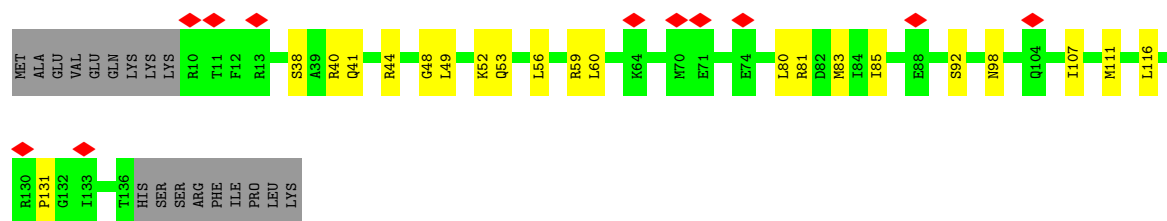


- Molecule 11: 40S ribosomal protein S11

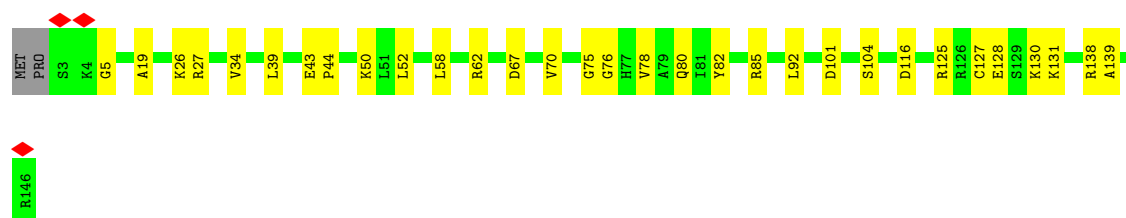
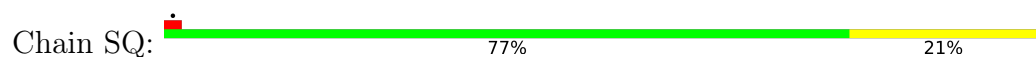


- Molecule 12: 40S ribosomal protein S15

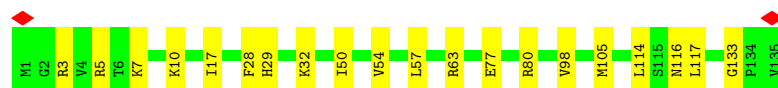
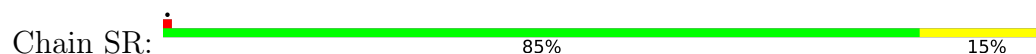




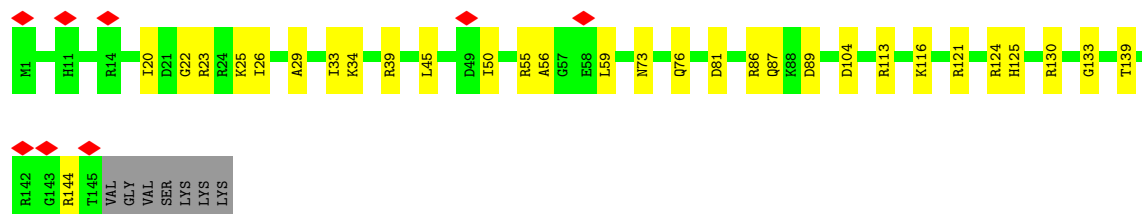
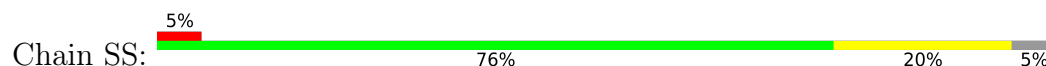
- Molecule 13: 40S ribosomal protein S16



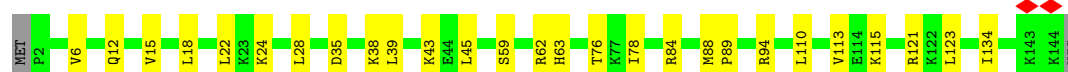
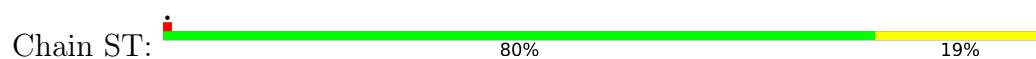
- Molecule 14: 40S ribosomal protein S17



- Molecule 15: 40S ribosomal protein S18

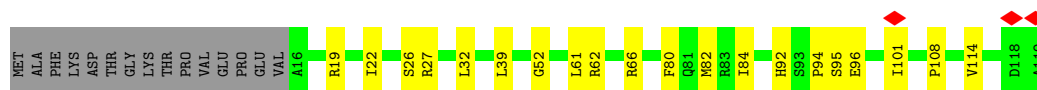


- Molecule 16: 40S ribosomal protein S19



- Molecule 17: 40S ribosomal protein S20

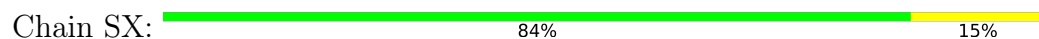




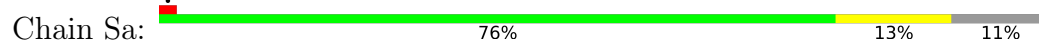
- Molecule 18: 40S ribosomal protein S21



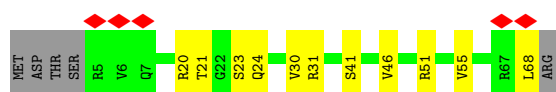
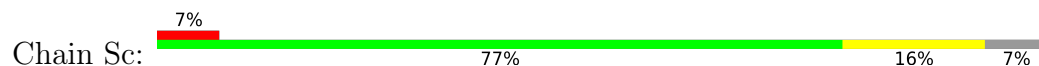
- Molecule 19: 40S ribosomal protein S23



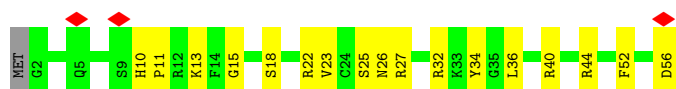
- Molecule 20: 40S ribosomal protein S26



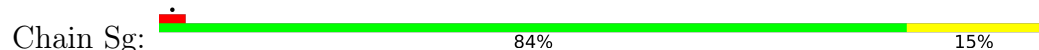
- Molecule 21: 40S ribosomal protein S28



- Molecule 22: 40S ribosomal protein S29



- Molecule 23: Receptor of activated protein C kinase 1



- Molecule 34: 40S ribosomal protein S30



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	9897	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.072	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	481.32, 481.32, 481.32	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.146, 1.146, 1.146	Depositor

5 Model quality

5.1 Standard geometry

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

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	Ln	0.26	0/231	0.52	0/294
2	S2	0.24	0/41241	0.38	5/64258 (0.0%)
3	SA	0.21	0/1784	0.46	0/2424
4	SB	0.18	0/1765	0.50	0/2362
5	SD	0.20	0/1793	0.51	0/2414
6	SE	0.22	0/2118	0.49	2/2849 (0.1%)
7	SF	0.34	0/1481	0.77	1/1988 (0.1%)
8	SH	0.21	0/1519	0.54	0/2033
9	SI	0.20	0/1715	0.51	0/2287
10	SK	0.19	0/851	0.46	0/1147
11	SL	0.27	0/1202	0.55	0/1606
12	SP	0.16	0/1065	0.48	0/1423
13	SQ	0.21	0/1160	0.52	0/1553
14	SR	0.31	0/1105	0.62	0/1484
15	SS	0.20	0/1216	0.53	0/1628
16	ST	0.17	0/1131	0.43	0/1515
17	SU	0.21	0/831	0.51	0/1115
18	SV	0.19	0/643	0.53	1/860 (0.1%)
19	SX	0.19	0/1116	0.45	0/1490
20	Sa	0.20	0/836	0.46	0/1121
21	Sc	0.21	0/508	0.48	0/680
22	Sd	0.20	0/470	0.57	0/623
23	Sg	0.19	0/2493	0.52	0/3394
24	SC	0.22	0/1762	0.51	0/2381
25	SG	0.21	0/1946	0.51	0/2590
26	SJ	0.20	0/1550	0.45	0/2069
27	SM	0.15	0/950	0.45	0/1275
28	SN	0.22	0/1232	0.55	2/1656 (0.1%)
29	SO	0.21	0/1023	0.45	0/1372
30	SW	0.22	0/1051	0.43	0/1406
31	SY	0.18	0/1039	0.46	0/1381
32	SZ	0.19	0/604	0.47	0/810

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Sb	0.24	0/665	0.60	0/891
34	Se	0.20	0/465	0.51	0/612
35	Sf	0.15	0/507	0.48	0/673
36	JD	0.11	0/435	0.35	0/581
37	JC	0.15	0/4006	0.42	0/5429
All	All	0.23	0/85509	0.45	11/123674 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	SK	0	1
13	SQ	0	1
All	All	0	2

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	SV	78	ILE	N-CA-C	-10.33	103.89	113.71
7	SF	67	PRO	CA-N-CD	-7.52	101.48	112.00
2	S2	291	G	C2'-C3'-O3'	6.99	124.19	113.70
2	S2	501	C	N1-C1'-C2'	6.55	121.83	112.00
2	S2	289	G	C4'-C3'-O3'	-6.02	103.96	113.00
2	S2	291	G	C4'-C3'-C2'	-5.90	96.70	102.60
28	SN	45	LEU	CA-C-N	5.80	128.45	120.39
28	SN	45	LEU	C-N-CA	5.80	128.45	120.39
6	SE	156	VAL	CA-C-N	5.57	130.31	122.46
6	SE	156	VAL	C-N-CA	5.57	130.31	122.46
2	S2	1453	C	N1-C1'-C2'	5.12	119.67	112.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	SK	29	MET	Peptide
13	SQ	43	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Ln	230	0	276	5	0
2	S2	36896	0	18603	434	0
3	SA	1747	0	1751	19	0
4	SB	1738	0	1809	27	0
5	SD	1765	0	1865	34	0
6	SE	2076	0	2177	38	0
7	SF	1461	0	1511	30	0
8	SH	1497	0	1590	25	0
9	SI	1686	0	1772	22	0
10	SK	827	0	854	18	0
11	SL	1182	0	1253	16	0
12	SP	1045	0	1095	14	0
13	SQ	1142	0	1213	19	0
14	SR	1090	0	1149	13	0
15	SS	1198	0	1261	22	0
16	ST	1112	0	1146	21	0
17	SU	821	0	883	13	0
18	SV	636	0	637	7	0
19	SX	1098	0	1167	15	0
20	Sa	821	0	870	11	0
21	Sc	506	0	536	9	0
22	Sd	459	0	451	14	0
23	Sg	2436	0	2393	29	0
24	SC	1725	0	1813	26	0
25	SG	1923	0	2089	39	0
26	SJ	1525	0	1640	25	0
27	SM	940	0	965	12	0
28	SN	1208	0	1294	17	0
29	SO	1010	0	1034	14	0
30	SW	1034	0	1080	11	0
31	SY	1022	0	1088	19	0
32	SZ	598	0	656	7	0
33	Sb	651	0	672	12	0
34	Se	459	0	503	8	0
35	Sf	497	0	497	3	0
36	JD	429	0	415	3	0
37	JC	3941	0	4101	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	Sa	1	0	0	0	0
38	Sb	1	0	0	0	0
38	Sd	1	0	0	0	0
38	Sf	1	0	0	0	0
All	All	80435	0	64109	928	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (928) 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)
2:S2:834:C:N4	2:S2:839:C:H42	1.25	1.31
2:S2:886:A:N6	2:S2:901:G:C4	2.11	1.19
2:S2:24:C:H42	2:S2:650:A:N6	1.50	1.10
2:S2:24:C:N4	2:S2:650:A:H61	1.49	1.10
2:S2:533:A:H61	2:S2:550:C:N4	1.53	1.07
2:S2:834:C:H42	2:S2:839:C:N4	1.53	1.07
2:S2:1534:C:C2	2:S2:1598:G:N2	2.26	1.04
2:S2:1287:A:H62	2:S2:1312:G:N2	1.56	1.02
2:S2:140:C:H42	2:S2:313:A:N6	1.59	1.01
2:S2:140:C:N4	2:S2:313:A:H61	1.57	1.01
2:S2:1050:A:H62	2:S2:1068:G:H21	1.04	1.00
2:S2:1287:A:N6	2:S2:1312:G:H21	1.60	1.00
2:S2:1609:C:H42	2:S2:1630:A:H61	1.02	0.99
2:S2:1609:C:N4	2:S2:1630:A:H61	1.60	0.98
2:S2:1236:G:H21	2:S2:1522:A:N6	1.62	0.97
2:S2:533:A:H61	2:S2:550:C:H42	1.00	0.97
2:S2:533:A:N6	2:S2:550:C:H42	1.63	0.97
2:S2:1726:G:H1	2:S2:1808:U:H3	1.03	0.97
2:S2:1050:A:H62	2:S2:1068:G:N2	1.63	0.97
2:S2:1609:C:H42	2:S2:1630:A:N6	1.63	0.96
2:S2:834:C:N4	2:S2:839:C:N4	2.09	0.94
2:S2:1236:G:H21	2:S2:1522:A:H61	1.13	0.94
2:S2:834:C:N3	2:S2:839:C:N3	2.16	0.94
2:S2:1756:C:N4	2:S2:1776:G:H22	1.65	0.93
2:S2:1756:C:H42	2:S2:1776:G:N2	1.66	0.92
2:S2:696:G:N2	2:S2:737:G:H1	1.66	0.91
2:S2:925:G:H1	2:S2:1017:U:H3	1.14	0.90
2:S2:696:G:H21	2:S2:737:G:H1	0.94	0.90
2:S2:1287:A:H62	2:S2:1312:G:H21	0.90	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:694:G:C6	2:S2:737:G:N2	2.41	0.89
2:S2:1417:C:H42	2:S2:1422:G:N2	1.71	0.88
2:S2:1752:C:C4	2:S2:1779:G:N2	2.43	0.87
2:S2:1756:C:H42	2:S2:1776:G:H22	0.86	0.85
2:S2:748:C:H42	2:S2:795:A:N6	1.74	0.84
2:S2:528:A:N1	2:S2:558:G:C6	2.48	0.82
2:S2:1050:A:N6	2:S2:1068:G:H21	1.77	0.82
2:S2:1236:G:N2	2:S2:1522:A:H61	1.77	0.81
2:S2:834:C:H42	2:S2:839:C:H42	0.82	0.81
2:S2:1417:C:H42	2:S2:1422:G:H22	1.25	0.81
2:S2:694:G:O6	2:S2:737:G:C2	2.34	0.81
2:S2:528:A:C2	2:S2:558:G:N1	2.51	0.79
2:S2:912:C:C4	2:S2:914:U:C2	2.71	0.79
2:S2:924:G:H1	2:S2:1018:U:H3	1.31	0.79
2:S2:1417:C:N4	2:S2:1422:G:H22	1.80	0.78
2:S2:989:C:N4	2:S2:1001:A:C2	2.52	0.78
2:S2:810:A:N6	2:S2:851:C:N4	2.32	0.77
2:S2:532:C:C2	2:S2:552:G:N2	2.53	0.76
2:S2:1230:C:O2	2:S2:1665:G:N2	2.19	0.76
2:S2:886:A:N6	2:S2:901:G:C5	2.54	0.75
2:S2:1416:C:N4	2:S2:1417:C:N4	2.33	0.75
2:S2:1416:C:C4	2:S2:1417:C:N4	2.54	0.75
23:Sg:153:CYS:SG	23:Sg:155:ARG:NH1	2.59	0.74
3:SA:2:SER:HB3	3:SA:59:LEU:HD22	1.68	0.74
2:S2:1609:C:N3	2:S2:1630:A:N1	2.35	0.74
24:SC:209:VAL:HG21	24:SC:233:LEU:HD11	1.69	0.74
2:S2:1605:G:H21	2:S2:1634:A:H62	1.35	0.74
2:S2:528:A:C2	2:S2:558:G:C6	2.76	0.74
2:S2:955:A:N6	2:S2:971:G:N2	2.36	0.73
2:S2:748:C:N4	2:S2:795:A:H61	1.85	0.73
2:S2:1166:G:H1	2:S2:1193:U:H3	1.38	0.72
2:S2:47:G:H1'	37:JC:428:LYS:HG2	1.72	0.71
2:S2:748:C:N4	2:S2:795:A:N6	2.38	0.71
25:SG:50:VAL:HG12	25:SG:113:ILE:HG22	1.72	0.71
2:S2:1756:C:N4	2:S2:1775:U:C4	2.59	0.71
3:SA:205:ARG:HH22	3:SA:213:GLU:HG2	1.54	0.71
6:SE:68:ARG:HG3	6:SE:76:VAL:HG11	1.73	0.71
9:SI:12:ARG:HE	9:SI:18:ARG:HG3	1.55	0.71
9:SI:29:LEU:HD11	9:SI:31:ARG:HH21	1.55	0.71
2:S2:834:C:O2	2:S2:839:C:O2	2.08	0.71
2:S2:1756:C:N4	2:S2:1775:U:N3	2.38	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:SB:62:LEU:HA	4:SB:65:ARG:HE	1.57	0.70
17:SU:61:LEU:HB2	17:SU:82:MET:HB3	1.73	0.69
2:S2:1709:G:C6	2:S2:1826:G:C6	2.81	0.69
16:ST:88:MET:HE3	16:ST:89:PRO:HD2	1.74	0.68
2:S2:913:A:H62	8:SH:120:ARG:HD2	1.59	0.68
2:S2:140:C:N3	2:S2:313:A:N1	2.42	0.68
2:S2:377:G:H5'	9:SI:98:LYS:HB3	1.76	0.68
2:S2:912:C:N4	2:S2:914:U:N3	2.42	0.67
3:SA:108:PHE:HB3	3:SA:140:VAL:HG21	1.75	0.67
29:SO:34:PHE:HB3	29:SO:41:PHE:HB2	1.76	0.67
6:SE:19:MET:HB2	6:SE:51:ARG:HH22	1.59	0.67
2:S2:1417:C:N3	2:S2:1422:G:N1	2.43	0.67
19:SX:67:ARG:HG3	19:SX:115:ILE:HG12	1.76	0.67
2:S2:694:G:O6	2:S2:737:G:N2	2.28	0.67
23:Sg:45:LEU:O	23:Sg:47:ARG:NH1	2.27	0.67
8:SH:10:LYS:HZ1	8:SH:14:GLU:HB2	1.59	0.67
13:SQ:58:LEU:HB3	13:SQ:62:ARG:HD2	1.76	0.67
2:S2:878:G:O6	2:S2:908:A:N1	2.28	0.66
29:SO:75:MET:SD	29:SO:79:GLN:NE2	2.69	0.66
11:SL:55:TYR:OH	11:SL:116:CYS:SG	2.54	0.66
2:S2:955:A:H62	2:S2:971:G:N2	1.94	0.66
22:Sd:11:PRO:HB2	22:Sd:13:LYS:HG3	1.77	0.66
6:SE:153:LEU:HD13	25:SG:216:ARG:HD3	1.79	0.65
2:S2:886:A:C6	2:S2:901:G:N3	2.64	0.65
2:S2:1534:C:O2	2:S2:1598:G:N2	2.29	0.65
7:SF:80:GLY:HA2	7:SF:83:ASN:HB2	1.77	0.65
10:SK:4:PRO:O	10:SK:8:ARG:NH1	2.29	0.65
2:S2:1416:C:N4	2:S2:1417:C:H41	1.92	0.65
37:JC:25:LEU:HA	37:JC:56:GLU:HB3	1.78	0.65
2:S2:694:G:N7	2:S2:696:G:N2	2.45	0.65
2:S2:157:U:H4'	25:SG:59:GLN:HA	1.79	0.65
30:SW:66:THR:HG23	30:SW:68:ARG:HG3	1.78	0.65
2:S2:1259:A:N6	2:S2:1519:U:OP1	2.30	0.65
2:S2:533:A:N6	2:S2:550:C:N4	2.31	0.65
12:SP:83:MET:HB3	12:SP:116:LEU:HD23	1.79	0.65
5:SD:103:GLU:OE1	5:SD:106:ARG:NH2	2.28	0.64
15:SS:23:ARG:O	15:SS:55:ARG:NH1	2.30	0.64
37:JC:359:GLN:O	37:JC:363:HIS:ND1	2.29	0.64
2:S2:532:C:O2	2:S2:552:G:N2	2.31	0.64
2:S2:746:C:H1'	2:S2:798:A:H61	1.63	0.63
2:S2:1709:G:C5	2:S2:1826:G:N1	2.66	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:SE:198:ARG:HB3	6:SE:208:VAL:HG22	1.79	0.63
37:JC:230:ILE:HG12	37:JC:251:THR:HG23	1.80	0.63
37:JC:307:LEU:HD21	37:JC:508:LYS:HB2	1.81	0.63
2:S2:886:A:N6	2:S2:901:G:N3	2.46	0.63
19:SX:134:TYR:O	34:Se:13:ARG:NH2	2.32	0.63
37:JC:452:VAL:HG22	37:JC:458:VAL:HG22	1.79	0.63
2:S2:1546:G:H21	2:S2:1670:C:H1'	1.64	0.62
2:S2:124:U:OP1	6:SE:148:ARG:NH2	2.32	0.62
2:S2:1656:G:H1	2:S2:1668:U:H3	1.47	0.62
2:S2:1658:G:OP2	2:S2:1660:C:N4	2.32	0.62
2:S2:1709:G:O6	2:S2:1826:G:C6	2.53	0.62
19:SX:94:ILE:HG12	19:SX:125:VAL:HG11	1.79	0.62
32:SZ:99:LEU:HD21	32:SZ:102:LYS:HB2	1.81	0.62
2:S2:1177:U:H5''	37:JC:252:ARG:HH22	1.64	0.62
2:S2:1700:C:N3	2:S2:1834:A:N1	2.48	0.62
15:SS:73:ASN:HB3	15:SS:76:GLN:HE22	1.65	0.62
24:SC:191:VAL:HG11	24:SC:236:PHE:HA	1.80	0.62
37:JC:191:LEU:HB2	37:JC:212:ASN:HD21	1.65	0.62
2:S2:1743:G:H21	2:S2:1791:A:H62	1.47	0.61
7:SF:67:PRO:HD2	7:SF:70:GLU:HB2	1.81	0.61
11:SL:104:LYS:O	19:SX:11:ARG:NH2	2.33	0.61
2:S2:140:C:H42	2:S2:313:A:H61	0.76	0.61
24:SC:94:ILE:HG23	24:SC:159:LYS:HE2	1.82	0.61
2:S2:804:U:H3	2:S2:859:G:H1	1.48	0.61
2:S2:1550:G:H3'	2:S2:1579:A:H61	1.66	0.61
5:SD:101:GLN:HG2	5:SD:126:ILE:HD11	1.82	0.61
17:SU:80:PHE:HB3	22:Sd:52:PHE:HB3	1.83	0.61
8:SH:144:ILE:HB	30:SW:52:ILE:HB	1.83	0.60
24:SC:65:LYS:HD2	24:SC:273:LEU:HD13	1.83	0.60
4:SB:40:ASN:ND2	4:SB:75:GLN:OE1	2.34	0.60
37:JC:102:ARG:HA	37:JC:131:LEU:HA	1.83	0.60
23:Sg:44:LYS:HB2	23:Sg:56:GLN:HB2	1.82	0.60
26:SJ:3:VAL:HB	26:SJ:5:ARG:HD3	1.83	0.60
2:S2:570:C:H4'	31:SY:36:PRO:HG3	1.83	0.60
6:SE:106:LYS:HD2	6:SE:108:ARG:HH12	1.67	0.60
12:SP:44:ARG:HH12	12:SP:49:LEU:HA	1.65	0.60
2:S2:912:C:N4	2:S2:914:U:C2	2.69	0.60
2:S2:1533:A:N6	2:S2:1602:U:C2	2.69	0.60
16:ST:22:LEU:HD12	16:ST:28:LEU:HD22	1.83	0.60
2:S2:1605:G:N2	2:S2:1634:A:H62	2.00	0.60
8:SH:145:ARG:NH2	8:SH:146:VAL:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:SP:44:ARG:NH1	12:SP:48:GLY:O	2.34	0.60
37:JC:330:ARG:HA	37:JC:334:PRO:HB3	1.83	0.60
2:S2:329:G:H2'	2:S2:330:G:C8	2.37	0.60
2:S2:1083:A:N7	2:S2:1841:C:O2'	2.35	0.60
2:S2:1756:C:N3	2:S2:1776:G:N1	2.46	0.59
2:S2:1588:A:H2'	2:S2:1589:A:H8	1.66	0.59
2:S2:67:C:H5''	25:SG:162:LEU:HD11	1.85	0.59
2:S2:1533:A:N6	2:S2:1602:U:N3	2.51	0.59
2:S2:1091:C:HO2'	30:SW:2:VAL:N	1.99	0.59
2:S2:1752:C:N3	2:S2:1779:G:C2	2.70	0.59
2:S2:1791:A:H5''	25:SG:75:LEU:HD11	1.85	0.59
23:Sg:152:SER:OG	23:Sg:168:CYS:SG	2.60	0.59
26:SJ:82:VAL:HG21	26:SJ:92:MET:HE1	1.84	0.59
28:SN:5:HIS:HB3	28:SN:117:LEU:HD23	1.85	0.58
6:SE:54:TYR:O	31:SY:15:ASN:ND2	2.36	0.58
6:SE:247:THR:OG1	6:SE:250:GLU:OE1	2.19	0.58
37:JC:363:HIS:HA	37:JC:367:CYS:HB2	1.84	0.58
2:S2:671:A:H4'	2:S2:672:A:H5''	1.85	0.58
17:SU:82:MET:HE2	17:SU:84:ILE:HD11	1.85	0.58
2:S2:822:U:H3	2:S2:826:A:H62	1.49	0.58
5:SD:76:ARG:HB2	10:SK:22:VAL:HG11	1.85	0.58
8:SH:87:PHE:HB3	8:SH:90:LYS:HD2	1.84	0.58
26:SJ:158:ASP:OD1	26:SJ:159:PHE:N	2.36	0.58
27:SM:121:LYS:HA	27:SM:124:ILE:HD12	1.86	0.58
29:SO:30:VAL:HG12	29:SO:94:HIS:HB2	1.85	0.58
2:S2:989:C:C4	2:S2:1001:A:C2	2.91	0.58
23:Sg:73:SER:OG	23:Sg:117:ASN:ND2	2.35	0.58
28:SN:46:THR:OG1	28:SN:86:GLU:OE1	2.19	0.58
2:S2:73:C:H1'	2:S2:74:G:H2'	1.86	0.57
23:Sg:87:LEU:HB2	23:Sg:101:PHE:HB2	1.86	0.57
33:Sb:49:HIS:ND1	33:Sb:69:GLY:O	2.36	0.57
5:SD:40:ARG:HB3	5:SD:47:GLU:HB2	1.86	0.57
15:SS:86:ARG:HH21	15:SS:89:ASP:HA	1.69	0.57
2:S2:1549:U:OP1	22:Sd:34:TYR:OH	2.22	0.57
2:S2:1588:A:H2'	2:S2:1589:A:C8	2.39	0.57
27:SM:35:ILE:HA	27:SM:38:ALA:HB3	1.87	0.57
20:Sa:87:ARG:NH1	20:Sa:91:ALA:O	2.37	0.57
7:SF:52:SER:HA	13:SQ:50:LYS:HZ1	1.70	0.57
2:S2:1261:C:O2	22:Sd:10:HIS:NE2	2.33	0.57
31:SY:74:MET:SD	31:SY:90:ARG:NH2	2.78	0.57
37:JC:50:PRO:O	37:JC:76:GLN:NE2	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:SB:49:VAL:HG21	4:SB:62:LEU:HB3	1.87	0.57
10:SK:32:HIS:HB3	10:SK:35:LEU:HB2	1.87	0.56
37:JC:117:GLY:H	37:JC:121:GLY:HA3	1.69	0.56
2:S2:847:A:OP1	6:SE:108:ARG:NH2	2.39	0.56
2:S2:1113:A:C6	2:S2:1121:G:C6	2.94	0.56
17:SU:19:ARG:HH11	17:SU:92:HIS:HB3	1.70	0.56
17:SU:95:SER:OG	17:SU:96:GLU:OE1	2.24	0.56
2:S2:1050:A:C6	2:S2:1069:U:C4	2.94	0.56
2:S2:1092:G:OP2	28:SN:9:LYS:NZ	2.39	0.56
2:S2:1709:G:C5	2:S2:1826:G:C2	2.93	0.56
23:Sg:10:THR:HG22	23:Sg:308:ARG:HG3	1.87	0.56
2:S2:528:A:C2	2:S2:558:G:C2	2.94	0.56
2:S2:1015:U:OP2	33:Sb:20:LYS:NZ	2.38	0.56
2:S2:1021:U:OP1	28:SN:132:LYS:NZ	2.39	0.56
31:SY:14:THR:HG22	31:SY:21:LYS:HG2	1.88	0.56
31:SY:102:THR:OG1	31:SY:106:GLN:OE1	2.23	0.56
2:S2:532:C:O2	2:S2:552:G:C2	2.58	0.56
2:S2:919:A:H5'	28:SN:16:LEU:HD21	1.86	0.56
2:S2:1231:C:H42	2:S2:1527:C:H42	1.52	0.56
25:SG:51:ARG:HH21	25:SG:112:VAL:HG11	1.70	0.56
2:S2:1228:A:H2'	2:S2:1229:G:H8	1.71	0.56
2:S2:1264:C:O2	2:S2:1517:G:N2	2.34	0.56
2:S2:1528:G:O2'	2:S2:1666:C:OP1	2.23	0.55
8:SH:145:ARG:NH2	30:SW:50:PHE:O	2.39	0.55
2:S2:165:G:OP2	2:S2:165:G:N2	2.37	0.55
2:S2:218:U:O2	9:SI:184:ARG:NH1	2.37	0.55
5:SD:114:ALA:HB3	5:SD:117:ARG:HD3	1.88	0.55
15:SS:121:ARG:HG2	15:SS:125:HIS:HE1	1.69	0.55
2:S2:955:A:N6	2:S2:971:G:H21	2.03	0.55
12:SP:49:LEU:HD23	12:SP:53:GLN:HB3	1.89	0.55
2:S2:697:G:OP2	2:S2:733:C:N4	2.40	0.55
2:S2:1700:C:C2	2:S2:1834:A:N6	2.75	0.55
5:SD:135:GLU:HG3	5:SD:153:VAL:HG12	1.89	0.55
37:JC:554:ARG:HE	37:JC:562:LEU:HD13	1.72	0.55
2:S2:943:U:H2'	2:S2:944:A:H8	1.72	0.55
2:S2:1421:A:H5''	2:S2:1422:G:H2'	1.87	0.55
2:S2:1679:A:OP1	7:SF:60:ARG:NH2	2.40	0.55
35:Sf:138:ARG:HA	35:Sf:150:PHE:H	1.71	0.55
2:S2:1542:C:H5''	16:ST:62:ARG:HH22	1.72	0.55
2:S2:1700:C:O2	2:S2:1834:A:N6	2.40	0.55
37:JC:341:VAL:HG22	37:JC:550:VAL:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:810:A:C6	2:S2:851:C:C4	2.95	0.55
2:S2:951:C:O2'	29:SO:50:LYS:NZ	2.39	0.55
2:S2:1477:U:H5'	14:SR:3:ARG:HH12	1.72	0.55
3:SA:76:VAL:HG12	3:SA:123:VAL:HB	1.89	0.55
5:SD:123:LEU:HD11	5:SD:152:PHE:HB3	1.89	0.55
23:Sg:201:SER:HB3	23:Sg:206:LEU:HB2	1.89	0.55
37:JC:130:GLN:HA	37:JC:154:ARG:HE	1.71	0.55
2:S2:1521:C:O2	2:S2:1522:A:N1	2.39	0.54
5:SD:29:LEU:HD21	5:SD:69:LEU:HD11	1.89	0.54
6:SE:11:ARG:HA	6:SE:28:ALA:HB2	1.89	0.54
2:S2:67:C:N4	25:SG:168:LYS:O	2.39	0.54
2:S2:1709:G:C8	2:S2:1826:G:N2	2.75	0.54
2:S2:56:G:OP1	31:SY:111:LYS:NZ	2.40	0.54
2:S2:659:G:HO2'	2:S2:662:G:HO2'	1.56	0.54
2:S2:1541:G:H4'	16:ST:15:VAL:HG11	1.87	0.54
2:S2:1700:C:N3	2:S2:1834:A:C6	2.76	0.54
6:SE:255:ARG:HH22	26:SJ:79:ARG:HH22	1.53	0.54
2:S2:928:G:H2'	2:S2:929:G:C8	2.42	0.54
2:S2:886:A:C5	2:S2:901:G:C2	2.96	0.54
2:S2:1700:C:C4	2:S2:1834:A:N1	2.75	0.54
3:SA:77:ILE:HG12	3:SA:99:ILE:HB	1.89	0.54
4:SB:27:LYS:O	4:SB:51:ARG:NE	2.40	0.54
23:Sg:152:SER:HG	23:Sg:168:CYS:HG	1.56	0.54
25:SG:55:GLY:HA3	25:SG:63:MET:HE3	1.90	0.54
27:SM:52:LEU:HB3	27:SM:76:LEU:HD21	1.89	0.54
2:S2:588:G:OP2	2:S2:588:G:N2	2.35	0.54
2:S2:604:A:N3	2:S2:639:C:O2'	2.41	0.54
2:S2:619:A:N6	19:SX:114:ASP:OD1	2.35	0.54
5:SD:27:ARG:NH1	10:SK:62:PHE:O	2.40	0.54
25:SG:58:LYS:HE2	25:SG:105:ASN:HA	1.89	0.54
37:JC:442:LEU:HD21	37:JC:463:PRO:HD3	1.89	0.54
2:S2:1033:G:N1	2:S2:1080:A:O2'	2.37	0.54
3:SA:66:VAL:HG11	3:SA:185:MET:HB2	1.88	0.54
25:SG:159:ARG:HD2	25:SG:171:THR:HB	1.88	0.54
2:S2:351:G:OP1	9:SI:7:ASN:ND2	2.40	0.54
2:S2:1337:C:H2'	2:S2:1338:G:H8	1.73	0.54
13:SQ:82:TYR:HD1	13:SQ:85:ARG:HD3	1.73	0.54
2:S2:989:C:C4	2:S2:1001:A:N1	2.76	0.54
4:SB:90:ASP:OD1	4:SB:91:VAL:N	2.41	0.54
8:SH:29:GLU:OE1	8:SH:86:LYS:NZ	2.41	0.54
8:SH:177:TYR:O	8:SH:181:THR:OG1	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:145:G:H2'	2:S2:146:G:C8	2.43	0.53
12:SP:85:ILE:HG13	12:SP:111:MET:HG2	1.90	0.53
2:S2:528:A:N1	2:S2:558:G:O6	2.42	0.53
2:S2:582:C:OP1	26:SJ:162:ARG:NH1	2.41	0.53
2:S2:913:A:N6	8:SH:119:SER:O	2.41	0.53
2:S2:1204:A:O2'	2:S2:1700:C:OP2	2.24	0.53
5:SD:126:ILE:HG21	5:SD:188:ILE:HD12	1.91	0.53
2:S2:1854:U:H2'	2:S2:1855:G:H8	1.73	0.53
26:SJ:114:VAL:HG23	26:SJ:126:ALA:HB1	1.90	0.53
5:SD:45:ARG:HH21	5:SD:85:GLU:HB2	1.74	0.53
10:SK:15:LEU:HD13	10:SK:21:MET:HE1	1.91	0.53
2:S2:563:G:H1	2:S2:592:C:H5	1.57	0.53
2:S2:981:A:H2'	2:S2:982:G:C8	2.44	0.53
28:SN:147:SER:HB2	37:JC:84:ARG:HH21	1.74	0.53
5:SD:30:ALA:HB1	5:SD:106:ARG:HH22	1.73	0.53
8:SH:10:LYS:NZ	8:SH:12:ASN:OD1	2.30	0.53
25:SG:2:LYS:HB2	25:SG:108:VAL:HG22	1.89	0.53
37:JC:483:VAL:HG13	37:JC:496:MET:HE2	1.91	0.53
10:SK:49:MET:HE3	10:SK:58:VAL:HG21	1.90	0.53
15:SS:26:ILE:HG23	15:SS:45:LEU:HD21	1.91	0.53
18:SV:16:LYS:NZ	24:SC:257:LYS:O	2.40	0.53
23:Sg:79:LEU:HD11	23:Sg:87:LEU:HD23	1.90	0.53
2:S2:1177:U:H4'	37:JC:252:ARG:HH12	1.73	0.53
2:S2:1660:C:P	22:Sd:32:ARG:HH21	2.31	0.53
2:S2:1737:G:OP1	25:SG:94:ARG:NH2	2.41	0.53
9:SI:150:ASP:HA	9:SI:153:LYS:HD2	1.90	0.53
37:JC:102:ARG:HG3	37:JC:103:VAL:HG23	1.91	0.53
2:S2:317:C:OP2	25:SG:183:ARG:NH2	2.37	0.53
24:SC:196:ILE:HB	24:SC:223:TYR:HB2	1.90	0.53
25:SG:137:ARG:HH11	25:SG:178:ARG:HH22	1.57	0.53
26:SJ:81:LEU:HB3	26:SJ:87:LEU:HD13	1.91	0.53
2:S2:151:C:O2	25:SG:132:ARG:NH1	2.42	0.53
24:SC:146:GLU:HG3	24:SC:148:ALA:H	1.74	0.53
37:JC:74:LEU:HD13	37:JC:77:LEU:HD13	1.90	0.53
2:S2:162:C:O3'	25:SG:95:LYS:NZ	2.42	0.52
7:SF:171:GLU:HG3	32:SZ:106:GLN:HE22	1.73	0.52
2:S2:1034:A:H61	2:S2:1843:G:H1'	1.75	0.52
2:S2:1396:A:O2'	2:S2:1398:G:N7	2.41	0.52
7:SF:168:THR:HG22	7:SF:170:ALA:H	1.74	0.52
7:SF:170:ALA:HB3	32:SZ:106:GLN:HE21	1.74	0.52
24:SC:85:SER:OG	24:SC:85:SER:O	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:SM:53:ALA:HA	27:SM:79:VAL:HB	1.92	0.52
2:S2:1228:A:O2'	2:S2:1634:A:N3	2.34	0.52
2:S2:1650:A:H5''	13:SQ:139:ALA:HB2	1.91	0.52
3:SA:2:SER:OG	18:SV:78:ILE:O	2.27	0.52
37:JC:201:LEU:HD23	37:JC:204:LEU:HD22	1.90	0.52
9:SI:76:THR:HG22	9:SI:108:PRO:HG2	1.91	0.52
2:S2:463:C:O2	2:S2:466:G:N2	2.37	0.52
2:S2:1454:A:H2	2:S2:1476:A:H1'	1.75	0.52
2:S2:1486:A:H2'	2:S2:1487:A:H8	1.74	0.52
6:SE:206:ASP:HB3	6:SE:222:LEU:HD23	1.92	0.52
5:SD:40:ARG:HH11	17:SU:108:PRO:HG3	1.74	0.52
9:SI:66:SER:H	9:SI:188:TYR:HA	1.75	0.52
19:SX:124:LYS:HA	19:SX:129:SER:HA	1.91	0.52
4:SB:62:LEU:HD11	4:SB:91:VAL:HG22	1.91	0.52
5:SD:64:ARG:HA	5:SD:67:ARG:HE	1.75	0.52
13:SQ:85:ARG:NH2	13:SQ:116:ASP:OD2	2.42	0.52
2:S2:526:A:OP1	34:Se:31:ARG:NH1	2.43	0.52
2:S2:913:A:OP2	8:SH:99:ARG:NH1	2.41	0.52
2:S2:989:C:O2	20:Sa:32:LYS:NZ	2.43	0.52
2:S2:1680:G:H4'	21:Sc:20:ARG:HD3	1.91	0.52
15:SS:23:ARG:HB3	32:SZ:48:VAL:HG21	1.92	0.52
1:Ln:6:ARG:NH2	2:S2:1169:G:OP1	2.42	0.52
2:S2:370:G:O2'	9:SI:10:LYS:NZ	2.43	0.52
2:S2:1605:G:H21	2:S2:1634:A:N6	2.04	0.52
2:S2:1615:U:O4	12:SP:40:ARG:NH2	2.42	0.52
2:S2:1166:G:N7	19:SX:25:LYS:NZ	2.57	0.52
11:SL:33:LEU:HD12	11:SL:34:PRO:HD2	1.91	0.52
18:SV:12:TYR:O	24:SC:248:TYR:OH	2.28	0.52
20:Sa:11:ALA:HB3	20:Sa:33:ASP:HB2	1.91	0.52
2:S2:630:U:OP2	5:SD:143:ARG:NH2	2.42	0.51
2:S2:1464:C:OP2	14:SR:63:ARG:NH2	2.43	0.51
27:SM:32:ALA:HB2	27:SM:112:LYS:HE3	1.91	0.51
37:JC:397:LEU:HD22	37:JC:409:ALA:HB2	1.92	0.51
2:S2:455:A:H2'	2:S2:456:C:C6	2.46	0.51
2:S2:1554:C:O2	10:SK:24:LYS:NZ	2.42	0.51
2:S2:1674:G:H4'	7:SF:77:MET:HE1	1.91	0.51
17:SU:22:ILE:HG12	17:SU:114:VAL:HG12	1.92	0.51
1:Ln:15:ARG:HH12	2:S2:1182:A:H5''	1.75	0.51
2:S2:1236:G:N2	2:S2:1522:A:N6	2.40	0.51
2:S2:1545:A:H2'	2:S2:1546:G:C8	2.44	0.51
2:S2:1595:U:H2'	2:S2:1596:U:C6	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:1756:C:C4	2:S2:1775:U:N3	2.79	0.51
8:SH:145:ARG:HA	30:SW:51:GLU:HG2	1.92	0.51
24:SC:169:TYR:OH	24:SC:175:GLY:O	2.28	0.51
37:JC:387:LEU:HD13	37:JC:451:LEU:HD21	1.92	0.51
2:S2:747:U:N3	2:S2:796:G:N1	2.58	0.51
2:S2:1541:G:N3	16:ST:12:GLN:NE2	2.58	0.51
2:S2:1589:A:N3	2:S2:1653:U:O2'	2.38	0.51
6:SE:11:ARG:HH21	6:SE:21:ASP:H	1.58	0.51
37:JC:571:ASP:O	37:JC:583:ARG:NH2	2.44	0.51
2:S2:326:C:O2	2:S2:327:G:N2	2.44	0.51
2:S2:959:G:OP1	29:SO:104:ARG:NH1	2.42	0.51
2:S2:1401:A:H4'	17:SU:52:GLY:HA3	1.91	0.51
2:S2:1220:A:N3	2:S2:1677:U:O2'	2.38	0.51
14:SR:17:ILE:HD11	14:SR:54:VAL:HG13	1.93	0.51
37:JC:237:LEU:HD12	37:JC:243:GLU:HA	1.92	0.51
1:Ln:20:MET:HE1	2:S2:1817:G:H1'	1.93	0.51
2:S2:1005:G:OP2	4:SB:162:ARG:NH2	2.43	0.51
5:SD:101:GLN:HA	5:SD:104:SER:HB3	1.92	0.51
21:Sc:31:ARG:NH2	21:Sc:41:SER:OG	2.44	0.51
28:SN:26:LEU:HD23	28:SN:28:LEU:H	1.75	0.51
11:SL:151:THR:OG1	11:SL:152:LYS:N	2.43	0.51
12:SP:92:SER:HB2	12:SP:107:ILE:HD13	1.93	0.51
13:SQ:127:CYS:SG	13:SQ:128:GLU:N	2.84	0.51
23:Sg:111:VAL:O	23:Sg:155:ARG:NH2	2.42	0.51
24:SC:69:LEU:HB3	24:SC:74:LYS:HB2	1.92	0.51
8:SH:103:LYS:HG2	8:SH:116:ARG:HH12	1.76	0.50
8:SH:158:LEU:HD12	8:SH:189:PHE:HE1	1.77	0.50
9:SI:98:LYS:HG3	9:SI:178:ARG:HG2	1.93	0.50
15:SS:22:GLY:HA2	15:SS:56:ALA:HB3	1.94	0.50
16:ST:35:ASP:N	16:ST:35:ASP:OD1	2.44	0.50
23:Sg:149:GLU:OE2	23:Sg:171:ASP:N	2.45	0.50
2:S2:14:C:OP1	24:SC:190:SER:OG	2.26	0.50
2:S2:1228:A:H2'	2:S2:1229:G:C8	2.47	0.50
5:SD:177:LEU:HD12	5:SD:182:LEU:HD13	1.92	0.50
7:SF:125:SER:HA	7:SF:138:ALA:HA	1.93	0.50
9:SI:34:ALA:HB2	9:SI:56:ARG:HD2	1.92	0.50
37:JC:114:LEU:HD13	37:JC:120:LEU:HD13	1.93	0.50
2:S2:921:G:OP2	33:Sb:21:LYS:NZ	2.44	0.50
2:S2:107:A:H2'	2:S2:108:G:C8	2.47	0.50
2:S2:639:C:H2'	2:S2:640:A:H8	1.76	0.50
16:ST:18:LEU:HD23	16:ST:134:ILE:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:SV:14:PRO:HG3	24:SC:248:TYR:CZ	2.47	0.50
2:S2:49:C:H2'	2:S2:472:C:H41	1.75	0.50
2:S2:943:U:H2'	2:S2:944:A:C8	2.45	0.50
2:S2:1032:C:H5''	28:SN:109:LYS:HD3	1.94	0.50
2:S2:1422:G:N2	2:S2:1424:G:O6	2.44	0.50
2:S2:1726:G:O6	2:S2:1808:U:O4	2.30	0.50
2:S2:1764:G:H5'	2:S2:1765:C:H5''	1.94	0.50
13:SQ:34:VAL:HG23	13:SQ:70:VAL:HB	1.93	0.50
16:ST:115:LYS:HE3	16:ST:121:ARG:HH21	1.76	0.50
24:SC:165:VAL:HG21	24:SC:217:ALA:HB1	1.94	0.50
25:SG:32:MET:HG2	25:SG:52:ILE:HG22	1.94	0.50
37:JC:394:PRO:HB2	37:JC:410:LYS:HB3	1.94	0.50
4:SB:52:THR:HG23	4:SB:57:ILE:HA	1.92	0.50
5:SD:45:ARG:NH1	5:SD:82:GLY:O	2.45	0.50
13:SQ:58:LEU:HD13	13:SQ:92:LEU:HD23	1.94	0.50
15:SS:34:LYS:NZ	15:SS:104:ASP:OD1	2.39	0.50
13:SQ:19:ALA:HB2	13:SQ:75:GLY:HA3	1.94	0.50
22:Sd:15:GLY:O	22:Sd:18:SER:OG	2.30	0.50
2:S2:1236:G:O2'	12:SP:131:PRO:O	2.30	0.50
29:SO:103:ASN:HB2	29:SO:142:ARG:HG2	1.92	0.50
6:SE:100:ARG:HB2	6:SE:114:ILE:HD13	1.93	0.49
6:SE:122:LYS:NZ	6:SE:124:CYS:SG	2.74	0.49
2:S2:886:A:C6	2:S2:901:G:C4	2.94	0.49
16:ST:76:THR:HB	16:ST:94:ARG:HB3	1.94	0.49
2:S2:886:A:N6	2:S2:901:G:N9	2.58	0.49
2:S2:1299:A:OP1	12:SP:59:ARG:NH1	2.44	0.49
6:SE:181:CYS:SG	6:SE:182:MET:N	2.86	0.49
7:SF:128:ILE:O	21:Sc:23:SER:OG	2.31	0.49
8:SH:186:ASN:ND2	8:SH:188:GLU:OE2	2.45	0.49
2:S2:45:A:C2	37:JC:428:LYS:HD3	2.48	0.49
2:S2:1541:G:H5''	16:ST:59:SER:HB2	1.94	0.49
4:SB:190:PRO:O	4:SB:195:LYS:NZ	2.45	0.49
7:SF:20:PHE:HZ	7:SF:93:VAL:HG12	1.78	0.49
25:SG:208:GLU:HA	25:SG:211:LYS:HE3	1.94	0.49
2:S2:508:A:H3'	2:S2:509:G:H8	1.77	0.49
2:S2:928:G:N2	33:Sb:68:GLY:O	2.40	0.49
5:SD:192:TRP:NE1	5:SD:201:LYS:O	2.42	0.49
23:Sg:31:ILE:HG22	23:Sg:43:TRP:HB2	1.94	0.49
2:S2:410:G:C6	2:S2:431:G:N1	2.80	0.49
2:S2:1617:G:N1	2:S2:1620:A:OP2	2.45	0.49
33:Sb:23:ARG:NH1	33:Sb:27:SER:OG	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Sb:23:ARG:NH2	33:Sb:29:ASN:OD1	2.45	0.49
2:S2:440:G:OP1	2:S2:1798:C:O2'	2.30	0.49
2:S2:888:U:H2'	2:S2:900:C:H42	1.78	0.49
2:S2:912:C:N3	2:S2:914:U:O2	2.46	0.49
2:S2:1756:C:O2	2:S2:1776:G:O6	2.31	0.49
2:S2:886:A:C6	2:S2:901:G:C2	3.01	0.49
2:S2:989:C:N3	2:S2:1001:A:C6	2.80	0.49
5:SD:6:SER:O	5:SD:10:LYS:N	2.46	0.49
2:S2:10:G:OP2	36:JD:591:ARG:NH2	2.43	0.49
14:SR:98:VAL:HG21	14:SR:117:LEU:HD12	1.95	0.49
20:Sa:52:ASP:OD2	29:SO:117:ARG:NH2	2.46	0.49
23:Sg:29:ASP:HA	23:Sg:47:ARG:HH22	1.77	0.49
23:Sg:107:ASP:HB2	23:Sg:125:ARG:HD2	1.95	0.49
2:S2:1709:G:C6	2:S2:1826:G:N1	2.81	0.48
7:SF:52:SER:HA	13:SQ:50:LYS:NZ	2.27	0.48
21:Sc:23:SER:OG	21:Sc:24:GLN:OE1	2.26	0.48
2:S2:433:A:H5''	9:SI:22:HIS:HB3	1.95	0.48
2:S2:695:C:N4	2:S2:736:C:O2'	2.46	0.48
10:SK:3:MET:HG3	10:SK:8:ARG:NH1	2.28	0.48
23:Sg:40:ILE:HD11	23:Sg:66:VAL:HG21	1.95	0.48
2:S2:1857:G:H3'	29:SO:146:ARG:NH2	2.28	0.48
10:SK:46:MET:O	10:SK:50:GLN:N	2.42	0.48
2:S2:78:C:O2	25:SG:175:LYS:NZ	2.40	0.48
7:SF:120:GLY:O	7:SF:193:LYS:NZ	2.40	0.48
8:SH:39:GLN:HG3	8:SH:75:ILE:HG21	1.94	0.48
14:SR:114:LEU:HG	14:SR:116:ASN:H	1.78	0.48
15:SS:20:ILE:HD11	15:SS:33:ILE:HG13	1.95	0.48
28:SN:19:ARG:NH1	28:SN:21:SER:OG	2.46	0.48
2:S2:1779:G:H2'	2:S2:1780:G:C8	2.49	0.48
2:S2:1842:C:H2'	2:S2:1843:G:C8	2.49	0.48
6:SE:166:THR:HG23	6:SE:168:LYS:H	1.78	0.48
6:SE:182:MET:HG3	6:SE:192:ILE:HG12	1.95	0.48
15:SS:81:ASP:OD1	15:SS:81:ASP:N	2.40	0.48
24:SC:66:LEU:HD11	24:SC:81:ILE:HG23	1.96	0.48
2:S2:860:G:OP1	8:SH:107:LYS:NZ	2.47	0.48
2:S2:1010:G:H2'	2:S2:1011:A:C8	2.48	0.48
6:SE:71:LYS:HE2	6:SE:74:GLY:HA2	1.96	0.48
9:SI:194:GLU:HG2	11:SL:10:TYR:CE2	2.49	0.48
12:SP:60:LEU:HD12	12:SP:92:SER:HB3	1.96	0.48
23:Sg:44:LYS:N	23:Sg:54:ILE:O	2.43	0.48
24:SC:88:ILE:HB	24:SC:93:ILE:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:SJ:81:LEU:HA	26:SJ:84:ILE:HG22	1.95	0.48
2:S2:410:G:O6	2:S2:431:G:C6	2.67	0.48
2:S2:1534:C:C2	2:S2:1598:G:C2	3.00	0.48
5:SD:105:LEU:HD23	5:SD:184:ILE:HG21	1.95	0.48
19:SX:40:PRO:O	19:SX:77:ASN:ND2	2.44	0.48
28:SN:87:ASP:OD1	28:SN:87:ASP:N	2.46	0.48
31:SY:86:GLU:OE2	31:SY:90:ARG:NE	2.36	0.48
37:JC:78:HIS:ND1	37:JC:100:ALA:O	2.37	0.48
2:S2:1113:A:N6	2:S2:1121:G:O6	2.47	0.48
10:SK:59:LYS:HE2	10:SK:70:TYR:HD2	1.78	0.48
23:Sg:111:VAL:HA	23:Sg:122:SER:HA	1.95	0.48
2:S2:566:U:H3	2:S2:584:G:H1	1.61	0.48
2:S2:808:A:H2	2:S2:855:G:H22	1.62	0.48
2:S2:1598:G:H1'	7:SF:166:ILE:HG23	1.96	0.48
7:SF:140:ASP:HB2	21:Sc:46:VAL:HG12	1.95	0.48
13:SQ:128:GLU:OE2	13:SQ:138:ARG:NH1	2.47	0.48
26:SJ:50:LEU:HA	26:SJ:53:ILE:HD12	1.96	0.48
28:SN:147:SER:O	37:JC:84:ARG:NH2	2.47	0.48
33:Sb:67:THR:OG1	33:Sb:70:LYS:O	2.25	0.48
2:S2:467:G:H4'	25:SG:72:ARG:HH12	1.77	0.47
37:JC:91:LEU:HB2	37:JC:111:LEU:HD11	1.96	0.47
37:JC:411:GLU:HA	37:JC:414:ARG:HE	1.79	0.47
2:S2:16:G:H2'	2:S2:17:C:C6	2.49	0.47
2:S2:24:C:N3	2:S2:650:A:N1	2.62	0.47
6:SE:63:LYS:HE2	31:SY:85:ASN:HA	1.96	0.47
29:SO:31:CYS:HB2	29:SO:93:LEU:HD13	1.96	0.47
2:S2:955:A:N6	2:S2:971:G:C2	2.83	0.47
2:S2:1648:G:H5''	13:SQ:125:ARG:HB2	1.96	0.47
7:SF:49:LEU:HD23	7:SF:50:PRO:HD2	1.95	0.47
7:SF:179:ASN:HB2	7:SF:187:SER:HB3	1.96	0.47
9:SI:57:ALA:HB2	9:SI:183:GLY:HA2	1.96	0.47
14:SR:5:ARG:HB2	14:SR:10:LYS:HE2	1.96	0.47
24:SC:94:ILE:HG21	24:SC:159:LYS:HB3	1.95	0.47
26:SJ:84:ILE:HD11	26:SJ:148:ILE:HG21	1.95	0.47
2:S2:693:A:C2	2:S2:694:G:O6	2.68	0.47
2:S2:885:U:H3	2:S2:901:G:H1	1.62	0.47
2:S2:1598:G:H8	32:SZ:81:GLY:HA3	1.78	0.47
5:SD:100:ALA:O	5:SD:104:SER:N	2.46	0.47
13:SQ:130:LYS:NZ	13:SQ:131:LYS:O	2.44	0.47
1:Ln:11:ARG:HD2	2:S2:1183:A:H5'	1.97	0.47
2:S2:526:A:H5'	34:Se:31:ARG:HH22	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:1723:G:H2'	2:S2:1724:A:C8	2.50	0.47
13:SQ:101:ASP:OD1	13:SQ:104:SER:N	2.46	0.47
26:SJ:120:ALA:HB2	26:SJ:129:LEU:HD22	1.96	0.47
2:S2:5:U:H2'	2:S2:6:G:H8	1.80	0.47
2:S2:640:A:H2'	2:S2:641:A:C8	2.50	0.47
2:S2:1010:G:H2'	2:S2:1011:A:H8	1.80	0.47
2:S2:1337:C:H5'	22:Sd:44:ARG:HH22	1.80	0.47
6:SE:162:ILE:HG22	6:SE:169:ILE:HA	1.97	0.47
7:SF:20:PHE:CZ	7:SF:93:VAL:HG12	2.49	0.47
8:SH:72:PHE:O	8:SH:76:GLN:N	2.48	0.47
30:SW:26:LEU:HD21	30:SW:60:LYS:HE2	1.97	0.47
2:S2:1097:G:H4'	3:SA:32:PHE:CG	2.50	0.47
2:S2:1227:G:H22	2:S2:1531:A:H2	1.63	0.47
17:SU:27:ARG:HD3	17:SU:82:MET:HE3	1.97	0.47
25:SG:102:VAL:HG23	25:SG:106:LEU:HD23	1.97	0.47
2:S2:1050:A:N6	2:S2:1068:G:N2	2.43	0.47
4:SB:57:ILE:HG22	4:SB:59:SER:H	1.80	0.47
6:SE:204:SER:OG	6:SE:205:PHE:N	2.48	0.47
7:SF:74:ASN:O	7:SF:77:MET:HG2	2.15	0.47
2:S2:161:U:O3'	25:SG:87:ARG:NH2	2.48	0.46
2:S2:1230:C:H2'	2:S2:1231:C:H6	1.79	0.46
2:S2:1752:C:N3	2:S2:1779:G:N1	2.62	0.46
9:SI:11:ARG:NH1	9:SI:15:GLY:O	2.41	0.46
19:SX:68:LYS:HB3	19:SX:91:LEU:HD13	1.98	0.46
26:SJ:113:GLN:HG3	26:SJ:149:VAL:HG11	1.96	0.46
26:SJ:160:SER:O	26:SJ:163:SER:OG	2.29	0.46
2:S2:1480:A:O2'	22:Sd:56:ASP:OXT	2.32	0.46
23:Sg:106:LYS:HE2	23:Sg:126:ASP:HA	1.97	0.46
2:S2:913:A:N6	8:SH:120:ARG:HD2	2.28	0.46
23:Sg:110:SER:OG	23:Sg:155:ARG:NH2	2.47	0.46
2:S2:307:G:N7	9:SI:44:HIS:ND1	2.63	0.46
2:S2:1144:A:H2'	2:S2:1145:A:C8	2.51	0.46
2:S2:1785:C:O2'	2:S2:1786:U:O4'	2.31	0.46
19:SX:135:LYS:HG3	19:SX:137:LYS:HG2	1.96	0.46
37:JC:305:GLY:O	37:JC:578:HIS:NE2	2.49	0.46
2:S2:207:G:H3'	2:S2:208:G:H8	1.80	0.46
4:SB:109:LYS:HG3	4:SB:113:MET:HE2	1.98	0.46
2:S2:65:C:OP1	25:SG:136:LYS:NZ	2.48	0.46
2:S2:819:G:OP2	26:SJ:80:ARG:NH1	2.48	0.46
2:S2:924:G:O6	2:S2:1018:U:O4	2.34	0.46
6:SE:175:PHE:HE1	6:SE:225:ILE:HG21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:SF:40:ALA:HB3	7:SF:67:PRO:HA	1.97	0.46
15:SS:25:LYS:O	15:SS:29:ALA:N	2.48	0.46
37:JC:434:GLY:HA2	37:JC:437:ARG:HD2	1.98	0.46
17:SU:26:SER:HB3	17:SU:32:LEU:HD12	1.97	0.46
2:S2:429:C:OP1	6:SE:10:LYS:NZ	2.47	0.46
2:S2:613:G:N2	2:S2:626:G:OP1	2.43	0.46
2:S2:1147:C:OP1	20:Sa:6:ARG:NH1	2.49	0.46
2:S2:1550:G:O2'	2:S2:1558:C:O2	2.28	0.46
9:SI:178:ARG:HE	9:SI:181:GLN:HG3	1.80	0.46
23:Sg:99:ARG:NH2	23:Sg:134:THR:O	2.49	0.46
37:JC:401:PRO:HG2	37:JC:404:ARG:HB2	1.97	0.46
2:S2:433:A:H2'	2:S2:434:G:C8	2.51	0.46
3:SA:8:LEU:HD13	3:SA:191:ARG:HH12	1.81	0.46
11:SL:77:VAL:HG23	11:SL:123:GLY:H	1.81	0.46
18:SV:15:ARG:NH1	24:SC:83:LEU:O	2.47	0.46
37:JC:110:ALA:N	37:JC:139:ASN:OD1	2.49	0.46
37:JC:209:LEU:HD13	37:JC:214:LEU:HD11	1.98	0.46
25:SG:67:VAL:HB	25:SG:99:GLY:HA2	1.97	0.46
3:SA:212:LYS:HA	3:SA:212:LYS:HD3	1.77	0.45
2:S2:527:C:H2'	2:S2:528:A:C8	2.50	0.45
2:S2:562:U:C5	26:SJ:172:ARG:HD3	2.51	0.45
2:S2:857:U:H2'	2:S2:858:A:C8	2.50	0.45
2:S2:1743:G:N2	2:S2:1791:A:H62	2.13	0.45
3:SA:8:LEU:HD12	3:SA:59:LEU:HD11	1.97	0.45
7:SF:165:ASN:OD1	7:SF:166:ILE:N	2.49	0.45
12:SP:52:LYS:HE2	12:SP:80:LEU:HD11	1.98	0.45
2:S2:1605:G:OP1	16:ST:84:ARG:NH2	2.45	0.45
4:SB:65:ARG:HB3	29:SO:48:SER:HB2	1.97	0.45
7:SF:127:ARG:HB3	7:SF:136:ARG:HG2	1.98	0.45
25:SG:168:LYS:HD2	25:SG:169:PRO:HD2	1.98	0.45
28:SN:118:ILE:HD13	28:SN:121:ARG:HH21	1.82	0.45
2:S2:1202:U:O2'	24:SC:115:GLN:O	2.26	0.45
15:SS:39:ARG:HH12	16:ST:38:LYS:HD2	1.81	0.45
27:SM:89:VAL:HG13	27:SM:91:LEU:HD23	1.98	0.45
2:S2:1861:G:H5''	20:Sa:3:LYS:HA	1.99	0.45
5:SD:226:GLN:HG2	23:Sg:186:THR:HG23	1.98	0.45
9:SI:194:GLU:HG2	11:SL:10:TYR:HE2	1.82	0.45
30:SW:111:MET:HE2	30:SW:111:MET:HB3	1.87	0.45
32:SZ:104:ARG:H	32:SZ:104:ARG:HG2	1.58	0.45
2:S2:1050:A:N6	2:S2:1068:G:C2	2.83	0.45
2:S2:1387:G:N1	5:SD:206:ASP:OD2	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:1513:C:H2'	2:S2:1514:G:H8	1.81	0.45
2:S2:1752:C:C4	2:S2:1779:G:C2	3.05	0.45
5:SD:31:GLU:HA	5:SD:107:TYR:HE2	1.81	0.45
27:SM:40:LYS:HE3	35:Sf:130:VAL:HA	1.98	0.45
37:JC:557:ASP:OD1	37:JC:561:SER:N	2.49	0.45
2:S2:12:U:H2'	2:S2:13:C:C6	2.52	0.45
2:S2:109:U:O2	11:SL:71:ARG:NH2	2.50	0.45
2:S2:410:G:C6	2:S2:431:G:C6	3.04	0.45
2:S2:866:U:H2'	2:S2:867:G:C8	2.52	0.45
2:S2:1521:C:O2	2:S2:1522:A:C2	2.69	0.45
3:SA:206:ASP:HB3	3:SA:209:GLU:HG2	1.98	0.45
8:SH:145:ARG:NH2	30:SW:49:GLU:HB3	2.31	0.45
10:SK:65:ARG:NH1	22:Sd:25:SER:OG	2.50	0.45
25:SG:218:LYS:HB3	25:SG:218:LYS:HE2	1.73	0.45
26:SJ:33:GLY:HA3	34:Se:38:TYR:CG	2.51	0.45
2:S2:834:C:C2	2:S2:839:C:N3	2.84	0.45
2:S2:919:A:O2'	2:S2:1020:A:N1	2.40	0.45
2:S2:1752:C:H42	2:S2:1778:C:H42	1.64	0.45
2:S2:1779:G:H2'	2:S2:1780:G:H8	1.81	0.45
3:SA:118:GLU:HB2	24:SC:65:LYS:NZ	2.31	0.45
8:SH:121:THR:HG23	8:SH:124:ALA:H	1.81	0.45
2:S2:104:A:H62	2:S2:356:C:H5	1.65	0.45
2:S2:119:U:H2'	2:S2:120:U:H6	1.81	0.45
2:S2:186:C:H2'	2:S2:187:G:C8	2.52	0.45
2:S2:752:G:OP1	2:S2:792:C:O2'	2.34	0.45
2:S2:996:A:H2'	2:S2:997:A:C8	2.51	0.45
2:S2:1486:A:H2'	2:S2:1487:A:C8	2.52	0.45
6:SE:100:ARG:NH2	6:SE:121:TYR:O	2.37	0.45
2:S2:1410:C:H2'	2:S2:1411:G:C8	2.52	0.45
2:S2:1705:C:H2'	2:S2:1706:G:C8	2.52	0.45
20:Sa:60:ASP:OD1	20:Sa:60:ASP:N	2.49	0.45
2:S2:852:G:O2'	11:SL:97:ARG:NH1	2.50	0.44
2:S2:1729:U:H3	2:S2:1805:G:H1	1.64	0.44
9:SI:83:TYR:HB3	9:SI:101:ILE:HB	2.00	0.44
37:JC:124:GLU:HG2	37:JC:150:ARG:HH22	1.82	0.44
37:JC:130:GLN:HB2	37:JC:154:ARG:HH21	1.82	0.44
2:S2:28:U:H2'	2:S2:29:G:H8	1.81	0.44
2:S2:818:A:OP1	26:SJ:80:ARG:NH2	2.42	0.44
2:S2:905:C:H2'	2:S2:906:U:C6	2.52	0.44
2:S2:1013:U:OP1	2:S2:1129:G:O2'	2.35	0.44
2:S2:1236:G:N2	2:S2:1522:A:C6	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:SB:129:THR:HG23	4:SB:131:ASP:H	1.81	0.44
12:SP:38:SER:H	12:SP:41:GLN:NE2	2.15	0.44
30:SW:93:LEU:HB2	30:SW:94:LEU:HD22	1.99	0.44
37:JC:154:ARG:HB2	37:JC:180:LEU:HD12	1.98	0.44
2:S2:618:C:H41	19:SX:67:ARG:NH2	2.14	0.44
2:S2:955:A:C6	2:S2:971:G:N2	2.86	0.44
2:S2:1612:G:O2'	15:SS:87:GLN:OE1	2.25	0.44
2:S2:1730:U:O4	2:S2:1731:A:N6	2.50	0.44
31:SY:20:ARG:HD2	31:SY:22:GLN:HB3	1.99	0.44
2:S2:550:C:H2'	2:S2:551:U:C6	2.53	0.44
2:S2:825:A:H2'	2:S2:826:A:C8	2.53	0.44
11:SL:68:ILE:HG13	11:SL:143:LEU:HD21	1.98	0.44
28:SN:83:ASP:OD1	28:SN:83:ASP:N	2.50	0.44
33:Sb:33:MET:HE2	33:Sb:48:SER:HA	1.99	0.44
37:JC:169:PRO:HG2	37:JC:172:LEU:HG	1.99	0.44
2:S2:223:C:H2'	2:S2:224:A:C8	2.51	0.44
2:S2:1709:G:O6	2:S2:1826:G:O6	2.34	0.44
2:S2:1723:G:H2'	2:S2:1724:A:H8	1.82	0.44
4:SB:123:ALA:HB2	4:SB:165:ARG:HG3	2.00	0.44
6:SE:181:CYS:HA	6:SE:227:VAL:HA	2.00	0.44
10:SK:37:ASP:OD1	10:SK:37:ASP:N	2.46	0.44
23:Sg:36:ARG:HG2	23:Sg:65:PHE:CG	2.53	0.44
25:SG:227:GLN:HG2	25:SG:231:ARG:HH21	1.82	0.44
2:S2:54:A:OP1	31:SY:111:LYS:NZ	2.48	0.44
2:S2:1488:C:O2'	2:S2:1490:G:OP2	2.22	0.44
2:S2:1593:C:H2'	2:S2:1594:A:H8	1.83	0.44
11:SL:75:GLY:HA3	11:SL:88:ILE:HD12	2.00	0.44
16:ST:113:VAL:HG22	16:ST:123:LEU:HD23	1.99	0.44
2:S2:907:G:H2'	2:S2:908:A:C8	2.52	0.44
2:S2:1275:G:H22	2:S2:1506:A:P	2.40	0.44
2:S2:1337:C:H2'	2:S2:1338:G:C8	2.53	0.44
5:SD:16:ILE:HD11	22:Sd:36:LEU:HD13	2.00	0.44
12:SP:56:LEU:HD23	12:SP:83:MET:HE3	1.99	0.44
17:SU:66:ARG:HD2	17:SU:66:ARG:HA	1.83	0.44
27:SM:58:GLU:HB3	27:SM:61:TYR:HB3	1.98	0.44
4:SB:30:TRP:CE2	29:SO:19:PRO:HD3	2.53	0.44
7:SF:47:LYS:HB3	7:SF:47:LYS:HE3	1.57	0.44
7:SF:85:LYS:O	7:SF:89:THR:HG23	2.18	0.44
16:ST:115:LYS:HG2	16:ST:121:ARG:HE	1.82	0.44
25:SG:26:THR:HG21	25:SG:40:ALA:HB3	1.99	0.44
6:SE:106:LYS:NZ	6:SE:251:GLU:OE2	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:SI:157:LYS:HA	9:SI:157:LYS:HD2	1.82	0.44
19:SX:51:VAL:HG22	19:SX:98:ASP:H	1.83	0.44
26:SJ:162:ARG:NH2	31:SY:30:PRO:O	2.51	0.44
27:SM:41:ALA:HB1	27:SM:47:ALA:HB2	1.99	0.44
37:JC:457:ASP:OD2	37:JC:469:LYS:NZ	2.47	0.44
11:SL:96:ILE:HD12	19:SX:10:ALA:HB1	1.99	0.43
15:SS:130:ARG:HD3	15:SS:130:ARG:HA	1.81	0.43
20:Sa:79:ILE:HD13	20:Sa:84:VAL:HG23	2.00	0.43
2:S2:532:C:C2	2:S2:552:G:C2	3.06	0.43
2:S2:591:U:H5''	2:S2:593:C:H5'	1.99	0.43
2:S2:1780:G:H3'	2:S2:1781:A:H8	1.82	0.43
3:SA:120:ARG:HD2	24:SC:266:TYR:HB3	2.00	0.43
14:SR:28:PHE:CE2	14:SR:32:LYS:HD3	2.53	0.43
15:SS:113:ARG:HA	15:SS:116:LYS:HG2	2.00	0.43
24:SC:233:LEU:HA	24:SC:233:LEU:HD12	1.78	0.43
2:S2:912:C:N4	2:S2:914:U:C4	2.87	0.43
2:S2:1177:U:H2'	2:S2:1178:U:C6	2.53	0.43
9:SI:188:TYR:OH	11:SL:12:LYS:NZ	2.51	0.43
29:SO:85:CYS:HB3	29:SO:90:ILE:HB	2.01	0.43
37:JC:117:GLY:HA2	37:JC:123:ALA:HB3	2.00	0.43
3:SA:10:MET:HG2	3:SA:55:TRP:CD2	2.53	0.43
2:S2:691:G:OP2	2:S2:691:G:N2	2.52	0.43
2:S2:748:C:N3	2:S2:795:A:N1	2.66	0.43
2:S2:810:A:N1	2:S2:851:C:C4	2.87	0.43
2:S2:1533:A:N6	2:S2:1602:U:H3	2.15	0.43
2:S2:1711:U:H2'	2:S2:1712:A:C8	2.52	0.43
6:SE:32:SER:HB3	6:SE:81:THR:HG23	1.99	0.43
31:SY:63:HIS:CE1	31:SY:68:LYS:HG2	2.54	0.43
1:Ln:12:ARG:NH1	2:S2:1848:U:O4	2.51	0.43
2:S2:5:U:H2'	2:S2:6:G:C8	2.54	0.43
2:S2:1438:A:H2'	2:S2:1439:A:C8	2.54	0.43
6:SE:213:ALA:HB3	6:SE:244:ILE:HD11	2.01	0.43
13:SQ:26:LYS:HG3	13:SQ:67:ASP:HB2	2.01	0.43
15:SS:26:ILE:HD13	15:SS:56:ALA:HA	2.00	0.43
27:SM:123:VAL:O	27:SM:127:TYR:N	2.49	0.43
31:SY:9:THR:HG22	31:SY:25:ILE:HG12	2.00	0.43
34:Se:50:GLY:HA2	36:JD:610:GLU:HB2	1.99	0.43
2:S2:1113:A:N1	2:S2:1121:G:C6	2.87	0.43
13:SQ:5:GLY:HA3	13:SQ:27:ARG:HH11	1.83	0.43
19:SX:66:ILE:HG21	34:Se:5:SER:HB2	2.00	0.43
30:SW:38:LEU:HD13	30:SW:41:MET:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:46:A:H4'	2:S2:47:G:H5''	2.01	0.43
8:SH:160:LYS:HB3	8:SH:160:LYS:HE2	1.83	0.43
11:SL:35:ARG:HB3	11:SL:37:TYR:CE1	2.54	0.43
14:SR:77:GLU:HB2	14:SR:80:ARG:HH21	1.84	0.43
18:SV:28:ASP:O	24:SC:85:SER:OG	2.35	0.43
20:Sa:29:CYS:HB2	29:SO:146:ARG:HG3	2.01	0.43
3:SA:77:ILE:HD12	3:SA:122:LEU:HD11	2.01	0.43
4:SB:137:LEU:HG	4:SB:215:VAL:HG22	2.01	0.43
23:Sg:32:LEU:HD12	23:Sg:71:ILE:HD11	1.99	0.43
34:Se:28:LYS:HB3	34:Se:28:LYS:HE3	1.84	0.43
2:S2:650:A:OP2	19:SX:108:LYS:NZ	2.41	0.43
2:S2:1711:U:H2'	2:S2:1712:A:H8	1.83	0.43
4:SB:38:MET:HE1	4:SB:231:LEU:HD21	2.01	0.43
11:SL:65:ASN:O	11:SL:132:ARG:NH1	2.51	0.43
16:ST:28:LEU:HD13	16:ST:110:LEU:HD22	2.01	0.43
2:S2:106:C:H2'	2:S2:107:A:H8	1.84	0.42
2:S2:1101:U:H2'	2:S2:1102:G:C8	2.54	0.42
3:SA:5:LEU:HB2	3:SA:8:LEU:HB2	2.01	0.42
8:SH:58:LYS:HE3	8:SH:58:LYS:HA	2.01	0.42
16:ST:43:LYS:HD3	16:ST:43:LYS:HA	1.71	0.42
37:JC:323:VAL:HG22	37:JC:387:LEU:HB2	2.00	0.42
2:S2:72:C:N4	2:S2:74:G:O6	2.52	0.42
2:S2:562:U:H1'	26:SJ:132:GLN:HG2	2.01	0.42
2:S2:1777:G:H2'	2:S2:1778:C:H6	1.84	0.42
5:SD:29:LEU:HD13	5:SD:58:VAL:HG22	2.01	0.42
15:SS:86:ARG:NE	15:SS:89:ASP:OD1	2.52	0.42
16:ST:24:LYS:HB3	16:ST:24:LYS:HE3	1.79	0.42
25:SG:10:THR:HB	25:SG:128:THR:HA	2.00	0.42
2:S2:507:G:O6	31:SY:105:LYS:NZ	2.47	0.42
2:S2:570:C:O2'	31:SY:34:THR:O	2.33	0.42
2:S2:1069:U:H2'	2:S2:1070:A:H8	1.84	0.42
2:S2:1081:U:OP1	2:S2:1184:G:O2'	2.35	0.42
6:SE:151:ASP:OD1	25:SG:216:ARG:NH1	2.53	0.42
8:SH:82:GLU:O	8:SH:86:LYS:N	2.44	0.42
16:ST:39:LEU:HD23	16:ST:39:LEU:HA	1.84	0.42
2:S2:1280:G:H2'	2:S2:1281:G:H8	1.84	0.42
37:JC:311:VAL:HB	37:JC:583:ARG:HA	2.01	0.42
2:S2:1231:C:OP2	15:SS:139:THR:OG1	2.33	0.42
2:S2:1757:G:H8	2:S2:1758:G:H1'	1.85	0.42
5:SD:67:ARG:HD2	10:SK:96:ARG:HB3	2.00	0.42
5:SD:150:MET:HE3	5:SD:152:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:SS:124:ARG:HA	15:SS:124:ARG:HD2	1.76	0.42
16:ST:63:HIS:CE1	16:ST:78:ILE:HD11	2.54	0.42
2:S2:1284:A:H4'	2:S2:1285:G:H3'	2.00	0.42
2:S2:1658:G:H2'	2:S2:1659:U:O4'	2.19	0.42
2:S2:1700:C:N4	2:S2:1834:A:C2	2.88	0.42
6:SE:43:PRO:HG2	6:SE:46:ILE:HG12	2.02	0.42
6:SE:115:THR:HG23	6:SE:118:GLU:H	1.83	0.42
23:Sg:213:ASP:OD1	23:Sg:213:ASP:N	2.53	0.42
25:SG:194:LEU:HB3	25:SG:198:ARG:HH21	1.85	0.42
28:SN:17:PRO:HD3	33:Sb:28:PRO:HG3	2.02	0.42
2:S2:28:U:H2'	2:S2:29:G:C8	2.54	0.42
2:S2:1051:G:H2'	2:S2:1052:A:C8	2.55	0.42
2:S2:1740:C:H5''	9:SI:58:LEU:HD11	2.01	0.42
4:SB:88:THR:HA	4:SB:98:THR:HA	2.02	0.42
4:SB:181:LEU:HA	4:SB:184:VAL:HG22	2.00	0.42
5:SD:49:ILE:HG13	5:SD:87:TYR:HB2	2.01	0.42
14:SR:29:HIS:HA	14:SR:32:LYS:NZ	2.34	0.42
31:SY:116:LYS:HA	31:SY:116:LYS:HD2	1.86	0.42
34:Se:46:VAL:HG12	34:Se:48:THR:HG23	2.01	0.42
2:S2:197:U:OP2	2:S2:203:G:N2	2.40	0.42
2:S2:1866:A:N3	20:Sa:87:ARG:NH2	2.68	0.42
10:SK:80:ARG:NH1	10:SK:89:ILE:O	2.52	0.42
13:SQ:39:LEU:HD23	13:SQ:52:LEU:HD23	2.02	0.42
15:SS:50:ILE:HG21	15:SS:59:LEU:HD21	2.02	0.42
21:Sc:21:THR:HB	21:Sc:68:LEU:HD11	2.01	0.42
26:SJ:37:LEU:HD22	26:SJ:42:GLU:HB3	2.02	0.42
31:SY:76:TYR:OH	31:SY:85:ASN:O	2.29	0.42
37:JC:556:VAL:HG12	37:JC:562:LEU:HA	2.01	0.42
2:S2:329:G:H2'	2:S2:330:G:H8	1.83	0.42
2:S2:921:G:C4	33:Sb:22:LYS:HG2	2.54	0.42
4:SB:128:LYS:HB2	4:SB:134:LEU:HD13	2.01	0.42
4:SB:152:LYS:HD3	14:SR:133:GLY:HA3	2.01	0.42
20:Sa:4:LYS:HE2	20:Sa:5:ARG:HH22	1.84	0.42
35:Sf:137:ASP:N	35:Sf:137:ASP:OD1	2.50	0.42
2:S2:51:U:H2'	2:S2:52:G:C8	2.55	0.42
2:S2:106:C:H2'	2:S2:107:A:C8	2.55	0.42
2:S2:509:G:H2'	2:S2:510:G:H8	1.85	0.42
2:S2:639:C:H2'	2:S2:640:A:C8	2.55	0.42
2:S2:1189:A:H2'	2:S2:1190:A:H8	1.85	0.42
10:SK:15:LEU:HG	10:SK:79:LEU:HD11	2.02	0.42
21:Sc:30:VAL:HG11	21:Sc:46:VAL:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:SC:104:ASP:HB3	24:SC:130:ILE:HD12	2.02	0.42
27:SM:46:GLN:HE21	27:SM:112:LYS:HD3	1.85	0.42
28:SN:55:ARG:HH22	33:Sb:51:GLN:NE2	2.18	0.42
33:Sb:42:LYS:HG2	33:Sb:57:VAL:HG12	2.01	0.42
5:SD:137:VAL:HG22	5:SD:151:LYS:HG3	2.02	0.41
6:SE:153:LEU:O	6:SE:174:LYS:NZ	2.53	0.41
7:SF:61:PHE:CE2	21:Sc:51:ARG:HG3	2.55	0.41
8:SH:157:HIS:HB3	8:SH:190:PRO:HG3	2.01	0.41
25:SG:91:GLU:OE2	25:SG:93:LYS:HE3	2.20	0.41
26:SJ:22:LYS:HD2	26:SJ:22:LYS:HA	1.79	0.41
37:JC:310:ARG:HB2	37:JC:547:LEU:HD11	2.02	0.41
2:S2:115:U:H2'	2:S2:116:U:C6	2.56	0.41
2:S2:693:A:C5	2:S2:739:C:H4'	2.55	0.41
2:S2:900:C:H5'	2:S2:901:G:C8	2.55	0.41
2:S2:1332:A:N3	5:SD:141:LYS:NZ	2.58	0.41
2:S2:1373:C:OP1	14:SR:7:LYS:HG3	2.20	0.41
4:SB:224:GLU:HG3	4:SB:227:LYS:NZ	2.35	0.41
6:SE:73:ASP:HA	6:SE:164:LEU:HD13	2.02	0.41
25:SG:7:PHE:CE2	25:SG:9:ALA:HB3	2.55	0.41
25:SG:58:LYS:HA	25:SG:107:SER:OG	2.21	0.41
30:SW:37:PHE:HD1	30:SW:41:MET:HE2	1.85	0.41
36:JD:609:TYR:CZ	36:JD:613:LEU:HD11	2.55	0.41
2:S2:98:C:OP2	2:S2:426:A:O2'	2.29	0.41
2:S2:328:U:O2'	2:S2:329:G:O5'	2.33	0.41
2:S2:643:A:OP1	26:SJ:38:ARG:NH2	2.53	0.41
4:SB:64:GLY:HA2	4:SB:87:ILE:HD11	2.02	0.41
7:SF:50:PRO:HG2	7:SF:90:VAL:HG23	2.01	0.41
10:SK:95:ARG:NH2	10:SK:97:SER:O	2.41	0.41
2:S2:573:U:N3	2:S2:576:A:OP2	2.39	0.41
2:S2:1546:G:N2	2:S2:1670:C:O2	2.53	0.41
2:S2:1844:U:H2'	2:S2:1845:A:C8	2.55	0.41
4:SB:145:LYS:HB2	4:SB:145:LYS:HE3	1.78	0.41
17:SU:39:LEU:HD13	17:SU:101:ILE:HG22	2.03	0.41
23:Sg:217:MET:HB3	23:Sg:226:HIS:CD2	2.55	0.41
37:JC:35:VAL:HA	37:JC:38:ALA:HB3	2.02	0.41
37:JC:175:PRO:HA	37:JC:200:HIS:HB3	2.03	0.41
2:S2:51:U:H2'	2:S2:52:G:H8	1.84	0.41
2:S2:690:G:H2'	2:S2:691:G:N3	2.35	0.41
2:S2:1101:U:H2'	2:S2:1102:G:H8	1.85	0.41
4:SB:127:VAL:HG21	4:SB:176:VAL:HB	2.03	0.41
4:SB:134:LEU:HB3	4:SB:218:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:SF:19:LEU:C	7:SF:21:GLY:H	2.28	0.41
23:Sg:66:VAL:HA	23:Sg:82:SER:HA	2.02	0.41
26:SJ:53:ILE:HG21	26:SJ:81:LEU:HD21	2.02	0.41
2:S2:29:G:H2'	2:S2:30:C:C6	2.56	0.41
2:S2:429:C:H2'	2:S2:430:C:H6	1.86	0.41
2:S2:561:A:H2'	2:S2:562:U:C6	2.56	0.41
2:S2:694:G:C5	2:S2:737:G:N2	2.88	0.41
2:S2:1669:G:H4'	17:SU:62:ARG:HH12	1.84	0.41
3:SA:51:LEU:H	14:SR:105:MET:HE3	1.85	0.41
18:SV:17:CYS:HB2	18:SV:56:CYS:HB3	2.03	0.41
37:JC:106:LEU:HB2	37:JC:136:LEU:HD23	2.01	0.41
37:JC:149:ALA:HB1	37:JC:177:ALA:HB1	2.02	0.41
2:S2:810:A:C6	2:S2:851:C:N4	2.89	0.41
2:S2:829:C:OP1	6:SE:22:LYS:N	2.42	0.41
2:S2:1007:C:O2'	28:SN:104:ARG:NH2	2.53	0.41
2:S2:1514:G:H2'	2:S2:1515:G:C8	2.55	0.41
2:S2:1593:C:H2'	2:S2:1594:A:C8	2.56	0.41
2:S2:609:U:H2'	2:S2:610:G:H8	1.85	0.41
2:S2:1539:U:H2'	2:S2:1540:G:C8	2.56	0.41
2:S2:1719:A:H8	2:S2:1814:G:H21	1.68	0.41
2:S2:1777:G:H2'	2:S2:1778:C:C6	2.56	0.41
24:SC:91:SER:HB2	24:SC:156:ILE:HG23	2.02	0.41
27:SM:55:ASN:HD21	27:SM:82:ASN:H	1.69	0.41
2:S2:289:G:P	6:SE:155:LYS:HZ1	2.44	0.41
2:S2:300:U:H2'	2:S2:301:A:C8	2.56	0.41
2:S2:382:C:H2'	2:S2:383:G:H8	1.86	0.41
2:S2:1256:G:OP2	22:Sd:40:ARG:NH1	2.54	0.41
2:S2:1598:G:H1'	7:SF:166:ILE:HD12	2.03	0.41
2:S2:1740:C:H2'	2:S2:1741:U:C6	2.56	0.41
3:SA:222:VAL:HG23	3:SA:223:THR:HG23	2.03	0.41
6:SE:124:CYS:HA	6:SE:142:HIS:HE1	1.86	0.41
11:SL:150:GLY:O	28:SN:133:ARG:NH2	2.54	0.41
12:SP:81:ARG:HH12	12:SP:98:ASN:HA	1.84	0.41
14:SR:57:LEU:HD23	14:SR:57:LEU:HA	1.95	0.41
23:Sg:110:SER:O	23:Sg:123:GLY:N	2.54	0.41
25:SG:229:ALA:HA	25:SG:232:ARG:HG2	2.03	0.41
29:SO:82:ALA:HB1	29:SO:86:LYS:HE3	2.02	0.41
2:S2:1405:A:H2'	2:S2:1406:G:O4'	2.21	0.41
2:S2:1521:C:O2'	15:SS:144:ARG:NH2	2.54	0.41
2:S2:1623:A:O5'	15:SS:133:GLY:HA3	2.21	0.41
6:SE:222:LEU:HA	6:SE:225:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:SK:64:TRP:CD1	22:Sd:23:VAL:HG13	2.56	0.41
22:Sd:26:ASN:OD1	22:Sd:27:ARG:N	2.54	0.41
23:Sg:154:VAL:HG12	23:Sg:167:SER:HA	2.03	0.41
25:SG:48:TYR:OH	25:SG:119:LYS:O	2.36	0.41
25:SG:181:THR:HG22	25:SG:183:ARG:H	1.86	0.41
26:SJ:108:ARG:HA	26:SJ:108:ARG:HD2	1.82	0.41
31:SY:112:ASN:HA	31:SY:115:LYS:HD3	2.02	0.41
2:S2:498:C:H2'	2:S2:499:G:C8	2.56	0.40
2:S2:750:C:H41	2:S2:793:G:H21	1.69	0.40
2:S2:839:C:O2'	2:S2:841:G:O4'	2.39	0.40
2:S2:1230:C:O2	2:S2:1665:G:C2	2.74	0.40
2:S2:1752:C:C2	2:S2:1779:G:N1	2.90	0.40
2:S2:1866:A:H2'	2:S2:1867:U:C6	2.56	0.40
2:S2:492:C:N4	2:S2:507:G:OP2	2.47	0.40
2:S2:912:C:N3	2:S2:914:U:C2	2.88	0.40
2:S2:1539:U:H2'	2:S2:1540:G:H8	1.87	0.40
2:S2:1615:U:H2'	2:S2:1616:U:C6	2.56	0.40
2:S2:1673:U:H5''	13:SQ:78:VAL:HG12	2.03	0.40
2:S2:1780:G:H3'	2:S2:1781:A:C8	2.57	0.40
13:SQ:76:GLY:O	13:SQ:80:GLN:HG2	2.21	0.40
2:S2:1388:A:H61	5:SD:161:GLY:HA3	1.86	0.40
2:S2:1845:A:H2'	2:S2:1846:G:C8	2.57	0.40
7:SF:87:LEU:HD22	7:SF:87:LEU:HA	1.77	0.40
25:SG:78:SER:OG	25:SG:79:LYS:N	2.54	0.40
32:SZ:102:LYS:HA	32:SZ:107:VAL:HG12	2.02	0.40
2:S2:17:C:H2'	2:S2:18:C:H6	1.87	0.40
2:S2:168:C:O2'	25:SG:133:LEU:O	2.39	0.40
2:S2:374:G:H2'	2:S2:375:U:C6	2.57	0.40
7:SF:34:SER:HA	21:Sc:55:VAL:HG23	2.04	0.40
16:ST:6:VAL:HG21	16:ST:62:ARG:HG3	2.02	0.40
24:SC:74:LYS:HB3	24:SC:269:PHE:CE2	2.56	0.40
2:S2:1538:C:H4'	16:ST:45:LEU:HD12	2.04	0.40
2:S2:1784:G:H2'	2:S2:1785:C:C6	2.57	0.40
4:SB:167:LYS:HE2	4:SB:200:ALA:HB1	2.04	0.40
5:SD:16:ILE:HD13	22:Sd:22:ARG:NH1	2.36	0.40
10:SK:58:VAL:HG12	10:SK:71:LEU:HA	2.03	0.40
26:SJ:162:ARG:NH2	31:SY:31:GLY:HA2	2.37	0.40
37:JC:497:ASP:OD1	37:JC:566:TYR:OH	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Ln	22/25 (88%)	22 (100%)	0	0	100	100
3	SA	220/295 (75%)	214 (97%)	6 (3%)	0	100	100
4	SB	212/264 (80%)	206 (97%)	6 (3%)	0	100	100
5	SD	225/243 (93%)	219 (97%)	6 (3%)	0	100	100
6	SE	260/263 (99%)	249 (96%)	11 (4%)	0	100	100
7	SF	180/204 (88%)	165 (92%)	12 (7%)	3 (2%)	7	28
8	SH	182/194 (94%)	173 (95%)	9 (5%)	0	100	100
9	SI	204/208 (98%)	194 (95%)	10 (5%)	0	100	100
10	SK	96/165 (58%)	90 (94%)	6 (6%)	0	100	100
11	SL	140/158 (89%)	134 (96%)	6 (4%)	0	100	100
12	SP	125/145 (86%)	122 (98%)	3 (2%)	0	100	100
13	SQ	142/146 (97%)	131 (92%)	10 (7%)	1 (1%)	18	47
14	SR	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
15	SS	143/152 (94%)	137 (96%)	6 (4%)	0	100	100
16	ST	141/145 (97%)	138 (98%)	3 (2%)	0	100	100
17	SU	102/119 (86%)	93 (91%)	8 (8%)	1 (1%)	12	40
18	SV	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
19	SX	139/143 (97%)	133 (96%)	6 (4%)	0	100	100
20	Sa	100/115 (87%)	97 (97%)	2 (2%)	1 (1%)	12	40
21	Sc	62/69 (90%)	59 (95%)	3 (5%)	0	100	100
22	Sd	53/56 (95%)	49 (92%)	4 (8%)	0	100	100
23	Sg	311/317 (98%)	289 (93%)	22 (7%)	0	100	100
24	SC	220/293 (75%)	213 (97%)	7 (3%)	0	100	100
25	SG	235/249 (94%)	228 (97%)	7 (3%)	0	100	100
26	SJ	183/194 (94%)	177 (97%)	5 (3%)	1 (0%)	24	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	SM	120/132 (91%)	112 (93%)	8 (7%)	0	100	100
28	SN	148/151 (98%)	144 (97%)	4 (3%)	0	100	100
29	SO	133/151 (88%)	125 (94%)	8 (6%)	0	100	100
30	SW	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
31	SY	123/133 (92%)	121 (98%)	2 (2%)	0	100	100
32	SZ	73/125 (58%)	67 (92%)	6 (8%)	0	100	100
33	Sb	81/84 (96%)	72 (89%)	9 (11%)	0	100	100
34	Se	56/59 (95%)	48 (86%)	8 (14%)	0	100	100
35	Sf	59/156 (38%)	55 (93%)	4 (7%)	0	100	100
36	JD	48/1096 (4%)	48 (100%)	0	0	100	100
37	JC	506/583 (87%)	488 (96%)	18 (4%)	0	100	100
All	All	5385/7180 (75%)	5141 (96%)	237 (4%)	7 (0%)	49	78

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	SQ	44	PRO
7	SF	80	GLY
7	SF	20	PHE
7	SF	52	SER
20	Sa	46	GLU
26	SJ	122	SER
17	SU	94	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Ln	23/24 (96%)	23 (100%)	0	100	100
3	SA	184/243 (76%)	184 (100%)	0	100	100
4	SB	195/231 (84%)	195 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	SD	190/202 (94%)	190 (100%)	0	100	100
6	SE	224/225 (100%)	224 (100%)	0	100	100
7	SF	156/170 (92%)	147 (94%)	9 (6%)	18	45
8	SH	166/174 (95%)	166 (100%)	0	100	100
9	SI	178/180 (99%)	178 (100%)	0	100	100
10	SK	89/136 (65%)	89 (100%)	0	100	100
11	SL	130/142 (92%)	128 (98%)	2 (2%)	57	69
12	SP	113/130 (87%)	113 (100%)	0	100	100
13	SQ	119/121 (98%)	119 (100%)	0	100	100
14	SR	122/122 (100%)	121 (99%)	1 (1%)	73	77
15	SS	126/132 (96%)	126 (100%)	0	100	100
16	ST	113/115 (98%)	113 (100%)	0	100	100
17	SU	94/107 (88%)	94 (100%)	0	100	100
18	SV	67/67 (100%)	67 (100%)	0	100	100
19	SX	113/115 (98%)	113 (100%)	0	100	100
20	Sa	89/98 (91%)	89 (100%)	0	100	100
21	Sc	57/62 (92%)	57 (100%)	0	100	100
22	Sd	48/49 (98%)	48 (100%)	0	100	100
23	Sg	272/275 (99%)	272 (100%)	0	100	100
24	SC	188/225 (84%)	188 (100%)	0	100	100
25	SG	207/218 (95%)	207 (100%)	0	100	100
26	SJ	161/168 (96%)	161 (100%)	0	100	100
27	SM	102/108 (94%)	102 (100%)	0	100	100
28	SN	130/131 (99%)	130 (100%)	0	100	100
29	SO	105/119 (88%)	105 (100%)	0	100	100
30	SW	112/113 (99%)	112 (100%)	0	100	100
31	SY	109/115 (95%)	109 (100%)	0	100	100
32	SZ	66/103 (64%)	66 (100%)	0	100	100
33	Sb	75/76 (99%)	75 (100%)	0	100	100
34	Se	47/48 (98%)	47 (100%)	0	100	100
35	Sf	54/140 (39%)	54 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	JD	46/948 (5%)	46 (100%)	0	100	100
37	JC	437/487 (90%)	437 (100%)	0	100	100
All	All	4707/6119 (77%)	4695 (100%)	12 (0%)	84	84

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	SF	18	LYS
7	SF	19	LEU
7	SF	47	LYS
7	SF	49	LEU
7	SF	52	SER
7	SF	70	GLU
7	SF	86	LYS
7	SF	87	LEU
7	SF	91	ARG
11	SL	37	TYR
11	SL	38	LYS
14	SR	50	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	Ln	22	GLN
3	SA	164	ASN
3	SA	169	HIS
4	SB	40	ASN
4	SB	43	ASN
4	SB	75	GLN
4	SB	92	GLN
4	SB	101	HIS
4	SB	118	GLN
5	SD	4	GLN
6	SE	36	HIS
6	SE	98	ASN
7	SF	110	GLN
8	SH	126	HIS
9	SI	22	HIS
12	SP	103	ASN
14	SR	31	ASN

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Mol	Chain	Res	Type
14	SR	48	ASN
16	ST	137	GLN
23	Sg	20	GLN
23	Sg	119	GLN
23	Sg	196	ASN
24	SC	113	GLN
26	SJ	154	GLN
30	SW	24	GLN
30	SW	56	HIS
30	SW	90	GLN
32	SZ	103	HIS
32	SZ	112	ASN
36	JD	636	ASN
37	JC	130	GLN
37	JC	445	ASN
37	JC	447	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	S2	1715/1869 (91%)	435 (25%)	8 (0%)

All (435) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	S2	4	C
2	S2	8	U
2	S2	14	C
2	S2	17	C
2	S2	25	A
2	S2	26	U
2	S2	33	G
2	S2	41	G
2	S2	42	A
2	S2	44	U
2	S2	46	A
2	S2	49	C
2	S2	56	G
2	S2	58	C
2	S2	59	U
2	S2	62	G

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Mol	Chain	Res	Type
2	S2	64	A
2	S2	65	C
2	S2	66	G
2	S2	67	C
2	S2	68	A
2	S2	72	C
2	S2	73	C
2	S2	74	G
2	S2	75	G
2	S2	76	U
2	S2	77	A
2	S2	103	A
2	S2	113	G
2	S2	114	G
2	S2	115	U
2	S2	116	U
2	S2	118	C
2	S2	126	G
2	S2	130	G
2	S2	143	U
2	S2	149	A
2	S2	154	U
2	S2	156	G
2	S2	159	A
2	S2	160	U
2	S2	161	U
2	S2	162	C
2	S2	163	U
2	S2	170	A
2	S2	182	C
2	S2	190	G
2	S2	196	C
2	S2	197	U
2	S2	198	U
2	S2	200	G
2	S2	203	G
2	S2	204	G
2	S2	206	G
2	S2	208	G
2	S2	214	U
2	S2	289	G
2	S2	290	U

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Mol	Chain	Res	Type
2	S2	291	G
2	S2	292	A
2	S2	294	U
2	S2	295	C
2	S2	302	A
2	S2	305	U
2	S2	306	C
2	S2	307	G
2	S2	308	G
2	S2	309	G
2	S2	310	C
2	S2	311	C
2	S2	318	A
2	S2	319	C
2	S2	323	C
2	S2	324	C
2	S2	325	C
2	S2	326	C
2	S2	327	G
2	S2	328	U
2	S2	329	G
2	S2	332	G
2	S2	335	G
2	S2	339	A
2	S2	347	G
2	S2	357	C
2	S2	362	C
2	S2	364	A
2	S2	368	U
2	S2	369	C
2	S2	381	C
2	S2	385	G
2	S2	386	C
2	S2	398	A
2	S2	400	C
2	S2	408	A
2	S2	409	C
2	S2	426	A
2	S2	436	G
2	S2	438	G
2	S2	445	A
2	S2	448	A

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Mol	Chain	Res	Type
2	S2	449	A
2	S2	450	C
2	S2	452	G
2	S2	464	A
2	S2	465	A
2	S2	466	G
2	S2	467	G
2	S2	470	G
2	S2	471	G
2	S2	472	C
2	S2	474	G
2	S2	482	G
2	S2	483	C
2	S2	487	U
2	S2	488	U
2	S2	492	C
2	S2	493	A
2	S2	500	A
2	S2	501	C
2	S2	504	G
2	S2	516	A
2	S2	525	A
2	S2	529	A
2	S2	531	A
2	S2	532	C
2	S2	533	A
2	S2	536	A
2	S2	537	C
2	S2	542	U
2	S2	546	G
2	S2	547	G
2	S2	556	U
2	S2	557	U
2	S2	558	G
2	S2	559	G
2	S2	563	G
2	S2	564	A
2	S2	583	C
2	S2	589	G
2	S2	590	A
2	S2	591	U
2	S2	596	U

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Mol	Chain	Res	Type
2	S2	604	A
2	S2	607	U
2	S2	608	C
2	S2	614	C
2	S2	617	G
2	S2	623	G
2	S2	626	G
2	S2	627	U
2	S2	628	A
2	S2	631	U
2	S2	643	A
2	S2	644	G
2	S2	655	A
2	S2	660	C
2	S2	664	A
2	S2	668	A
2	S2	669	A
2	S2	671	A
2	S2	672	A
2	S2	673	G
2	S2	687	C
2	S2	688	U
2	S2	689	U
2	S2	690	G
2	S2	692	G
2	S2	693	A
2	S2	694	G
2	S2	695	C
2	S2	696	G
2	S2	697	G
2	S2	698	G
2	S2	732	U
2	S2	736	C
2	S2	737	G
2	S2	738	C
2	S2	749	U
2	S2	751	G
2	S2	752	G
2	S2	788	G
2	S2	791	C
2	S2	792	C
2	S2	794	A

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Mol	Chain	Res	Type
2	S2	797	C
2	S2	798	A
2	S2	811	A
2	S2	821	G
2	S2	822	U
2	S2	823	U
2	S2	824	C
2	S2	827	A
2	S2	830	A
2	S2	834	C
2	S2	835	C
2	S2	836	G
2	S2	837	A
2	S2	838	G
2	S2	839	C
2	S2	840	C
2	S2	841	G
2	S2	842	C
2	S2	847	A
2	S2	869	A
2	S2	873	G
2	S2	874	G
2	S2	877	C
2	S2	878	G
2	S2	880	G
2	S2	882	U
2	S2	883	U
2	S2	888	U
2	S2	889	U
2	S2	891	G
2	S2	893	U
2	S2	894	G
2	S2	896	U
2	S2	897	U
2	S2	898	U
2	S2	899	U
2	S2	900	C
2	S2	901	G
2	S2	913	A
2	S2	914	U
2	S2	917	U
2	S2	920	A

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Mol	Chain	Res	Type
2	S2	922	A
2	S2	933	G
2	S2	955	A
2	S2	956	G
2	S2	957	A
2	S2	963	A
2	S2	970	G
2	S2	971	G
2	S2	990	A
2	S2	992	A
2	S2	999	G
2	S2	1001	A
2	S2	1017	U
2	S2	1023	A
2	S2	1030	A
2	S2	1042	A
2	S2	1045	U
2	S2	1047	C
2	S2	1061	U
2	S2	1062	A
2	S2	1073	U
2	S2	1074	C
2	S2	1078	C
2	S2	1083	A
2	S2	1085	C
2	S2	1086	G
2	S2	1087	A
2	S2	1089	G
2	S2	1109	C
2	S2	1115	U
2	S2	1116	C
2	S2	1118	C
2	S2	1119	A
2	S2	1132	C
2	S2	1133	A
2	S2	1135	C
2	S2	1138	C
2	S2	1153	C
2	S2	1154	U
2	S2	1155	U
2	S2	1195	A
2	S2	1203	G

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Mol	Chain	Res	Type
2	S2	1207	G
2	S2	1208	A
2	S2	1210	G
2	S2	1215	C
2	S2	1216	C
2	S2	1217	A
2	S2	1221	G
2	S2	1224	G
2	S2	1227	G
2	S2	1240	A
2	S2	1242	U
2	S2	1243	U
2	S2	1251	A
2	S2	1253	A
2	S2	1256	G
2	S2	1257	G
2	S2	1259	A
2	S2	1260	A
2	S2	1264	C
2	S2	1265	A
2	S2	1269	G
2	S2	1273	C
2	S2	1274	G
2	S2	1275	G
2	S2	1277	C
2	S2	1283	C
2	S2	1284	A
2	S2	1285	G
2	S2	1286	G
2	S2	1287	A
2	S2	1294	G
2	S2	1295	A
2	S2	1298	G
2	S2	1302	G
2	S2	1303	C
2	S2	1308	U
2	S2	1312	G
2	S2	1348	G
2	S2	1371	U
2	S2	1372	U
2	S2	1378	A
2	S2	1382	A

Continued on next page...

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Mol	Chain	Res	Type
2	S2	1397	U
2	S2	1409	A
2	S2	1412	C
2	S2	1414	A
2	S2	1415	C
2	S2	1419	C
2	S2	1420	G
2	S2	1421	A
2	S2	1422	G
2	S2	1423	C
2	S2	1424	G
2	S2	1433	C
2	S2	1434	C
2	S2	1435	C
2	S2	1436	C
2	S2	1438	A
2	S2	1452	A
2	S2	1454	A
2	S2	1462	U
2	S2	1463	U
2	S2	1464	C
2	S2	1484	A
2	S2	1489	A
2	S2	1490	G
2	S2	1494	U
2	S2	1495	G
2	S2	1497	G
2	S2	1498	A
2	S2	1499	U
2	S2	1505	U
2	S2	1507	G
2	S2	1508	A
2	S2	1509	U
2	S2	1520	G
2	S2	1521	C
2	S2	1533	A
2	S2	1537	A
2	S2	1544	C
2	S2	1547	C
2	S2	1553	C
2	S2	1556	A
2	S2	1558	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	S2	1560	U
2	S2	1570	G
2	S2	1574	C
2	S2	1580	A
2	S2	1585	U
2	S2	1587	G
2	S2	1588	A
2	S2	1594	A
2	S2	1599	U
2	S2	1600	G
2	S2	1601	A
2	S2	1606	G
2	S2	1614	A
2	S2	1621	U
2	S2	1623	A
2	S2	1634	A
2	S2	1638	G
2	S2	1640	A
2	S2	1643	U
2	S2	1644	C
2	S2	1648	G
2	S2	1654	G
2	S2	1661	A
2	S2	1663	A
2	S2	1665	G
2	S2	1671	G
2	S2	1684	C
2	S2	1698	C
2	S2	1699	A
2	S2	1715	A
2	S2	1719	A
2	S2	1721	U
2	S2	1722	G
2	S2	1723	G
2	S2	1726	G
2	S2	1729	U
2	S2	1731	A
2	S2	1742	C
2	S2	1743	G
2	S2	1744	G
2	S2	1745	A
2	S2	1752	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	S2	1753	C
2	S2	1754	G
2	S2	1757	G
2	S2	1758	G
2	S2	1761	U
2	S2	1772	C
2	S2	1773	C
2	S2	1774	C
2	S2	1775	U
2	S2	1776	G
2	S2	1777	G
2	S2	1781	A
2	S2	1783	C
2	S2	1784	G
2	S2	1786	U
2	S2	1798	C
2	S2	1801	A
2	S2	1804	U
2	S2	1807	C
2	S2	1809	A
2	S2	1812	U
2	S2	1814	G
2	S2	1821	U
2	S2	1822	A
2	S2	1823	A
2	S2	1824	A
2	S2	1825	A
2	S2	1826	G
2	S2	1829	G
2	S2	1831	A
2	S2	1835	A
2	S2	1838	U
2	S2	1849	G
2	S2	1850	A
2	S2	1852	C
2	S2	1861	G
2	S2	1862	G
2	S2	1863	A
2	S2	1864	U
2	S2	1865	C
2	S2	1867	U

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	S2	72	C
2	S2	158	A
2	S2	291	G
2	S2	466	G
2	S2	500	A
2	S2	688	U
2	S2	954	U
2	S2	1434	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

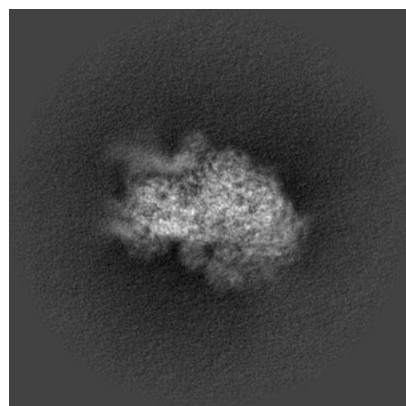
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38549. These allow visual inspection of the internal detail of the map and identification of artifacts.

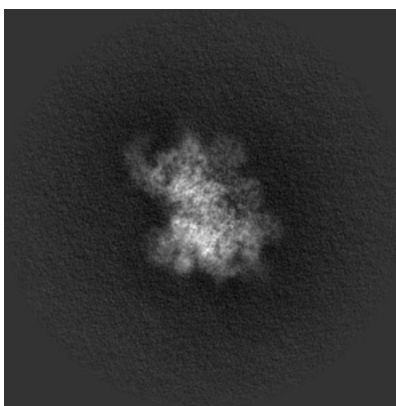
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

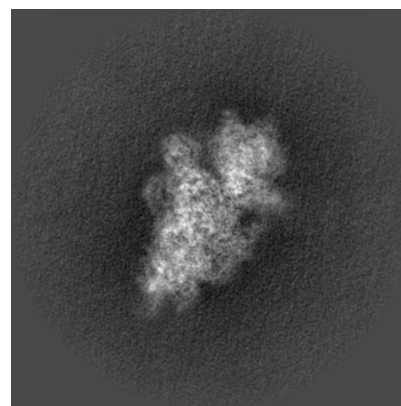
6.1.1 Primary map



X

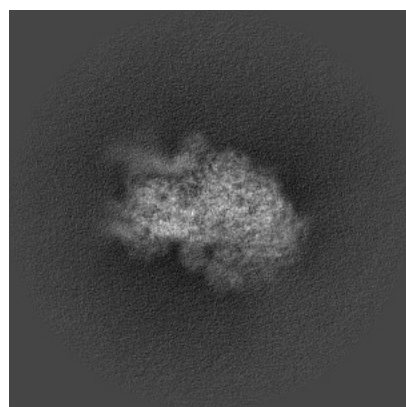


Y

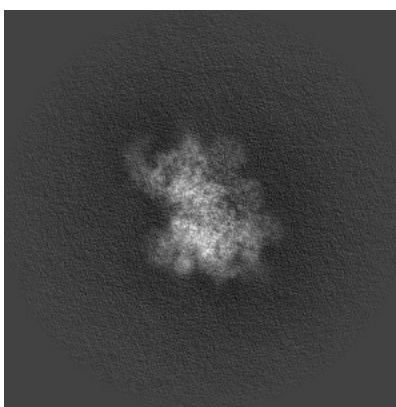


Z

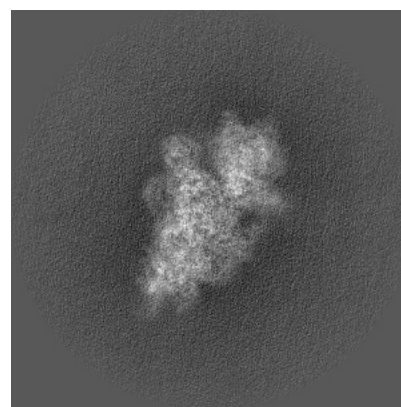
6.1.2 Raw map



X



Y

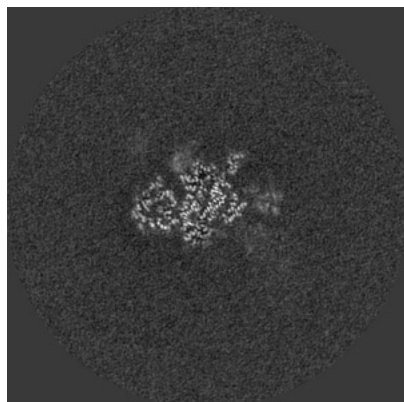


Z

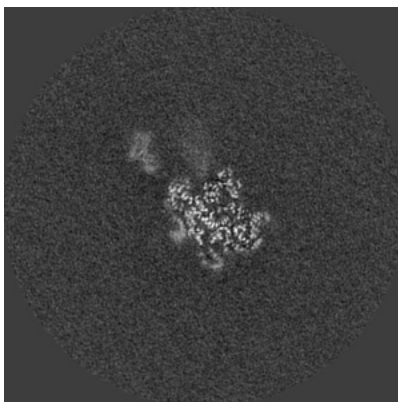
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

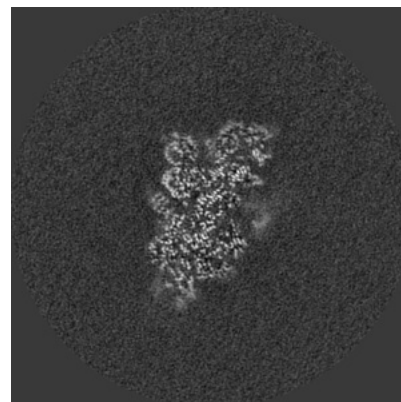
6.2.1 Primary map



X Index: 210

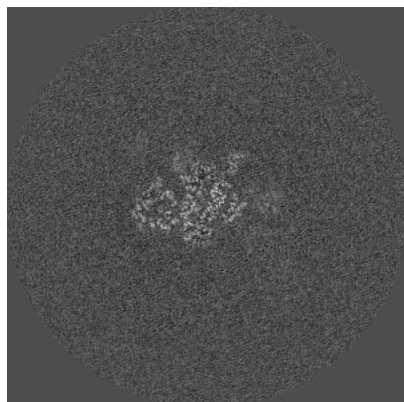


Y Index: 210

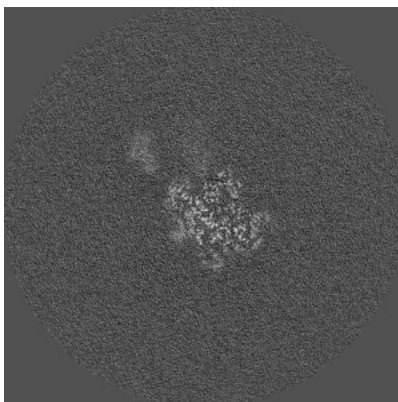


Z Index: 210

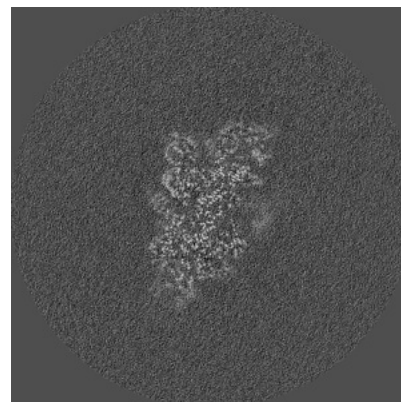
6.2.2 Raw map



X Index: 210



Y Index: 210

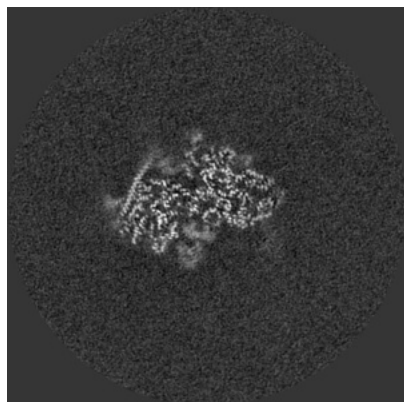


Z Index: 210

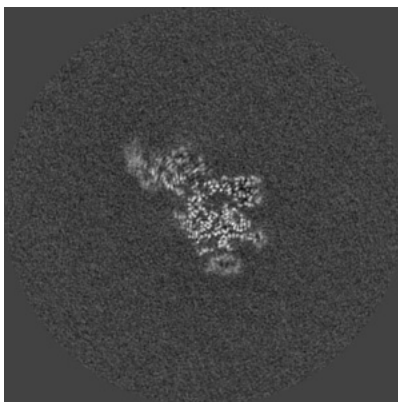
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

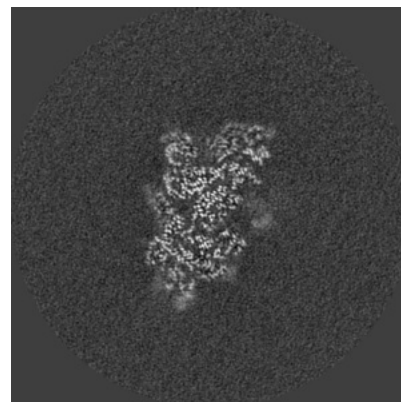
6.3.1 Primary map



X Index: 179

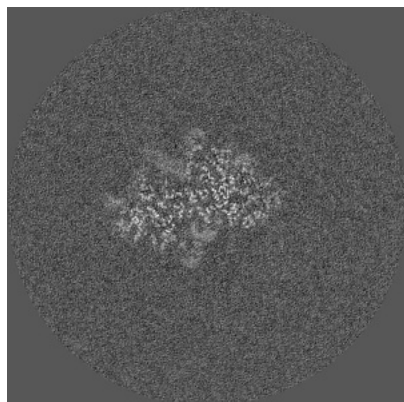


Y Index: 232

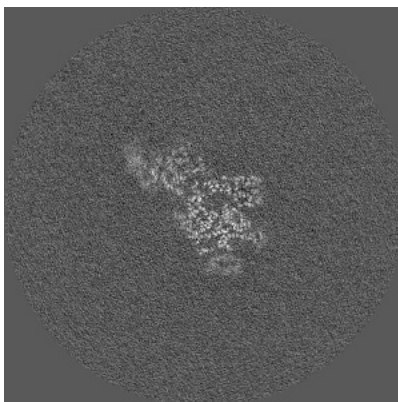


Z Index: 212

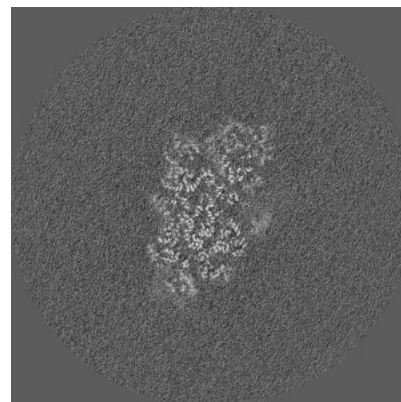
6.3.2 Raw map



X Index: 182



Y Index: 232

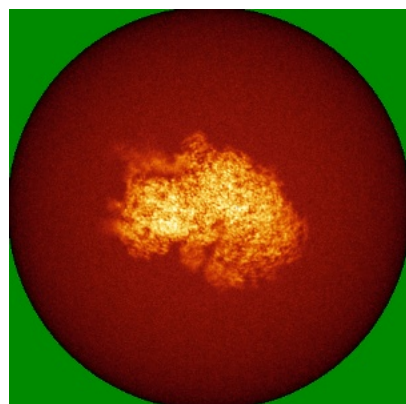


Z Index: 208

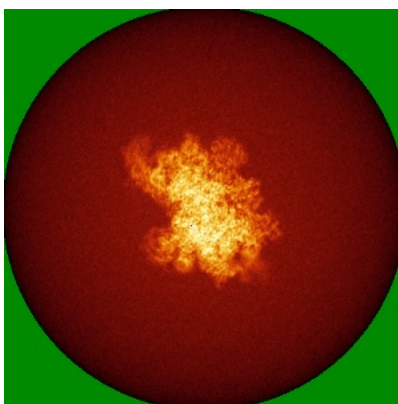
The images above show the largest variance slices of the map in three orthogonal directions.

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

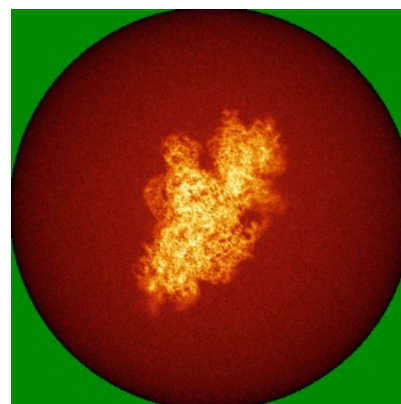
6.4.1 Primary map



X

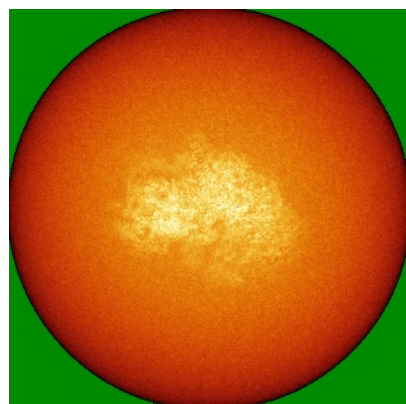


Y

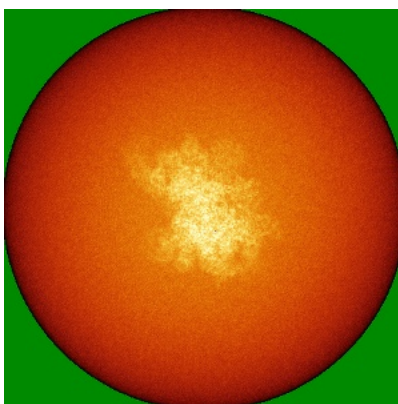


Z

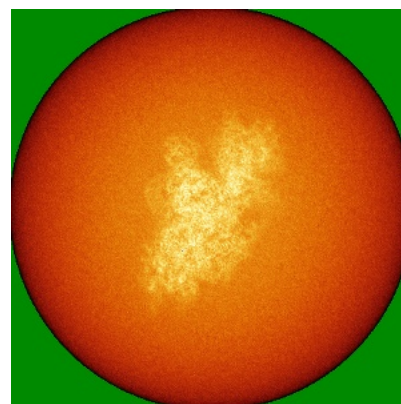
6.4.2 Raw map



X



Y

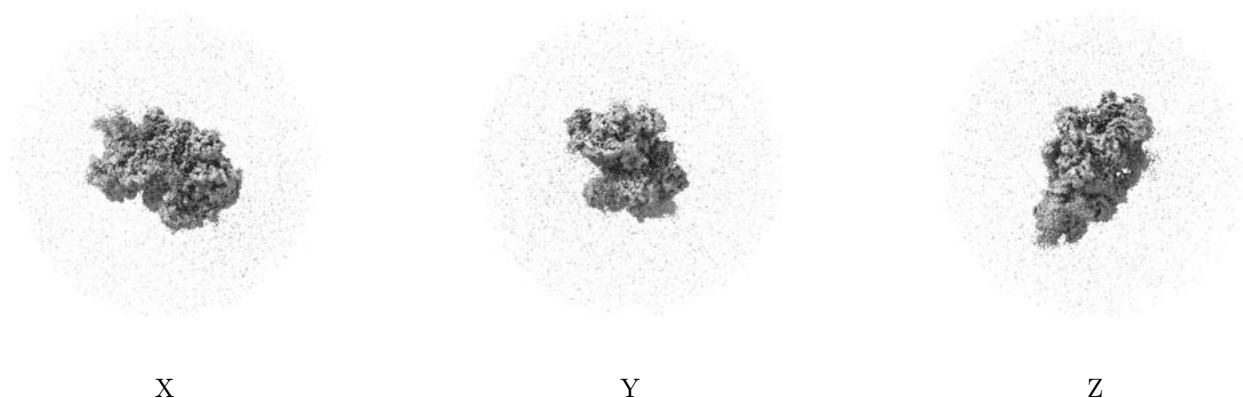


Z

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

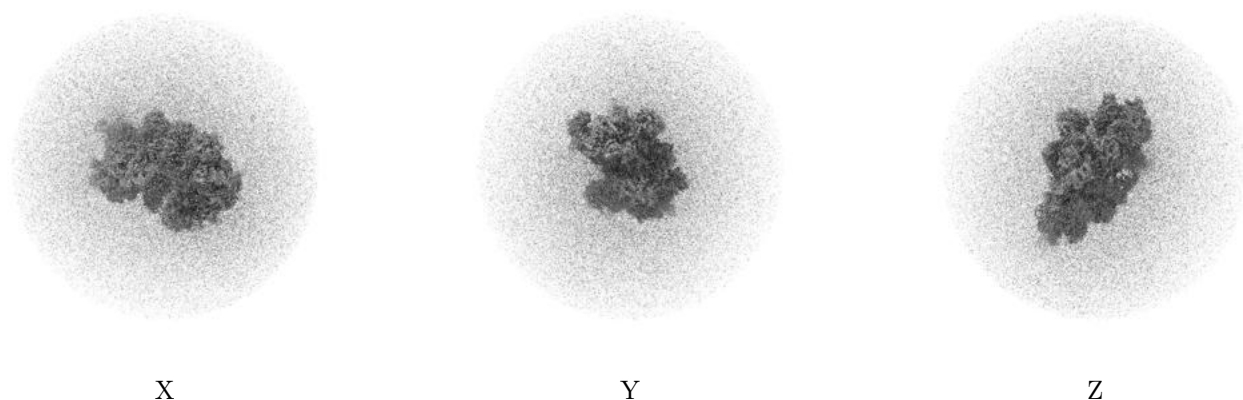
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

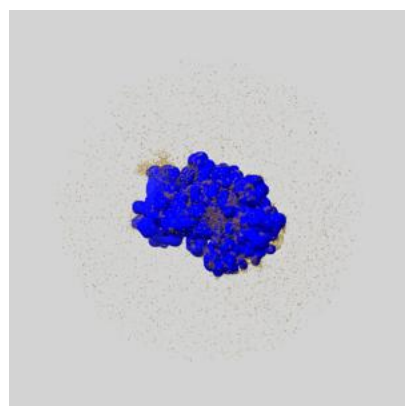
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

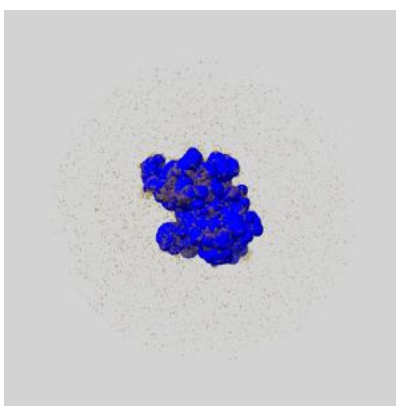
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

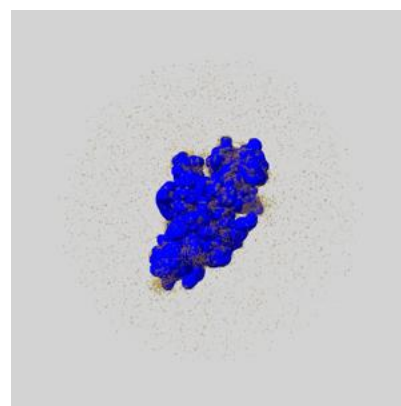
6.6.1 emd_38549_msk_1.map [i](#)



X



Y

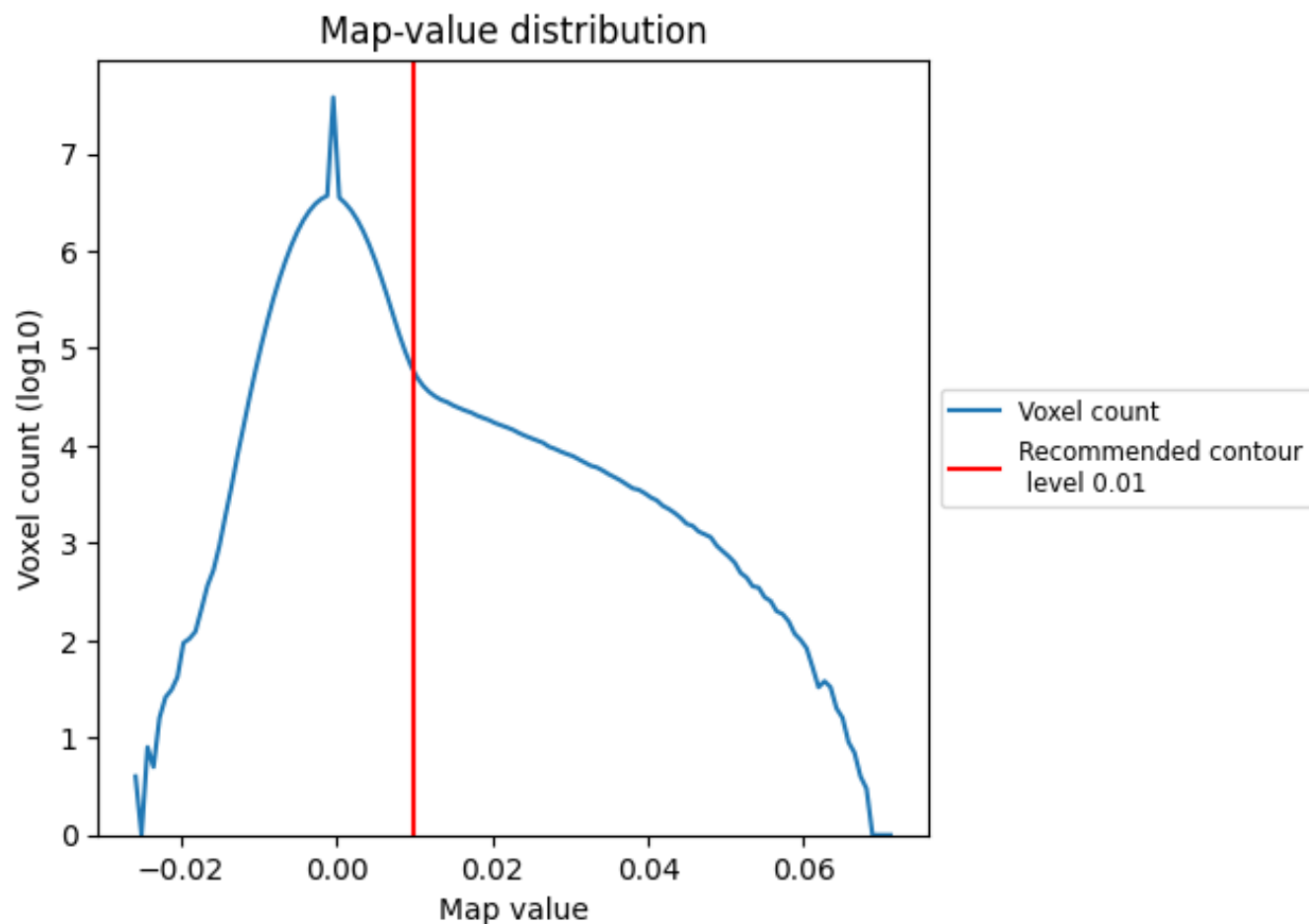


Z

7 Map analysis [i](#)

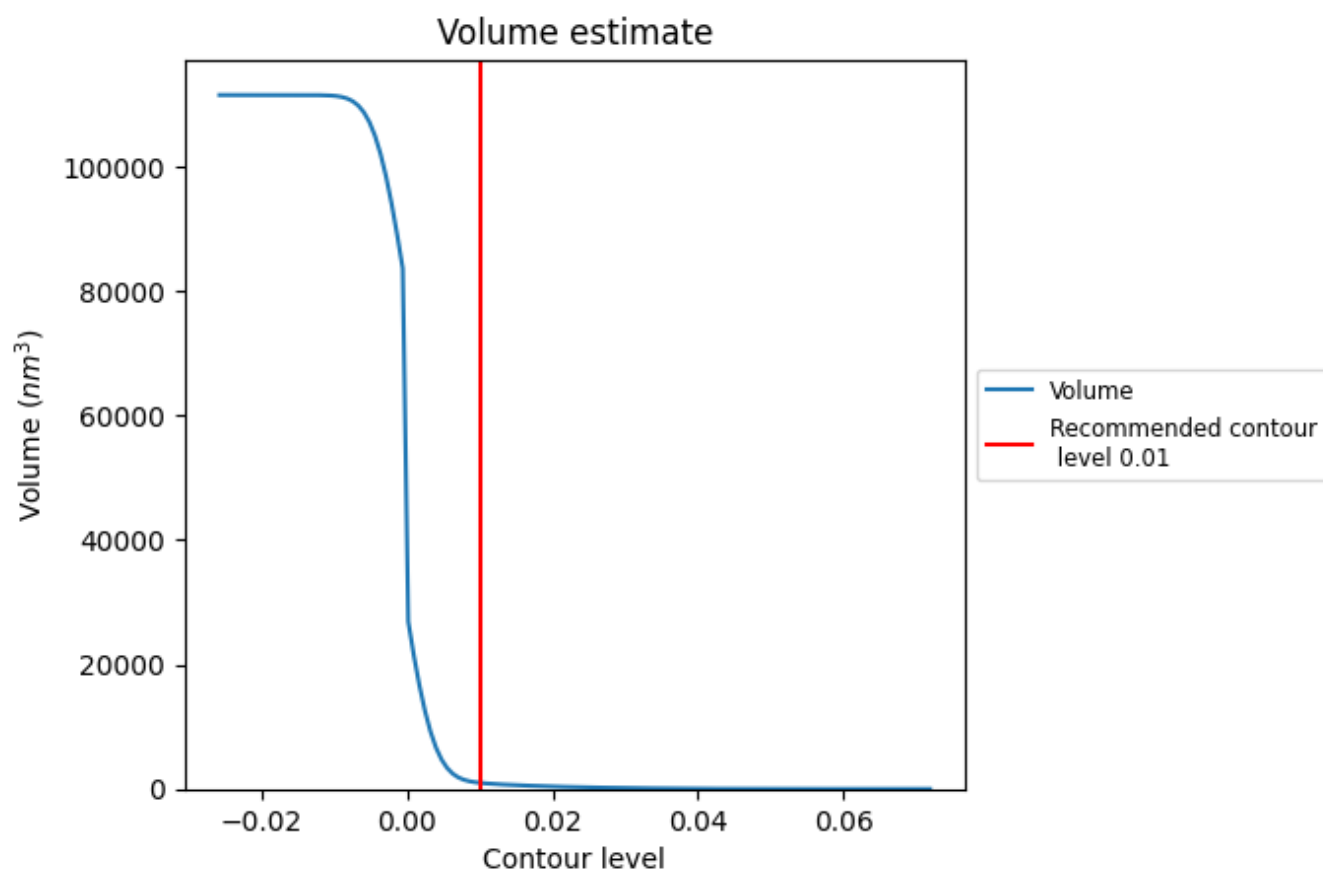
This section contains the results of statistical analysis of the map.

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.

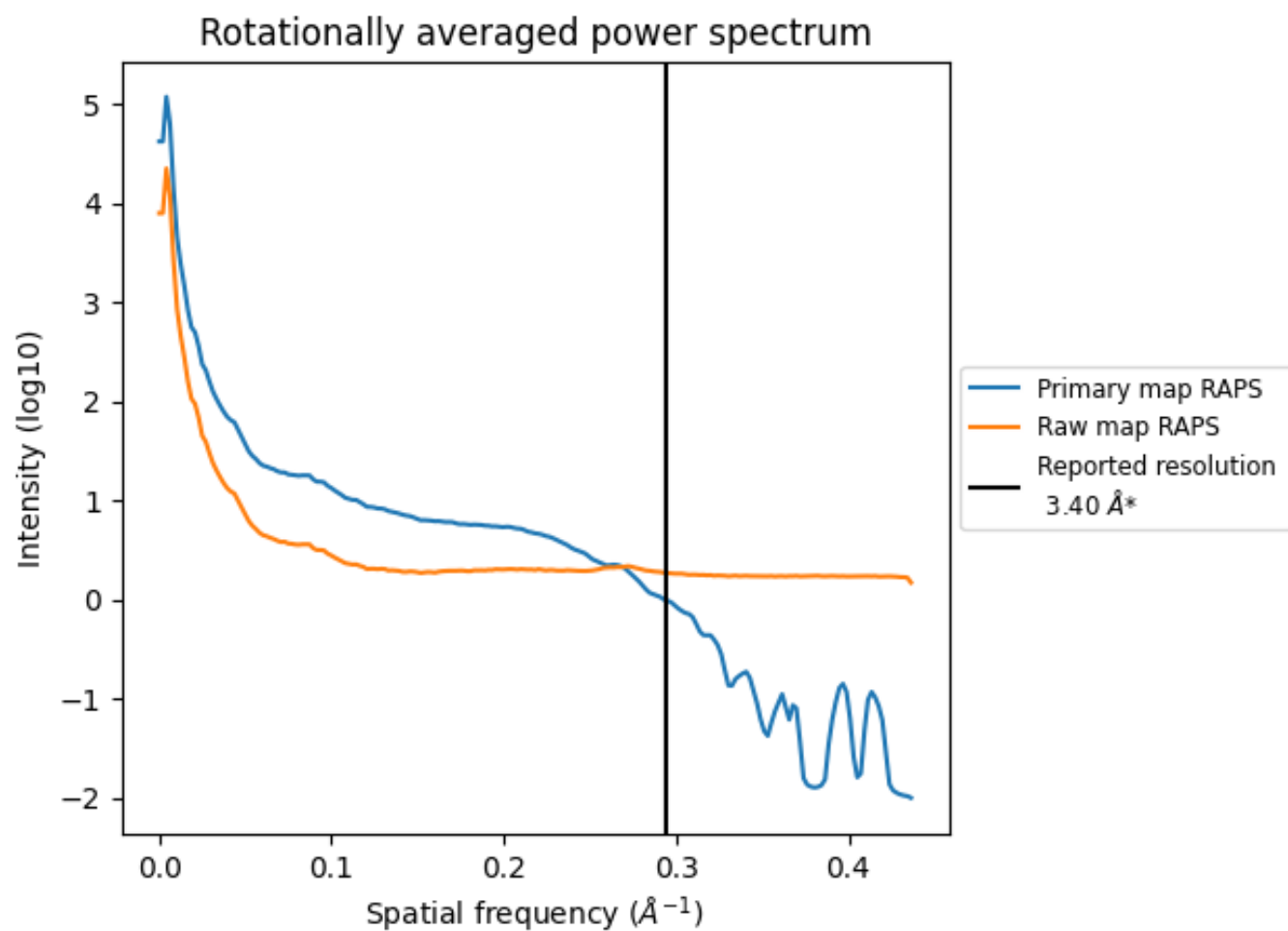
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 985 nm³; this corresponds to an approximate mass of 890 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 ⓘ

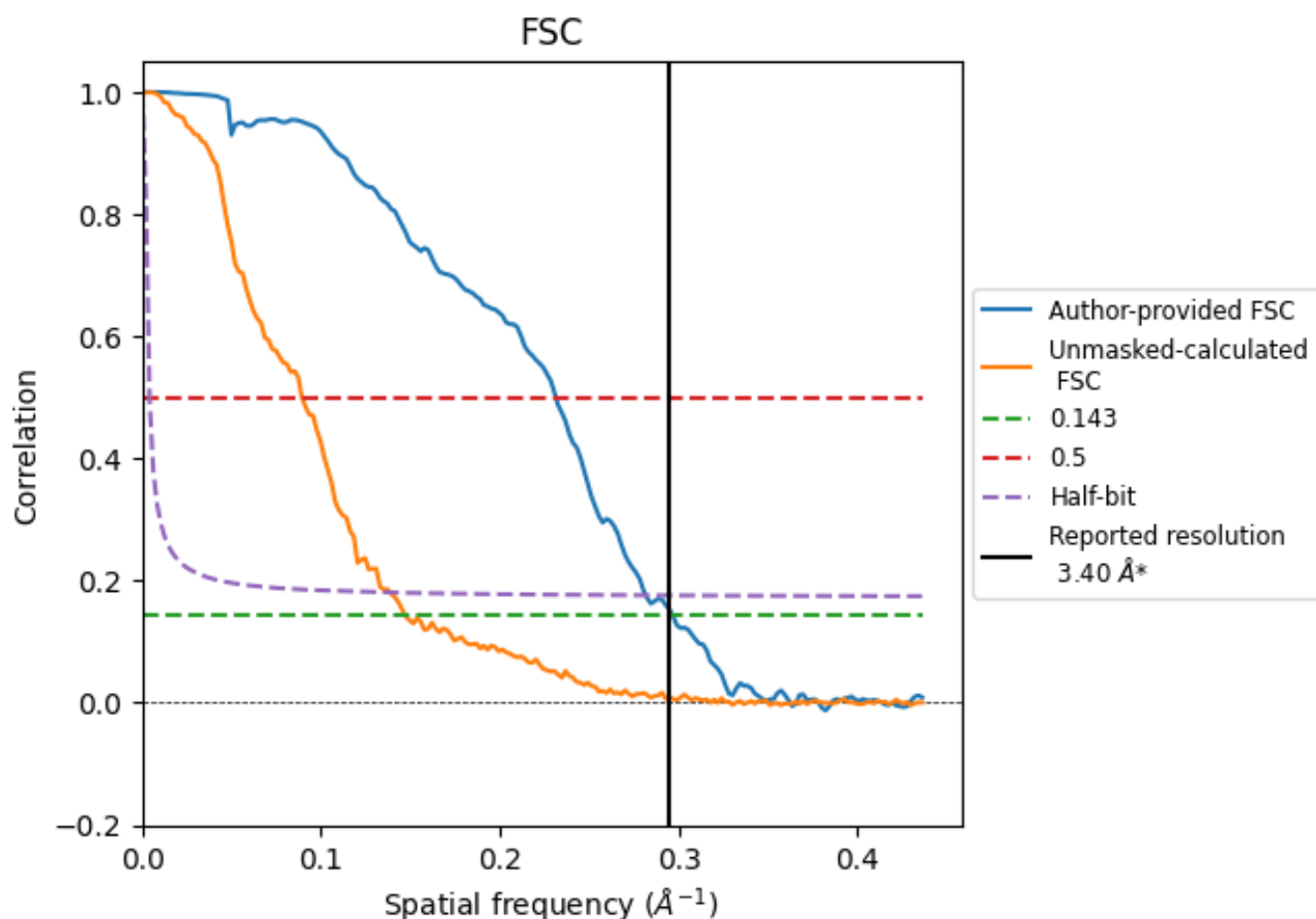


*Reported resolution corresponds to spatial frequency of 0.294 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

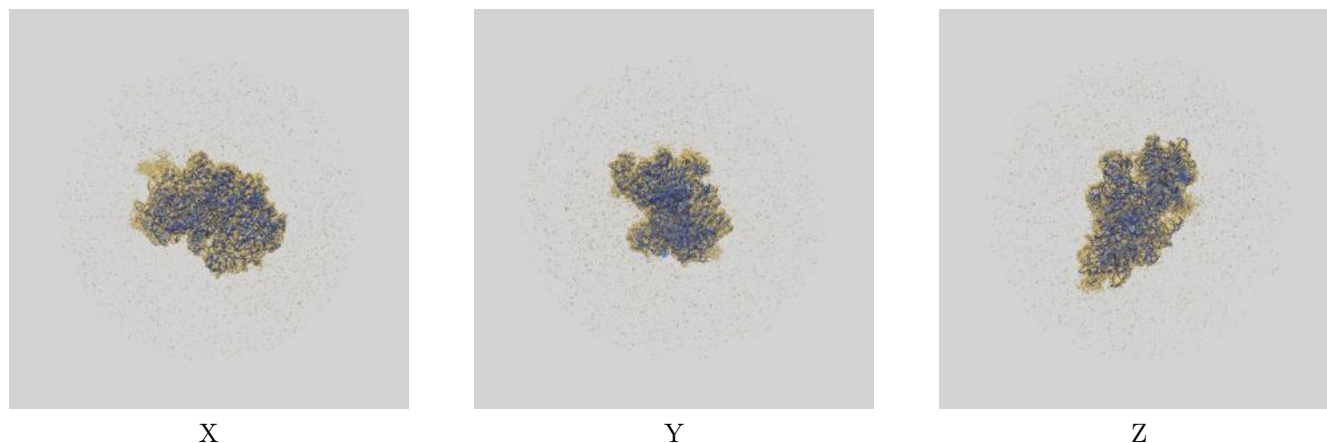
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.37	4.32	3.55
Unmasked-calculated*	6.79	11.19	7.21

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.79 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

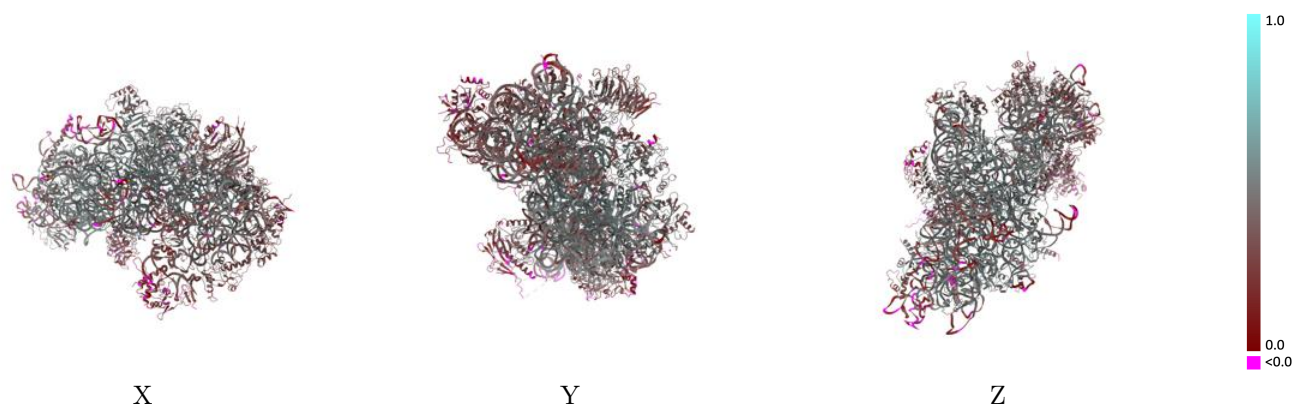
This section contains information regarding the fit between EMDB map EMD-38549 and PDB model 8XP3. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



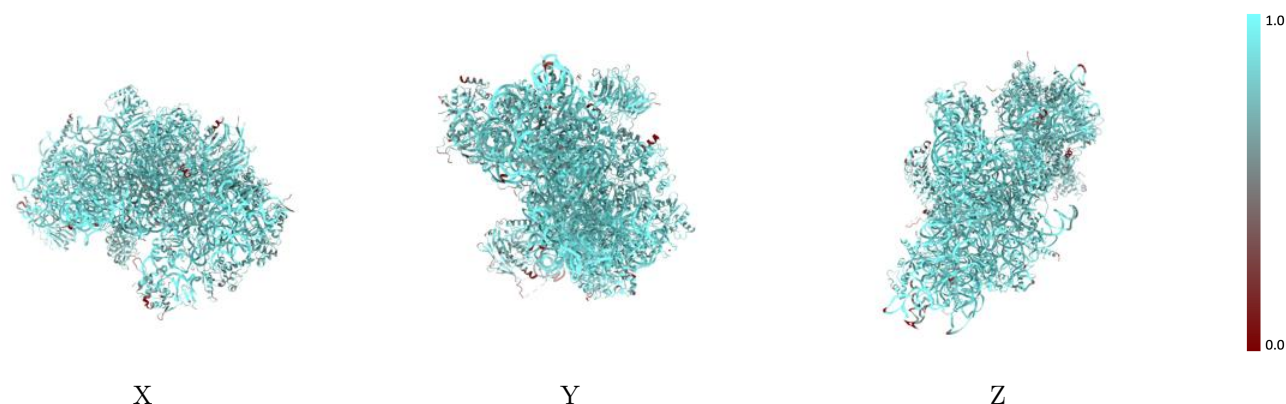
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



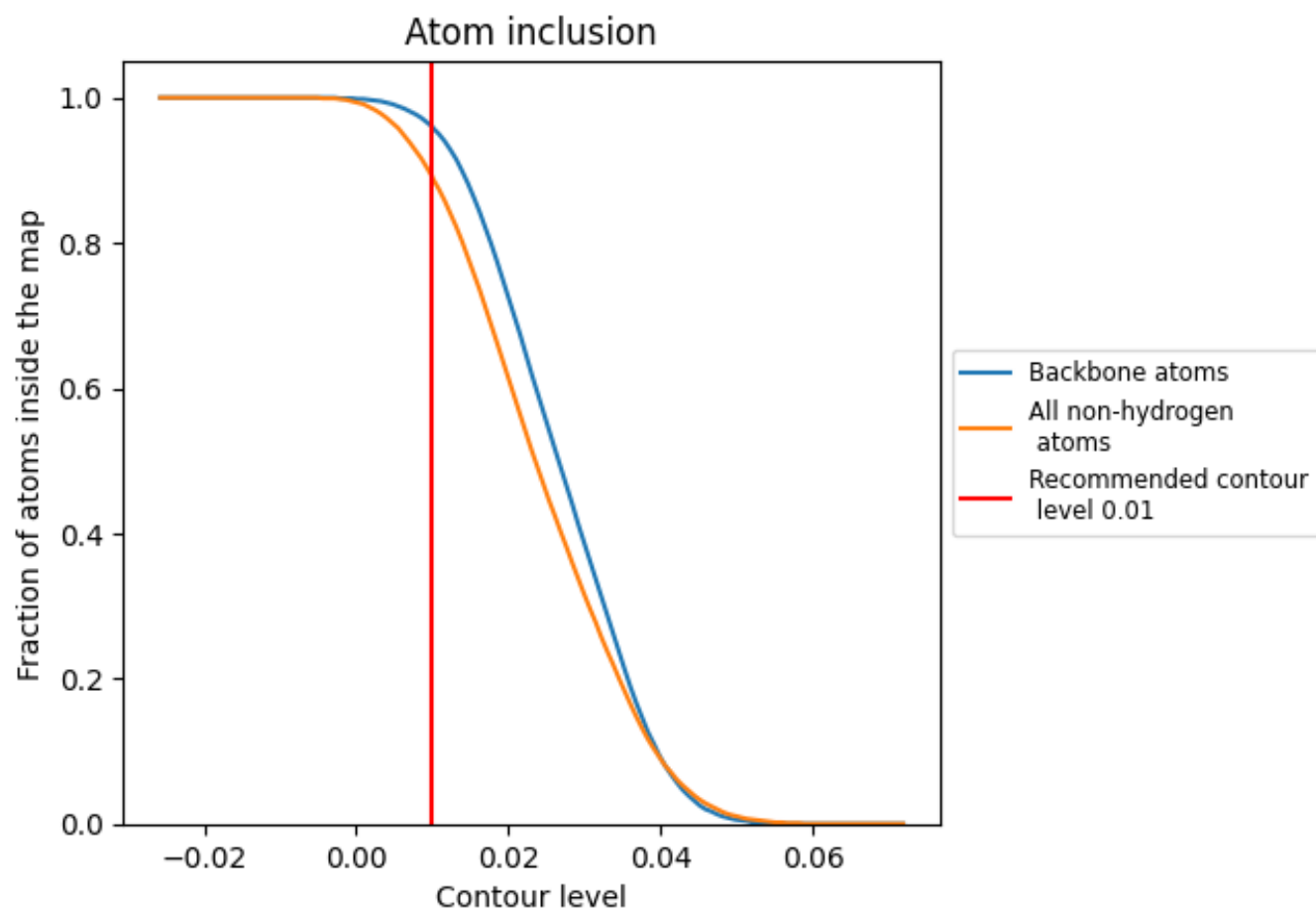
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8910	 0.4130
JC	 0.7490	 0.2460
JD	 0.4830	 0.2700
Ln	 0.6510	 0.3420
S2	 0.9600	 0.4400
SA	 0.8750	 0.4570
SB	 0.8680	 0.4400
SC	 0.8910	 0.4880
SD	 0.7890	 0.3590
SE	 0.9010	 0.4910
SF	 0.8070	 0.3640
SG	 0.8720	 0.3990
SH	 0.8500	 0.3900
SI	 0.8920	 0.4420
SJ	 0.8850	 0.4730
SK	 0.7970	 0.3010
SL	 0.8940	 0.4860
SM	 0.6630	 0.1520
SN	 0.8870	 0.4600
SO	 0.8540	 0.4270
SP	 0.7330	 0.2940
SQ	 0.8290	 0.4140
SR	 0.8260	 0.4230
SS	 0.7420	 0.3090
ST	 0.8210	 0.3730
SU	 0.7970	 0.3740
SV	 0.9070	 0.4850
SW	 0.9080	 0.5120
SX	 0.9040	 0.4930
SY	 0.8900	 0.4530
SZ	 0.7080	 0.2750
Sa	 0.8760	 0.4650
Sb	 0.8770	 0.4590
Sc	 0.7650	 0.3410
Sd	 0.8530	 0.4100



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Chain	Atom inclusion	Q-score
Se	 0.8150	 0.4040
Sf	 0.6900	 0.1820
Sg	 0.8330	 0.3370