



Full wwPDB EM Validation Report ⓘ

Jun 25, 2026 – 07:32 PM EDT

PDB ID : 8FLD / pdb_00008fld
EMDB ID : EMD-29275
Title : Human nuclear pre-60S ribosomal subunit (State L1)
Authors : Vanden Broeck, A.; Klinge, S.
Deposited on : 2022-12-21
Resolution : 2.58 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
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

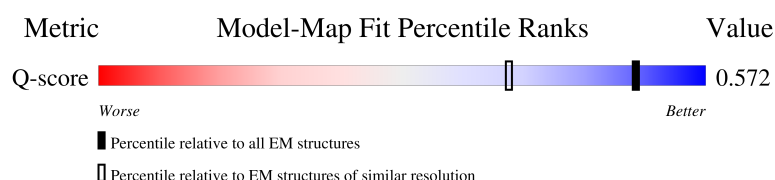
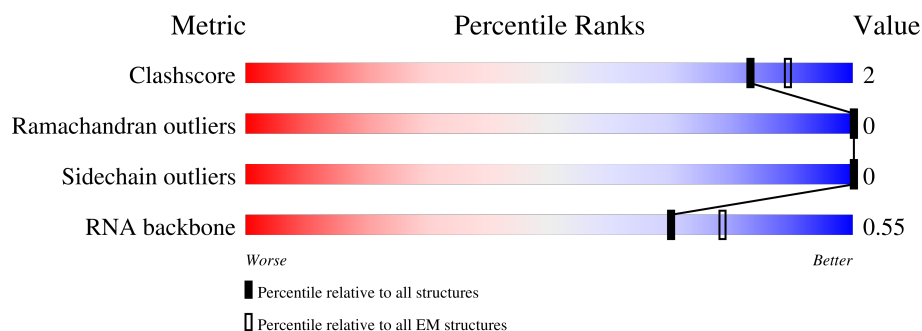
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.58 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.



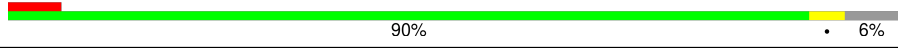
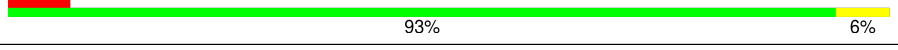
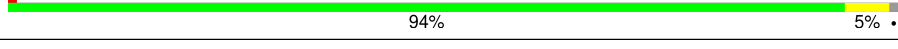
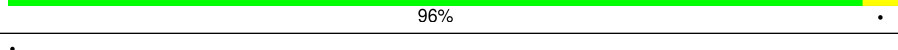
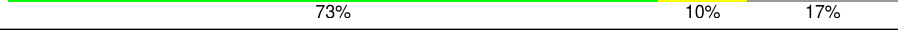
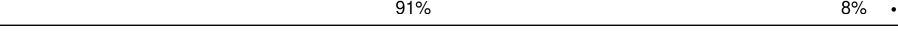
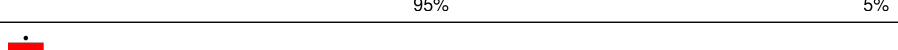
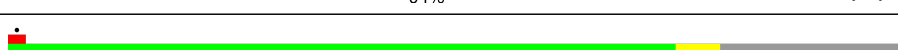
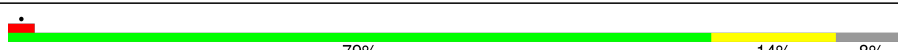
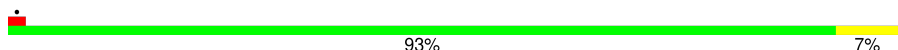
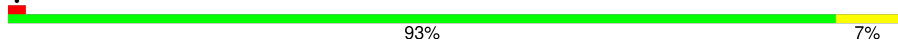
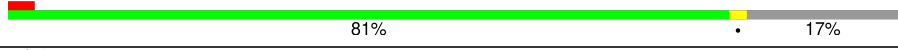
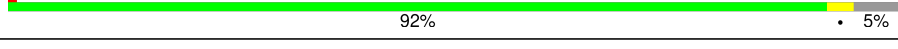
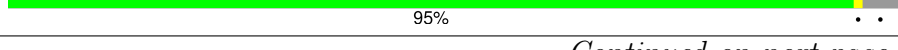
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7675 (2.08 - 3.08)

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	BE	214	
2	L1	157	
3	L2	1167	

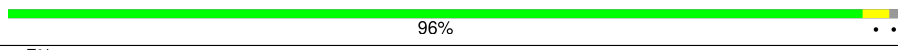
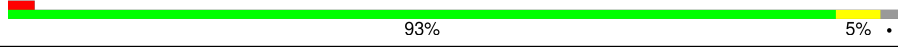
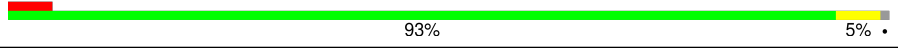
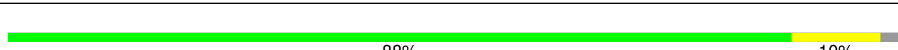
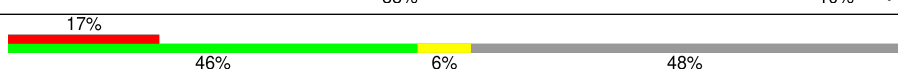
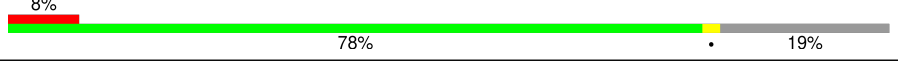
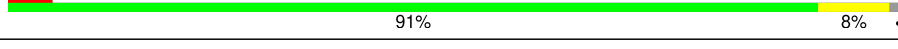
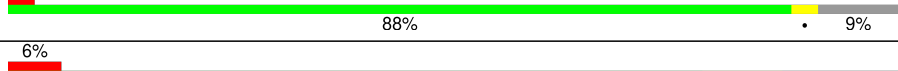
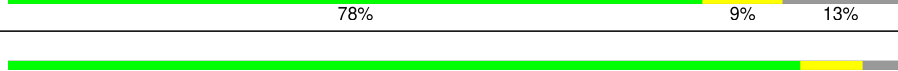
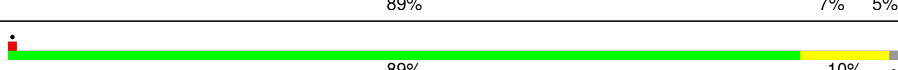
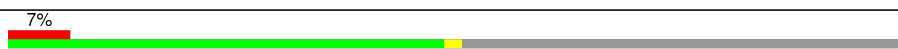
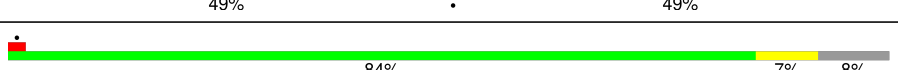
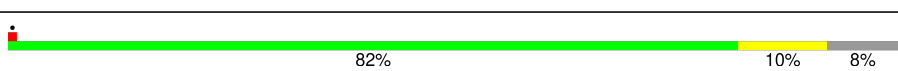
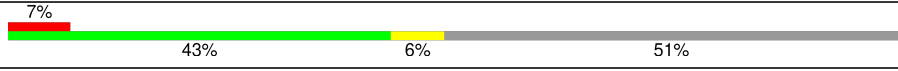
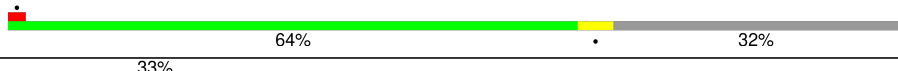
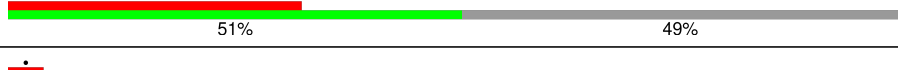
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	L3	5070	
5	L4	121	
6	L5	178	
7	L6	211	
8	L7	203	
9	L8	215	
10	L9	204	
11	LA	184	
12	LB	188	
13	LC	176	
14	LD	196	
15	LE	160	
16	LF	128	
17	LG	140	
18	LH	156	
19	LI	145	
20	LJ	136	
21	LK	148	
22	LL	137	
23	LM	159	
24	LN	403	
25	LO	115	
26	LP	125	
27	LQ	135	
28	LR	117	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	LS	123	
30	LT	110	
31	LU	105	
32	LV	106	
33	LW	97	
34	LX	92	
35	LY	70	
36	LZ	51	
37	NK	129	
38	NL	478	
39	NP	134	
40	SA	427	
41	SB	297	
42	SC	288	
43	SD	248	
44	SE	266	
45	SF	257	
46	SG	192	
47	SH	293	
48	SI	255	
49	SK	245	
50	SL	490	
51	SM	588	
52	SQ	239	
53	SR	634	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	SV	163	

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 148569 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 L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	BE	160	Total	C	N	O	S	0	0
			1295	827	242	218	8		

- Molecule 2 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L1	154	Total	C	N	O	P	0	0
			3278	1463	581	1080	154		

- Molecule 3 is a RNA chain called ITS2 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L2	72	Total	C	N	O	P	0	0
			1535	683	278	502	72		

- Molecule 4 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L3	3372	Total	C	N	O	P	0	0
			72381	32259	13258	23492	3372		

- Molecule 5 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L4	120	Total	C	N	O	P	0	0
			2561	1141	456	844	120		

- Molecule 6 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L5	168	Total	C	N	O	S	0	0
			1349	853	251	239	6		

- Molecule 7 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L6	210	Total	C	N	O	S	0	0
			1701	1064	352	281	4		

- Molecule 8 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L7	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 9 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L8	135	Total	C	N	O	S	0	0
			1111	713	213	178	7		

- Molecule 10 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L9	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 11 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LA	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 12 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LB	187	Total	C	N	O	S	0	0
			1512	944	314	249	5		

- Molecule 13 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LC	176	Total	C	N	O	S	0	0
			1461	930	284	236	11		

- Molecule 14 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LD	154	Total	C	N	O	S	0	0
			1289	805	277	198	9		

- Molecule 15 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LE	154	Total	C	N	O	S	0	0
			1264	803	246	210	5		

- Molecule 16 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LF	103	Total	C	N	O	S	0	0
			842	538	148	154	2		

- Molecule 17 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LG	139	Total	C	N	O	S	0	0
			1034	648	199	182	5		

- Molecule 18 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LH	143	Total	C	N	O	S	0	0
			1156	740	220	195	1		

- Molecule 19 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LI	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 20 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LJ	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 21 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LK	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 22 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LL	125	Total	C	N	O	S	0	0
			1002	622	207	168	5		

- Molecule 23 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LM	94	Total	C	N	O	S	0	0
			775	483	170	118	4		

- Molecule 24 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LN	402	Total	C	N	O	S	0	0
			3239	2061	608	556	14		

- Molecule 25 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LO	95	Total	C	N	O	S	0	0
			738	468	131	133	6		

- Molecule 26 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LP	106	Total	C	N	O	S	0	0
			879	555	170	152	2		

- Molecule 27 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LQ	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 28 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LR	112	Total	C	N	O	S	0	0
			888	555	183	144	6		

- Molecule 29 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LS	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 30 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LT	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 31 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LU	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 32 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LV	104	Total	C	N	O	S	0	0
			851	533	174	138	6		

- Molecule 33 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LW	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 34 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LX	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 35 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	LY	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 36 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	LZ	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 37 is a protein called Protein LLP homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	NK	67	Total	C	N	O	S	0	0
			581	363	128	88	2		

- Molecule 38 is a protein called Ribosome biogenesis protein NOP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	NL	323	Total	C	N	O	S	0	0
			2666	1658	531	475	2		

- Molecule 39 is a protein called Zinc finger protein 593.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	NP	108	Total	C	N	O	S	0	0
			876	537	182	153	4		

- Molecule 40 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	SA	358	Total	C	N	O	S	0	0
			2853	1797	570	473	13		

- Molecule 41 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	SB	292	Total	C	N	O	S	0	0
			2376	1499	433	430	14		

- Molecule 42 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	SC	217	Total	C	N	O	S	0	0
			1747	1124	332	287	4		

- Molecule 43 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	SD	225	Total	C	N	O	S	0	0
			1870	1202	358	301	9		

- Molecule 44 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	SE	231	Total	C	N	O	S	1	0
			1869	1191	361	313	4		

- Molecule 45 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	SF	245	Total	C	N	O	S	0	0
			1876	1177	383	310	6		

- Molecule 46 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	SG	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 47 is a protein called MKI67 FHA domain-interacting nucleolar phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	SH	150	Total	C	N	O	S	1	0
			1275	824	227	220	4		

- Molecule 48 is a protein called 60S ribosomal protein L7-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SI	234	Total	C	N	O	S	1	0
			1937	1254	363	316	4		

- Molecule 49 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SK	226	Total	C	N	O	S	0	0
			1721	1070	296	343	12		

- Molecule 50 is a protein called Ribosomal L1 domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SL	238	Total	C	N	O	S	0	0
			1917	1227	337	347	6		

- Molecule 51 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SM	399	Total	C	N	O	S	0	0
			3278	2120	576	571	11		

- Molecule 52 is a protein called mRNA turnover protein 4 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	SQ	123	Total	C	N	O	0	0
			610	364	123	123		

- Molecule 53 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SR	243	Total	C	N	O	S	0	0
			2002	1238	377	375	12		

- Molecule 54 is a protein called Probable ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SV	139	Total	C	N	O	S	0	0
			1184	754	229	191	10		

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
55	L1	5	Total	Mg	0
			5	5	
55	L3	72	Total	Mg	0
			72	72	
55	L4	3	Total	Mg	0
			3	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
55	LG	1	Total 1	Mg 1	0
55	LQ	1	Total 1	Mg 1	0
55	LR	1	Total 1	Mg 1	0
55	LT	1	Total 1	Mg 1	0
55	LW	1	Total 1	Mg 1	0
55	SA	1	Total 1	Mg 1	0
55	SF	1	Total 1	Mg 1	0

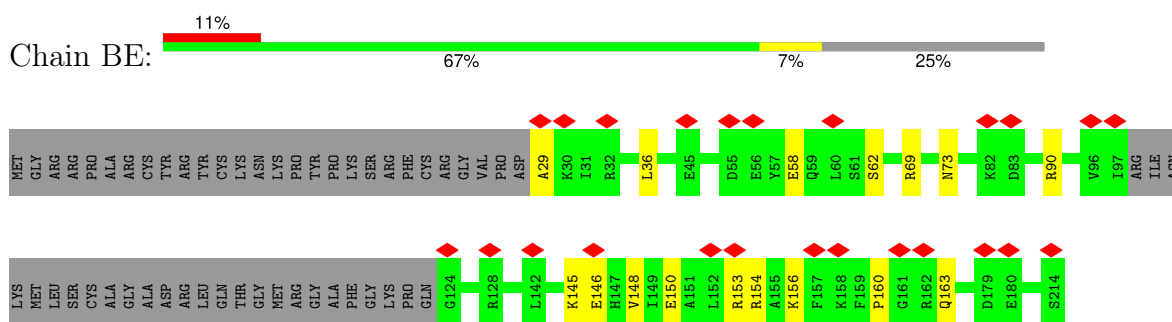
- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
56	LR	1	Total 1	Zn 1	0
56	LV	1	Total 1	Zn 1	0
56	LW	1	Total 1	Zn 1	0
56	LX	1	Total 1	Zn 1	0
56	NP	1	Total 1	Zn 1	0
56	SV	1	Total 1	Zn 1	0

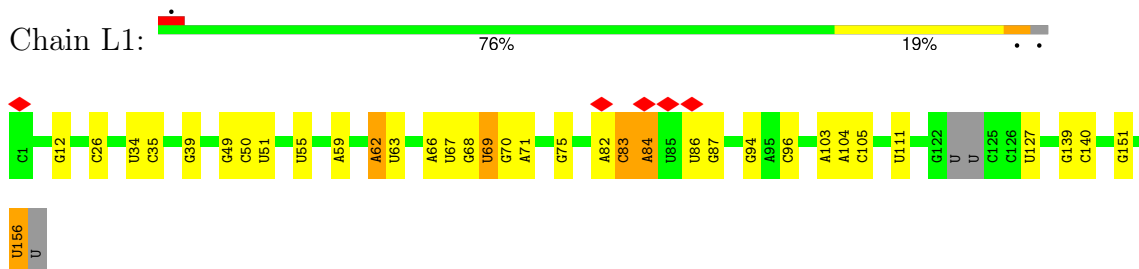
3 Residue-property plots [i](#)

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.

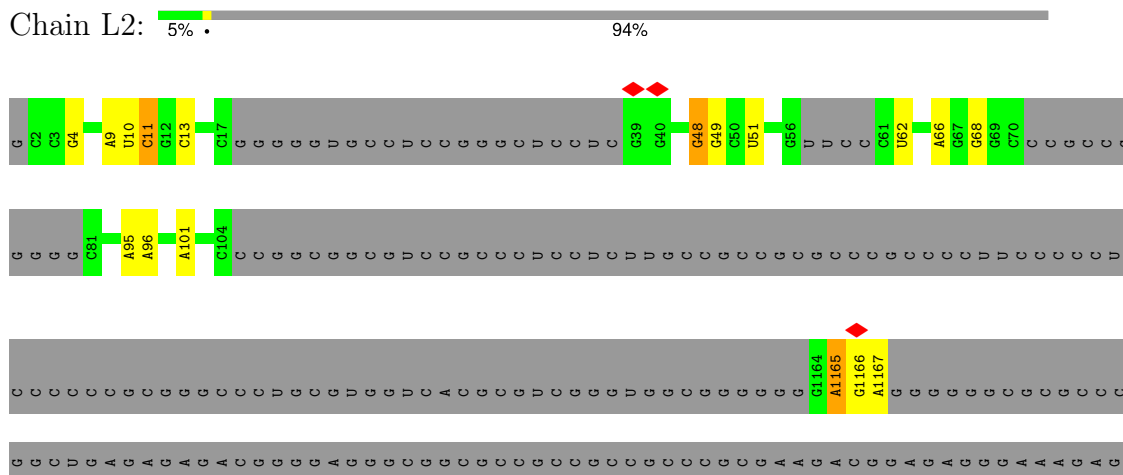
- Molecule 1: 60S ribosomal protein L10



- Molecule 2: 5.8S rRNA



- Molecule 3: ITS2 rRNA





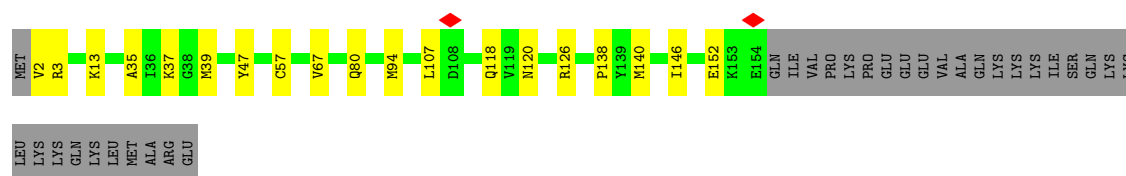






- Molecule 11: 60S ribosomal protein L17

Chain LA:  73% 10% 17%



- Molecule 12: 60S ribosomal protein L18

Chain LB:  91% 8% .



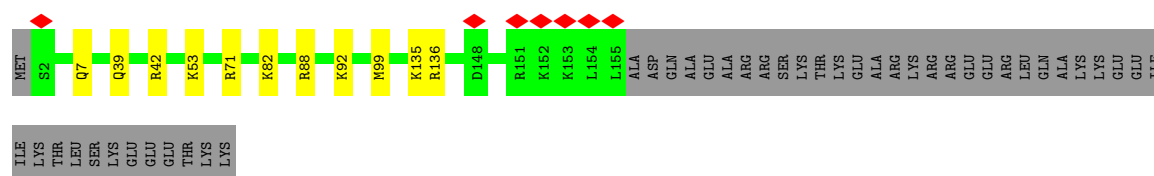
- Molecule 13: 60S ribosomal protein L18a

Chain LC:  95% 5%



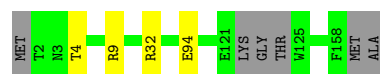
- Molecule 14: 60S ribosomal protein L19

Chain LD:  73% 6% 21%



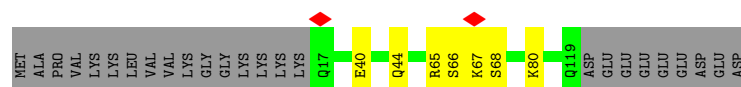
- Molecule 15: 60S ribosomal protein L21

Chain LE:  94% . .

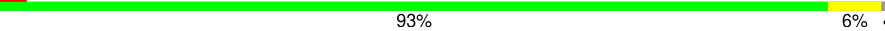


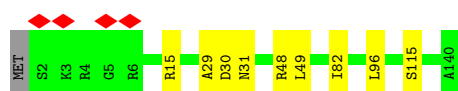
- Molecule 16: 60S ribosomal protein L22

Chain LF:  75% 5% 20%



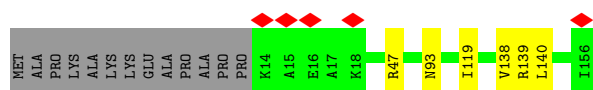
- Molecule 17: 60S ribosomal protein L23

Chain LG:  93% 6%



- Molecule 18: 60S ribosomal protein L23a

Chain LH:  88% 8%



- Molecule 19: 60S ribosomal protein L26

Chain LI:  79% 14% 8%

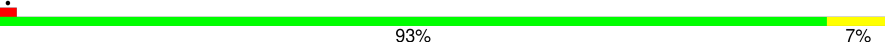


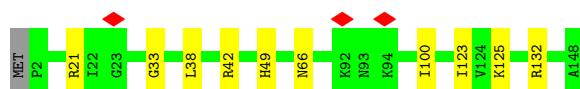
- Molecule 20: 60S ribosomal protein L27

Chain LJ:  88% 11%



- Molecule 21: 60S ribosomal protein L27a

Chain LK:  93% 7%



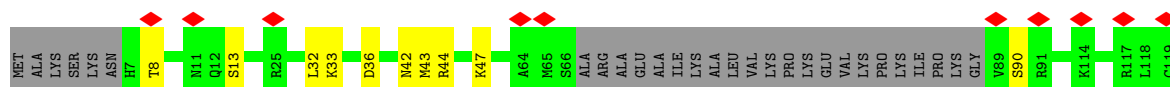
- Molecule 22: 60S ribosomal protein L28

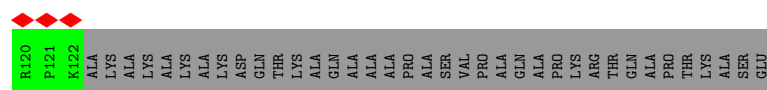
Chain LL:  84% 7% 9%



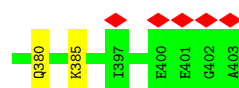
- Molecule 23: 60S ribosomal protein L29

Chain LM:  8% 53% 6% 41%

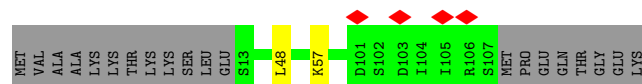
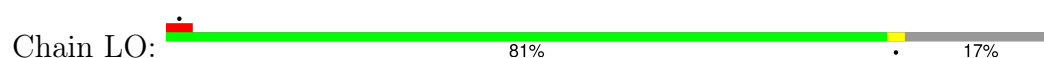




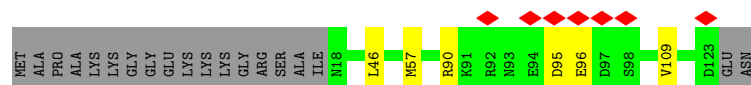
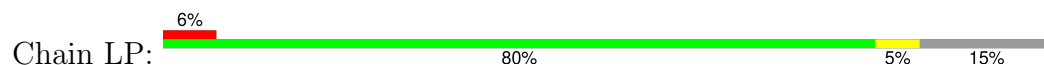
- Molecule 24: 60S ribosomal protein L3



- Molecule 25: 60S ribosomal protein L30



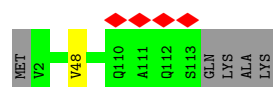
- Molecule 26: 60S ribosomal protein L31



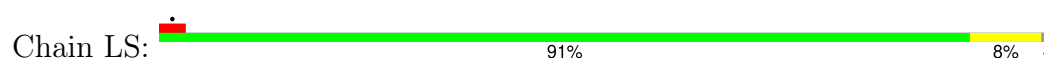
- Molecule 27: 60S ribosomal protein L32

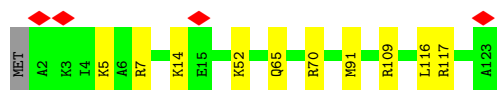


- Molecule 28: 60S ribosomal protein L34



- Molecule 29: 60S ribosomal protein L35





- Molecule 30: 60S ribosomal protein L35a

Chain LT: 96%



- Molecule 31: 60S ribosomal protein L36

Chain LU: 7% 86% 11%



- Molecule 32: 60S ribosomal protein L36a

Chain LV: 93% 5%



- Molecule 33: 60S ribosomal protein L37

Chain LW: 81% 7% 11%



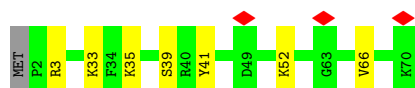
- Molecule 34: 60S ribosomal protein L37a

Chain LX: 5% 93% 5%



- Molecule 35: 60S ribosomal protein L38

Chain LY: 89% 10%

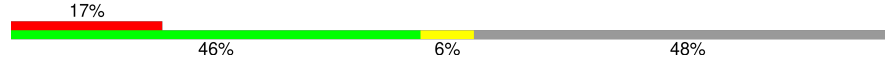


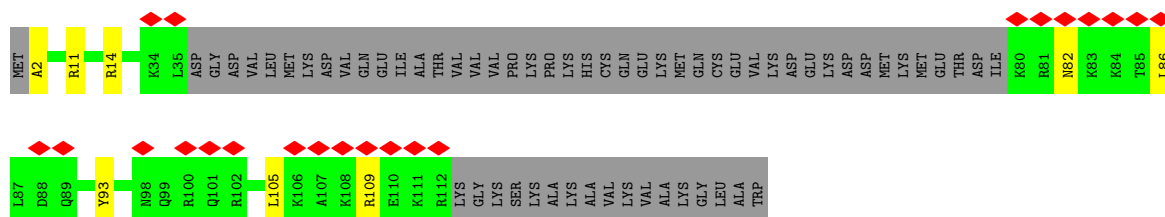
- Molecule 36: 60S ribosomal protein L39

Chain LZ:  88% 10%



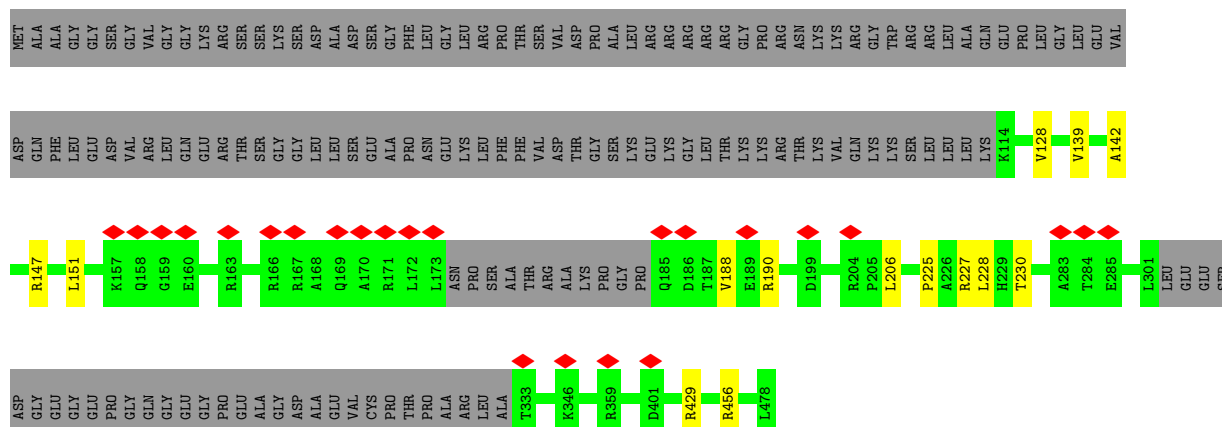
- Molecule 37: Protein LLP homolog

Chain NK:  17% 46% 6% 48%



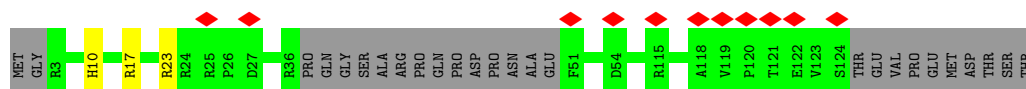
- Molecule 38: Ribosome biogenesis protein NOP53

Chain NL:  5% 65% 32%



- Molecule 39: Zinc finger protein 593

Chain NP:  8% 78% 19%

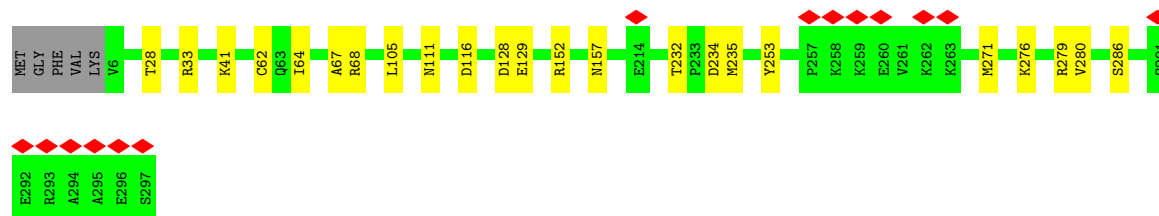


- Molecule 40: 60S ribosomal protein L4

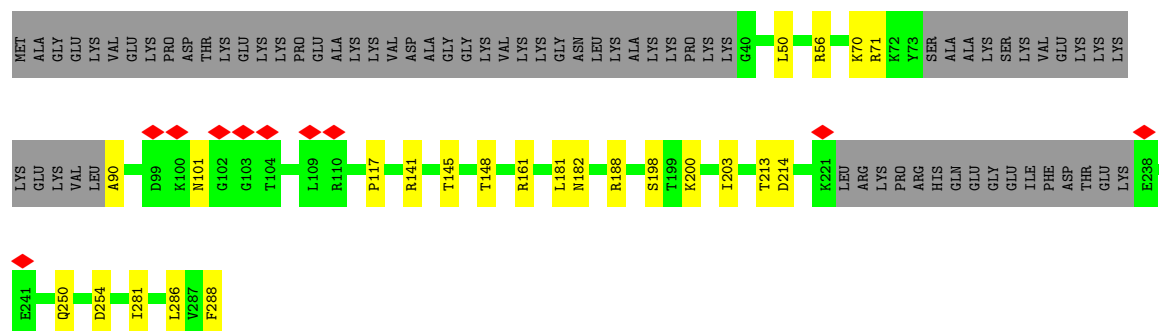
Chain SA:  77% 7% 16%



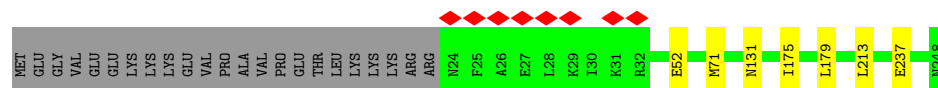
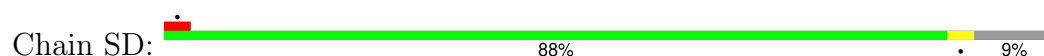
- Molecule 41: 60S ribosomal protein L5



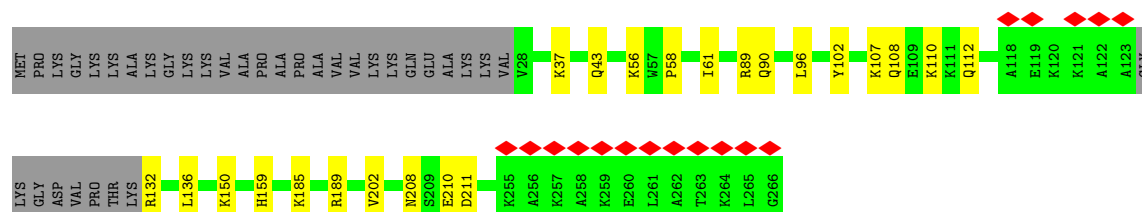
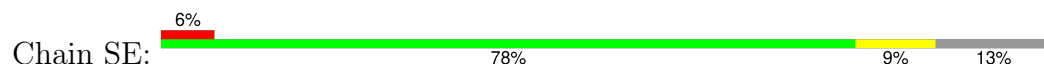
- Molecule 42: 60S ribosomal protein L6



- Molecule 43: 60S ribosomal protein L7



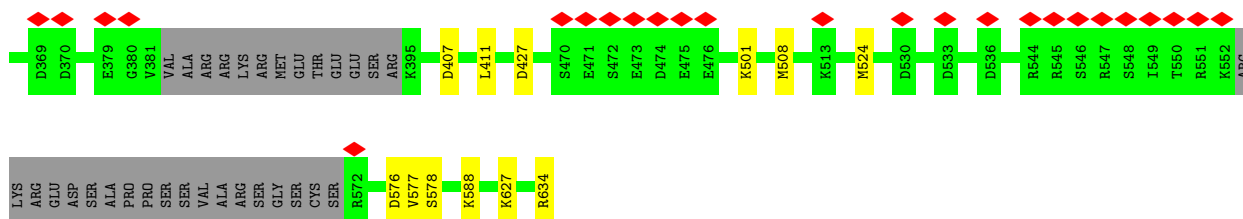
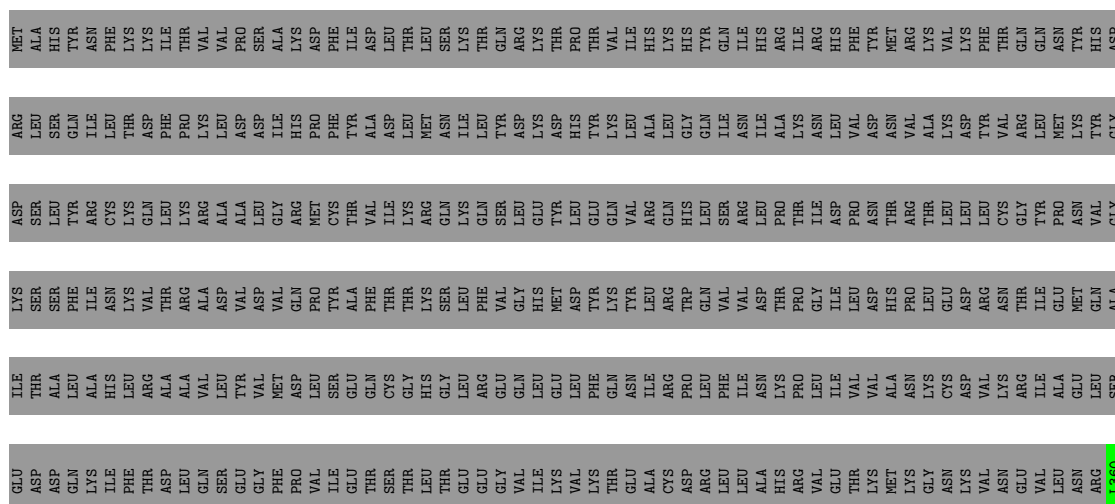
- Molecule 44: 60S ribosomal protein L7a



- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| M1 | A2 | M21 | D44 | T45 | V49 | H50 | Q79 | L88 | I94 | R95 | R96 | E99 | A103 | V107 | D112 | H118 | T125 | E126 | R139 | Q145 | S155 | N156 | P163 | T185 | L215 | E246 | ALA | GLN | PRO | SER | THR | ILE | ALA | THR | SER | MET | ARG | ASP | SER |
|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

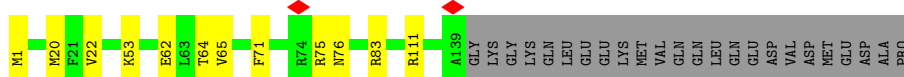
- Molecule 53: GTP-binding protein 4

Chain SR:



- Molecule 54: Probable ribosome biogenesis protein RLP24

Chain SV:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	88174	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	11.150	Depositor
Minimum map value	-0.181	Depositor
Average map value	0.047	Depositor
Map value standard deviation	0.194	Depositor
Recommended contour level	0.95	Depositor
Map size ($\text{\AA}$)	514.56, 514.56, 514.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.072, 1.072, 1.072	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UR3, HIC, 1MA, A2M, PSU, OMC, MG, 6MZ, OMU, ZN, OMG

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	BE	0.17	0/1323	0.34	0/1767
2	L1	0.40	0/3589	0.31	0/5589
3	L2	0.29	0/1709	0.33	0/2653
4	L3	0.35	1/78428 (0.0%)	0.31	1/122316 (0.0%)
5	L4	0.51	0/2861	0.36	0/4459
6	L5	0.27	0/1372	0.35	0/1836
7	L6	0.25	0/1732	0.32	0/2315
8	L7	0.32	0/1682	0.34	0/2250
9	L8	0.28	0/1133	0.31	0/1516
10	L9	0.35	0/1746	0.35	0/2338
11	LA	0.28	0/1268	0.33	0/1701
12	LB	0.35	1/1536 (0.1%)	0.38	0/2052
13	LC	0.35	0/1501	0.41	0/2013
14	LD	0.25	0/1305	0.31	0/1727
15	LE	0.37	0/1291	0.41	0/1724
16	LF	0.21	0/856	0.32	0/1149
17	LG	0.27	0/1048	0.38	0/1402
18	LH	0.28	0/1175	0.33	0/1572
19	LI	0.28	0/1132	0.38	0/1504
20	LJ	0.30	0/1130	0.31	0/1507
21	LK	0.32	0/1191	0.34	0/1591
22	LL	0.24	0/1017	0.33	0/1364
23	LM	0.26	0/788	0.35	0/1040
24	LN	0.26	0/3294	0.35	0/4406
25	LO	0.22	0/748	0.26	0/1004
26	LP	0.25	0/894	0.33	0/1204
27	LQ	0.28	0/1071	0.31	0/1429
28	LR	0.26	0/898	0.35	0/1197
29	LS	0.28	0/1023	0.32	0/1351
30	LT	0.29	0/895	0.36	0/1198
31	LU	0.24	0/843	0.32	0/1115
32	LV	0.35	0/864	0.38	0/1140

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	LW	0.32	0/720	0.48	0/952
34	LX	0.23	0/718	0.32	0/953
35	LY	0.21	0/575	0.29	0/761
36	LZ	0.31	0/454	0.36	0/599
37	NK	0.20	0/587	0.29	0/767
38	NL	0.24	0/2705	0.30	0/3624
39	NP	0.20	0/893	0.31	0/1194
40	SA	0.28	0/2907	0.34	0/3905
41	SB	0.35	0/2421	0.35	0/3241
42	SC	0.21	0/1781	0.32	0/2388
43	SD	0.30	0/1905	0.35	0/2539
44	SE	0.35	0/1903	0.41	0/2559
45	SF	0.28	0/1914	0.37	0/2567
46	SG	0.29	0/1537	0.33	0/2066
47	SH	0.27	0/1309	0.34	0/1756
48	SI	0.28	0/1980	0.34	0/2656
49	SK	0.24	0/1745	0.35	0/2374
50	SL	0.23	0/1949	0.37	0/2621
51	SM	0.33	0/3357	0.33	0/4529
52	SQ	0.09	0/608	0.27	0/845
53	SR	0.20	0/2026	0.33	0/2690
54	SV	0.30	0/1207	0.41	0/1600
All	All	0.33	2/156544 (0.0%)	0.33	1/228615 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	LB	157	GLY	C-N	-5.45	1.25	1.33
4	L3	2415	OMU	O3'-P	5.05	1.61	1.56

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	4305	G	C4'-C3'-O3'	5.70	117.95	109.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BE	1295	0	1331	11	0
2	L1	3278	0	1665	21	0
3	L2	1535	0	789	11	0
4	L3	72381	0	36675	307	0
5	L4	2561	0	1295	10	0
6	L5	1349	0	1383	5	0
7	L6	1701	0	1818	15	0
8	L7	1650	0	1794	8	0
9	L8	1111	0	1174	7	0
10	L9	1701	0	1749	7	0
11	LA	1242	0	1269	12	0
12	LB	1512	0	1628	11	0
13	LC	1461	0	1502	7	0
14	LD	1289	0	1429	11	0
15	LE	1264	0	1328	3	0
16	LF	842	0	864	5	0
17	LG	1034	0	1097	8	0
18	LH	1156	0	1268	4	0
19	LI	1115	0	1205	15	0
20	LJ	1107	0	1182	8	0
21	LK	1162	0	1213	10	0
22	LL	1002	0	1068	8	0
23	LM	775	0	841	11	0
24	LN	3239	0	3377	23	0
25	LO	738	0	774	1	0
26	LP	879	0	924	4	0
27	LQ	1053	0	1147	4	0
28	LR	888	0	977	1	0
29	LS	1015	0	1148	10	0
30	LT	876	0	912	3	0
31	LU	832	0	917	10	0
32	LV	851	0	920	5	0
33	LW	705	0	737	6	0
34	LX	708	0	756	6	0
35	LY	569	0	637	6	0
36	LZ	444	0	483	4	0
37	NK	581	0	656	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	NL	2666	0	2774	11	0
39	NP	876	0	881	3	0
40	SA	2853	0	3028	26	0
41	SB	2376	0	2403	16	0
42	SC	1747	0	1897	17	0
43	SD	1870	0	1996	6	0
44	SE	1869	0	2014	19	0
45	SF	1876	0	1970	14	0
46	SG	1518	0	1601	12	0
47	SH	1275	0	1304	4	0
48	SI	1937	0	2070	14	0
49	SK	1721	0	1695	14	0
50	SL	1917	0	2018	18	0
51	SM	3278	0	3332	16	0
52	SQ	610	0	257	1	0
53	SR	2002	0	2072	12	0
54	SV	1184	0	1248	10	0
55	L1	5	0	0	0	0
55	L3	72	0	0	0	0
55	L4	3	0	0	0	0
55	LG	1	0	0	0	0
55	LQ	1	0	0	0	0
55	LR	1	0	0	0	0
55	LT	1	0	0	0	0
55	LW	1	0	0	0	0
55	SA	1	0	0	0	0
55	SF	1	0	0	0	0
56	LR	1	0	0	0	0
56	LV	1	0	0	0	0
56	LW	1	0	0	0	0
56	LX	1	0	0	0	0
56	NP	1	0	0	0	0
56	SV	1	0	0	0	0
All	All	148569	0	112492	613	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 2.

All (613) 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:L1:51:U:OP2	36:LZ:21:ARG:NH2	2.06	0.88
5:L4:40:U:O2	6:L5:75:ARG:NH1	2.06	0.88
4:L3:2520:C:O2	4:L3:2640:G:N2	2.08	0.84
4:L3:2898:G:OP2	14:LD:135:LYS:NZ	2.11	0.83
32:LV:23:VAL:HG12	32:LV:70:LEU:HD23	1.59	0.83
4:L3:2470:C:O2'	44:SE:56:LYS:NZ	2.13	0.82
4:L3:1176:C:O3'	41:SB:279:ARG:NH1	2.12	0.82
5:L4:72:U:O2	5:L4:103:A:N6	2.13	0.82
38:NL:429:ARG:NH1	48:SI:183:GLU:OE2	2.12	0.81
44:SE:96:LEU:HD11	44:SE:189:ARG:HE	1.43	0.81
4:L3:309:C:OP2	31:LU:32:ARG:NH1	2.14	0.81
4:L3:4156:G:OP2	4:L3:4157:A:O2'	1.99	0.80
4:L3:1480:C:O2'	4:L3:1482:G:OP2	2.00	0.80
4:L3:155:C:OP1	29:LS:109:ARG:NH2	2.15	0.80
2:L1:75:OMG:OP2	19:LI:74:TYR:OH	2.00	0.79
4:L3:690:C:OP1	22:LL:87:ARG:NH1	2.15	0.79
5:L4:55:A:O2'	6:L5:151:ILE:O	2.00	0.79
4:L3:3867:A2M:H8	4:L3:3867:A2M:H5''	1.63	0.78
4:L3:3605:C:OP2	14:LD:71:ARG:NH1	2.16	0.77
4:L3:2318:G:N2	4:L3:2321:G:OP2	2.16	0.77
44:SE:108:GLN:O	44:SE:112:GLN:NE2	2.18	0.77
3:L2:1167:A:O3'	4:L3:1:C:OP2	2.03	0.76
4:L3:981:C:OP2	42:SC:71:ARG:NH2	2.19	0.76
4:L3:1693:U:OP2	12:LB:49:LYS:NZ	2.18	0.76
4:L3:1214:C:N4	23:LM:90:SER:O	2.18	0.76
4:L3:404:U:O3'	19:LI:87:ARG:NH2	2.18	0.76
4:L3:4299:PSU:OP1	23:LM:33:LYS:NZ	2.18	0.76
4:L3:508:G:O2'	4:L3:510:U:OP2	2.04	0.76
12:LB:64:SER:OG	12:LB:89:ASP:OD2	2.04	0.75
40:SA:297:GLU:OE1	40:SA:300:ARG:NH2	2.19	0.75
4:L3:695:G:O2'	4:L3:697:G:OP2	2.03	0.75
20:LJ:21:ARG:NH1	20:LJ:47:ASP:OD1	2.20	0.75
29:LS:14:LYS:NZ	29:LS:65:GLN:OE1	2.20	0.75
4:L3:1646:A:OP2	40:SA:80:ARG:NH1	2.19	0.75
12:LB:128:LEU:HD23	40:SA:298:ILE:HD11	1.69	0.74
4:L3:119:G:O4'	44:SE:132:ARG:NH1	2.20	0.74
4:L3:194:C:O2'	19:LI:121:ARG:NH1	2.20	0.74
4:L3:2601:A:N6	4:L3:2744:A:OP2	2.21	0.74
16:LF:40:GLU:OE1	16:LF:65:ARG:NH1	2.21	0.74
4:L3:1562:G:N2	4:L3:1565:A:OP2	2.21	0.72
4:L3:2773:G:OP1	35:LY:39:SER:OG	2.06	0.72
4:L3:2407:G:O6	36:LZ:2:SER:N	2.23	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L5:84:GLU:OE2	6:L5:92:TYR:OH	2.03	0.72
4:L3:408:A:O2'	4:L3:411:G:OP2	2.06	0.72
50:SL:204:ASN:O	50:SL:212:SER:OG	2.08	0.72
8:L7:182:GLU:OE2	9:L8:119:ARG:NH2	2.23	0.71
4:L3:1364:U:O2	40:SA:234:LYS:NZ	2.22	0.71
40:SA:13:GLU:N	40:SA:155:GLU:OE2	2.22	0.71
51:SM:265:TYR:OH	51:SM:358:LYS:O	2.07	0.71
2:L1:66:A:OP1	29:LS:7:ARG:NE	2.23	0.71
4:L3:4765:G:OP1	46:SG:23:ARG:NE	2.22	0.71
11:LA:47:TYR:OH	11:LA:57:CYS:O	2.06	0.71
4:L3:4124:G:N2	44:SE:43:GLN:O	2.23	0.71
2:L1:156:U:OP2	44:SE:89:ARG:NH2	2.24	0.71
4:L3:1364:U:OP2	7:L6:36:ARG:NH2	2.24	0.70
19:LI:50:ARG:NH1	19:LI:112:ASP:OD1	2.24	0.70
24:LN:223:THR:HG22	24:LN:338:VAL:HG23	1.74	0.69
38:NL:139:VAL:HG13	38:NL:142:ALA:HB2	1.75	0.69
4:L3:2922:G:O2'	4:L3:3275:A:N6	2.25	0.69
4:L3:684:G:O2'	42:SC:101:ASN:ND2	2.25	0.69
50:SL:77:GLU:OE2	50:SL:79:ARG:NH2	2.25	0.69
4:L3:1744:PSU:H2'	4:L3:1745:G:H8	1.57	0.69
4:L3:5002:U:OP2	24:LN:385:LYS:NZ	2.24	0.69
44:SE:96:LEU:HD11	44:SE:189:ARG:NE	2.08	0.69
4:L3:3938:G:N2	4:L3:4171:C:OP2	2.26	0.69
13:LC:84:TYR:HE1	13:LC:93:MET:HE3	1.56	0.69
51:SM:33:ASP:OD1	51:SM:36:ARG:NH2	2.26	0.68
4:L3:1071:C:O2	42:SC:70:LYS:NZ	2.23	0.68
4:L3:2626:U:OP2	53:SR:501:LYS:NZ	2.26	0.68
4:L3:2475:G:O6	18:LH:47:ARG:NH1	2.27	0.68
4:L3:1378:C:O2	7:L6:158:ARG:NH1	2.27	0.68
4:L3:1433:A:N6	4:L3:1451:G:O2'	2.27	0.68
1:BE:29:ALA:N	1:BE:62:SER:HG	1.92	0.68
4:L3:3700:C:O2'	4:L3:3774:A:N3	2.26	0.68
7:L6:164:GLU:OE1	21:LK:125:LYS:NZ	2.21	0.68
49:SK:96:ARG:O	54:SV:76:ASN:ND2	2.27	0.68
4:L3:4927:G:OP2	4:L3:4927:G:N2	2.20	0.68
4:L3:1724:G:N2	23:LM:13:SER:O	2.24	0.67
14:LD:39:GLN:OE1	14:LD:42:ARG:NH1	2.27	0.67
20:LJ:9:LYS:NZ	20:LJ:83:THR:O	2.22	0.67
4:L3:4678:G:OP2	37:NK:14:ARG:NH1	2.27	0.67
4:L3:1255:A:OP1	4:L3:1257:A:N6	2.28	0.67
4:L3:4626:A:OP2	24:LN:224:LYS:NZ	2.24	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:NL:456:ARG:NH2	51:SM:213:THR:O	2.28	0.67
5:L4:23:A:N3	5:L4:118:C:O2'	2.27	0.67
17:LG:96:LEU:HD11	54:SV:22:VAL:HG23	1.75	0.67
4:L3:4500:PSU:H2'	4:L3:4501:U:C6	2.31	0.66
11:LA:2:VAL:HG23	11:LA:3:ARG:H	1.61	0.66
4:L3:3776:G:OP2	4:L3:3776:G:N2	2.24	0.66
4:L3:2262:G:OP2	22:LL:98:ARG:NH1	2.29	0.66
38:NL:227:ARG:O	38:NL:230:THR:HG22	1.96	0.66
4:L3:2263:A:OP1	22:LL:107:ARG:NH2	2.29	0.66
4:L3:1325:C:H2'	4:L3:1326:A2M:H5'	1.77	0.66
4:L3:2841:G:OP1	39:NP:10:HIS:NE2	2.25	0.66
4:L3:1317:U:OP1	21:LK:21:ARG:NH2	2.29	0.65
4:L3:1961:G:HO2'	4:L3:2024:G:H1	1.43	0.65
4:L3:502:C:O2'	4:L3:503:C:OP1	2.09	0.65
44:SE:90:GLN:NE2	48:SI:62:GLU:OE2	2.29	0.65
4:L3:1734:G:N2	4:L3:1735:U:O4	2.25	0.65
4:L3:935:A:O2'	9:L8:46:ARG:NH1	2.30	0.65
4:L3:4678:G:N7	37:NK:11:ARG:NH2	2.44	0.65
4:L3:4476:C:O2'	46:SG:173:ARG:NH2	2.30	0.64
46:SG:129:ARG:NH1	46:SG:156:ASN:OD1	2.30	0.64
4:L3:2258:C:N3	42:SC:90:ALA:N	2.46	0.64
4:L3:197:A:N3	4:L3:222:C:O2'	2.31	0.63
4:L3:1280:C:O2'	40:SA:321:ASN:OD1	2.13	0.63
51:SM:357:ASP:OD2	51:SM:359:SER:OG	2.16	0.63
2:L1:87:G:OP2	29:LS:5:LYS:NZ	2.32	0.63
4:L3:2448:G:O2'	45:SF:21:LYS:NZ	2.29	0.63
4:L3:1646:A:O2'	33:LW:49:TRP:O	2.15	0.63
4:L3:4928:C:O4'	9:L8:121:ARG:NH1	2.30	0.63
4:L3:1744:PSU:H2'	4:L3:1745:G:C8	2.33	0.63
4:L3:2438:A:O2'	4:L3:2440:U:OP2	2.11	0.63
24:LN:160:ILE:HD11	24:LN:190:VAL:HG13	1.81	0.63
20:LJ:22:LYS:NZ	20:LJ:132:GLN:O	2.27	0.62
42:SC:281:ILE:CG2	42:SC:286:LEU:HD11	2.29	0.62
4:L3:375:G:OP2	33:LW:52:LYS:NZ	2.28	0.62
4:L3:407:A:O2'	4:L3:410:A:OP1	2.14	0.62
48:SI:101:ARG:NH1	48:SI:122:LYS:O	2.32	0.62
4:L3:1508:A:OP1	40:SA:110:ARG:NH2	2.33	0.62
24:LN:110:ILE:O	24:LN:115:LYS:NZ	2.33	0.62
4:L3:4717:A:OP2	24:LN:30:LYS:NZ	2.32	0.62
4:L3:2545:U:O2'	4:L3:2547:G:N7	2.32	0.62
44:SE:136:LEU:HD22	44:SE:202:VAL:CG1	2.30	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:SL:82:LEU:HD12	50:SL:203:LEU:HD11	1.81	0.62
4:L3:1398:A:OP2	4:L3:1420:A:N6	2.33	0.61
50:SL:191:SER:O	50:SL:195:ASN:ND2	2.33	0.61
4:L3:1326:A2M:H2'	4:L3:1327:C:C6	2.35	0.61
12:LB:88:ASP:OD1	12:LB:89:ASP:N	2.32	0.61
4:L3:2848:G:O2'	4:L3:3838:U:O4	2.09	0.61
4:L3:4117:U:O4'	44:SE:43:GLN:NE2	2.33	0.61
24:LN:219:VAL:HG11	24:LN:337:VAL:CG2	2.31	0.61
4:L3:2923:A:O2'	35:LY:52:LYS:NZ	2.34	0.61
4:L3:3838:U:OP2	39:NP:23:ARG:NH2	2.33	0.61
2:L1:84:A:N6	19:LI:114:ASP:OD2	2.34	0.61
7:L6:62:PRO:O	7:L6:63:THR:OG1	2.13	0.61
7:L6:129:ARG:NH1	29:LS:116:LEU:O	2.34	0.61
4:L3:1493:G:OP1	23:LM:44:ARG:NH2	2.33	0.61
4:L3:3715:PSU:H2'	4:L3:3716:C:O4'	2.00	0.61
42:SC:161:ARG:O	42:SC:182:ASN:ND2	2.33	0.61
1:BE:160:PRO:O	1:BE:163:GLN:NE2	2.34	0.60
4:L3:1326:A2M:H2'	4:L3:1327:C:H6	1.66	0.60
4:L3:1743:A:O2'	4:L3:1744:PSU:H5''	2.00	0.60
23:LM:32:LEU:HD13	23:LM:43:MET:HE1	1.84	0.60
19:LI:34:LEU:HD22	19:LI:44:VAL:HG23	1.82	0.60
2:L1:71:A:OP2	2:L1:83:C:N4	2.35	0.60
2:L1:96:C:OP1	29:LS:70:ARG:NH1	2.33	0.60
4:L3:3718:A2M:H2	4:L3:3934:G:O4'	2.01	0.60
30:LT:40:GLU:OE1	30:LT:40:GLU:N	2.35	0.60
38:NL:128:VAL:O	44:SE:150:LYS:NZ	2.31	0.59
4:L3:1468:C:H5''	21:LK:132:ARG:HH12	1.66	0.59
4:L3:4314:C:O2'	23:LM:36:ASP:OD1	2.18	0.59
2:L1:67:U:OP2	29:LS:7:ARG:NH2	2.34	0.59
4:L3:2326:G:OP1	27:LQ:108:ARG:NH2	2.34	0.59
4:L3:369:G:N2	4:L3:372:A:OP2	2.31	0.59
4:L3:1629:G:N1	45:SF:208:GLU:OE1	2.33	0.59
4:L3:4536:OMC:HM22	4:L3:4537:C:O4'	2.02	0.59
34:LX:26:VAL:HG21	45:SF:180:LEU:HD11	1.84	0.59
4:L3:2480:G:OP1	51:SM:22:LYS:NZ	2.36	0.59
4:L3:4633:G:O2'	4:L3:4635:A:OP2	2.15	0.58
8:L7:190:ASP:OD1	8:L7:191:LYS:N	2.37	0.58
23:LM:32:LEU:CD1	23:LM:43:MET:HE1	2.33	0.58
3:L2:95:A:N6	50:SL:140:LYS:O	2.34	0.58
16:LF:40:GLU:OE2	16:LF:44:GLN:NE2	2.37	0.58
9:L8:104:MET:HE3	9:L8:109:ARG:HG2	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:LI:51:LYS:NZ	19:LI:71:VAL:O	2.36	0.58
50:SL:89:ARG:NH2	50:SL:198:ILE:O	2.37	0.58
4:L3:453:G:H1	4:L3:1293:G:H22	1.51	0.58
4:L3:4637:OMG:H2'	4:L3:4638:U:C6	2.39	0.57
7:L6:63:THR:HG21	21:LK:66:ASN:HB3	1.86	0.57
24:LN:219:VAL:HG11	24:LN:337:VAL:HG21	1.87	0.57
46:SG:128:MET:HA	46:SG:128:MET:HE2	1.86	0.57
4:L3:496:G:O2'	4:L3:497:G:OP1	2.22	0.57
2:L1:69:PSU:H2'	2:L1:70:G:O4'	2.04	0.57
48:SI:105:ILE:HD13	48:SI:116:ILE:HD13	1.87	0.57
4:L3:2588:C:OP1	4:L3:2768:C:O2'	2.20	0.57
33:LW:15:THR:HG23	33:LW:16:HIS:ND1	2.19	0.57
49:SK:103:ALA:O	49:SK:107:VAL:HG23	2.04	0.57
4:L3:2351:OMC:HM23	40:SA:95:MET:HG3	1.86	0.57
4:L3:3827:G:O2'	4:L3:3829:G:OP2	2.21	0.57
4:L3:3725:G:O6	31:LU:71:LYS:NZ	2.36	0.56
4:L3:4524:G:C2	24:LN:252:ALA:HB1	2.40	0.56
5:L4:117:G:OP1	41:SB:253:TYR:OH	2.17	0.56
4:L3:151:G:OP1	10:L9:49:ARG:NH2	2.39	0.56
4:L3:4934:A:O2'	4:L3:4935:C:OP2	2.16	0.56
40:SA:156:ASP:OD2	40:SA:255:SER:OG	2.21	0.56
48:SI:237:MET:HE1	48:SI:254:LEU:HD21	1.87	0.56
4:L3:397:G:H2'	4:L3:398:A2M:H5'	1.87	0.56
10:L9:115:VAL:HG22	10:L9:134:LEU:CD2	2.36	0.56
42:SC:250:GLN:NE2	42:SC:254:ASP:OD2	2.36	0.56
3:L2:66:A:OP2	47:SH:168:LYS:NZ	2.36	0.55
4:L3:2536:A:O2'	4:L3:2641:A:N1	2.33	0.55
12:LB:154:LYS:NZ	12:LB:159:PRO:O	2.39	0.55
4:L3:4517:A:OP2	24:LN:2:SER:OG	2.25	0.55
24:LN:371:THR:HG23	24:LN:380:GLN:NE2	2.22	0.55
38:NL:190:ARG:NH2	51:SM:117:ASP:OD1	2.39	0.55
4:L3:131:C:N4	4:L3:138:G:O6	2.40	0.55
4:L3:2299:G:OP1	40:SA:182:LYS:NZ	2.35	0.55
4:L3:4664:A:OP1	24:LN:376:HIS:NE2	2.36	0.55
17:LG:96:LEU:HD11	54:SV:22:VAL:CG2	2.37	0.55
26:LP:95:ASP:OD1	26:LP:96:GLU:N	2.39	0.55
35:LY:3:ARG:NH2	35:LY:41:TYR:OH	2.39	0.55
2:L1:50:C:O2'	53:SR:578:SER:OG	2.25	0.55
3:L2:68:G:OP2	47:SH:164:ARG:NH2	2.40	0.55
4:L3:2590:G:O2'	4:L3:2755:A:N6	2.36	0.54
4:L3:4590:A2M:HM'2	4:L3:4591:U:H5'	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L3:1534:A2M:HM'3	4:L3:1637:A:C4	2.42	0.54
4:L3:4580:U:O2'	24:LN:182:GLU:OE2	2.08	0.54
4:L3:1515:A:OP1	21:LK:33:GLY:N	2.40	0.54
4:L3:1874:A:O2'	4:L3:4219:A:N3	2.34	0.54
13:LC:84:TYR:CE1	13:LC:93:MET:HE3	2.39	0.54
46:SG:87:GLY:O	46:SG:186:THR:OG1	2.19	0.54
1:BE:153:ARG:O	1:BE:156:LYS:HG2	2.08	0.54
4:L3:1741:G:H3'	4:L3:1742:A:H5'	1.90	0.54
24:LN:69:LYS:NZ	53:SR:411:LEU:O	2.38	0.54
31:LU:66:ASP:O	31:LU:87:ARG:NH1	2.40	0.54
45:SF:36:GLU:OE1	45:SF:163:ARG:NH1	2.39	0.54
53:SR:524:MET:HE2	53:SR:524:MET:HA	1.89	0.54
8:L7:189:ILE:HD11	9:L8:119:ARG:HG2	1.90	0.54
20:LJ:68:ILE:O	20:LJ:115:LYS:NZ	2.38	0.54
46:SG:41:ILE:HD12	46:SG:73:ILE:HD11	1.89	0.54
38:NL:225:PRO:HD2	38:NL:228:LEU:HD12	1.89	0.53
46:SG:41:ILE:CD1	46:SG:73:ILE:HD11	2.39	0.53
4:L3:4088:C:OP1	45:SF:37:ARG:NH2	2.41	0.53
4:L3:1621:A:OP2	33:LW:30:GLN:NE2	2.42	0.53
4:L3:2483:G:O2'	4:L3:2485:U:OP2	2.25	0.53
41:SB:234:ASP:OD1	41:SB:235:MET:N	2.42	0.53
4:L3:399:G:O2'	4:L3:400:A2M:H5'	2.08	0.53
4:L3:1438:U:O2'	4:L3:1439:C:OP1	2.23	0.53
4:L3:1238:A:O2'	43:SD:52:GLU:OE2	2.26	0.53
4:L3:4724:A:O2'	24:LN:104:THR:HG22	2.09	0.53
22:LL:23:GLN:CD	22:LL:25:TYR:HH	2.12	0.53
4:L3:2815:A2M:H2'	4:L3:2816:G:C8	2.44	0.53
4:L3:3867:A2M:H8	4:L3:3867:A2M:C5'	2.36	0.53
4:L3:2860:C:OP1	39:NP:17:ARG:NH2	2.42	0.53
4:L3:4529:G:O2'	4:L3:4530:UR3:H5'	2.08	0.53
5:L4:12:U:O3'	5:L4:109:U:O2'	2.24	0.53
34:LX:69:TRP:NE1	45:SF:173:GLY:O	2.41	0.53
4:L3:4989:U:OP1	4:L3:4991:U:O2'	2.27	0.53
42:SC:198:SER:N	42:SC:288:PHE:O	2.41	0.52
50:SL:80:VAL:HG13	50:SL:203:LEU:HD12	1.91	0.52
4:L3:52:G:OP2	33:LW:48:ASN:ND2	2.42	0.52
4:L3:1088:C:O2'	43:SD:71:MET:HE1	2.09	0.52
4:L3:2835:A:O2'	24:LN:228:TYR:O	2.28	0.52
5:L4:7:G:OP1	41:SB:33:ARG:NH1	2.43	0.52
18:LH:93:ASN:O	18:LH:139:ARG:NH1	2.42	0.52
4:L3:4322:G:N2	4:L3:4325:A:OP2	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LJ:30:ASP:O	20:LJ:39:SER:OG	2.17	0.52
1:BE:58:GLU:N	1:BE:58:GLU:OE1	2.43	0.52
4:L3:308:G:OP2	4:L3:308:G:N2	2.28	0.52
4:L3:412:G:O6	53:SR:588:LYS:NZ	2.29	0.52
30:LT:110:ILE:O	42:SC:141:ARG:NH2	2.42	0.52
36:LZ:23:ILE:HD12	36:LZ:27:ILE:HD11	1.92	0.52
4:L3:2695:A:OP1	35:LY:35:LYS:NZ	2.43	0.52
32:LV:23:VAL:HG12	32:LV:70:LEU:CD2	2.34	0.52
50:SL:158:ASP:OD2	50:SL:160:ARG:NH2	2.42	0.52
50:SL:255:THR:HG22	50:SL:256:GLU:N	2.25	0.51
4:L3:3661:G:N7	45:SF:152:SER:OG	2.43	0.51
4:L3:4139:G:H21	4:L3:4140:C:N4	2.07	0.51
4:L3:121:A:OP1	44:SE:110:LYS:NZ	2.35	0.51
50:SL:82:LEU:CD1	50:SL:203:LEU:HD11	2.40	0.51
53:SR:427:ASP:OD2	54:SV:83:ARG:NH1	2.44	0.51
4:L3:1178:G:H21	41:SB:286:SER:HB3	1.74	0.51
4:L3:2639:U:O2'	4:L3:2694:G:O6	2.28	0.51
4:L3:4377:G:O6	21:LK:42:ARG:NH2	2.44	0.51
4:L3:1366:G:N2	4:L3:1371:A:OP2	2.43	0.51
14:LD:7:GLN:N	14:LD:7:GLN:OE1	2.43	0.51
19:LI:67:ILE:O	19:LI:84:ARG:NH2	2.43	0.51
21:LK:38:LEU:O	21:LK:42:ARG:NH1	2.42	0.51
22:LL:112:ARG:NH1	42:SC:117:PRO:O	2.42	0.51
4:L3:398:A2M:O5'	4:L3:398:A2M:H8	2.09	0.51
4:L3:1325:C:C2'	4:L3:1326:A2M:H5'	2.40	0.51
4:L3:2787:A2M:HM'3	4:L3:2790:U:OP2	2.10	0.51
4:L3:2692:U:OP1	35:LY:33:LYS:NZ	2.31	0.50
14:LD:99:MET:HE2	14:LD:99:MET:HA	1.92	0.50
42:SC:145:THR:O	42:SC:148:THR:HG23	2.10	0.50
4:L3:2632:PSU:H2'	4:L3:2633:U:C6	2.47	0.50
43:SD:175:ILE:HG23	43:SD:179:LEU:HD12	1.94	0.50
4:L3:151:G:OP2	10:L9:4:TYR:OH	2.21	0.50
3:L2:13:C:OP1	48:SI:86:HIS:NE2	2.35	0.50
31:LU:63:VAL:HG12	31:LU:63:VAL:O	2.12	0.50
51:SM:169:MET:HE1	51:SM:341:GLU:OE2	2.12	0.50
4:L3:1577:G:OP1	34:LX:17:ARG:NH2	2.43	0.50
14:LD:53:LYS:HG2	53:SR:508:MET:HE1	1.92	0.50
41:SB:111:ASN:ND2	41:SB:116:ASP:OD2	2.45	0.50
1:BE:145:LYS:O	1:BE:148:VAL:HG22	2.12	0.50
4:L3:2562:G:O2'	4:L3:2565:A:N6	2.45	0.50
4:L3:4220:6MZ:H2'	4:L3:4222:G:H5''	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L3:453:G:H1	4:L3:1293:G:N2	2.09	0.49
4:L3:4126:C:OP1	44:SE:37:LYS:NZ	2.32	0.49
29:LS:91:MET:HE1	33:LW:78:PHE:CD2	2.47	0.49
50:SL:255:THR:HG22	50:SL:256:GLU:H	1.77	0.49
1:BE:150:GLU:OE2	1:BE:154:ARG:NE	2.44	0.49
4:L3:4883:C:N4	42:SC:181:LEU:O	2.35	0.49
4:L3:1534:A2M:HM'2	4:L3:1535:C:C6	2.48	0.49
44:SE:159:HIS:ND1	44:SE:185:LYS:HA	2.28	0.49
4:L3:1778:C:O2'	4:L3:1779:PSU:H5''	2.13	0.49
17:LG:115:SER:OG	49:SK:145:GLN:OE1	2.26	0.49
26:LP:109:VAL:HG13	26:LP:109:VAL:O	2.12	0.49
4:L3:152:U:OP1	10:L9:49:ARG:NH1	2.46	0.49
4:L3:4546:A:N7	45:SF:215:ASN:ND2	2.60	0.49
49:SK:21:ASN:ND2	49:SK:112:ASP:OD2	2.45	0.49
9:L8:11:ARG:NH1	9:L8:58:THR:O	2.44	0.49
51:SM:356:TRP:HB2	51:SM:360:LEU:HD23	1.95	0.49
2:L1:84:A:N6	2:L1:87:G:O6	2.46	0.49
51:SM:59:THR:HG22	51:SM:59:THR:O	2.13	0.49
4:L3:294:G:OP2	32:LV:43:ARG:NH1	2.38	0.49
11:LA:138:PRO:HB3	11:LA:140:MET:HE3	1.94	0.49
49:SK:44:ASP:OD1	49:SK:45:THR:N	2.46	0.49
12:LB:70:MET:HE1	12:LB:137:VAL:HB	1.96	0.48
51:SM:414:PHE:O	51:SM:417:VAL:HG22	2.13	0.48
4:L3:4500:PSU:H2'	4:L3:4501:U:H6	1.78	0.48
4:L3:5053:U:O2'	4:L3:5054:C:OP2	2.25	0.48
4:L3:62:A:N3	4:L3:77:U:O2'	2.40	0.48
4:L3:937:U:OP1	9:L8:46:ARG:NH1	2.46	0.48
4:L3:3824:A:H2	34:LX:16:THR:HG22	1.79	0.48
24:LN:357:ARG:NE	53:SR:407:ASP:OD1	2.38	0.48
45:SF:101:VAL:C	45:SF:102:LEU:HD12	2.38	0.48
4:L3:2343:G:OP2	40:SA:109:ARG:NH2	2.46	0.48
4:L3:2424:OMG:HM23	4:L3:2424:OMG:H1'	1.54	0.48
4:L3:5039:U:OP1	54:SV:111:ARG:NH1	2.46	0.48
51:SM:140:MET:HE1	51:SM:220:MET:HE3	1.95	0.48
4:L3:4190:U:O2'	4:L3:4382:G:OP2	2.23	0.48
12:LB:122:THR:OG1	12:LB:124:ASP:OD1	2.25	0.48
4:L3:2422:OMC:H1'	4:L3:2422:OMC:HM23	1.50	0.48
34:LX:26:VAL:HG22	45:SF:178:PRO:HD2	1.95	0.48
11:LA:35:ALA:O	11:LA:39:MET:HE3	2.13	0.48
49:SK:2:ALA:HB1	49:SK:215:LEU:HD11	1.96	0.48
51:SM:286:VAL:HG12	51:SM:287:VAL:HG23	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L3:1548:G:O2'	4:L3:2812:A:N3	2.44	0.48
6:L5:120:ASP:OD2	6:L5:122:SER:OG	2.32	0.48
15:LE:94:GLU:OE1	15:LE:94:GLU:N	2.45	0.48
4:L3:5001:PSU:H2'	4:L3:5002:U:O4'	2.13	0.48
17:LG:96:LEU:HD13	54:SV:20:MET:SD	2.54	0.48
23:LM:43:MET:HE3	23:LM:47:LYS:NZ	2.29	0.48
24:LN:223:THR:HG22	24:LN:338:VAL:CG2	2.41	0.48
3:L2:48:G:O2'	48:SI:79:ARG:NH1	2.46	0.48
4:L3:1677:PSU:H4'	4:L3:1680:G:C2	2.49	0.48
4:L3:3852:A:H2'	4:L3:3853:PSU:H5''	1.95	0.48
50:SL:165:LEU:HB3	50:SL:169:ILE:HD12	1.95	0.48
7:L6:100:PRO:O	31:LU:25:ARG:NH1	2.42	0.47
3:L2:4:G:O6	48:SI:70:ARG:NH2	2.43	0.47
4:L3:2876:OMG:HM22	4:L3:2877:G:H5'	1.96	0.47
4:L3:4593:C:OP2	37:NK:2:ALA:N	2.47	0.47
24:LN:370:THR:O	24:LN:370:THR:HG22	2.14	0.47
40:SA:318:PRO:HB2	40:SA:325:MET:HE2	1.95	0.47
44:SE:102:TYR:OH	44:SE:211:ASP:OD2	2.29	0.47
46:SG:105:ILE:HD13	46:SG:136:VAL:HG23	1.97	0.47
18:LH:119:ILE:HD12	18:LH:140:LEU:HD22	1.95	0.47
41:SB:128:ASP:OD1	41:SB:129:GLU:N	2.46	0.47
19:LI:2:LYS:NZ	19:LI:7:VAL:O	2.41	0.47
4:L3:1676:C:OP2	4:L3:1677:PSU:N1	2.46	0.47
4:L3:1860:PSU:H2'	4:L3:1861:U:C6	2.49	0.47
4:L3:2097:U:O3'	4:L3:2098:G:H4'	2.15	0.47
4:L3:2579:G:N2	4:L3:2582:A:OP2	2.30	0.47
4:L3:4305:G:O2'	4:L3:4306:OMU:O5'	2.29	0.47
40:SA:8:ILE:HD11	40:SA:24:LEU:HD13	1.95	0.47
48:SI:153:ASN:ND2	51:SM:263:GLY:O	2.48	0.47
51:SM:170:HIS:HB3	51:SM:283:LEU:HD11	1.97	0.47
3:L2:1165:A:O2'	3:L2:1167:A:OP1	2.26	0.47
4:L3:198:A:OP2	19:LI:126:ARG:NH2	2.48	0.47
2:L1:75:OMG:HM23	2:L1:75:OMG:H1'	1.43	0.47
16:LF:66:SER:OG	16:LF:67:LYS:N	2.47	0.47
40:SA:287:THR:O	40:SA:287:THR:HG22	2.15	0.47
4:L3:265:C:H2'	38:NL:151:LEU:HD21	1.96	0.47
4:L3:1573:G:OP1	14:LD:92:LYS:NZ	2.44	0.47
4:L3:3723:A:H2'	4:L3:3724:A2M:H8	1.97	0.47
10:L9:165:THR:HG23	10:L9:168:GLY:H	1.79	0.47
4:L3:287:U:O2'	10:L9:91:GLN:OE1	2.31	0.46
4:L3:2364:OMG:HM23	4:L3:2364:OMG:H1'	1.44	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L3:4910:G:N2	8:L7:106:ASP:O	2.48	0.46
17:LG:30:ASP:OD1	17:LG:31:ASN:N	2.45	0.46
4:L3:2363:A2M:H2'	4:L3:2364:OMG:O4'	2.15	0.46
4:L3:3730:PSU:H2'	4:L3:3731:C:C6	2.50	0.46
17:LG:48:ARG:HG2	17:LG:49:LEU:N	2.29	0.46
49:SK:99:GLU:OE1	49:SK:125:THR:OG1	2.32	0.46
2:L1:62:A:OP1	29:LS:52:LYS:NZ	2.47	0.46
2:L1:68:G:O2'	2:L1:69:PSU:H5''	2.16	0.46
4:L3:295:A:OP2	32:LV:39:ARG:NH1	2.44	0.46
4:L3:2843:U:O2'	4:L3:4632:U:OP1	2.32	0.46
4:L3:3830:A2M:HM'3	4:L3:3830:A2M:H1'	1.58	0.46
4:L3:3852:A:N7	4:L3:3853:PSU:N1	2.63	0.46
4:L3:3868:G:O2'	4:L3:3869:OMC:H5''	2.14	0.46
50:SL:253:VAL:CG1	50:SL:263:ILE:HD11	2.45	0.46
7:L6:100:PRO:O	31:LU:25:ARG:NH2	2.46	0.46
8:L7:84:VAL:HG11	8:L7:102:LEU:HD22	1.98	0.46
12:LB:128:LEU:HD23	40:SA:298:ILE:CD1	2.43	0.46
42:SC:203:ILE:O	42:SC:203:ILE:HG22	2.15	0.46
2:L1:83:C:N3	19:LI:50:ARG:NH2	2.64	0.46
4:L3:1316:OMG:HM22	4:L3:1316:OMG:H1'	1.56	0.46
22:LL:5:LEU:HB2	40:SA:287:THR:HG21	1.98	0.46
44:SE:58:PRO:HD2	44:SE:61:ILE:HD12	1.96	0.46
47:SH:135:ASN:OD1	47:SH:136:ILE:N	2.48	0.46
2:L1:83:C:O2'	2:L1:84:A:N7	2.47	0.46
4:L3:1677:PSU:H4'	4:L3:1680:G:N1	2.30	0.46
2:L1:12:G:H21	11:LA:120:ASN:ND2	2.13	0.46
4:L3:2896:G:OP1	14:LD:136:ARG:NH2	2.49	0.46
4:L3:4260:U:H2'	4:L3:4261:C:C6	2.51	0.46
31:LU:50:PHE:O	31:LU:55:ARG:NH1	2.49	0.46
49:SK:163:PRO:HG3	49:SK:185:THR:HG22	1.98	0.46
4:L3:267:G:N7	38:NL:147:ARG:NH1	2.64	0.46
4:L3:1595:G:N2	53:SR:634:ARG:OXT	2.34	0.46
4:L3:4618:OMG:HM22	4:L3:4619:U:H5'	1.98	0.46
50:SL:156:LEU:HD23	50:SL:181:VAL:CG2	2.46	0.46
4:L3:1654:G:N2	4:L3:1678:C:OP1	2.47	0.46
4:L3:2837:OMU:HM23	4:L3:2837:OMU:H1'	1.52	0.46
21:LK:100:ILE:HD13	21:LK:123:ILE:HB	1.98	0.46
6:L5:100:SER:N	6:L5:104:ASN:O	2.44	0.46
4:L3:3681:G:OP2	45:SF:128:ARG:NH2	2.49	0.45
3:L2:9:A:N3	3:L2:11:C:O2'	2.41	0.45
4:L3:2362:U:H2'	4:L3:2363:A2M:H8	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L3:2804:OMC:HM23	4:L3:2804:OMC:H1'	1.57	0.45
4:L3:4494:OMG:O5'	4:L3:4494:OMG:H8	1.99	0.45
37:NK:93:TYR:OH	37:NK:109:ARG:NH1	2.50	0.45
45:SF:142:GLU:HG3	45:SF:143:THR:HG23	1.97	0.45
7:L6:63:THR:HG22	7:L6:64:VAL:N	2.31	0.45
50:SL:123:ILE:HD13	50:SL:194:ILE:HD12	1.98	0.45
4:L3:3925:OMU:HM23	4:L3:3925:OMU:H1'	1.60	0.45
46:SG:92:MET:HE2	46:SG:146:LEU:HD12	1.98	0.45
4:L3:222:C:OP2	40:SA:165:LYS:NZ	2.22	0.45
4:L3:2042:A:O2'	4:L3:2043:A:O4'	2.31	0.45
53:SR:576:ASP:OD1	53:SR:577:VAL:N	2.49	0.45
4:L3:1252:C:N4	4:L3:1259:G:N3	2.65	0.45
4:L3:2859:G:H21	4:L3:3837:C:H1'	1.82	0.45
4:L3:3724:A2M:H2'	4:L3:3725:G:C8	2.51	0.45
4:L3:3887:OMC:H6	4:L3:3887:OMC:C5'	2.30	0.45
19:LI:32:SER:OG	19:LI:101:PRO:O	2.21	0.45
40:SA:284:MET:HE2	40:SA:287:THR:HA	1.99	0.45
4:L3:748:G:N2	13:LC:147:ASP:O	2.45	0.45
4:L3:2340:C:H4'	40:SA:42:THR:HG23	1.99	0.45
7:L6:107:THR:HG22	31:LU:18:THR:HB	1.98	0.45
7:L6:126:LEU:HD11	29:LS:117:ARG:HG2	1.99	0.45
4:L3:1468:C:OP1	21:LK:132:ARG:NH2	2.43	0.45
4:L3:5021:C:O2	4:L3:5023:C:N4	2.50	0.45
46:SG:86:LEU:HD22	46:SG:188:GLN:O	2.17	0.45
4:L3:3729:U:O2'	4:L3:3730:PSU:H5''	2.17	0.44
4:L3:4571:A2M:H8	4:L3:4571:A2M:O5'	2.17	0.44
5:L4:48:G:O2'	5:L4:49:A:C8	2.67	0.44
37:NK:82:ASN:O	37:NK:86:LEU:N	2.47	0.44
4:L3:121:A:OP2	44:SE:107:LYS:NZ	2.51	0.44
4:L3:1250:C:N4	4:L3:1261:G:O6	2.50	0.44
4:L3:2322:G:OP2	27:LQ:34:ASN:ND2	2.49	0.44
4:L3:442:G:OP1	30:LT:68:ARG:NH1	2.44	0.44
4:L3:1741:G:H3'	4:L3:1742:A:C5'	2.47	0.44
4:L3:4499:OMG:HM23	4:L3:4499:OMG:H1'	1.53	0.44
7:L6:7:GLY:O	21:LK:49:HIS:NE2	2.49	0.44
40:SA:209:ILE:HB	40:SA:229:LEU:HD13	1.99	0.44
19:LI:22:PRO:HD2	19:LI:25:ILE:HD13	2.00	0.44
3:L2:4:G:N7	48:SI:70:ARG:NH1	2.63	0.44
4:L3:2021:G:OP1	52:SQ:70:ASN:N	2.48	0.44
4:L3:3641:U:OP2	4:L3:3646:A:N6	2.43	0.44
4:L3:3744:OMG:HM23	4:L3:3744:OMG:H1'	1.45	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:LD:53:LYS:CG	53:SR:508:MET:HE1	2.47	0.44
23:LM:43:MET:HE3	23:LM:47:LYS:HZ1	1.82	0.44
41:SB:152:ARG:O	41:SB:157:ASN:ND2	2.49	0.44
4:L3:4296:PSU:H2'	4:L3:4297:G:O4'	2.17	0.44
49:SK:155:SER:OG	49:SK:156:ASN:N	2.51	0.44
4:L3:3887:OMC:H6	4:L3:3887:OMC:H5'	1.81	0.44
4:L3:4226:G:O2'	4:L3:4227:OMU:H5''	2.17	0.44
12:LB:95:VAL:HG13	12:LB:95:VAL:O	2.17	0.44
47:SH:81:ARG:HG2	47:SH:82:THR:HG23	2.00	0.44
4:L3:3841:OMC:HM23	4:L3:3841:OMC:H1'	1.59	0.44
44:SE:208:ASN:HB3	44:SE:210:GLU:OE1	2.18	0.44
46:SG:118:LEU:HD21	46:SG:177:ASP:OD2	2.18	0.44
11:LA:118:GLN:NE2	11:LA:120:ASN:OD1	2.51	0.43
20:LJ:10:VAL:HG11	20:LJ:129:TRP:HZ3	1.83	0.43
4:L3:2691:U:C2	4:L3:2692:U:C5	3.05	0.43
31:LU:74:LYS:O	31:LU:78:GLY:N	2.49	0.43
49:SK:79:GLN:OE1	54:SV:1:MET:N	2.48	0.43
4:L3:2724:G:O2'	4:L3:2726:G:OP2	2.26	0.43
41:SB:62:CYS:HB3	41:SB:105:LEU:HD22	2.00	0.43
4:L3:1427:A:C2	12:LB:138:LEU:HD23	2.54	0.43
4:L3:1727:U:OP1	43:SD:131:ASN:ND2	2.52	0.43
4:L3:2380:G:N2	4:L3:2425:U:OP1	2.37	0.43
4:L3:2487:G:O2'	4:L3:2488:C:O5'	2.36	0.43
4:L3:3722:G:OP2	31:LU:68:ARG:NE	2.50	0.43
17:LG:29:ALA:HB3	17:LG:82:ILE:HD11	2.01	0.43
2:L1:26:C:O2'	40:SA:53:ALA:O	2.33	0.43
11:LA:13:LYS:HA	11:LA:107:LEU:HD11	2.00	0.43
7:L6:63:THR:HG22	7:L6:64:VAL:H	1.84	0.43
35:LY:66:VAL:HG13	35:LY:66:VAL:O	2.18	0.43
46:SG:113:GLU:OE1	46:SG:115:ARG:NH2	2.52	0.43
48:SI:210:GLU:OE1	48:SI:210:GLU:N	2.43	0.43
4:L3:1398:A:H61	4:L3:1501:C:N4	2.17	0.43
4:L3:2363:A2M:HM'3	4:L3:2363:A2M:H1'	1.66	0.43
4:L3:2838:G:O2'	4:L3:2839:PSU:H5''	2.19	0.43
10:L9:103:GLU:OE1	10:L9:165:THR:HG21	2.18	0.43
1:BE:36:LEU:HD13	1:BE:73:ASN:HB2	2.01	0.43
4:L3:2072:C:O2'	43:SD:213:LEU:O	2.37	0.43
4:L3:2781:G:O2'	36:LZ:3:SER:O	2.36	0.43
4:L3:4266:G:H2'	4:L3:4266:G:N3	2.34	0.43
24:LN:340:THR:OG1	24:LN:343:ARG:NH1	2.51	0.43
50:SL:78:LEU:HD21	50:SL:80:VAL:HG12	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L3:1340:OMC:H1'	4:L3:1340:OMC:HM23	1.51	0.43
4:L3:1352:C:O2'	4:L3:1356:U:OP1	2.35	0.43
41:SB:232:THR:OG1	41:SB:234:ASP:OD1	2.36	0.43
4:L3:1591:U:OP2	4:L3:2856:C:O2'	2.25	0.42
4:L3:4202:U:O2'	4:L3:4203:A:OP2	2.32	0.42
24:LN:360:LEU:HD12	24:LN:360:LEU:O	2.19	0.42
40:SA:322:LEU:O	40:SA:325:MET:N	2.52	0.42
1:BE:36:LEU:HD11	1:BE:69:ARG:HG2	1.99	0.42
1:BE:146:GLU:OE1	1:BE:146:GLU:N	2.45	0.42
4:L3:431:G:H21	4:L3:3888:G:H3'	1.82	0.42
4:L3:1781:PSU:C2'	4:L3:1782:PSU:H5''	2.49	0.42
4:L3:3924:C:O2'	4:L3:3925:OMU:H5''	2.18	0.42
4:L3:4941:G:OP2	42:SC:188:ARG:NH2	2.44	0.42
11:LA:94:MET:HE1	11:LA:146:ILE:HB	2.01	0.42
4:L3:4530:UR3:H6	4:L3:4530:UR3:O5'	2.19	0.42
41:SB:67:ALA:O	41:SB:68:ARG:NH1	2.52	0.42
54:SV:71:PHE:O	54:SV:75:ARG:NH2	2.52	0.42
4:L3:4227:OMU:HM23	4:L3:4227:OMU:H1'	1.88	0.42
4:L3:4371:G:OP1	32:LV:59:LYS:NZ	2.51	0.42
40:SA:137:VAL:CG1	40:SA:144:ILE:HD13	2.49	0.42
4:L3:4575:G:O2'	4:L3:5069:U:OP1	2.35	0.42
4:L3:4759:C:OP2	8:L7:171:LYS:NZ	2.27	0.42
15:LE:4:THR:HG22	15:LE:9:ARG:HD2	2.00	0.42
4:L3:160:G:N2	4:L3:276:C:O2	2.52	0.42
4:L3:2562:G:N2	4:L3:2565:A:OP2	2.47	0.42
42:SC:148:THR:HG22	42:SC:200:LYS:HG2	2.02	0.42
4:L3:1326:A2M:HM'3	4:L3:1326:A2M:H1'	1.59	0.42
4:L3:2434:G:O2'	4:L3:2527:A:N1	2.43	0.42
4:L3:4637:OMG:HM23	4:L3:4637:OMG:H1'	1.73	0.42
8:L7:113:ASP:OD1	8:L7:113:ASP:N	2.52	0.42
4:L3:1174:G:H22	4:L3:1186:U:H3	1.67	0.42
5:L4:11:A:N1	5:L4:66:G:O2'	2.43	0.42
13:LC:38:VAL:HG13	43:SD:237:GLU:OE1	2.20	0.42
18:LH:138:VAL:O	18:LH:138:VAL:HG23	2.19	0.42
4:L3:1554:A:OP2	34:LX:4:ARG:NE	2.49	0.42
4:L3:4392:OMG:H1'	4:L3:4392:OMG:HM23	1.57	0.42
4:L3:5022:U:O2'	4:L3:5023:C:OP2	2.37	0.42
11:LA:126:ARG:HG3	11:LA:140:MET:HE1	2.02	0.42
19:LI:34:LEU:HD22	19:LI:44:VAL:CG2	2.49	0.42
3:L2:10:U:OP2	50:SL:163:ARG:NH1	2.51	0.42
4:L3:511:C:O3'	7:L6:165:LYS:NZ	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L3:911:U:H2'	4:L3:912:G:O4'	2.20	0.42
4:L3:1627:G:O6	45:SF:3:ARG:NH2	2.53	0.42
4:L3:2306:G:OP1	27:LQ:128:ARG:NH1	2.52	0.42
4:L3:2580:U:OP1	20:LJ:36:ARG:NH1	2.43	0.42
4:L3:4389:C:OP2	53:SR:627:LYS:NZ	2.52	0.42
26:LP:57:MET:SD	26:LP:90:ARG:NH1	2.93	0.42
4:L3:1633:G:O2'	4:L3:1634:A:OP2	2.34	0.41
4:L3:4618:OMG:H5''	17:LG:15:ARG:HB2	2.02	0.41
22:LL:20:ARG:NH1	27:LQ:78:LEU:O	2.53	0.41
37:NK:86:LEU:HB3	37:NK:105:LEU:HD21	2.02	0.41
49:SK:88:LEU:HD12	49:SK:94:ILE:HD11	2.01	0.41
49:SK:49:VAL:HG12	49:SK:50:HIS:O	2.20	0.41
4:L3:72:C:N3	7:L6:60:ARG:NH1	2.68	0.41
4:L3:2725:A:N6	14:LD:88:ARG:O	2.53	0.41
4:L3:2815:A2M:H2'	4:L3:2816:G:H8	1.83	0.41
11:LA:67:VAL:O	11:LA:80:GLN:NE2	2.44	0.41
4:L3:1877:G:H1'	23:LM:8:THR:HG23	2.02	0.41
4:L3:2296:G:O2'	40:SA:242:PRO:O	2.37	0.41
4:L3:3867:A2M:HM'3	4:L3:3867:A2M:H1'	1.76	0.41
15:LE:32:ARG:O	41:SB:41:LYS:NZ	2.40	0.41
28:LR:48:VAL:O	28:LR:48:VAL:HG22	2.20	0.41
49:SK:126:GLU:OE1	49:SK:139:ARG:NH2	2.50	0.41
4:L3:1814:C:O2'	23:LM:42:ASN:OD1	2.31	0.41
4:L3:3623:C:O2	14:LD:82:LYS:NZ	2.53	0.41
4:L3:4201:G:O2'	4:L3:4202:U:OP2	2.30	0.41
38:NL:188:VAL:O	51:SM:163:ARG:NH1	2.50	0.41
42:SC:50:LEU:HD22	42:SC:56:ARG:HA	2.03	0.41
48:SI:98:PHE:HB2	48:SI:152:PRO:HG3	2.03	0.41
1:BE:29:ALA:N	1:BE:62:SER:OG	2.53	0.41
4:L3:2861:OMC:HM23	4:L3:2861:OMC:H1'	1.59	0.41
12:LB:95:VAL:HG13	12:LB:116:ALA:HB2	2.03	0.41
24:LN:122:TRP:CH2	24:LN:127:LYS:HG3	2.55	0.41
50:SL:88:ILE:HD13	50:SL:201:THR:CG2	2.51	0.41
4:L3:425:U:OP1	11:LA:37:LYS:NZ	2.43	0.41
4:L3:2372:U:O2'	26:LP:46:LEU:HD13	2.20	0.41
4:L3:4156:G:P	4:L3:4157:A:HO2'	2.35	0.41
13:LC:45:TRP:CZ3	13:LC:54:MET:HE2	2.56	0.41
24:LN:248:LEU:HD23	24:LN:248:LEU:H	1.86	0.41
54:SV:53:LYS:NZ	54:SV:62:GLU:OE2	2.27	0.41
2:L1:39:G:O2'	2:L1:104:A:N1	2.53	0.41
4:L3:1577:G:O2'	4:L3:1612:G:H4'	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L3:3825:A2M:HM'3	4:L3:3825:A2M:H1'	1.83	0.41
4:L3:100:C:C2	4:L3:101:A:C8	3.09	0.41
4:L3:1742:A:H1'	4:L3:1744:PSU:OP2	2.21	0.41
4:L3:1881:C:O2	4:L3:1881:C:H2'	2.21	0.41
4:L3:1933:G:H2'	4:L3:1934:A:C8	2.56	0.41
4:L3:2415:OMU:HM21	4:L3:2416:G:O2'	2.21	0.41
8:L7:27:VAL:O	8:L7:101:ARG:NH1	2.53	0.41
20:LJ:29:ILE:O	20:LJ:31:ASP:N	2.52	0.41
25:LO:48:LEU:HD23	25:LO:57:LYS:HG2	2.03	0.41
40:SA:141:GLY:O	40:SA:182:LYS:NZ	2.51	0.41
41:SB:271:MET:HE2	41:SB:276:LYS:CG	2.50	0.41
48:SI:78:LEU:HD13	48:SI:111:LEU:HD23	2.03	0.41
54:SV:64:THR:HG23	54:SV:65:VAL:N	2.36	0.41
2:L1:139:G:H2'	2:L1:140:C:O4'	2.21	0.40
4:L3:346:G:OP1	19:LI:8:THR:HG23	2.21	0.40
4:L3:2621:A:OP1	16:LF:80:LYS:NZ	2.52	0.40
11:LA:107:LEU:HD12	11:LA:152:GLU:OE1	2.21	0.40
13:LC:173:ASN:ND2	13:LC:175:PHE:O	2.51	0.40
22:LL:64:ILE:HD11	22:LL:96:MET:HE2	2.02	0.40
4:L3:4227:OMU:H6	4:L3:4227:OMU:O5'	2.21	0.40
4:L3:4280:A:N6	41:SB:28:THR:O	2.48	0.40
13:LC:45:TRP:HA	13:LC:48:VAL:HG12	2.03	0.40
49:SK:107:VAL:HG13	49:SK:118:HIS:HB2	2.02	0.40
4:L3:106:A:H2'	4:L3:107:G:O4'	2.21	0.40
4:L3:2341:A:O2'	4:L3:2342:G:O5'	2.34	0.40
4:L3:4591:U:H2'	4:L3:4592:C:C6	2.56	0.40
16:LF:67:LYS:O	16:LF:68:SER:OG	2.26	0.40
41:SB:64:ILE:HG13	41:SB:105:LEU:HD21	2.03	0.40
42:SC:213:THR:HG22	42:SC:214:ASP:H	1.86	0.40
1:BE:90:ARG:NH2	4:L3:1784:U:OP1	2.54	0.40
4:L3:4526:U:H2'	4:L3:4527:G:C8	2.56	0.40
5:L4:63:C:H1'	41:SB:280:VAL:HG11	2.04	0.40
38:NL:206:LEU:O	38:NL:206:LEU:HD12	2.22	0.40
45:SF:102:LEU:HB2	45:SF:107:MET:HE2	2.02	0.40
48:SI:166:GLN:OE1	48:SI:173:THR:HG21	2.21	0.40
4:L3:2493:G:O4'	51:SM:36:ARG:NH1	2.54	0.40
4:L3:3903:A:OP2	40:SA:71:ARG:NH2	2.53	0.40
44:SE:96:LEU:CD1	44:SE:189:ARG:HE	2.24	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	BE	156/214 (73%)	149 (96%)	7 (4%)	0	100	100
6	L5	166/178 (93%)	164 (99%)	2 (1%)	0	100	100
7	L6	208/211 (99%)	203 (98%)	5 (2%)	0	100	100
8	L7	199/203 (98%)	196 (98%)	3 (2%)	0	100	100
9	L8	133/215 (62%)	130 (98%)	3 (2%)	0	100	100
10	L9	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
11	LA	151/184 (82%)	146 (97%)	5 (3%)	0	100	100
12	LB	185/188 (98%)	180 (97%)	5 (3%)	0	100	100
13	LC	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
14	LD	152/196 (78%)	152 (100%)	0	0	100	100
15	LE	150/160 (94%)	145 (97%)	5 (3%)	0	100	100
16	LF	101/128 (79%)	99 (98%)	2 (2%)	0	100	100
17	LG	137/140 (98%)	132 (96%)	5 (4%)	0	100	100
18	LH	141/156 (90%)	140 (99%)	1 (1%)	0	100	100
19	LI	132/145 (91%)	130 (98%)	2 (2%)	0	100	100
20	LJ	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
21	LK	145/148 (98%)	142 (98%)	3 (2%)	0	100	100
22	LL	123/137 (90%)	120 (98%)	3 (2%)	0	100	100
23	LM	90/159 (57%)	87 (97%)	3 (3%)	0	100	100
24	LN	399/403 (99%)	383 (96%)	16 (4%)	0	100	100
25	LO	93/115 (81%)	93 (100%)	0	0	100	100
26	LP	104/125 (83%)	101 (97%)	3 (3%)	0	100	100
27	LQ	126/135 (93%)	126 (100%)	0	0	100	100
28	LR	110/117 (94%)	110 (100%)	0	0	100	100
29	LS	120/123 (98%)	120 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	LT	107/110 (97%)	106 (99%)	1 (1%)	0	100	100
31	LU	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
32	LV	102/106 (96%)	98 (96%)	4 (4%)	0	100	100
33	LW	84/97 (87%)	83 (99%)	1 (1%)	0	100	100
34	LX	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
35	LY	67/70 (96%)	67 (100%)	0	0	100	100
36	LZ	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
37	NK	63/129 (49%)	62 (98%)	1 (2%)	0	100	100
38	NL	317/478 (66%)	315 (99%)	2 (1%)	0	100	100
39	NP	104/134 (78%)	102 (98%)	2 (2%)	0	100	100
40	SA	356/427 (83%)	350 (98%)	6 (2%)	0	100	100
41	SB	290/297 (98%)	287 (99%)	3 (1%)	0	100	100
42	SC	211/288 (73%)	202 (96%)	9 (4%)	0	100	100
43	SD	223/248 (90%)	216 (97%)	7 (3%)	0	100	100
44	SE	228/266 (86%)	225 (99%)	3 (1%)	0	100	100
45	SF	243/257 (95%)	232 (96%)	11 (4%)	0	100	100
46	SG	188/192 (98%)	184 (98%)	4 (2%)	0	100	100
47	SH	149/293 (51%)	145 (97%)	4 (3%)	0	100	100
48	SI	231/255 (91%)	228 (99%)	3 (1%)	0	100	100
49	SK	224/245 (91%)	218 (97%)	6 (3%)	0	100	100
50	SL	236/490 (48%)	226 (96%)	10 (4%)	0	100	100
51	SM	393/588 (67%)	387 (98%)	6 (2%)	0	100	100
52	SQ	119/239 (50%)	118 (99%)	1 (1%)	0	100	100
53	SR	237/634 (37%)	235 (99%)	2 (1%)	0	100	100
54	SV	137/163 (84%)	136 (99%)	1 (1%)	0	100	100
All	All	8375/10550 (79%)	8201 (98%)	174 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BE	137/181 (76%)	137 (100%)	0	100	100
6	L5	142/149 (95%)	142 (100%)	0	100	100
7	L6	176/177 (99%)	176 (100%)	0	100	100
8	L7	173/174 (99%)	173 (100%)	0	100	100
9	L8	115/161 (71%)	115 (100%)	0	100	100
10	L9	171/172 (99%)	171 (100%)	0	100	100
11	LA	134/163 (82%)	134 (100%)	0	100	100
12	LB	164/165 (99%)	164 (100%)	0	100	100
13	LC	157/157 (100%)	157 (100%)	0	100	100
14	LD	138/175 (79%)	138 (100%)	0	100	100
15	LE	136/140 (97%)	136 (100%)	0	100	100
16	LF	93/115 (81%)	93 (100%)	0	100	100
17	LG	106/107 (99%)	106 (100%)	0	100	100
18	LH	124/133 (93%)	124 (100%)	0	100	100
19	LI	124/135 (92%)	124 (100%)	0	100	100
20	LJ	117/118 (99%)	117 (100%)	0	100	100
21	LK	120/121 (99%)	120 (100%)	0	100	100
22	LL	109/121 (90%)	109 (100%)	0	100	100
23	LM	80/126 (64%)	80 (100%)	0	100	100
24	LN	347/348 (100%)	347 (100%)	0	100	100
25	LO	80/97 (82%)	80 (100%)	0	100	100
26	LP	97/110 (88%)	97 (100%)	0	100	100
27	LQ	114/121 (94%)	114 (100%)	0	100	100
28	LR	96/100 (96%)	96 (100%)	0	100	100
29	LS	109/110 (99%)	109 (100%)	0	100	100
30	LT	88/89 (99%)	88 (100%)	0	100	100
31	LU	86/89 (97%)	86 (100%)	0	100	100
32	LV	92/94 (98%)	92 (100%)	0	100	100
33	LW	73/80 (91%)	73 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	LX	74/75 (99%)	74 (100%)	0	100	100
35	LY	64/65 (98%)	64 (100%)	0	100	100
36	LZ	47/48 (98%)	47 (100%)	0	100	100
37	NK	61/115 (53%)	61 (100%)	0	100	100
38	NL	280/402 (70%)	280 (100%)	0	100	100
39	NP	92/114 (81%)	92 (100%)	0	100	100
40	SA	298/348 (86%)	298 (100%)	0	100	100
41	SB	246/250 (98%)	246 (100%)	0	100	100
42	SC	192/252 (76%)	192 (100%)	0	100	100
43	SD	194/215 (90%)	194 (100%)	0	100	100
44	SE	198/223 (89%)	198 (100%)	0	100	100
45	SF	188/199 (94%)	188 (100%)	0	100	100
46	SG	169/171 (99%)	169 (100%)	0	100	100
47	SH	141/274 (52%)	141 (100%)	0	100	100
48	SI	210/228 (92%)	210 (100%)	0	100	100
49	SK	196/213 (92%)	196 (100%)	0	100	100
50	SL	221/437 (51%)	221 (100%)	0	100	100
51	SM	354/509 (70%)	354 (100%)	0	100	100
53	SR	218/574 (38%)	218 (100%)	0	100	100
54	SV	128/149 (86%)	128 (100%)	0	100	100
All	All	7269/8889 (82%)	7269 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	BE	92	HIS
1	BE	130	HIS
1	BE	147	HIS
6	L5	104	ASN
7	L6	104	ASN
8	L7	42	ASN
8	L7	50	ASN
9	L8	20	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	L8	34	ASN
9	L8	69	HIS
10	L9	109	HIS
11	LA	116	HIS
12	LB	7	HIS
12	LB	162	HIS
13	LC	122	HIS
14	LD	58	HIS
14	LD	141	HIS
15	LE	66	ASN
15	LE	98	HIS
16	LF	95	ASN
17	LG	27	ASN
18	LH	33	HIS
18	LH	107	HIS
19	LI	20	ASN
21	LK	19	HIS
22	LL	21	ASN
24	LN	42	HIS
24	LN	167	GLN
24	LN	203	GLN
24	LN	258	HIS
25	LO	40	GLN
25	LO	72	HIS
26	LP	121	ASN
27	LQ	52	GLN
27	LQ	126	ASN
28	LR	28	ASN
29	LS	101	ASN
30	LT	99	HIS
33	LW	13	ASN
34	LX	56	HIS
38	NL	124	ASN
38	NL	150	GLN
38	NL	216	GLN
38	NL	254	HIS
38	NL	365	HIS
39	NP	13	HIS
39	NP	99	GLN
40	SA	198	ASN
40	SA	310	HIS
41	SB	225	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	SB	244	HIS
42	SC	43	HIS
42	SC	101	ASN
42	SC	136	HIS
42	SC	190	HIS
42	SC	211	HIS
42	SC	245	GLN
43	SD	24	ASN
43	SD	63	GLN
43	SD	131	ASN
43	SD	163	ASN
44	SE	112	GLN
45	SF	22	HIS
46	SG	169	ASN
47	SH	119	HIS
47	SH	140	GLN
48	SI	136	ASN
49	SK	50	HIS
49	SK	68	HIS
51	SM	170	HIS
53	SR	436	HIS
53	SR	612	HIS
54	SV	39	ASN
54	SV	122	GLN
54	SV	132	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	L1	152/157 (96%)	17 (11%)	0
3	L2	67/1167 (5%)	9 (13%)	0
4	L3	3341/5070 (65%)	442 (13%)	6 (0%)
5	L4	119/121 (98%)	13 (10%)	1 (0%)
All	All	3679/6515 (56%)	481 (13%)	7 (0%)

All (481) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	L1	34	U
2	L1	35	C
2	L1	49	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L1	59	A
2	L1	62	A
2	L1	63	U
2	L1	82	A
2	L1	83	C
2	L1	84	A
2	L1	86	U
2	L1	94	G
2	L1	103	A
2	L1	105	C
2	L1	111	U
2	L1	127	U
2	L1	151	G
2	L1	156	U
3	L2	11	C
3	L2	48	G
3	L2	49	G
3	L2	51	U
3	L2	62	U
3	L2	96	A
3	L2	101	A
3	L2	1165	A
3	L2	1166	G
4	L3	2	G
4	L3	6	C
4	L3	39	A
4	L3	42	A
4	L3	48	G
4	L3	56	A
4	L3	58	G
4	L3	59	A
4	L3	64	A
4	L3	65	A
4	L3	69	A
4	L3	91	G
4	L3	98	A
4	L3	108	A
4	L3	109	G
4	L3	119	G
4	L3	159	C
4	L3	164	G
4	L3	167	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	L3	170	C
4	L3	171	U
4	L3	172	C
4	L3	173	C
4	L3	181	C
4	L3	197	A
4	L3	200	U
4	L3	209	U
4	L3	210	C
4	L3	218	A
4	L3	233	U
4	L3	234	G
4	L3	261	G
4	L3	263	G
4	L3	266	C
4	L3	274	C
4	L3	297	U
4	L3	316	U
4	L3	340	C
4	L3	349	A
4	L3	387	G
4	L3	409	G
4	L3	410	A
4	L3	412	G
4	L3	450	G
4	L3	452	A
4	L3	453	G
4	L3	454	U
4	L3	464	G
4	L3	467	U
4	L3	469	C
4	L3	472	C
4	L3	473	C
4	L3	492	U
4	L3	493	G
4	L3	496	G
4	L3	497	G
4	L3	499	G
4	L3	501	C
4	L3	502	C
4	L3	503	C
4	L3	504	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	L3	510	U
4	L3	511	C
4	L3	657	C
4	L3	658	C
4	L3	660	A
4	L3	667	A
4	L3	668	C
4	L3	669	C
4	L3	686	A
4	L3	697	G
4	L3	704	C
4	L3	729	G
4	L3	730	G
4	L3	731	G
4	L3	739	G
4	L3	741	C
4	L3	742	G
4	L3	746	A
4	L3	757	G
4	L3	913	U
4	L3	915	A
4	L3	917	A
4	L3	918	G
4	L3	926	G
4	L3	932	A
4	L3	933	G
4	L3	944	A
4	L3	945	U
4	L3	946	C
4	L3	959	G
4	L3	960	A
4	L3	971	U
4	L3	972	C
4	L3	1066	G
4	L3	1072	C
4	L3	1080	C
4	L3	1167	C
4	L3	1169	G
4	L3	1171	G
4	L3	1172	C
4	L3	1177	U
4	L3	1178	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	L3	1180	C
4	L3	1181	C
4	L3	1182	C
4	L3	1201	U
4	L3	1203	G
4	L3	1211	G
4	L3	1214	C
4	L3	1215	C
4	L3	1241	C
4	L3	1253	G
4	L3	1254	A
4	L3	1255	A
4	L3	1256	G
4	L3	1266	G
4	L3	1269	G
4	L3	1270	A
4	L3	1272	C
4	L3	1273	G
4	L3	1276	C
4	L3	1280	C
4	L3	1284	G
4	L3	1287	G
4	L3	1294	A
4	L3	1295	C
4	L3	1301	C
4	L3	1313	C
4	L3	1314	C
4	L3	1318	C
4	L3	1319	U
4	L3	1322	1MA
4	L3	1323	A
4	L3	1354	A
4	L3	1358	G
4	L3	1359	G
4	L3	1365	C
4	L3	1366	G
4	L3	1379	C
4	L3	1397	A
4	L3	1420	A
4	L3	1439	C
4	L3	1443	A
4	L3	1472	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	L3	1476	C
4	L3	1498	G
4	L3	1502	G
4	L3	1523	A
4	L3	1534	A2M
4	L3	1547	A
4	L3	1578	U
4	L3	1581	G
4	L3	1592	G
4	L3	1596	U
4	L3	1597	G
4	L3	1613	A
4	L3	1624	G
4	L3	1625	OMG
4	L3	1631	A
4	L3	1633	G
4	L3	1634	A
4	L3	1640	C
4	L3	1642	A
4	L3	1654	G
4	L3	1661	C
4	L3	1670	G
4	L3	1671	U
4	L3	1676	C
4	L3	1677	PSU
4	L3	1678	C
4	L3	1721	G
4	L3	1726	U
4	L3	1734	G
4	L3	1740	C
4	L3	1741	G
4	L3	1742	A
4	L3	1743	A
4	L3	1750	G
4	L3	1791	U
4	L3	1804	A
4	L3	1811	G
4	L3	1815	G
4	L3	1821	G
4	L3	1836	G
4	L3	1837	A
4	L3	1842	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	L3	1854	G
4	L3	1862	PSU
4	L3	1873	A
4	L3	1875	C
4	L3	1880	G
4	L3	1882	U
4	L3	1887	G
4	L3	1888	A
4	L3	1897	A
4	L3	1910	G
4	L3	1919	G
4	L3	1921	C
4	L3	1922	G
4	L3	1925	G
4	L3	1955	G
4	L3	1974	U
4	L3	1997	U
4	L3	2021	G
4	L3	2025	A
4	L3	2026	A
4	L3	2041	A
4	L3	2046	G
4	L3	2055	G
4	L3	2056	G
4	L3	2069	A
4	L3	2084	C
4	L3	2085	G
4	L3	2092	G
4	L3	2093	A
4	L3	2094	G
4	L3	2095	A
4	L3	2096	G
4	L3	2097	U
4	L3	2098	G
4	L3	2099	G
4	L3	2109	G
4	L3	2110	C
4	L3	2111	G
4	L3	2261	G
4	L3	2289	C
4	L3	2300	A
4	L3	2301	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	L3	2313	A
4	L3	2348	G
4	L3	2351	OMC
4	L3	2395	A
4	L3	2409	U
4	L3	2416	G
4	L3	2417	A
4	L3	2422	OMC
4	L3	2425	U
4	L3	2429	A
4	L3	2450	G
4	L3	2453	A
4	L3	2470	C
4	L3	2471	G
4	L3	2475	G
4	L3	2476	G
4	L3	2477	A
4	L3	2478	C
4	L3	2480	G
4	L3	2486	G
4	L3	2487	G
4	L3	2488	C
4	L3	2489	C
4	L3	2492	C
4	L3	2493	G
4	L3	2512	A
4	L3	2513	A
4	L3	2519	U
4	L3	2520	C
4	L3	2529	A
4	L3	2544	G
4	L3	2545	U
4	L3	2548	C
4	L3	2551	A
4	L3	2554	U
4	L3	2567	G
4	L3	2587	A
4	L3	2589	C
4	L3	2601	A
4	L3	2627	C
4	L3	2638	G
4	L3	2653	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	L3	2669	C
4	L3	2687	U
4	L3	2694	G
4	L3	2695	A
4	L3	2696	A
4	L3	2711	G
4	L3	2742	G
4	L3	2743	A
4	L3	2760	G
4	L3	2764	A
4	L3	2769	U
4	L3	2772	C
4	L3	2787	A2M
4	L3	2788	U
4	L3	2790	U
4	L3	2814	C
4	L3	2826	U
4	L3	2827	G
4	L3	2855	G
4	L3	2877	G
4	L3	2894	A
4	L3	2902	G
4	L3	2917	G
4	L3	2918	G
4	L3	3271	G
4	L3	3585	G
4	L3	3595	U
4	L3	3597	G
4	L3	3615	G
4	L3	3626	G
4	L3	3635	A
4	L3	3644	U
4	L3	3653	A
4	L3	3662	A
4	L3	3696	C
4	L3	3697	U
4	L3	3701	OMC
4	L3	3775	A
4	L3	3838	U
4	L3	3840	U
4	L3	3867	A2M
4	L3	3868	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	L3	3872	A
4	L3	3887	OMC
4	L3	3897	G
4	L3	3905	A
4	L3	3915	U
4	L3	3923	A
4	L3	3938	G
4	L3	4069	U
4	L3	4076	G
4	L3	4084	G
4	L3	4085	A
4	L3	4119	C
4	L3	4122	G
4	L3	4127	A
4	L3	4133	C
4	L3	4138	C
4	L3	4139	G
4	L3	4140	C
4	L3	4142	C
4	L3	4143	G
4	L3	4144	C
4	L3	4145	C
4	L3	4147	G
4	L3	4150	G
4	L3	4154	G
4	L3	4162	C
4	L3	4163	U
4	L3	4164	C
4	L3	4170	A
4	L3	4183	G
4	L3	4184	G
4	L3	4191	G
4	L3	4194	U
4	L3	4202	U
4	L3	4220	6MZ
4	L3	4222	G
4	L3	4229	U
4	L3	4233	A
4	L3	4235	G
4	L3	4251	A
4	L3	4254	G
4	L3	4266	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	L3	4267	G
4	L3	4268	A
4	L3	4273	A
4	L3	4281	A
4	L3	4295	U
4	L3	4305	G
4	L3	4306	OMU
4	L3	4314	C
4	L3	4329	G
4	L3	4330	G
4	L3	4332	C
4	L3	4339	A
4	L3	4373	G
4	L3	4376	A
4	L3	4377	G
4	L3	4378	A
4	L3	4387	C
4	L3	4453	C
4	L3	4464	A
4	L3	4466	C
4	L3	4475	G
4	L3	4491	G
4	L3	4495	G
4	L3	4498	OMU
4	L3	4512	U
4	L3	4513	A
4	L3	4519	C
4	L3	4523	A2M
4	L3	4524	G
4	L3	4532	PSU
4	L3	4545	G
4	L3	4548	A
4	L3	4549	G
4	L3	4556	U
4	L3	4557	U
4	L3	4558	U
4	L3	4560	C
4	L3	4567	G
4	L3	4584	A
4	L3	4590	A2M
4	L3	4608	G
4	L3	4636	PSU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	L3	4637	OMG
4	L3	4656	A
4	L3	4670	C
4	L3	4672	A
4	L3	4701	A
4	L3	4708	A
4	L3	4709	U
4	L3	4719	G
4	L3	4720	C
4	L3	4740	G
4	L3	4741	C
4	L3	4742	G
4	L3	4750	G
4	L3	4751	G
4	L3	4754	G
4	L3	4757	C
4	L3	4759	C
4	L3	4765	G
4	L3	4772	C
4	L3	4773	C
4	L3	4870	G
4	L3	4871	C
4	L3	4882	U
4	L3	4883	C
4	L3	4900	C
4	L3	4901	G
4	L3	4910	G
4	L3	4914	C
4	L3	4916	G
4	L3	4937	C
4	L3	4943	A
4	L3	4976	U
4	L3	4996	C
4	L3	5014	A
4	L3	5022	U
4	L3	5023	C
4	L3	5026	U
4	L3	5027	C
4	L3	5031	G
4	L3	5041	G
4	L3	5050	C
4	L3	5054	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	L3	5055	G
4	L3	5061	A
4	L3	5069	U
5	L4	10	C
5	L4	18	C
5	L4	49	A
5	L4	53	U
5	L4	54	A
5	L4	64	G
5	L4	66	G
5	L4	93	G
5	L4	97	G
5	L4	103	A
5	L4	110	G
5	L4	111	C
5	L4	120	U

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	L3	496	G
4	L3	502	C
4	L3	503	C
4	L3	1625	OMG
4	L3	1633	G
4	L3	2095	A
5	L4	109	U

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

110 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
4	OMU	L3	4306	4	19,22,23	1.90	5 (26%)	25,31,34	2.08	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PSU	L3	1677	4	18,21,22	1.07	2 (11%)	21,30,33	1.94	4 (19%)
4	PSU	L3	1683	4	18,21,22	1.22	3 (16%)	21,30,33	2.17	5 (23%)
4	PSU	L3	4296	4	18,21,22	1.09	2 (11%)	21,30,33	2.13	6 (28%)
24	HIC	LN	245	24	10,11,12	1.43	1 (10%)	9,14,16	1.24	1 (11%)
4	A2M	L3	3830	4	22,25,26	0.94	1 (4%)	30,36,39	2.07	9 (30%)
4	OMC	L3	4536	4	19,22,23	0.65	0	25,31,34	0.68	0
4	PSU	L3	3695	4	18,21,22	1.12	2 (11%)	21,30,33	1.98	5 (23%)
4	OMC	L3	3869	4	19,22,23	0.70	0	25,31,34	0.76	0
4	OMU	L3	2837	4	19,22,23	1.97	6 (31%)	25,31,34	1.92	5 (20%)
4	PSU	L3	3639	4	18,21,22	1.06	2 (11%)	21,30,33	1.89	4 (19%)
4	OMC	L3	2804	4	19,22,23	0.69	0	25,31,34	0.65	0
4	PSU	L3	1779	4	18,21,22	1.09	1 (5%)	21,30,33	2.01	6 (28%)
4	OMG	L3	4618	4	23,26,27	0.61	0	32,38,41	0.61	0
4	OMG	L3	1316	4	23,26,27	0.60	0	32,38,41	0.51	0
4	PSU	L3	4689	4	18,21,22	1.06	2 (11%)	21,30,33	1.93	3 (14%)
4	OMC	L3	3887	4	19,22,23	0.64	0	25,31,34	0.61	0
4	OMG	L3	4494	4	23,26,27	0.66	0	32,38,41	0.48	0
4	PSU	L3	4500	4	18,21,22	1.11	1 (5%)	21,30,33	1.97	5 (23%)
2	PSU	L1	69	2	18,21,22	1.09	2 (11%)	21,30,33	1.95	5 (23%)
4	A2M	L3	2363	55,4	22,25,26	1.01	1 (4%)	30,36,39	2.01	7 (23%)
4	PSU	L3	5010	4	18,21,22	1.06	2 (11%)	21,30,33	1.91	4 (19%)
4	OMC	L3	2351	55,4	19,22,23	0.73	1 (5%)	25,31,34	0.85	1 (4%)
4	PSU	L3	2632	4	18,21,22	1.06	1 (5%)	21,30,33	1.92	3 (14%)
4	PSU	L3	4628	4	18,21,22	1.00	2 (11%)	21,30,33	2.01	6 (28%)
4	PSU	L3	5001	4	18,21,22	1.13	3 (16%)	21,30,33	2.09	5 (23%)
4	A2M	L3	3867	4	22,25,26	0.91	1 (4%)	30,36,39	2.15	9 (30%)
4	1MA	L3	1322	4	21,25,26	0.50	0	30,37,40	0.75	1 (3%)
4	A2M	L3	400	4	22,25,26	0.92	1 (4%)	30,36,39	2.10	9 (30%)
4	PSU	L3	1792	4	18,21,22	1.04	2 (11%)	21,30,33	2.03	4 (19%)
4	PSU	L3	3715	4	18,21,22	1.08	2 (11%)	21,30,33	2.01	6 (28%)
4	PSU	L3	2508	4	18,21,22	1.03	2 (11%)	21,30,33	2.04	5 (23%)
4	PSU	L3	4576	4	18,21,22	1.10	2 (11%)	21,30,33	2.05	6 (28%)
4	A2M	L3	2401	4	22,25,26	0.94	1 (4%)	30,36,39	2.11	8 (26%)
4	PSU	L3	3734	4	18,21,22	1.08	1 (5%)	21,30,33	1.99	5 (23%)
4	OMG	L3	4228	4	23,26,27	0.75	0	32,38,41	0.61	0
4	OMC	L3	2824	4	19,22,23	0.65	0	25,31,34	0.66	0
4	OMC	L3	3701	4	19,22,23	0.59	0	25,31,34	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PSU	L3	3637	4	18,21,22	1.01	1 (5%)	21,30,33	1.98	5 (23%)
4	PSU	L3	3853	4	18,21,22	1.01	2 (11%)	21,30,33	1.89	5 (23%)
4	PSU	L3	4636	4	18,21,22	1.05	1 (5%)	21,30,33	2.14	6 (28%)
4	UR3	L3	4530	4	19,22,23	1.22	3 (15%)	26,32,35	1.49	2 (7%)
4	OMG	L3	4637	4	23,26,27	0.61	0	32,38,41	0.52	0
4	PSU	L3	4353	4	18,21,22	1.09	2 (11%)	21,30,33	2.07	6 (28%)
4	OMG	L3	4392	4	23,26,27	0.60	0	32,38,41	0.49	0
4	PSU	L3	3920	55,4	18,21,22	1.11	2 (11%)	21,30,33	1.93	4 (19%)
4	OMU	L3	4227	4	19,22,23	1.90	5 (26%)	25,31,34	1.87	5 (20%)
4	PSU	L3	4579	4	18,21,22	1.01	2 (11%)	21,30,33	1.83	4 (19%)
4	OMG	L3	2424	4	23,26,27	0.58	0	32,38,41	0.44	0
4	PSU	L3	3822	4	18,21,22	1.18	1 (5%)	21,30,33	1.96	5 (23%)
4	PSU	L3	4552	4	18,21,22	1.03	2 (11%)	21,30,33	2.01	5 (23%)
4	OMG	L3	4499	4	23,26,27	0.45	0	32,38,41	0.50	0
4	A2M	L3	3825	4	22,25,26	0.93	1 (4%)	30,36,39	2.13	7 (23%)
4	6MZ	L3	4220	4	22,25,26	1.14	1 (4%)	29,36,39	2.15	9 (31%)
4	PSU	L3	1582	4	18,21,22	1.03	2 (11%)	21,30,33	2.09	5 (23%)
4	PSU	L3	2839	4	18,21,22	1.06	2 (11%)	21,30,33	1.91	4 (19%)
4	OMC	L3	3841	4	19,22,23	0.65	0	25,31,34	0.75	1 (4%)
2	OMG	L1	75	2	23,26,27	0.54	0	32,38,41	0.52	0
4	PSU	L3	4312	4	18,21,22	1.07	2 (11%)	21,30,33	2.11	5 (23%)
4	OMU	L3	3925	4	19,22,23	1.89	6 (31%)	25,31,34	1.96	5 (20%)
4	PSU	L3	1536	4	18,21,22	1.04	2 (11%)	21,30,33	2.00	5 (23%)
4	A2M	L3	3724	4	22,25,26	0.89	0	30,36,39	2.02	7 (23%)
4	A2M	L3	4590	4	22,25,26	1.00	1 (4%)	30,36,39	2.01	10 (33%)
4	OMC	L3	2365	4	19,22,23	0.68	0	25,31,34	0.59	0
4	A2M	L3	1534	55,4	22,25,26	0.98	1 (4%)	30,36,39	2.15	9 (30%)
4	PSU	L3	3851	4	18,21,22	1.09	1 (5%)	21,30,33	1.95	4 (19%)
4	PSU	L3	4299	4	18,21,22	1.04	2 (11%)	21,30,33	2.11	3 (14%)
4	OMG	L3	4370	4	23,26,27	0.72	0	32,38,41	0.69	0
4	OMG	L3	1522	4	23,26,27	0.64	0	32,38,41	0.62	0
4	A2M	L3	2815	4	22,25,26	0.90	1 (4%)	30,36,39	2.06	7 (23%)
2	PSU	L1	55	2	18,21,22	1.05	2 (11%)	21,30,33	2.10	5 (23%)
4	PSU	L3	1744	4	18,21,22	1.09	1 (5%)	21,30,33	1.99	5 (23%)
4	OMC	L3	2422	55,4	19,22,23	0.64	0	25,31,34	0.80	1 (4%)
4	A2M	L3	398	4	22,25,26	0.94	1 (4%)	30,36,39	2.15	8 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PSU	L3	1782	4	18,21,22	1.09	1 (5%)	21,30,33	1.98	5 (23%)
4	OMU	L3	2415	4	19,22,23	1.95	6 (31%)	25,31,34	1.97	5 (20%)
4	A2M	L3	4571	4	22,25,26	0.93	1 (4%)	30,36,39	2.01	7 (23%)
4	OMG	L3	4623	4	23,26,27	0.60	0	32,38,41	0.54	0
4	OMG	L3	3899	4	23,26,27	0.62	0	32,38,41	0.58	0
4	A2M	L3	1871	4	22,25,26	0.88	0	30,36,39	2.15	8 (26%)
4	PSU	L3	4361	4	18,21,22	1.12	2 (11%)	21,30,33	2.06	5 (23%)
4	OMG	L3	3744	4	23,26,27	0.52	0	32,38,41	0.49	0
4	OMG	L3	1625	4	23,26,27	0.58	0	32,38,41	0.48	0
4	PSU	L3	4493	4	18,21,22	1.05	1 (5%)	21,30,33	2.02	2 (9%)
4	PSU	L3	1781	4	18,21,22	1.10	1 (5%)	21,30,33	1.99	5 (23%)
4	OMU	L3	4498	4	19,22,23	2.10	7 (36%)	25,31,34	1.80	5 (20%)
4	PSU	L3	4532	4	18,21,22	1.11	2 (11%)	21,30,33	2.11	5 (23%)
4	PSU	L3	4673	4	18,21,22	1.10	2 (11%)	21,30,33	1.99	5 (23%)
4	OMG	L3	3627	4	23,26,27	0.57	0	32,38,41	0.59	0
4	PSU	L3	4293	4	18,21,22	1.05	2 (11%)	21,30,33	1.76	4 (19%)
4	PSU	L3	1862	4	18,21,22	1.05	1 (5%)	21,30,33	2.00	5 (23%)
4	OMC	L3	4456	4	19,22,23	0.66	0	25,31,34	0.60	0
4	A2M	L3	1524	4	22,25,26	0.97	1 (4%)	30,36,39	2.20	8 (26%)
4	PSU	L3	4471	4	18,21,22	1.11	2 (11%)	21,30,33	1.95	5 (23%)
4	PSU	L3	4972	4	18,21,22	1.03	1 (5%)	21,30,33	1.90	4 (19%)
4	PSU	L3	4457	4	18,21,22	1.11	2 (11%)	21,30,33	2.03	5 (23%)
4	PSU	L3	3884	4	18,21,22	1.11	2 (11%)	21,30,33	2.02	5 (23%)
4	A2M	L3	1326	4	22,25,26	0.96	1 (4%)	30,36,39	2.14	8 (26%)
4	PSU	L3	4521	4	18,21,22	1.04	2 (11%)	21,30,33	1.94	4 (19%)
4	OMG	L3	2876	4	23,26,27	0.56	0	32,38,41	0.51	0
4	OMG	L3	2364	4	23,26,27	0.60	0	32,38,41	0.53	0
4	OMC	L3	1340	4	19,22,23	0.75	1 (5%)	25,31,34	0.72	0
4	PSU	L3	1860	4	18,21,22	1.01	2 (11%)	21,30,33	1.92	4 (19%)
4	PSU	L3	3730	4	18,21,22	1.08	1 (5%)	21,30,33	1.98	5 (23%)
4	OMC	L3	2861	4	19,22,23	0.62	0	25,31,34	0.63	0
4	A2M	L3	3718	4	22,25,26	0.99	1 (4%)	30,36,39	1.92	7 (23%)
4	PSU	L3	3844	4	18,21,22	1.12	2 (11%)	21,30,33	2.03	5 (23%)
4	A2M	L3	4523	4	22,25,26	0.91	1 (4%)	30,36,39	2.08	8 (26%)
4	A2M	L3	2787	4	22,25,26	0.94	1 (4%)	30,36,39	2.11	8 (26%)
4	OMU	L3	4620	4	19,22,23	1.93	5 (26%)	25,31,34	1.74	4 (16%)

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
4	OMU	L3	4306	4	-	4/9/27/28	0/2/2/2
4	PSU	L3	1677	4	-	3/7/25/26	0/2/2/2
4	PSU	L3	1683	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4296	4	-	0/7/25/26	0/2/2/2
24	HIC	LN	245	24	-	0/5/6/8	0/1/1/1
4	A2M	L3	3830	4	-	1/9/27/28	0/3/3/3
4	OMC	L3	4536	4	-	0/9/27/28	0/2/2/2
4	PSU	L3	3695	4	-	0/7/25/26	0/2/2/2
4	OMC	L3	3869	4	-	0/9/27/28	0/2/2/2
4	OMU	L3	2837	4	-	1/9/27/28	0/2/2/2
4	PSU	L3	3639	4	-	0/7/25/26	0/2/2/2
4	OMC	L3	2804	4	-	1/9/27/28	0/2/2/2
4	PSU	L3	1779	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	4618	4	-	4/9/27/28	0/3/3/3
4	OMG	L3	1316	4	-	1/9/27/28	0/3/3/3
4	PSU	L3	4689	4	-	0/7/25/26	0/2/2/2
4	OMC	L3	3887	4	-	2/9/27/28	0/2/2/2
4	OMG	L3	4494	4	-	0/9/27/28	0/3/3/3
4	PSU	L3	4500	4	-	0/7/25/26	0/2/2/2
2	PSU	L1	69	2	-	0/7/25/26	0/2/2/2
4	A2M	L3	2363	55,4	-	1/9/27/28	0/3/3/3
4	PSU	L3	5010	4	-	0/7/25/26	0/2/2/2
4	OMC	L3	2351	55,4	-	4/9/27/28	0/2/2/2
4	PSU	L3	2632	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4628	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	5001	4	-	0/7/25/26	0/2/2/2
4	A2M	L3	3867	4	-	3/9/27/28	0/3/3/3
4	1MA	L3	1322	4	-	2/7/25/26	0/3/3/3
4	A2M	L3	400	4	-	1/9/27/28	0/3/3/3
4	PSU	L3	1792	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	3715	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	2508	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4576	4	-	0/7/25/26	0/2/2/2
4	A2M	L3	2401	4	-	2/9/27/28	0/3/3/3
4	PSU	L3	3734	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	4228	4	-	0/9/27/28	0/3/3/3
4	OMC	L3	2824	4	-	0/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OMC	L3	3701	4	-	6/9/27/28	0/2/2/2
4	PSU	L3	3637	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	3853	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4636	4	-	1/7/25/26	0/2/2/2
4	UR3	L3	4530	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	4637	4	-	1/9/27/28	0/3/3/3
4	PSU	L3	4353	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	4392	4	-	1/9/27/28	0/3/3/3
4	PSU	L3	3920	55,4	-	0/7/25/26	0/2/2/2
4	OMU	L3	4227	4	-	0/9/27/28	0/2/2/2
4	PSU	L3	4579	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	2424	4	-	2/9/27/28	0/3/3/3
4	PSU	L3	3822	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4552	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	4499	4	-	1/9/27/28	0/3/3/3
4	A2M	L3	3825	4	-	1/9/27/28	0/3/3/3
4	6MZ	L3	4220	4	-	2/9/27/28	0/3/3/3
4	PSU	L3	1582	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	2839	4	-	3/7/25/26	0/2/2/2
4	OMC	L3	3841	4	-	1/9/27/28	0/2/2/2
2	OMG	L1	75	2	-	1/9/27/28	0/3/3/3
4	PSU	L3	4312	4	-	0/7/25/26	0/2/2/2
4	OMU	L3	3925	4	-	1/9/27/28	0/2/2/2
4	PSU	L3	1536	4	-	0/7/25/26	0/2/2/2
4	A2M	L3	3724	4	-	1/9/27/28	0/3/3/3
4	A2M	L3	4590	4	-	3/9/27/28	0/3/3/3
4	OMC	L3	2365	4	-	0/9/27/28	0/2/2/2
4	A2M	L3	1534	55,4	-	1/9/27/28	0/3/3/3
4	PSU	L3	3851	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4299	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	4370	4	-	0/9/27/28	0/3/3/3
4	OMG	L3	1522	4	-	0/9/27/28	0/3/3/3
4	A2M	L3	2815	4	-	1/9/27/28	0/3/3/3
2	PSU	L1	55	2	-	0/7/25/26	0/2/2/2
4	PSU	L3	1744	4	-	0/7/25/26	0/2/2/2
4	OMC	L3	2422	55,4	-	2/9/27/28	0/2/2/2
4	A2M	L3	398	4	-	1/9/27/28	0/3/3/3
4	PSU	L3	1782	4	-	0/7/25/26	0/2/2/2
4	OMU	L3	2415	4	-	0/9/27/28	0/2/2/2
4	A2M	L3	4571	4	-	1/9/27/28	0/3/3/3
4	OMG	L3	4623	4	-	0/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OMG	L3	3899	4	-	0/9/27/28	0/3/3/3
4	A2M	L3	1871	4	-	1/9/27/28	0/3/3/3
4	PSU	L3	4361	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	3744	4	-	1/9/27/28	0/3/3/3
4	OMG	L3	1625	4	-	2/9/27/28	0/3/3/3
4	PSU	L3	4493	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	1781	4	-	0/7/25/26	0/2/2/2
4	OMU	L3	4498	4	-	0/9/27/28	0/2/2/2
4	PSU	L3	4532	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4673	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	3627	4	-	0/9/27/28	0/3/3/3
4	PSU	L3	4293	4	-	1/7/25/26	0/2/2/2
4	PSU	L3	1862	4	-	2/7/25/26	0/2/2/2
4	OMC	L3	4456	4	-	0/9/27/28	0/2/2/2
4	A2M	L3	1524	4	-	2/9/27/28	0/3/3/3
4	PSU	L3	4471	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4972	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4457	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	3884	4	-	1/7/25/26	0/2/2/2
4	A2M	L3	1326	4	-	3/9/27/28	0/3/3/3
4	PSU	L3	4521	4	-	2/7/25/26	0/2/2/2
4	OMG	L3	2876	4	-	0/9/27/28	0/3/3/3
4	OMG	L3	2364	4	-	2/9/27/28	0/3/3/3
4	OMC	L3	1340	4	-	1/9/27/28	0/2/2/2
4	PSU	L3	1860	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	3730	4	-	0/7/25/26	0/2/2/2
4	OMC	L3	2861	4	-	1/9/27/28	0/2/2/2
4	A2M	L3	3718	4	-	1/9/27/28	0/3/3/3
4	PSU	L3	3844	4	-	1/7/25/26	0/2/2/2
4	A2M	L3	4523	4	-	2/9/27/28	0/3/3/3
4	A2M	L3	2787	4	-	5/9/27/28	0/3/3/3
4	OMU	L3	4620	4	-	0/9/27/28	0/2/2/2

All (150) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L3	4498	OMU	C6-N1	4.86	1.49	1.38
4	L3	4620	OMU	C6-N1	4.51	1.48	1.38
4	L3	2415	OMU	C6-N1	4.48	1.48	1.38
4	L3	2837	OMU	C6-N1	4.46	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L3	4498	OMU	C2-N1	4.32	1.45	1.38
4	L3	4227	OMU	C6-N1	4.31	1.48	1.38
4	L3	4306	OMU	C6-N1	4.31	1.48	1.38
4	L3	3925	OMU	C6-N1	4.29	1.48	1.38
4	L3	4498	OMU	C5-C4	4.18	1.52	1.43
4	L3	2837	OMU	C2-N1	3.94	1.44	1.38
4	L3	4620	OMU	C2-N1	3.92	1.44	1.38
4	L3	2837	OMU	C5-C4	3.89	1.52	1.43
4	L3	2415	OMU	C5-C4	3.84	1.52	1.43
4	L3	3822	PSU	C6-C5	3.83	1.39	1.35
4	L3	3925	OMU	C5-C4	3.73	1.51	1.43
4	L3	4306	OMU	C2-N1	3.71	1.44	1.38
4	L3	2415	OMU	C2-N1	3.62	1.44	1.38
4	L3	4620	OMU	C5-C4	3.61	1.51	1.43
4	L3	4227	OMU	C5-C4	3.55	1.51	1.43
4	L3	4500	PSU	C6-C5	3.54	1.39	1.35
4	L3	4227	OMU	C2-N1	3.53	1.44	1.38
4	L3	4220	6MZ	C6-N6	3.52	1.38	1.34
4	L3	1744	PSU	C6-C5	3.50	1.39	1.35
4	L3	1782	PSU	C6-C5	3.50	1.39	1.35
4	L3	4306	OMU	O4-C4	-3.50	1.17	1.24
4	L3	3695	PSU	C6-C5	3.46	1.39	1.35
4	L3	1779	PSU	C6-C5	3.44	1.39	1.35
4	L3	3925	OMU	C2-N1	3.43	1.43	1.38
4	L3	1781	PSU	C6-C5	3.40	1.39	1.35
4	L3	3730	PSU	C6-C5	3.31	1.39	1.35
4	L3	3734	PSU	C6-C5	3.30	1.38	1.35
4	L3	4532	PSU	C6-C5	3.30	1.38	1.35
4	L3	4306	OMU	C5-C4	3.27	1.50	1.43
4	L3	3844	PSU	C6-C5	3.25	1.38	1.35
4	L3	4457	PSU	C6-C5	3.21	1.38	1.35
4	L3	4471	PSU	C6-C5	3.21	1.38	1.35
4	L3	4361	PSU	C6-C5	3.20	1.38	1.35
4	L3	4972	PSU	C6-C5	3.17	1.38	1.35
4	L3	3715	PSU	C6-C5	3.17	1.38	1.35
4	L3	5010	PSU	C6-C5	3.16	1.38	1.35
4	L3	4636	PSU	C6-C5	3.15	1.38	1.35
4	L3	3884	PSU	C6-C5	3.15	1.38	1.35
4	L3	2632	PSU	C6-C5	3.15	1.38	1.35
4	L3	4576	PSU	C6-C5	3.14	1.38	1.35
4	L3	5001	PSU	C6-C5	3.13	1.38	1.35
4	L3	4530	UR3	C2-N1	-3.13	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L3	3851	PSU	C6-C5	3.11	1.38	1.35
2	L1	69	PSU	C6-C5	3.10	1.38	1.35
4	L3	4673	PSU	C6-C5	3.08	1.38	1.35
4	L3	4493	PSU	C6-C5	3.08	1.38	1.35
4	L3	4227	OMU	O4-C4	-3.08	1.18	1.24
4	L3	4530	UR3	C4-N3	-3.08	1.34	1.40
4	L3	1862	PSU	C6-C5	3.06	1.38	1.35
4	L3	2839	PSU	C6-C5	3.05	1.38	1.35
4	L3	4306	OMU	O2-C2	-3.01	1.17	1.23
4	L3	4620	OMU	O4-C4	-3.01	1.18	1.24
4	L3	3925	OMU	O4-C4	-3.01	1.18	1.24
4	L3	4227	OMU	O2-C2	-2.97	1.17	1.23
4	L3	2508	PSU	C6-C5	2.94	1.38	1.35
4	L3	2837	OMU	O4-C4	-2.94	1.18	1.24
4	L3	4521	PSU	C6-C5	2.93	1.38	1.35
4	L3	1860	PSU	C6-C5	2.91	1.38	1.35
4	L3	3920	PSU	C6-C5	2.88	1.38	1.35
4	L3	4552	PSU	C6-C5	2.88	1.38	1.35
4	L3	2415	OMU	O4-C4	-2.85	1.18	1.24
4	L3	3637	PSU	C6-C5	2.84	1.38	1.35
4	L3	4689	PSU	C6-C5	2.84	1.38	1.35
4	L3	3639	PSU	C6-C5	2.83	1.38	1.35
4	L3	4296	PSU	C6-C5	2.82	1.38	1.35
4	L3	1582	PSU	C6-C5	2.80	1.38	1.35
24	LN	245	HIC	CD2-CG	2.79	1.41	1.36
4	L3	4353	PSU	C6-C5	2.75	1.38	1.35
2	L1	55	PSU	C6-C5	2.73	1.38	1.35
4	L3	4498	OMU	O4-C4	-2.72	1.19	1.24
4	L3	3853	PSU	C6-C5	2.72	1.38	1.35
4	L3	4498	OMU	C2-N3	2.71	1.42	1.38
4	L3	4579	PSU	C6-C5	2.69	1.38	1.35
4	L3	1536	PSU	C6-C5	2.69	1.38	1.35
4	L3	4312	PSU	C6-C5	2.63	1.38	1.35
4	L3	2415	OMU	O2-C2	-2.61	1.18	1.23
4	L3	1677	PSU	O4'-C1'	-2.60	1.40	1.43
4	L3	2363	A2M	C5-N7	-2.58	1.34	1.39
4	L3	1792	PSU	C6-C5	2.57	1.38	1.35
4	L3	1534	A2M	C5-N7	-2.55	1.34	1.39
4	L3	4628	PSU	C6-C5	2.53	1.38	1.35
4	L3	3925	OMU	O2-C2	-2.51	1.18	1.23
4	L3	4293	PSU	C6-C5	2.51	1.38	1.35
4	L3	4620	OMU	O2-C2	-2.50	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L3	1683	PSU	C6-C5	2.48	1.38	1.35
4	L3	2787	A2M	C5-N7	-2.42	1.34	1.39
4	L3	3718	A2M	C5-N7	-2.41	1.34	1.39
4	L3	1683	PSU	C4-C5	-2.40	1.37	1.44
4	L3	4530	UR3	C2-N3	-2.39	1.34	1.39
4	L3	3920	PSU	C4-C5	-2.38	1.37	1.44
4	L3	4673	PSU	C4-C5	-2.35	1.37	1.44
4	L3	2837	OMU	C2-N3	2.35	1.42	1.38
4	L3	4296	PSU	C4-C5	-2.34	1.37	1.44
4	L3	4353	PSU	C4-C5	-2.32	1.37	1.44
4	L3	4590	A2M	C5-N7	-2.31	1.34	1.39
4	L3	1792	PSU	C4-C5	-2.31	1.37	1.44
4	L3	2837	OMU	O2-C2	-2.27	1.19	1.23
4	L3	4628	PSU	C4-C5	-2.26	1.38	1.44
4	L3	3830	A2M	C5-N7	-2.25	1.35	1.39
4	L3	2401	A2M	C5-N7	-2.23	1.35	1.39
4	L3	5001	PSU	C4-C5	-2.23	1.38	1.44
4	L3	4576	PSU	C4-C5	-2.22	1.38	1.44
4	L3	2415	OMU	C2-N3	2.22	1.41	1.38
4	L3	4579	PSU	C4-C5	-2.21	1.38	1.44
4	L3	1326	A2M	C5-N7	-2.20	1.35	1.39
4	L3	4571	A2M	C5-N7	-2.20	1.35	1.39
4	L3	3639	PSU	C4-C5	-2.19	1.38	1.44
4	L3	4293	PSU	C4-C5	-2.19	1.38	1.44
4	L3	3884	PSU	C4-C5	-2.19	1.38	1.44
2	L1	55	PSU	C4-C5	-2.18	1.38	1.44
4	L3	4299	PSU	C4-C5	-2.18	1.38	1.44
4	L3	3825	A2M	C5-N7	-2.18	1.35	1.39
4	L3	1524	A2M	C5-N7	-2.18	1.35	1.39
4	L3	1860	PSU	C4-C5	-2.16	1.38	1.44
4	L3	2508	PSU	C4-C5	-2.15	1.38	1.44
4	L3	4523	A2M	C5-N7	-2.14	1.35	1.39
4	L3	4471	PSU	C4-C5	-2.14	1.38	1.44
4	L3	1536	PSU	C4-C5	-2.14	1.38	1.44
4	L3	2815	A2M	C5-N7	-2.14	1.35	1.39
4	L3	4498	OMU	C4-N3	2.14	1.42	1.38
4	L3	2351	OMC	C4-N3	-2.14	1.30	1.34
4	L3	1340	OMC	C4-N3	-2.13	1.30	1.34
4	L3	2839	PSU	C4-C5	-2.13	1.38	1.44
4	L3	4552	PSU	C4-C5	-2.12	1.38	1.44
4	L3	3867	A2M	C5-N7	-2.11	1.35	1.39
4	L3	3715	PSU	C4-C5	-2.11	1.38	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L3	398	A2M	C5-N7	-2.11	1.35	1.39
4	L3	4521	PSU	C4-C5	-2.10	1.38	1.44
4	L3	1582	PSU	C4-C5	-2.09	1.38	1.44
4	L3	5001	PSU	O4'-C1'	-2.08	1.41	1.43
4	L3	3853	PSU	C4-C5	-2.07	1.38	1.44
4	L3	4457	PSU	C4-C5	-2.07	1.38	1.44
2	L1	69	PSU	C4-C5	-2.07	1.38	1.44
4	L3	1677	PSU	C6-C5	2.06	1.37	1.35
4	L3	5010	PSU	C4-C5	-2.06	1.38	1.44
4	L3	3925	OMU	C2-N3	2.06	1.41	1.38
4	L3	4689	PSU	C4-C5	-2.04	1.38	1.44
4	L3	4532	PSU	C4-C5	-2.04	1.38	1.44
4	L3	4299	PSU	C6-C5	2.04	1.37	1.35
4	L3	3695	PSU	C4-C5	-2.04	1.38	1.44
4	L3	4498	OMU	O2-C2	-2.04	1.19	1.23
4	L3	4312	PSU	C4-C5	-2.03	1.38	1.44
4	L3	1683	PSU	O4'-C1'	-2.02	1.41	1.43
4	L3	3844	PSU	C4-C5	-2.01	1.38	1.44
4	L3	400	A2M	C5-N7	-2.01	1.35	1.39
4	L3	4361	PSU	C4-C5	-2.00	1.38	1.44

All (429) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	3825	A2M	C5-C4-N3	-5.97	118.49	126.72
4	L3	4306	OMU	C4-N3-C2	-5.94	119.24	126.61
4	L3	3925	OMU	C4-N3-C2	-5.92	119.26	126.61
4	L3	1326	A2M	C5-C4-N3	-5.83	118.68	126.72
4	L3	1534	A2M	C5-C4-N3	-5.80	118.73	126.72
4	L3	2815	A2M	C5-C4-N3	-5.79	118.75	126.72
4	L3	2837	OMU	C4-N3-C2	-5.73	119.50	126.61
4	L3	2787	A2M	C5-C4-N3	-5.70	118.86	126.72
4	L3	4227	OMU	C4-N3-C2	-5.67	119.57	126.61
4	L3	2415	OMU	C4-N3-C2	-5.67	119.58	126.61
4	L3	4299	PSU	C4-N3-C2	-5.65	118.58	126.37
4	L3	1524	A2M	C5-C4-N3	-5.58	119.03	126.72
4	L3	4312	PSU	N1-C2-N3	5.57	121.04	115.17
4	L3	4296	PSU	C4-N3-C2	-5.49	118.80	126.37
4	L3	1683	PSU	C4-N3-C2	-5.47	118.83	126.37
4	L3	4493	PSU	C4-N3-C2	-5.44	118.88	126.37
4	L3	4571	A2M	C5-C4-N3	-5.43	119.24	126.72
4	L3	398	A2M	C5-C4-N3	-5.43	119.24	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	2363	A2M	C5-C4-N3	-5.43	119.24	126.72
4	L3	4523	A2M	C5-C4-N3	-5.42	119.26	126.72
4	L3	1871	A2M	C5-C4-N3	-5.41	119.26	126.72
4	L3	1582	PSU	C4-N3-C2	-5.38	118.97	126.37
4	L3	4498	OMU	C4-N3-C2	-5.36	119.96	126.61
4	L3	4532	PSU	N1-C2-N3	5.35	120.81	115.17
4	L3	4361	PSU	N1-C2-N3	5.35	120.81	115.17
4	L3	2401	A2M	C5-C4-N3	-5.31	119.40	126.72
4	L3	3718	A2M	C5-C4-N3	-5.30	119.42	126.72
4	L3	1677	PSU	C4-N3-C2	-5.30	119.08	126.37
4	L3	4636	PSU	N1-C2-N3	5.27	120.72	115.17
4	L3	1792	PSU	C4-N3-C2	-5.26	119.13	126.37
4	L3	5001	PSU	N1-C2-N3	5.25	120.71	115.17
4	L3	4636	PSU	C4-N3-C2	-5.25	119.14	126.37
4	L3	4353	PSU	N1-C2-N3	5.24	120.70	115.17
4	L3	3724	A2M	C5-C4-N3	-5.23	119.51	126.72
4	L3	3867	A2M	C5-C4-N3	-5.23	119.51	126.72
4	L3	4532	PSU	C4-N3-C2	-5.23	119.17	126.37
4	L3	4530	UR3	C4-N3-C2	-5.22	120.38	124.58
4	L3	400	A2M	C5-C4-N3	-5.21	119.54	126.72
4	L3	4220	6MZ	C5-C4-N3	-5.21	119.54	126.72
4	L3	4299	PSU	N1-C2-N3	5.21	120.66	115.17
4	L3	4312	PSU	C4-N3-C2	-5.21	119.20	126.37
4	L3	1683	PSU	N1-C2-N3	5.20	120.65	115.17
2	L1	55	PSU	C4-N3-C2	-5.19	119.23	126.37
4	L3	4457	PSU	N1-C2-N3	5.17	120.62	115.17
4	L3	3830	A2M	C5-C4-N3	-5.16	119.61	126.72
4	L3	3637	PSU	C4-N3-C2	-5.16	119.27	126.37
4	L3	2508	PSU	C4-N3-C2	-5.15	119.28	126.37
4	L3	3844	PSU	N1-C2-N3	5.14	120.59	115.17
4	L3	2632	PSU	C4-N3-C2	-5.13	119.31	126.37
4	L3	3884	PSU	N1-C2-N3	5.11	120.56	115.17
4	L3	1781	PSU	C4-N3-C2	-5.11	119.33	126.37
4	L3	4296	PSU	N1-C2-N3	5.10	120.55	115.17
4	L3	4552	PSU	C4-N3-C2	-5.08	119.37	126.37
4	L3	1862	PSU	C4-N3-C2	-5.08	119.38	126.37
2	L1	55	PSU	N1-C2-N3	5.07	120.52	115.17
4	L3	4493	PSU	N1-C2-N3	5.07	120.52	115.17
4	L3	4576	PSU	C4-N3-C2	-5.06	119.40	126.37
4	L3	4576	PSU	N1-C2-N3	5.05	120.49	115.17
4	L3	5001	PSU	C4-N3-C2	-5.05	119.42	126.37
4	L3	4689	PSU	C4-N3-C2	-5.04	119.42	126.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	4306	OMU	N3-C2-N1	5.04	121.45	114.89
4	L3	3825	A2M	N3-C4-N9	5.04	135.73	127.17
4	L3	4353	PSU	C4-N3-C2	-5.02	119.46	126.37
4	L3	4361	PSU	C4-N3-C2	-5.01	119.46	126.37
4	L3	1582	PSU	N1-C2-N3	5.01	120.45	115.17
4	L3	4552	PSU	N1-C2-N3	5.00	120.44	115.17
4	L3	3637	PSU	N1-C2-N3	5.00	120.44	115.17
4	L3	1779	PSU	N1-C2-N3	4.99	120.43	115.17
4	L3	4471	PSU	N1-C2-N3	4.99	120.43	115.17
4	L3	1536	PSU	C4-N3-C2	-4.99	119.50	126.37
4	L3	1862	PSU	N1-C2-N3	4.98	120.43	115.17
4	L3	3695	PSU	C4-N3-C2	-4.98	119.51	126.37
4	L3	1744	PSU	C4-N3-C2	-4.98	119.52	126.37
4	L3	4628	PSU	C4-N3-C2	-4.98	119.52	126.37
4	L3	3715	PSU	N1-C2-N3	4.97	120.41	115.17
4	L3	3851	PSU	C4-N3-C2	-4.96	119.54	126.37
4	L3	4673	PSU	C4-N3-C2	-4.96	119.54	126.37
4	L3	1781	PSU	N1-C2-N3	4.95	120.39	115.17
4	L3	1782	PSU	N1-C2-N3	4.95	120.39	115.17
4	L3	2508	PSU	N1-C2-N3	4.95	120.39	115.17
4	L3	3715	PSU	C4-N3-C2	-4.94	119.57	126.37
4	L3	4689	PSU	N1-C2-N3	4.94	120.38	115.17
4	L3	1779	PSU	C4-N3-C2	-4.93	119.58	126.37
4	L3	1792	PSU	N1-C2-N3	4.93	120.37	115.17
4	L3	1782	PSU	C4-N3-C2	-4.92	119.60	126.37
4	L3	4500	PSU	C4-N3-C2	-4.91	119.61	126.37
4	L3	3730	PSU	C4-N3-C2	-4.90	119.63	126.37
4	L3	3695	PSU	N1-C2-N3	4.89	120.33	115.17
4	L3	3734	PSU	N1-C2-N3	4.89	120.33	115.17
4	L3	4521	PSU	C4-N3-C2	-4.89	119.63	126.37
4	L3	4500	PSU	N1-C2-N3	4.89	120.33	115.17
4	L3	4673	PSU	N1-C2-N3	4.89	120.33	115.17
4	L3	3822	PSU	N1-C2-N3	4.89	120.33	115.17
4	L3	3920	PSU	C4-N3-C2	-4.89	119.64	126.37
4	L3	3734	PSU	C4-N3-C2	-4.88	119.65	126.37
4	L3	3851	PSU	N1-C2-N3	4.88	120.31	115.17
4	L3	1744	PSU	N1-C2-N3	4.87	120.31	115.17
4	L3	4521	PSU	N1-C2-N3	4.87	120.30	115.17
4	L3	4972	PSU	N1-C2-N3	4.85	120.29	115.17
4	L3	5010	PSU	C4-N3-C2	-4.85	119.69	126.37
4	L3	1536	PSU	N1-C2-N3	4.85	120.28	115.17
4	L3	4628	PSU	N1-C2-N3	4.84	120.28	115.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	2839	PSU	C4-N3-C2	-4.84	119.71	126.37
4	L3	2839	PSU	N1-C2-N3	4.83	120.26	115.17
4	L3	3730	PSU	N1-C2-N3	4.82	120.26	115.17
4	L3	4620	OMU	C4-N3-C2	-4.82	120.62	126.61
4	L3	3844	PSU	C4-N3-C2	-4.82	119.73	126.37
2	L1	69	PSU	N1-C2-N3	4.79	120.22	115.17
4	L3	1860	PSU	C4-N3-C2	-4.79	119.77	126.37
4	L3	3884	PSU	C4-N3-C2	-4.76	119.82	126.37
4	L3	5010	PSU	N1-C2-N3	4.75	120.18	115.17
2	L1	69	PSU	C4-N3-C2	-4.75	119.83	126.37
4	L3	1677	PSU	N1-C2-N3	4.74	120.17	115.17
4	L3	3639	PSU	C4-N3-C2	-4.74	119.85	126.37
4	L3	1860	PSU	N1-C2-N3	4.71	120.14	115.17
4	L3	4972	PSU	C4-N3-C2	-4.71	119.88	126.37
4	L3	4457	PSU	C4-N3-C2	-4.71	119.89	126.37
4	L3	4471	PSU	C4-N3-C2	-4.70	119.89	126.37
4	L3	2632	PSU	N1-C2-N3	4.70	120.12	115.17
4	L3	3853	PSU	C4-N3-C2	-4.69	119.91	126.37
4	L3	1534	A2M	N3-C4-N9	4.69	135.14	127.17
4	L3	3920	PSU	N1-C2-N3	4.68	120.11	115.17
4	L3	3822	PSU	C4-N3-C2	-4.64	119.97	126.37
4	L3	1524	A2M	N3-C4-N9	4.63	135.04	127.17
4	L3	3853	PSU	N1-C2-N3	4.61	120.03	115.17
4	L3	2363	A2M	N3-C4-N9	4.61	135.01	127.17
4	L3	2815	A2M	N3-C4-N9	4.60	135.00	127.17
4	L3	3639	PSU	N1-C2-N3	4.60	120.02	115.17
4	L3	398	A2M	N3-C4-N9	4.58	134.96	127.17
4	L3	4571	A2M	N3-C4-N9	4.58	134.96	127.17
4	L3	4523	A2M	N3-C4-N9	4.56	134.93	127.17
4	L3	4293	PSU	C4-N3-C2	-4.56	120.09	126.37
4	L3	1871	A2M	N3-C4-N9	4.55	134.90	127.17
4	L3	2787	A2M	N3-C4-N9	4.51	134.83	127.17
4	L3	1326	A2M	N3-C4-N9	4.50	134.82	127.17
4	L3	3718	A2M	N3-C4-N9	4.46	134.75	127.17
4	L3	4590	A2M	C5-C4-N3	-4.44	120.61	126.72
4	L3	4579	PSU	N1-C2-N3	4.43	119.84	115.17
4	L3	3867	A2M	N3-C4-N9	4.41	134.67	127.17
4	L3	4579	PSU	C4-N3-C2	-4.40	120.32	126.37
4	L3	2837	OMU	N3-C2-N1	4.36	120.57	114.89
4	L3	3724	A2M	N3-C4-N9	4.35	134.56	127.17
4	L3	4293	PSU	N1-C2-N3	4.35	119.75	115.17
4	L3	2415	OMU	N3-C2-N1	4.35	120.55	114.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	3724	A2M	N3-C2-N1	-4.33	122.03	128.58
4	L3	3925	OMU	N3-C2-N1	4.32	120.52	114.89
4	L3	400	A2M	N3-C4-N9	4.31	134.50	127.17
4	L3	2401	A2M	N3-C4-N9	4.30	134.47	127.17
4	L3	4590	A2M	N3-C2-N1	-4.29	122.08	128.58
4	L3	3830	A2M	N3-C2-N1	-4.29	122.09	128.58
4	L3	400	A2M	N3-C2-N1	-4.25	122.14	128.58
4	L3	3830	A2M	N3-C4-N9	4.24	134.37	127.17
4	L3	1524	A2M	N3-C2-N1	-4.22	122.20	128.58
4	L3	4227	OMU	C5-C4-N3	4.20	120.68	114.80
4	L3	2787	A2M	N3-C2-N1	-4.16	122.29	128.58
4	L3	2363	A2M	N3-C2-N1	-4.14	122.31	128.58
4	L3	4523	A2M	N3-C2-N1	-4.11	122.36	128.58
4	L3	4571	A2M	N3-C2-N1	-4.11	122.37	128.58
4	L3	2401	A2M	N3-C2-N1	-4.10	122.37	128.58
4	L3	1871	A2M	N3-C2-N1	-4.09	122.39	128.58
4	L3	4220	6MZ	N1-C2-N3	-4.06	122.44	128.58
4	L3	2815	A2M	N3-C2-N1	-4.02	122.49	128.58
4	L3	398	A2M	N3-C2-N1	-4.02	122.49	128.58
4	L3	3825	A2M	N3-C2-N1	-3.99	122.54	128.58
4	L3	4227	OMU	N3-C2-N1	3.99	120.08	114.89
4	L3	4498	OMU	N3-C2-N1	3.98	120.07	114.89
4	L3	3867	A2M	N3-C2-N1	-3.96	122.59	128.58
4	L3	4220	6MZ	C5-N7-C8	3.91	109.59	103.45
4	L3	1534	A2M	N3-C2-N1	-3.90	122.67	128.58
4	L3	4306	OMU	C5-C4-N3	3.90	120.26	114.80
4	L3	1524	A2M	C5-N7-C8	3.89	109.57	103.45
4	L3	3925	OMU	C5-C4-N3	3.89	120.25	114.80
4	L3	4220	6MZ	N3-C4-N9	3.89	133.78	127.17
4	L3	3718	A2M	N3-C2-N1	-3.82	122.80	128.58
4	L3	1326	A2M	N3-C2-N1	-3.81	122.82	128.58
4	L3	4620	OMU	N3-C2-N1	3.79	119.83	114.89
4	L3	2415	OMU	C5-C4-N3	3.77	120.08	114.80
4	L3	4590	A2M	N3-C4-N9	3.77	133.58	127.17
4	L3	3825	A2M	C2-N3-C4	3.76	121.01	111.83
4	L3	4620	OMU	C5-C4-N3	3.76	120.07	114.80
4	L3	4523	A2M	C5-N7-C8	3.74	109.33	103.45
4	L3	3825	A2M	C5-N7-C8	3.74	109.32	103.45
4	L3	4498	OMU	C5-C4-N3	3.73	120.03	114.80
4	L3	1326	A2M	C5-N7-C8	3.72	109.30	103.45
4	L3	2837	OMU	C5-C4-N3	3.71	119.99	114.80
4	L3	2815	A2M	C2-N3-C4	3.70	120.86	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	4590	A2M	C5-N7-C8	3.69	109.25	103.45
4	L3	2815	A2M	C5-N7-C8	3.69	109.25	103.45
4	L3	1871	A2M	C5-N7-C8	3.69	109.24	103.45
4	L3	2401	A2M	C5-N7-C8	3.67	109.22	103.45
4	L3	1534	A2M	C5-N7-C8	3.66	109.21	103.45
4	L3	1326	A2M	C2-N3-C4	3.66	120.77	111.83
4	L3	1524	A2M	C2-N3-C4	3.66	120.76	111.83
4	L3	2787	A2M	C2-N3-C4	3.65	120.75	111.83
4	L3	3830	A2M	C5-N7-C8	3.65	109.18	103.45
4	L3	398	A2M	C5-N7-C8	3.62	109.14	103.45
4	L3	398	A2M	C2'-C1'-N9	-3.59	107.84	113.75
4	L3	4571	A2M	C2-N3-C4	3.59	120.59	111.83
4	L3	3867	A2M	C5-N7-C8	3.58	109.07	103.45
4	L3	400	A2M	C5-N7-C8	3.58	109.07	103.45
4	L3	2787	A2M	C5-N7-C8	3.57	109.07	103.45
4	L3	1871	A2M	C2-N3-C4	3.57	120.54	111.83
4	L3	1534	A2M	C2-N3-C4	3.56	120.52	111.83
4	L3	3724	A2M	C2-N3-C4	3.55	120.50	111.83
4	L3	2401	A2M	C2-N3-C4	3.55	120.50	111.83
4	L3	400	A2M	C2-N3-C4	3.54	120.49	111.83
4	L3	4220	6MZ	C4-C5-N7	-3.53	106.55	110.58
4	L3	4523	A2M	C2-N3-C4	3.52	120.44	111.83
4	L3	3724	A2M	C5-N7-C8	3.52	108.98	103.45
4	L3	2363	A2M	C2-N3-C4	3.50	120.39	111.83
4	L3	4220	6MZ	C2-N3-C4	3.50	120.38	111.83
4	L3	4571	A2M	C5-N7-C8	3.50	108.94	103.45
4	L3	2363	A2M	C5-N7-C8	3.49	108.93	103.45
4	L3	3830	A2M	C2-N3-C4	3.48	120.32	111.83
4	L3	398	A2M	C2-N3-C4	3.47	120.32	111.83
4	L3	3867	A2M	C2-N3-C4	3.43	120.21	111.83
4	L3	4628	PSU	O2-C2-N1	-3.40	119.28	122.79
4	L3	2508	PSU	O2-C2-N1	-3.32	119.36	122.79
4	L3	3718	A2M	C2-N3-C4	3.32	119.94	111.83
4	L3	1536	PSU	O2-C2-N1	-3.30	119.39	122.79
4	L3	1326	A2M	C4-C5-N7	-3.29	106.82	110.58
4	L3	3718	A2M	C5-N7-C8	3.29	108.62	103.45
4	L3	2401	A2M	C2'-C1'-N9	-3.29	108.34	113.75
4	L3	4530	UR3	C5-C4-N3	3.26	119.33	115.04
4	L3	3853	PSU	O2-C2-N1	-3.24	119.45	122.79
4	L3	4457	PSU	C6-N1-C2	-3.22	119.70	122.69
4	L3	4457	PSU	O2-C2-N1	-3.22	119.47	122.79
4	L3	4590	A2M	C2-N3-C4	3.21	119.67	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	3884	PSU	C6-N1-C2	-3.20	119.72	122.69
4	L3	3822	PSU	O2-C2-N1	-3.16	119.53	122.79
4	L3	4220	6MZ	C9-N6-C6	-3.15	119.93	122.85
2	L1	55	PSU	O2-C2-N1	-3.15	119.54	122.79
4	L3	4312	PSU	O2-C2-N1	-3.15	119.54	122.79
4	L3	3730	PSU	O2-C2-N1	-3.14	119.55	122.79
4	L3	3844	PSU	O2-C2-N1	-3.14	119.55	122.79
4	L3	1871	A2M	C2'-C1'-N9	-3.14	108.58	113.75
4	L3	4636	PSU	O2-C2-N1	-3.14	119.55	122.79
4	L3	1524	A2M	C4-C5-N7	-3.10	107.03	110.58
4	L3	1677	PSU	O2-C2-N1	-3.09	119.60	122.79
4	L3	4296	PSU	O2-C2-N1	-3.07	119.62	122.79
4	L3	4299	PSU	O2-C2-N1	-3.07	119.62	122.79
4	L3	1582	PSU	O2-C2-N1	-3.06	119.63	122.79
4	L3	1860	PSU	O2-C2-N1	-3.05	119.65	122.79
4	L3	3884	PSU	O2-C2-N1	-3.04	119.65	122.79
4	L3	2837	OMU	O4-C4-C5	-3.04	119.91	125.16
4	L3	4579	PSU	O2-C2-N1	-3.04	119.65	122.79
4	L3	3925	OMU	O4-C4-C5	-3.04	119.92	125.16
4	L3	4579	PSU	C6-N1-C2	-3.03	119.88	122.69
4	L3	4636	PSU	C6-C5-C4	3.03	120.22	118.17
4	L3	1782	PSU	O2-C2-N1	-3.02	119.67	122.79
4	L3	1779	PSU	O2-C2-N1	-3.02	119.68	122.79
4	L3	1534	A2M	C4-C5-N7	-3.02	107.13	110.58
4	L3	1524	A2M	N9-C8-N7	-3.01	109.66	113.94
4	L3	4498	OMU	O4-C4-C5	-3.01	119.97	125.16
4	L3	4361	PSU	O2-C2-N1	-3.01	119.69	122.79
4	L3	1683	PSU	C6-C5-C4	3.00	120.20	118.17
24	LN	245	HIC	NE2-CE1-ND1	-3.00	111.52	112.66
4	L3	2415	OMU	O4-C4-C5	-2.98	120.02	125.16
4	L3	4227	OMU	O4-C4-C5	-2.98	120.03	125.16
4	L3	2815	A2M	C4-C5-N7	-2.98	107.18	110.58
4	L3	4532	PSU	O2-C2-N1	-2.98	119.72	122.79
4	L3	4500	PSU	O2-C2-N1	-2.97	119.73	122.79
4	L3	5001	PSU	C6-N1-C2	-2.96	119.94	122.69
4	L3	400	A2M	C2'-C1'-N9	-2.96	108.89	113.75
4	L3	4306	OMU	O4-C4-C5	-2.95	120.07	125.16
4	L3	2401	A2M	C4-C5-N7	-2.93	107.24	110.58
2	L1	69	PSU	O2-C2-N1	-2.92	119.78	122.79
4	L3	4590	A2M	N9-C8-N7	-2.89	109.83	113.94
4	L3	4523	A2M	N9-C8-N7	-2.89	109.83	113.94
4	L3	4590	A2M	C4-C5-N7	-2.89	107.28	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	1871	A2M	C4-C5-N7	-2.88	107.29	110.58
4	L3	3715	PSU	O2-C2-N1	-2.88	119.82	122.79
4	L3	3867	A2M	C2'-C1'-N9	-2.87	109.02	113.75
4	L3	3734	PSU	O2-C2-N1	-2.87	119.83	122.79
4	L3	4523	A2M	C4-C5-N7	-2.87	107.31	110.58
4	L3	3830	A2M	C4-C5-N7	-2.85	107.32	110.58
4	L3	398	A2M	C4-C5-N7	-2.85	107.33	110.58
4	L3	4571	A2M	C4-C5-N7	-2.84	107.33	110.58
4	L3	400	A2M	C4-C5-N7	-2.84	107.33	110.58
4	L3	3844	PSU	C6-N1-C2	-2.84	120.06	122.69
4	L3	2787	A2M	C4-C5-N7	-2.83	107.34	110.58
4	L3	4620	OMU	O4-C4-C5	-2.83	120.28	125.16
2	L1	55	PSU	C6-C5-C4	2.82	120.08	118.17
4	L3	1862	PSU	O2-C2-N1	-2.81	119.89	122.79
4	L3	3830	A2M	N9-C8-N7	-2.80	109.96	113.94
4	L3	4361	PSU	C6-N1-C2	-2.78	120.11	122.69
4	L3	1871	A2M	N9-C8-N7	-2.77	110.00	113.94
4	L3	2401	A2M	N9-C8-N7	-2.77	110.00	113.94
4	L3	4471	PSU	O2-C2-N1	-2.77	119.93	122.79
4	L3	3639	PSU	O2-C2-N1	-2.77	119.93	122.79
4	L3	4220	6MZ	C6-C5-N7	2.77	135.45	132.43
4	L3	3867	A2M	O4'-C1'-N9	2.77	113.40	108.09
4	L3	3825	A2M	C4-C5-N7	-2.76	107.43	110.58
4	L3	1744	PSU	O2-C2-N1	-2.75	119.95	122.79
4	L3	4353	PSU	O2-C2-N1	-2.75	119.95	122.79
4	L3	3724	A2M	C4-C5-N7	-2.75	107.44	110.58
4	L3	400	A2M	N9-C8-N7	-2.74	110.05	113.94
4	L3	3851	PSU	O2-C2-N1	-2.74	119.97	122.79
4	L3	4471	PSU	C6-N1-C2	-2.73	120.16	122.69
4	L3	1683	PSU	O2-C2-N1	-2.72	119.98	122.79
4	L3	3734	PSU	C6-C5-C4	2.71	120.01	118.17
4	L3	4972	PSU	C6-N1-C2	-2.71	120.17	122.69
4	L3	1582	PSU	C6-C5-C4	2.70	120.00	118.17
4	L3	4576	PSU	O2-C2-N1	-2.70	120.01	122.79
4	L3	5001	PSU	C6-C5-C4	2.70	119.99	118.17
4	L3	3867	A2M	C4-C5-N7	-2.69	107.50	110.58
4	L3	3867	A2M	N9-C8-N7	-2.69	110.12	113.94
4	L3	398	A2M	N9-C8-N7	-2.68	110.13	113.94
4	L3	4972	PSU	O2-C2-N1	-2.68	120.02	122.79
4	L3	2839	PSU	C6-N1-C2	-2.67	120.21	122.69
4	L3	4673	PSU	C6-N1-C2	-2.67	120.22	122.69
4	L3	3825	A2M	N9-C8-N7	-2.66	110.17	113.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L1	69	PSU	C6-N1-C2	-2.66	120.22	122.69
4	L3	3822	PSU	C6-N1-C2	-2.65	120.23	122.69
4	L3	1779	PSU	C6-N1-C2	-2.65	120.23	122.69
4	L3	4552	PSU	O2-C2-N1	-2.64	120.06	122.79
4	L3	3724	A2M	N9-C8-N7	-2.64	110.19	113.94
4	L3	4521	PSU	O2-C2-N1	-2.64	120.07	122.79
4	L3	3925	OMU	O2-C2-N1	-2.63	119.37	122.80
4	L3	2363	A2M	C4-C5-N7	-2.63	107.58	110.58
4	L3	1534	A2M	O4'-C1'-C2'	-2.63	102.07	106.59
4	L3	5010	PSU	O2-C2-N1	-2.62	120.08	122.79
4	L3	1792	PSU	O2-C2-N1	-2.62	120.09	122.79
4	L3	4220	6MZ	N9-C8-N7	-2.62	110.22	113.94
4	L3	1860	PSU	C6-N1-C2	-2.62	120.26	122.69
4	L3	2839	PSU	O2-C2-N1	-2.61	120.10	122.79
4	L3	5001	PSU	O2-C2-N1	-2.60	120.11	122.79
4	L3	3715	PSU	C6-N1-C2	-2.60	120.28	122.69
4	L3	2787	A2M	O4'-C1'-C2'	-2.59	102.13	106.59
4	L3	3718	A2M	C4-C5-N7	-2.57	107.64	110.58
4	L3	4312	PSU	C6-N1-C2	-2.56	120.31	122.69
4	L3	4576	PSU	C6-N1-C2	-2.56	120.32	122.69
4	L3	3830	A2M	C2'-C1'-N9	-2.56	109.55	113.75
4	L3	1781	PSU	O2-C2-N1	-2.55	120.16	122.79
4	L3	3822	PSU	C6-C5-C4	2.54	119.89	118.17
4	L3	4353	PSU	C6-C5-C4	2.54	119.89	118.17
4	L3	4532	PSU	C6-N1-C2	-2.53	120.34	122.69
4	L3	1683	PSU	C5-C6-N1	-2.53	118.63	122.14
4	L3	3695	PSU	O2-C2-N1	-2.53	120.18	122.79
4	L3	1744	PSU	C6-C5-C4	2.53	119.88	118.17
4	L3	1524	A2M	C2'-C1'-N9	-2.52	109.60	113.75
4	L3	2415	OMU	O2-C2-N1	-2.51	119.52	122.80
4	L3	4628	PSU	C6-N1-C2	-2.51	120.36	122.69
4	L3	5010	PSU	C6-N1-C2	-2.51	120.36	122.69
4	L3	4353	PSU	C6-N1-C2	-2.50	120.37	122.69
4	L3	4293	PSU	O2-C2-N1	-2.50	120.21	122.79
4	L3	4521	PSU	C6-N1-C2	-2.50	120.38	122.69
4	L3	4571	A2M	N9-C8-N7	-2.49	110.40	113.94
4	L3	2632	PSU	O2-C2-N1	-2.49	120.22	122.79
4	L3	1536	PSU	C6-N1-C2	-2.49	120.38	122.69
4	L3	4576	PSU	C6-C5-C4	2.48	119.85	118.17
4	L3	3695	PSU	C6-N1-C2	-2.48	120.39	122.69
4	L3	4532	PSU	C6-C5-C4	2.48	119.85	118.17
4	L3	1326	A2M	N9-C8-N7	-2.48	110.42	113.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	3639	PSU	C6-N1-C2	-2.47	120.39	122.69
4	L3	3853	PSU	C6-N1-C2	-2.47	120.40	122.69
4	L3	4689	PSU	C6-N1-C2	-2.47	120.40	122.69
4	L3	3920	PSU	O2-C2-N1	-2.46	120.25	122.79
4	L3	1782	PSU	C6-N1-C2	-2.45	120.41	122.69
4	L3	3844	PSU	C6-C5-C4	2.45	119.83	118.17
4	L3	2815	A2M	N9-C8-N7	-2.45	110.47	113.94
4	L3	4523	A2M	C2'-C1'-N9	-2.44	109.74	113.75
4	L3	1534	A2M	N9-C8-N7	-2.44	110.48	113.94
4	L3	3920	PSU	C6-N1-C2	-2.43	120.44	122.69
4	L3	4500	PSU	C6-N1-C2	-2.43	120.44	122.69
4	L3	3730	PSU	C6-N1-C2	-2.42	120.44	122.69
4	L3	2787	A2M	N9-C8-N7	-2.41	110.51	113.94
4	L3	4590	A2M	C2'-C1'-N9	-2.41	109.78	113.75
4	L3	2363	A2M	N9-C8-N7	-2.39	110.55	113.94
4	L3	1862	PSU	C6-N1-C2	-2.38	120.48	122.69
4	L3	3734	PSU	C6-N1-C2	-2.37	120.49	122.69
4	L3	4296	PSU	C6-C5-C4	2.36	119.76	118.17
4	L3	3637	PSU	C6-C5-C4	2.33	119.74	118.17
4	L3	1792	PSU	C6-C5-C4	2.32	119.74	118.17
4	L3	3851	PSU	C6-N1-C2	-2.31	120.55	122.69
4	L3	4552	PSU	C6-N1-C2	-2.31	120.55	122.69
2	L1	55	PSU	C6-N1-C2	-2.30	120.55	122.69
4	L3	4293	PSU	C6-N1-C2	-2.30	120.56	122.69
4	L3	3730	PSU	C6-C5-C4	2.30	119.72	118.17
2	L1	69	PSU	O4'-C1'-C2'	2.28	108.31	105.15
4	L3	3695	PSU	C6-C5-C4	2.28	119.71	118.17
4	L3	4673	PSU	O2-C2-N1	-2.28	120.44	122.79
4	L3	1744	PSU	C6-N1-C2	-2.28	120.58	122.69
4	L3	1534	A2M	C3'-C2'-C1'	-2.28	98.45	102.81
4	L3	4552	PSU	C6-C5-C4	2.27	119.71	118.17
4	L3	2837	OMU	O2-C2-N1	-2.27	119.84	122.80
4	L3	4498	OMU	O2-C2-N1	-2.26	119.86	122.80
4	L3	2508	PSU	C6-N1-C2	-2.25	120.60	122.69
4	L3	1322	1MA	N1-C6-N6	2.24	125.34	119.71
4	L3	4590	A2M	C2-N1-C6	2.24	122.41	118.73
4	L3	4500	PSU	C6-C5-C4	2.24	119.68	118.17
4	L3	1782	PSU	C6-C5-C4	2.23	119.68	118.17
4	L3	1677	PSU	C6-C5-C4	2.23	119.68	118.17
4	L3	3718	A2M	N9-C8-N7	-2.22	110.78	113.94
4	L3	4636	PSU	C6-N1-C2	-2.22	120.63	122.69
4	L3	4576	PSU	O4'-C1'-C2'	2.22	108.22	105.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	1781	PSU	C6-C5-C4	2.21	119.66	118.17
4	L3	2351	OMC	C1'-N1-C2	2.20	123.30	118.44
4	L3	3841	OMC	C1'-N1-C2	2.19	123.28	118.44
4	L3	1781	PSU	C6-N1-C2	-2.19	120.66	122.69
4	L3	1779	PSU	C6-C5-C4	2.18	119.65	118.17
4	L3	3715	PSU	O4'-C1'-C2'	2.18	108.16	105.15
4	L3	2422	OMC	C1'-N1-C2	2.16	123.22	118.44
4	L3	3637	PSU	O2-C2-N1	-2.15	120.57	122.79
4	L3	4457	PSU	C6-C5-C4	2.15	119.62	118.17
4	L3	3637	PSU	C6-N1-C2	-2.13	120.72	122.69
4	L3	4296	PSU	C6-N1-C2	-2.12	120.72	122.69
4	L3	3830	A2M	C5'-C4'-C3'	-2.12	107.57	115.21
4	L3	1536	PSU	C6-C5-C4	2.12	119.60	118.17
4	L3	3715	PSU	C6-C5-C4	2.10	119.59	118.17
4	L3	4312	PSU	C6-C5-C4	2.10	119.59	118.17
4	L3	4673	PSU	C6-C5-C4	2.09	119.58	118.17
4	L3	4590	A2M	C2'-C3'-C4'	-2.09	97.50	101.99
4	L3	1862	PSU	C6-C5-C4	2.08	119.58	118.17
4	L3	2508	PSU	C6-C5-C4	2.07	119.57	118.17
4	L3	4628	PSU	C6-C5-C4	2.06	119.57	118.17
4	L3	4636	PSU	O4'-C1'-C2'	2.06	108.00	105.15
4	L3	3884	PSU	C6-C5-C4	2.05	119.56	118.17
4	L3	4628	PSU	O4'-C1'-C2'	2.05	107.99	105.15
4	L3	4296	PSU	O4-C4-C5	-2.05	118.91	124.01
4	L3	1582	PSU	C5-C6-N1	-2.03	119.33	122.14
4	L3	400	A2M	C5'-C4'-C3'	-2.02	107.93	115.21
4	L3	4361	PSU	C6-C5-C4	2.02	119.54	118.17
4	L3	4353	PSU	O4'-C1'-C2'	2.02	107.94	105.15
4	L3	4471	PSU	C6-C5-C4	2.02	119.53	118.17
4	L3	4227	OMU	O2-C2-N1	-2.02	120.17	122.80
4	L3	1779	PSU	O4'-C1'-C2'	2.01	107.93	105.15
4	L3	3853	PSU	O4'-C1'-C2'	2.00	107.92	105.15
4	L3	1326	A2M	C5'-C4'-C3'	-2.00	108.01	115.21

There are no chirality outliers.

All (89) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L1	75	OMG	C1'-C2'-O2'-CM2
4	L3	398	A2M	C1'-C2'-O2'-CM'
4	L3	400	A2M	C1'-C2'-O2'-CM'
4	L3	1316	OMG	C1'-C2'-O2'-CM2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	L3	1326	A2M	C1'-C2'-O2'-CM'
4	L3	1340	OMC	C1'-C2'-O2'-CM2
4	L3	1871	A2M	C1'-C2'-O2'-CM'
4	L3	2363	A2M	C1'-C2'-O2'-CM'
4	L3	2364	OMG	C1'-C2'-O2'-CM2
4	L3	2422	OMC	C1'-C2'-O2'-CM2
4	L3	2424	OMG	C1'-C2'-O2'-CM2
4	L3	2787	A2M	C3'-C4'-C5'-O5'
4	L3	2804	OMC	C1'-C2'-O2'-CM2
4	L3	2815	A2M	C1'-C2'-O2'-CM'
4	L3	2837	OMU	C1'-C2'-O2'-CM2
4	L3	2861	OMC	C1'-C2'-O2'-CM2
4	L3	3701	OMC	C2'-C1'-N1-C6
4	L3	3718	A2M	C1'-C2'-O2'-CM'
4	L3	3724	A2M	C1'-C2'-O2'-CM'
4	L3	3744	OMG	C1'-C2'-O2'-CM2
4	L3	3825	A2M	C1'-C2'-O2'-CM'
4	L3	3830	A2M	C1'-C2'-O2'-CM'
4	L3	3841	OMC	C1'-C2'-O2'-CM2
4	L3	3867	A2M	O4'-C4'-C5'-O5'
4	L3	3867	A2M	C1'-C2'-O2'-CM'
4	L3	3887	OMC	C3'-C4'-C5'-O5'
4	L3	3887	OMC	O4'-C4'-C5'-O5'
4	L3	3925	OMU	C1'-C2'-O2'-CM2
4	L3	4392	OMG	C1'-C2'-O2'-CM2
4	L3	4499	OMG	C1'-C2'-O2'-CM2
4	L3	4523	A2M	O4'-C4'-C5'-O5'
4	L3	4571	A2M	C1'-C2'-O2'-CM'
4	L3	4636	PSU	C2'-C1'-C5-C4
4	L3	4637	OMG	C1'-C2'-O2'-CM2
4	L3	3701	OMC	C2'-C1'-N1-C2
4	L3	1862	PSU	C3'-C4'-C5'-O5'
4	L3	1862	PSU	O4'-C4'-C5'-O5'
4	L3	3867	A2M	C3'-C4'-C5'-O5'
4	L3	4220	6MZ	O4'-C4'-C5'-O5'
4	L3	4618	OMG	O4'-C4'-C5'-O5'
4	L3	1322	1MA	O4'-C4'-C5'-O5'
4	L3	2787	A2M	O4'-C4'-C5'-O5'
4	L3	3701	OMC	C3'-C4'-C5'-O5'
4	L3	3701	OMC	O4'-C4'-C5'-O5'
4	L3	4523	A2M	C3'-C4'-C5'-O5'
4	L3	4306	OMU	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	L3	4306	OMU	O4'-C4'-C5'-O5'
4	L3	2401	A2M	C3'-C4'-C5'-O5'
4	L3	4590	A2M	C4'-C5'-O5'-P
4	L3	1677	PSU	C3'-C4'-C5'-O5'
4	L3	1677	PSU	O4'-C4'-C5'-O5'
4	L3	4220	6MZ	C3'-C4'-C5'-O5'
4	L3	1326	A2M	C3'-C4'-C5'-O5'
4	L3	1625	OMG	C3'-C4'-C5'-O5'
4	L3	4618	OMG	C3'-C4'-C5'-O5'
4	L3	1322	1MA	C3'-C4'-C5'-O5'
4	L3	2401	A2M	O4'-C4'-C5'-O5'
4	L3	2839	PSU	O4'-C4'-C5'-O5'
4	L3	2839	PSU	C3'-C4'-C5'-O5'
4	L3	2787	A2M	C2'-C1'-N9-C8
4	L3	4590	A2M	C3'-C4'-C5'-O5'
4	L3	4293	PSU	O4'-C4'-C5'-O5'
4	L3	1677	PSU	O4'-C1'-C5-C4
4	L3	2839	PSU	O4'-C1'-C5-C4
4	L3	3884	PSU	O4'-C1'-C5-C4
4	L3	4521	PSU	O4'-C1'-C5-C4
4	L3	2787	A2M	C2'-C1'-N9-C4
4	L3	3701	OMC	O4'-C1'-N1-C2
4	L3	3701	OMC	O4'-C1'-N1-C6
4	L3	4306	OMU	C4'-C5'-O5'-P
4	L3	4618	OMG	C3'-C2'-O2'-CM2
4	L3	3844	PSU	C4'-C5'-O5'-P
4	L3	1524	A2M	O4'-C1'-N9-C8
4	L3	1534	A2M	C4'-C5'-O5'-P
4	L3	4618	OMG	C1'-C2'-O2'-CM2
4	L3	4521	PSU	O4'-C1'-C5-C6
4	L3	1524	A2M	O4'-C1'-N9-C4
4	L3	2351	OMC	C3'-C2'-O2'-CM2
4	L3	4590	A2M	C3'-C2'-O2'-CM'
4	L3	2364	OMG	O4'-C4'-C5'-O5'
4	L3	2424	OMG	O4'-C4'-C5'-O5'
4	L3	2351	OMC	C2'-C1'-N1-C6
4	L3	2787	A2M	O4'-C1'-N9-C8
4	L3	1326	A2M	O4'-C4'-C5'-O5'
4	L3	2422	OMC	O4'-C4'-C5'-O5'
4	L3	1625	OMG	O4'-C4'-C5'-O5'
4	L3	2351	OMC	O4'-C4'-C5'-O5'
4	L3	2351	OMC	C2'-C1'-N1-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	L3	4306	OMU	C2'-C1'-N1-C6

There are no ring outliers.

57 monomers are involved in 85 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L3	4306	OMU	1	0
4	L3	1677	PSU	3	0
4	L3	4296	PSU	1	0
4	L3	3830	A2M	1	0
4	L3	4536	OMC	1	0
4	L3	3869	OMC	1	0
4	L3	2837	OMU	1	0
4	L3	2804	OMC	1	0
4	L3	1779	PSU	1	0
4	L3	4618	OMG	2	0
4	L3	1316	OMG	1	0
4	L3	3887	OMC	2	0
4	L3	4494	OMG	1	0
4	L3	4500	PSU	2	0
2	L1	69	PSU	2	0
4	L3	2363	A2M	3	0
4	L3	2351	OMC	1	0
4	L3	2632	PSU	1	0
4	L3	5001	PSU	1	0
4	L3	3867	A2M	3	0
4	L3	400	A2M	1	0
4	L3	3715	PSU	1	0
4	L3	3853	PSU	2	0
4	L3	4530	UR3	2	0
4	L3	4637	OMG	2	0
4	L3	4392	OMG	1	0
4	L3	4227	OMU	3	0
4	L3	2424	OMG	1	0
4	L3	4499	OMG	1	0
4	L3	3825	A2M	1	0
4	L3	4220	6MZ	1	0
4	L3	2839	PSU	1	0
4	L3	3841	OMC	1	0
2	L1	75	OMG	2	0
4	L3	3925	OMU	2	0
4	L3	3724	A2M	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L3	4590	A2M	1	0
4	L3	1534	A2M	2	0
4	L3	4299	PSU	1	0
4	L3	2815	A2M	2	0
4	L3	1744	PSU	4	0
4	L3	2422	OMC	1	0
4	L3	398	A2M	2	0
4	L3	1782	PSU	1	0
4	L3	2415	OMU	1	0
4	L3	4571	A2M	1	0
4	L3	3744	OMG	1	0
4	L3	1781	PSU	1	0
4	L3	1326	A2M	5	0
4	L3	2876	OMG	1	0
4	L3	2364	OMG	2	0
4	L3	1340	OMC	1	0
4	L3	1860	PSU	1	0
4	L3	3730	PSU	2	0
4	L3	2861	OMC	1	0
4	L3	3718	A2M	1	0
4	L3	2787	A2M	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 93 ligands modelled in this entry, 93 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.

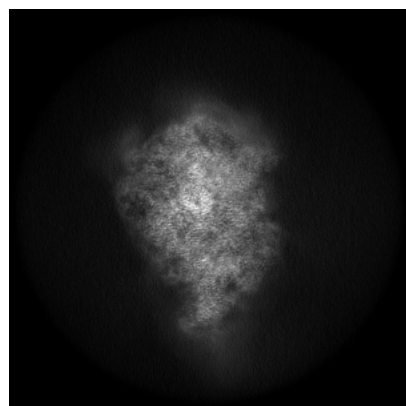
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29275. These allow visual inspection of the internal detail of the map and identification of artifacts.

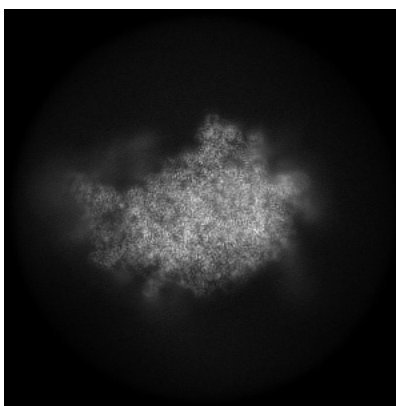
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

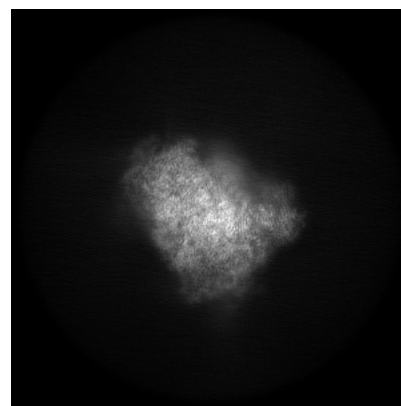
6.1.1 Primary map



X

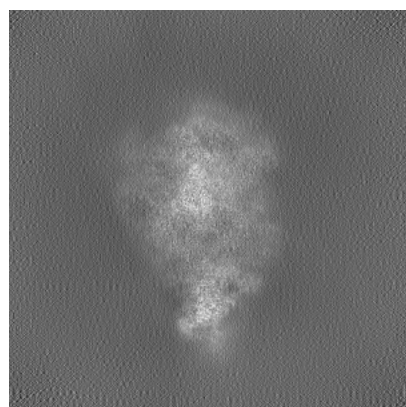


Y

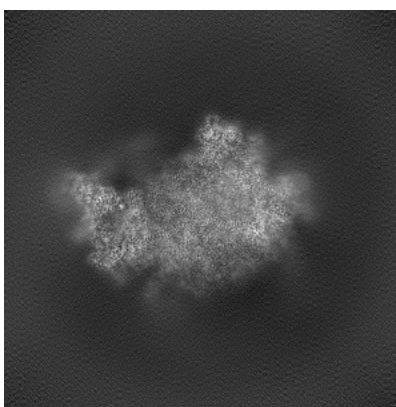


Z

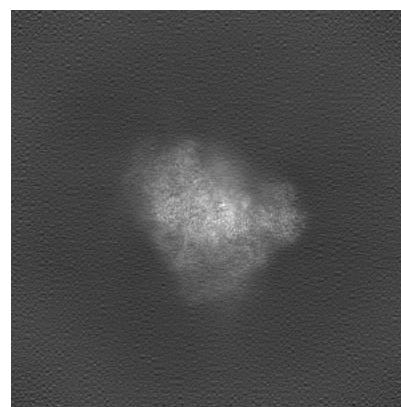
6.1.2 Raw map



X



Y

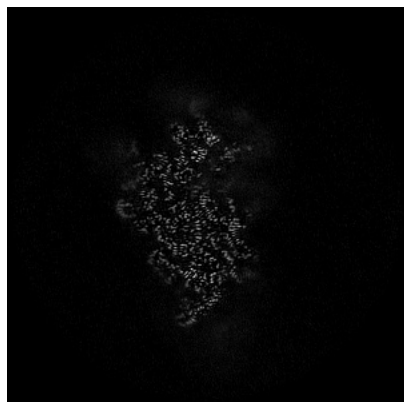


Z

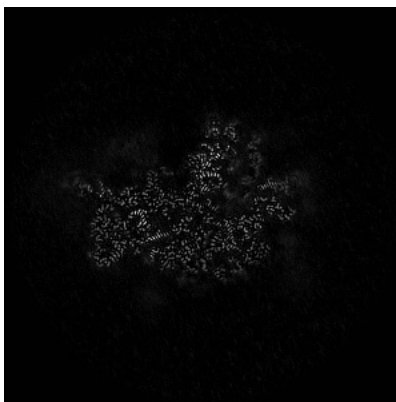
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

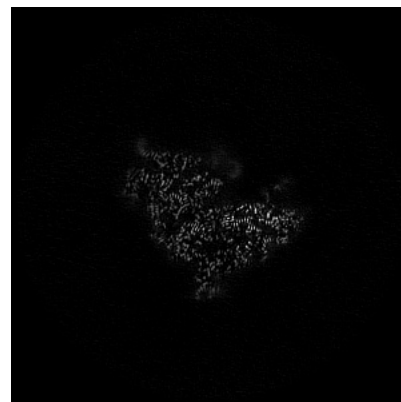
6.2.1 Primary map



X Index: 240

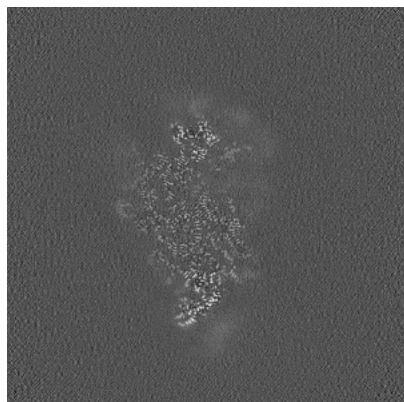


Y Index: 240

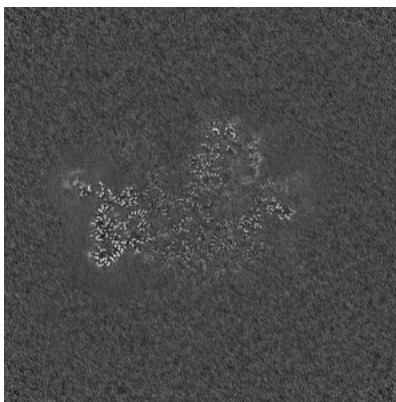


Z Index: 240

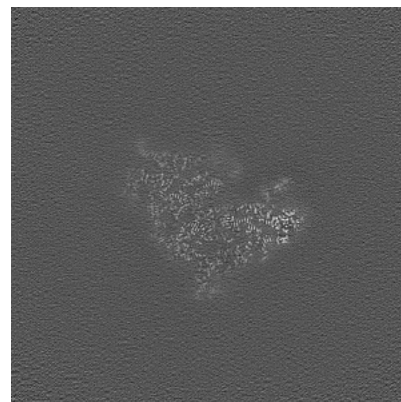
6.2.2 Raw map



X Index: 240



Y Index: 240

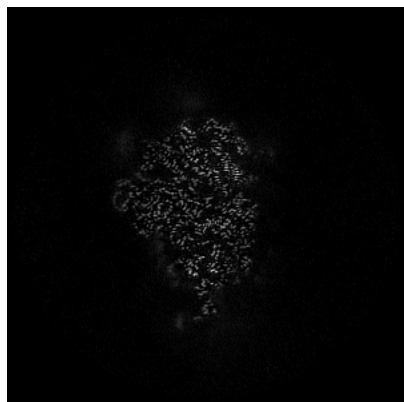


Z Index: 240

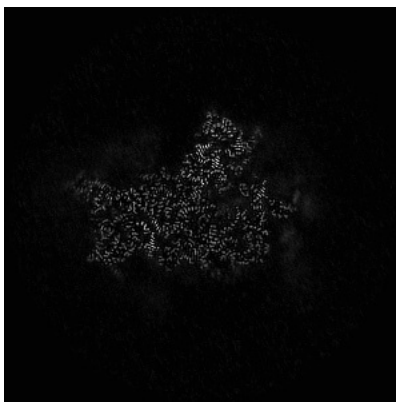
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

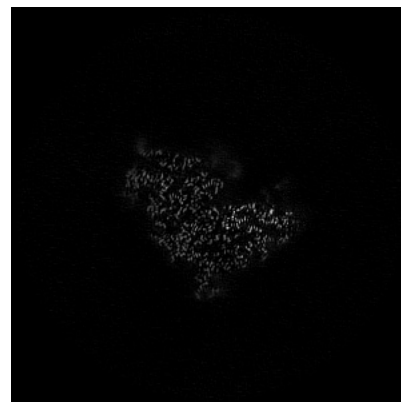
6.3.1 Primary map



X Index: 226

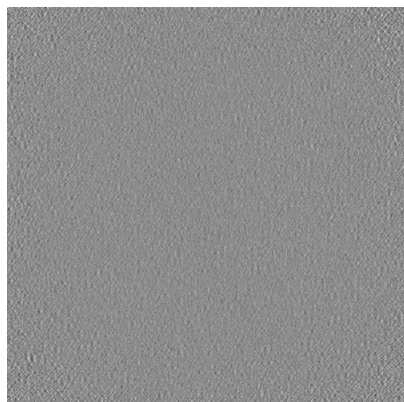


Y Index: 233

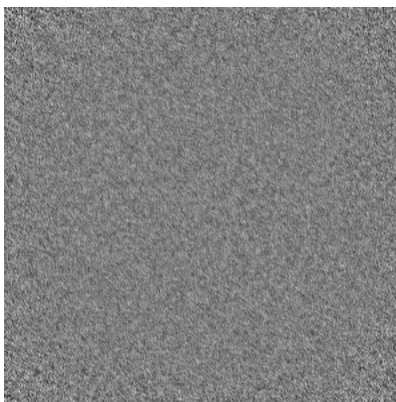


Z Index: 239

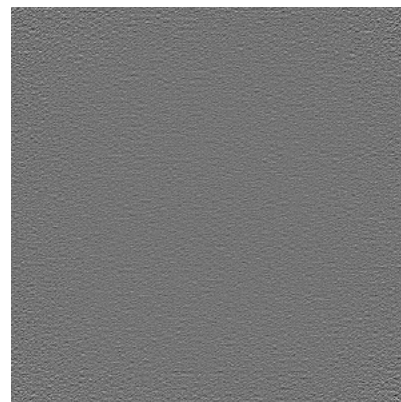
6.3.2 Raw map



X Index: 0



Y Index: 0

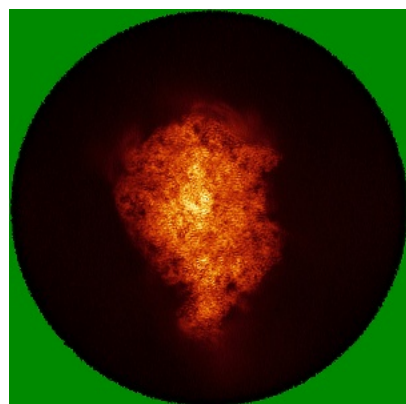


Z Index: 0

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

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

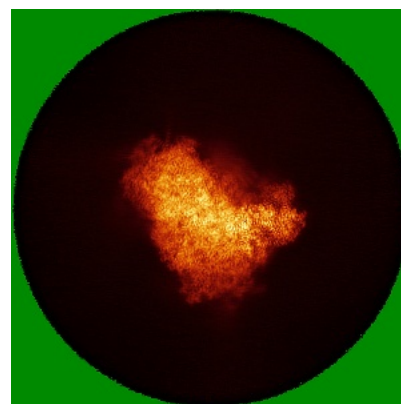
6.4.1 Primary map



X

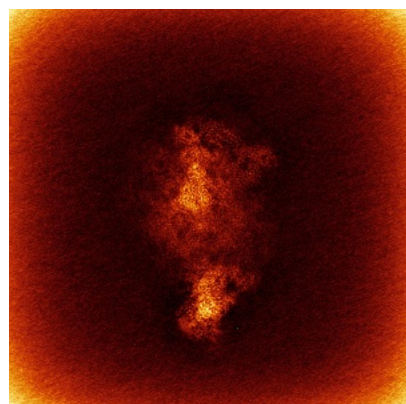


Y

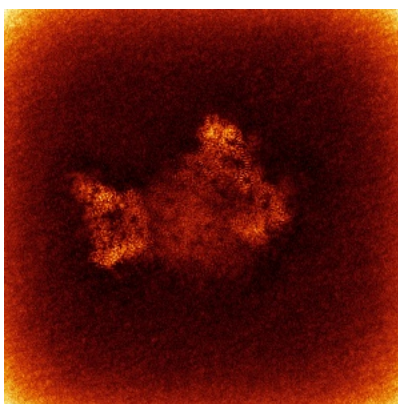


Z

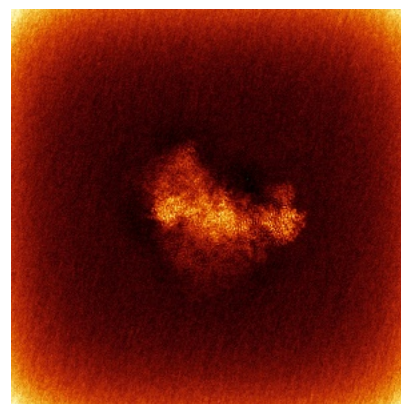
6.4.2 Raw map



X



Y

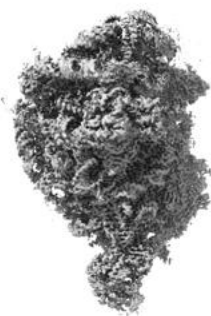


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



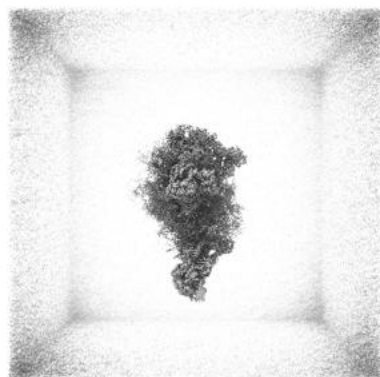
Y



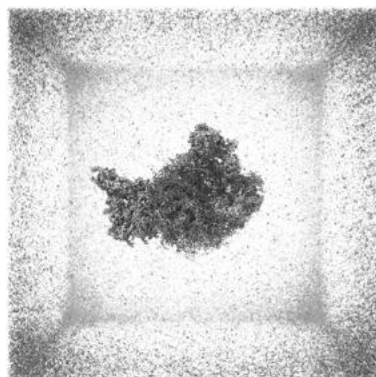
Z

The images above show the 3D surface view of the map at the recommended contour level 0.95. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

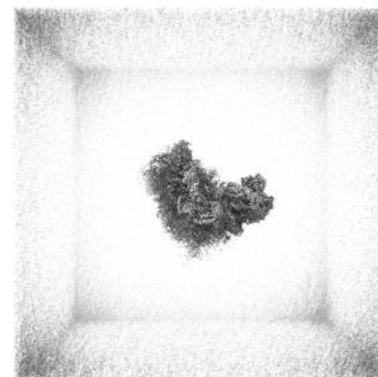
6.5.2 Raw map



X



Y



Z

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

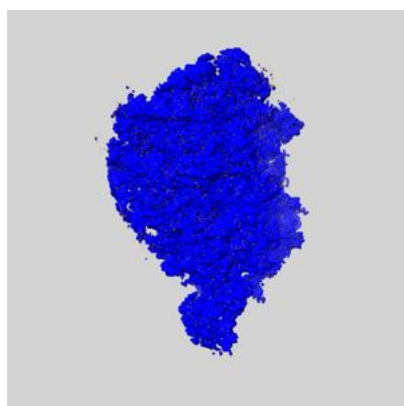
6.6 Mask visualisation [i](#)

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

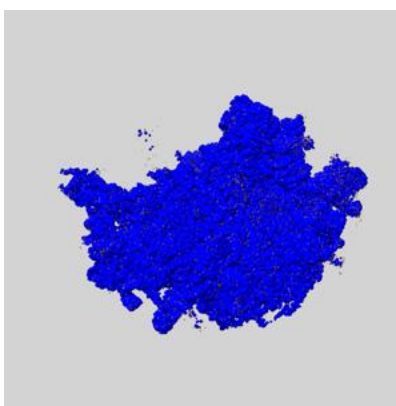
A mask typically either:

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

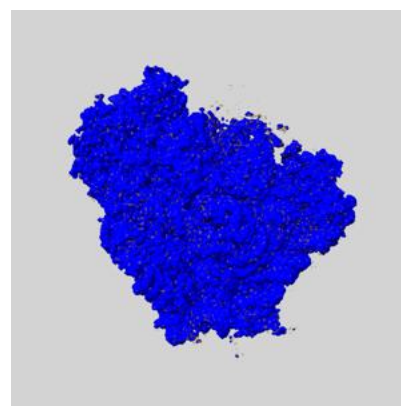
6.6.1 emd_29275_msk_1.map [i](#)



X



Y

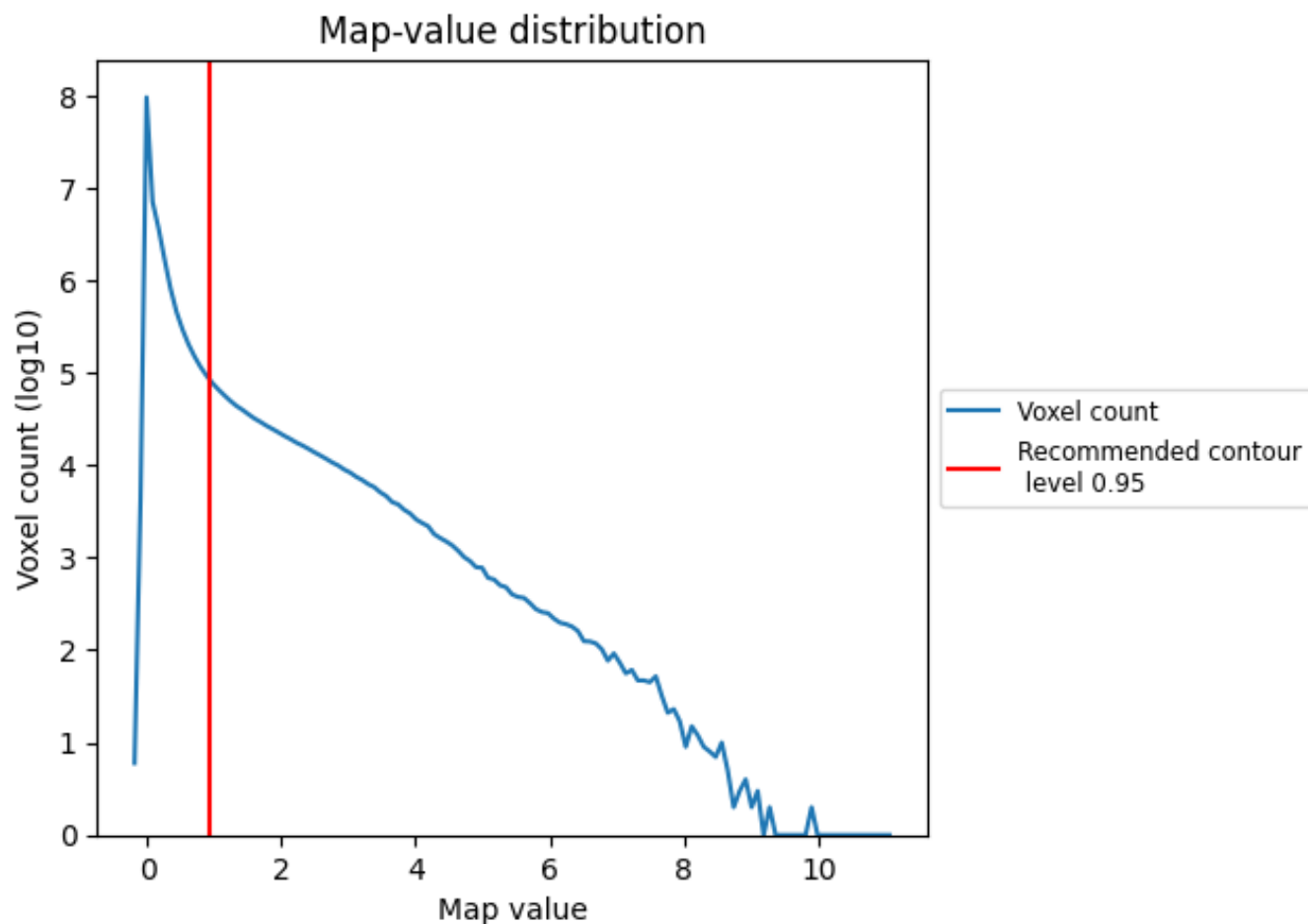


Z

7 Map analysis [i](#)

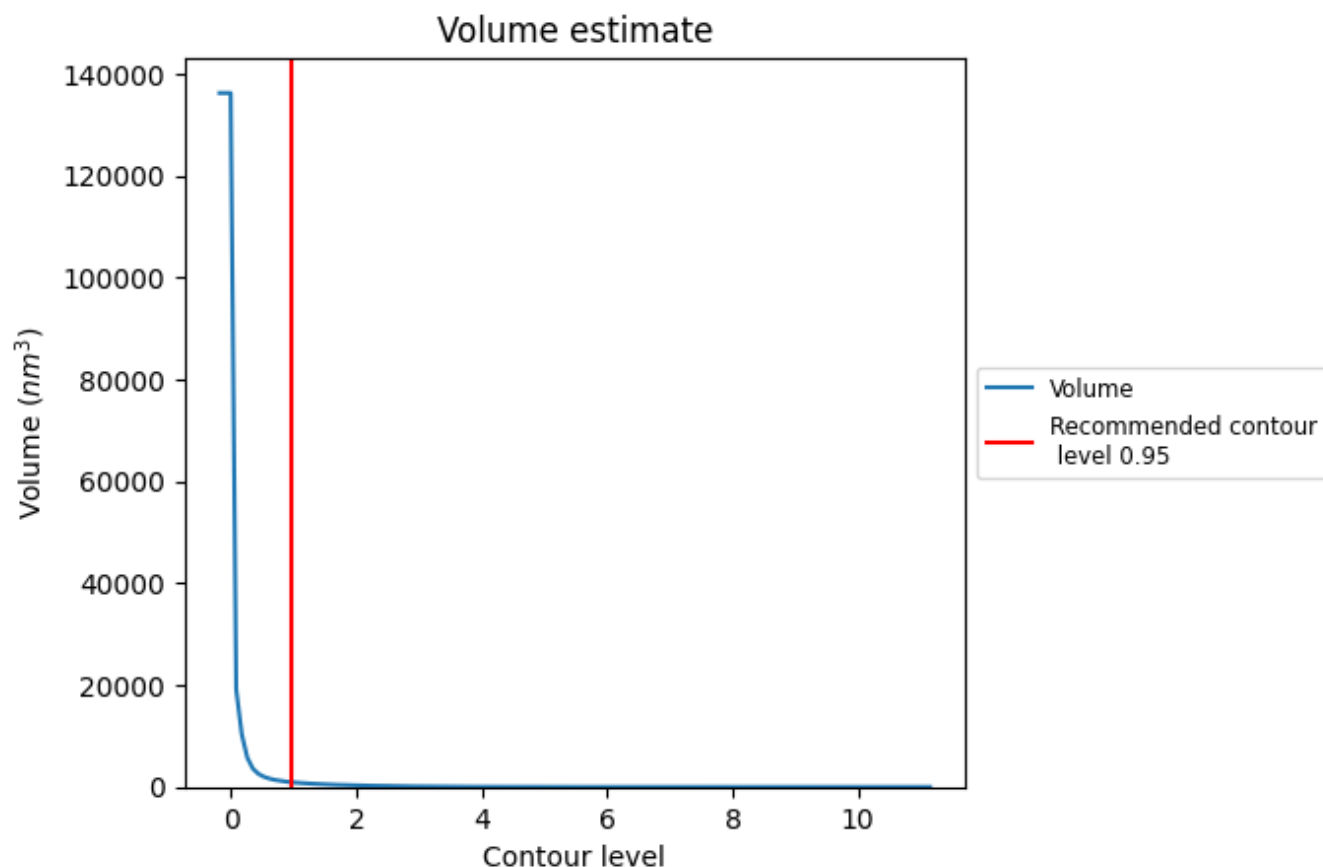
This section contains the results of statistical analysis of the map.

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.

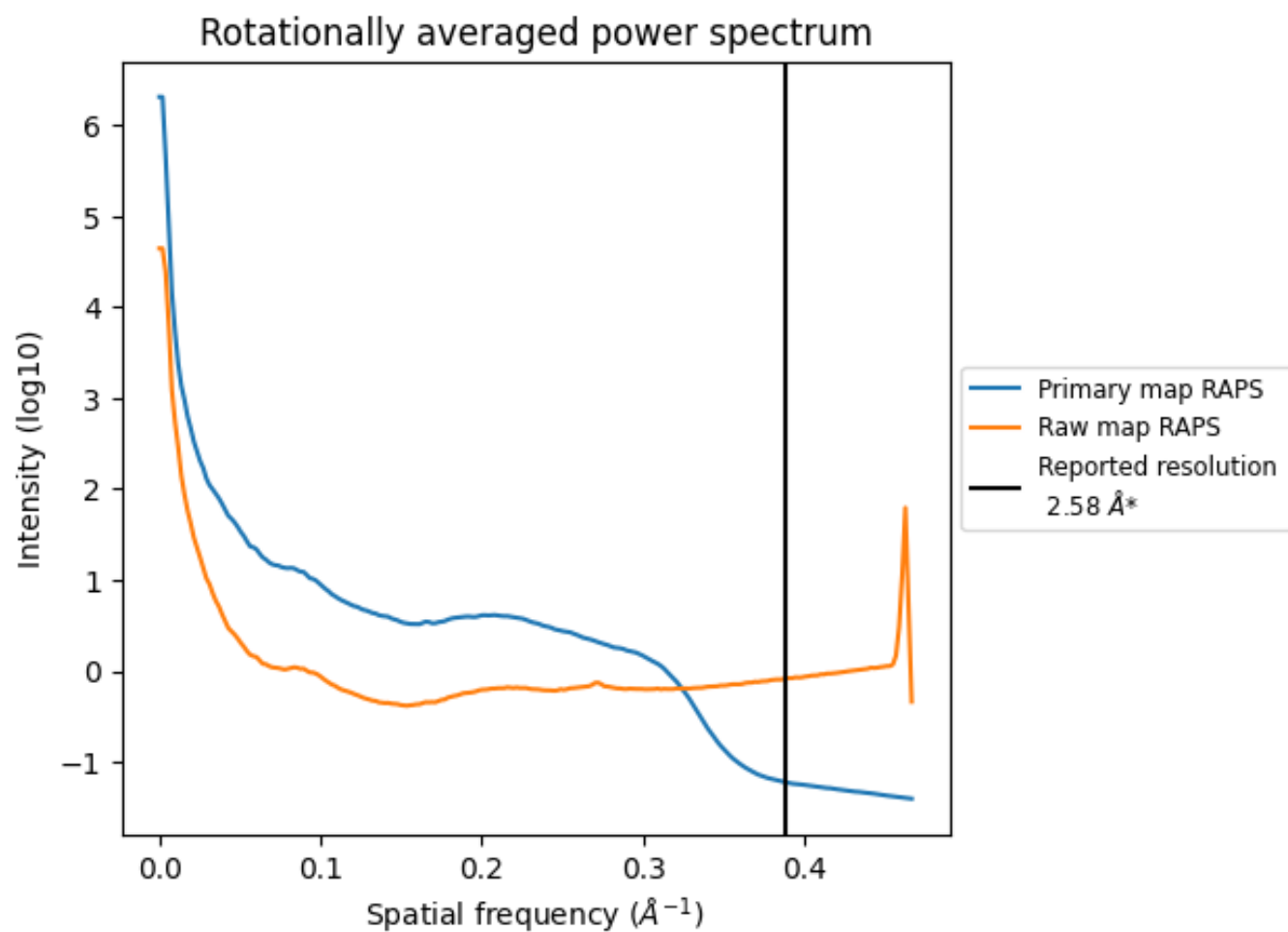
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 953 nm^3 ; this corresponds to an approximate mass of 861 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 ⓘ

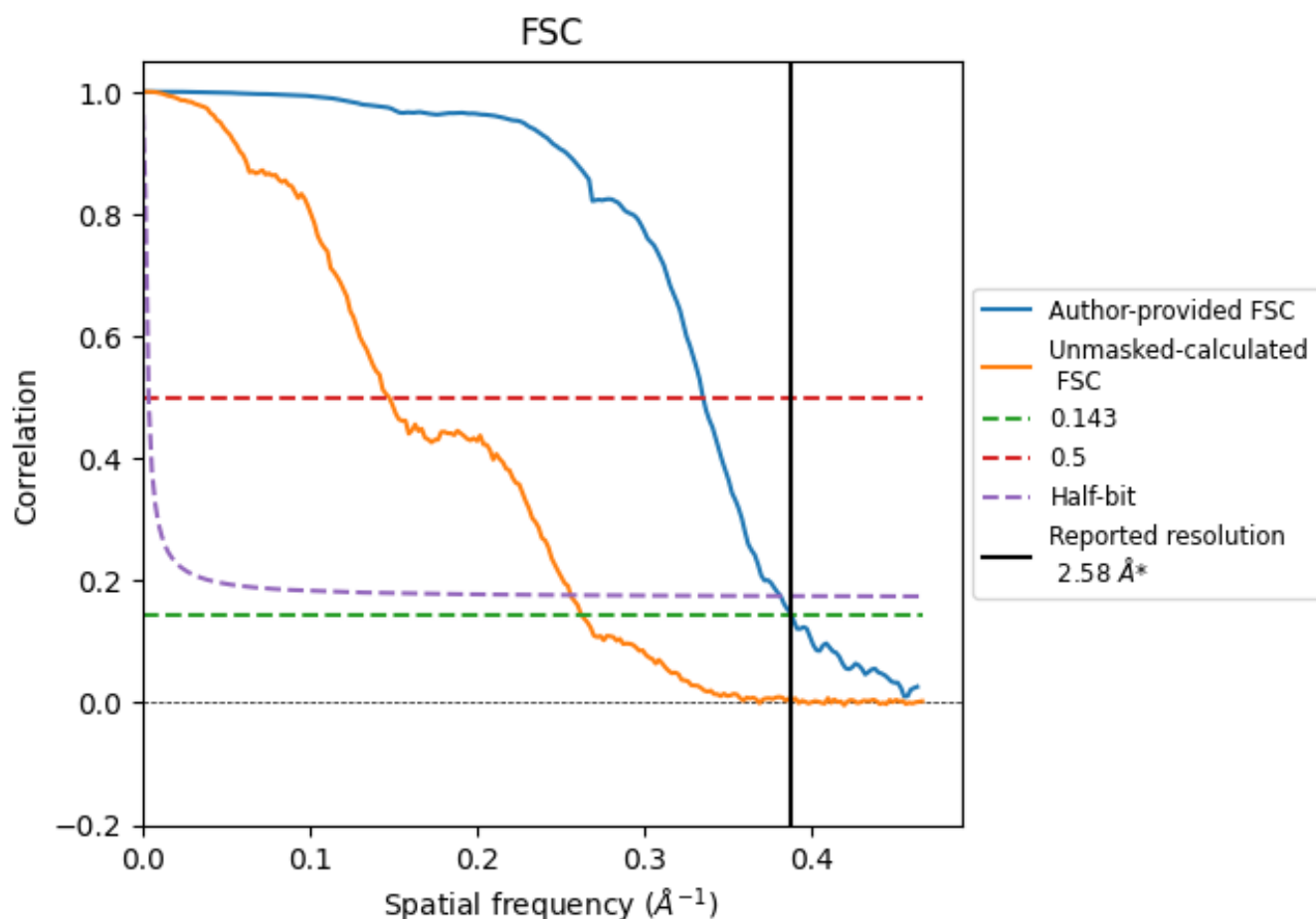


*Reported resolution corresponds to spatial frequency of 0.388 Å⁻¹

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 0.388 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

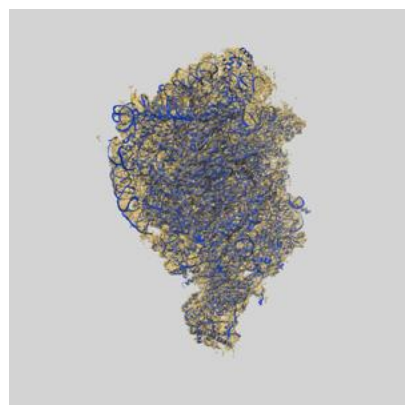
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.58	-	-
Author-provided FSC curve	2.58	2.98	2.62
Unmasked-calculated*	3.81	6.78	3.90

*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 3.81 differs from the reported value 2.58 by more than 10 %

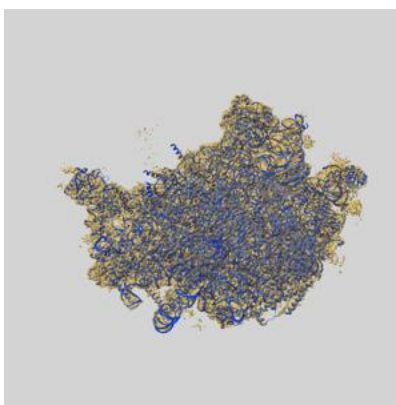
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29275 and PDB model 8FLD. Per-residue inclusion information can be found in section 3 on page 15.

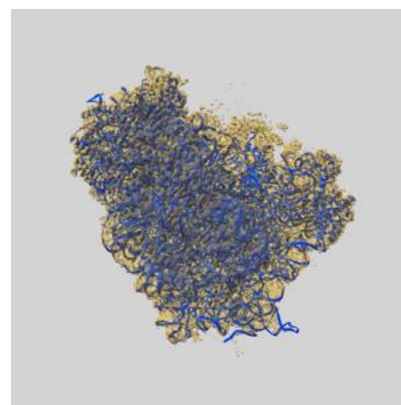
9.1 Map-model overlay [i](#)



X



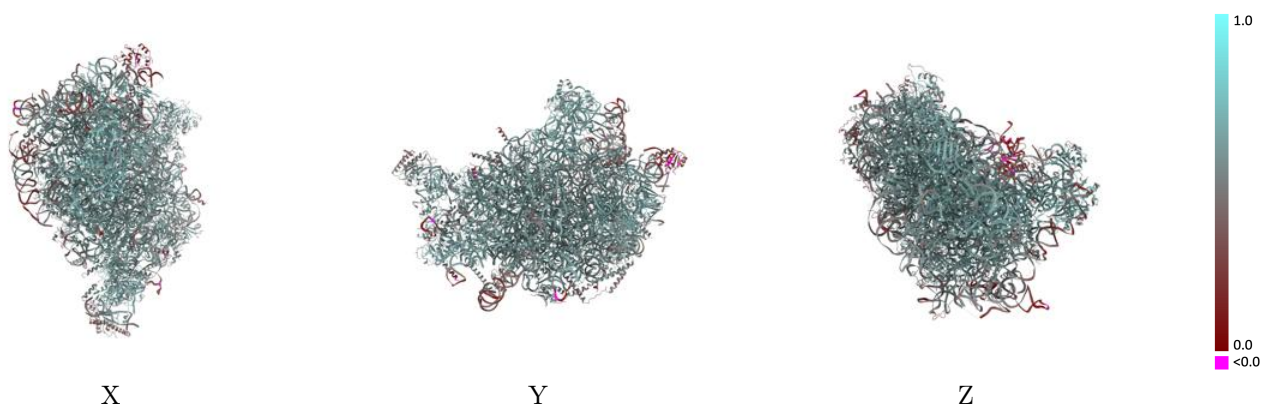
Y



Z

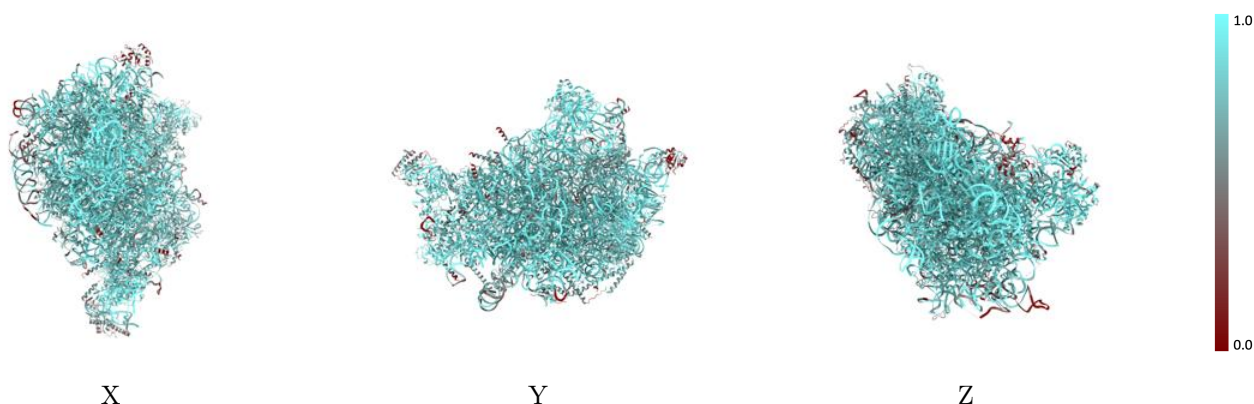
The images above show the 3D surface view of the map at the recommended contour level 0.95 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



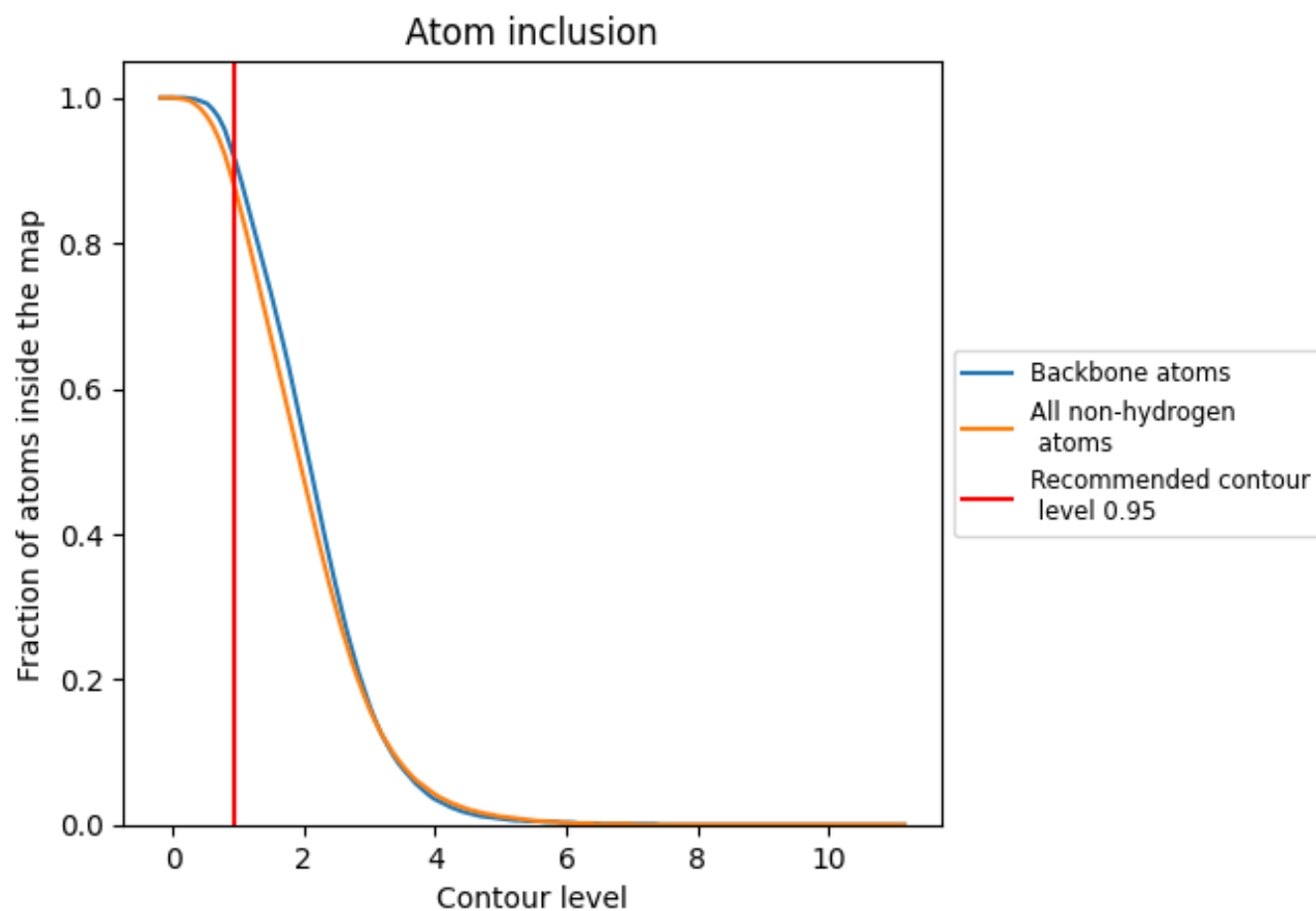
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.95).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 88% 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 (0.95) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8760	 0.5720
BE	 0.6410	 0.4570
L1	 0.9420	 0.6080
L2	 0.8700	 0.5540
L3	 0.9110	 0.5640
L4	 0.9910	 0.6370
L5	 0.8250	 0.5800
L6	 0.8080	 0.5640
L7	 0.9000	 0.6050
L8	 0.9130	 0.6070
L9	 0.9420	 0.6350
LA	 0.8630	 0.5860
LB	 0.8960	 0.6080
LC	 0.9620	 0.6470
LD	 0.8230	 0.5630
LE	 0.8980	 0.6140
LF	 0.7520	 0.5420
LG	 0.8620	 0.5980
LH	 0.8620	 0.6040
LI	 0.8170	 0.5720
LJ	 0.8760	 0.6020
LK	 0.9000	 0.6080
LL	 0.8610	 0.5790
LM	 0.7480	 0.5520
LN	 0.8560	 0.5850
LO	 0.7540	 0.5590
LP	 0.7990	 0.5580
LQ	 0.8660	 0.5940
LR	 0.8520	 0.5920
LS	 0.8210	 0.5810
LT	 0.8940	 0.6050
LU	 0.7710	 0.5530
LV	 0.8930	 0.6130
LW	 0.9170	 0.6140
LX	 0.7840	 0.5750



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
LY	 0.7270	 0.5350
LZ	 0.9080	 0.6090
NK	 0.6080	 0.5020
NL	 0.7570	 0.5540
NP	 0.7390	 0.5400
SA	 0.8730	 0.5920
SB	 0.8850	 0.6090
SC	 0.7680	 0.5410
SD	 0.8640	 0.5890
SE	 0.8690	 0.5980
SF	 0.8910	 0.6130
SG	 0.8860	 0.6030
SH	 0.7460	 0.5310
SI	 0.8450	 0.5860
SK	 0.8450	 0.5760
SL	 0.6710	 0.4970
SM	 0.9030	 0.6260
SQ	 0.3740	 0.2280
SR	 0.7000	 0.5120
SV	 0.7920	 0.5420