



Full wwPDB EM Validation Report ⓘ

Jun 26, 2026 – 02:37 AM EDT

PDB ID : 8FLC / pdb_00008flc
EMDB ID : EMD-29274
Title : Human nuclear pre-60S ribosomal subunit (State K3)
Authors : Vanden Broeck, A.; Klinge, S.
Deposited on : 2022-12-21
Resolution : 2.76 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:

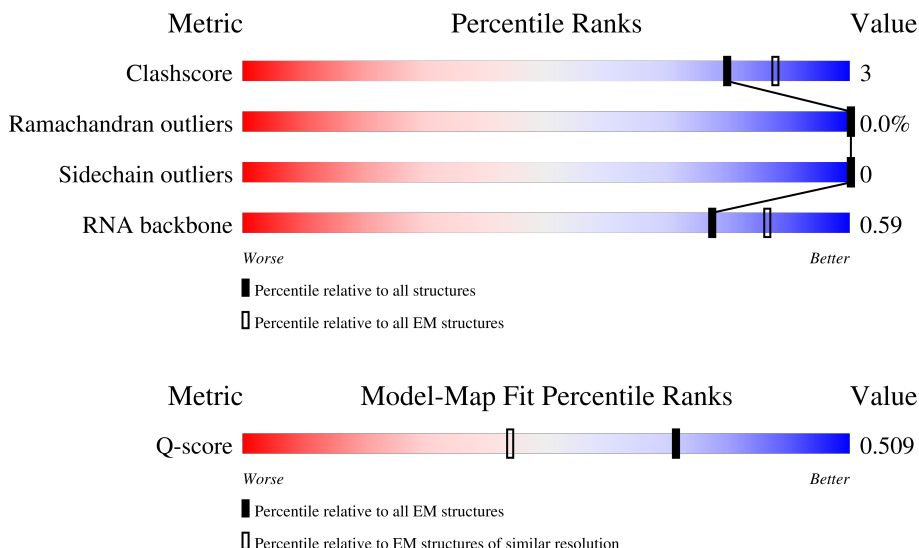
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.76 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.



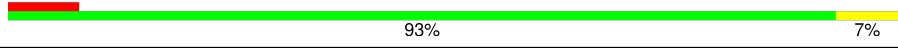
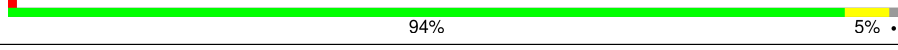
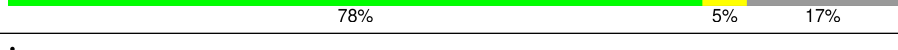
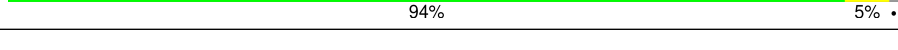
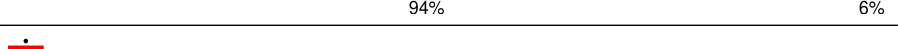
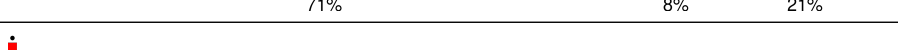
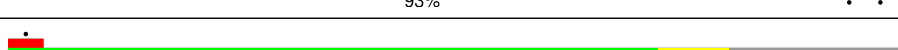
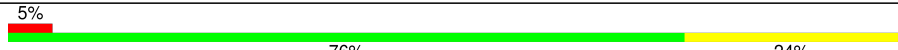
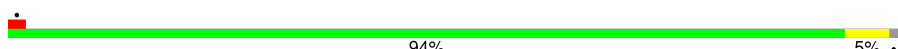
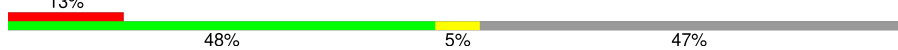
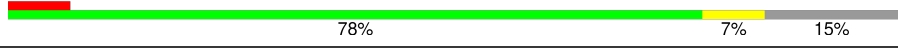
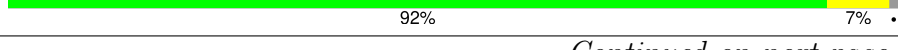
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10642 (2.26 - 3.26)

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	BA	165	
2	L1	157	
3	L3	5070	

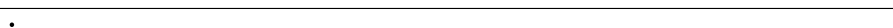
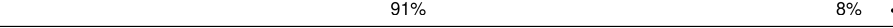
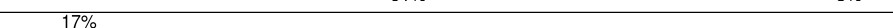
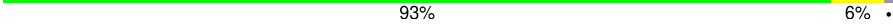
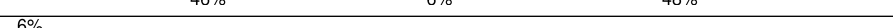
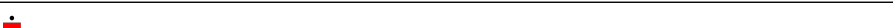
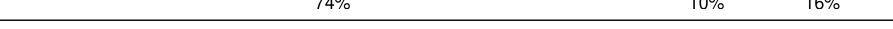
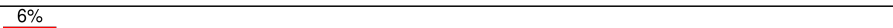
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	L4	121	
5	L5	178	
6	L6	211	
7	L7	203	
8	L8	215	
9	L9	204	
10	LA	184	
11	LB	188	
12	LC	176	
13	LD	196	
14	LE	160	
15	LF	128	
16	LG	140	
17	LH	156	
18	LI	145	
19	LJ	136	
20	LK	148	
21	LL	137	
22	LM	159	
23	LN	403	
24	LO	115	
25	LP	125	
26	LQ	135	
27	LR	117	
28	LS	123	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	LT	110	
30	LU	105	
31	LV	106	
32	LW	97	
33	LX	92	
34	LY	70	
35	LZ	51	
36	NK	129	
37	NP	134	
38	NR	203	
39	SA	427	
40	SB	297	
41	SC	288	
42	SD	248	
43	SE	266	
44	SF	257	
45	SG	192	
46	SK	245	
47	SQ	239	
48	SR	634	
49	SV	163	
50	VB	99	

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 139595 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 L12.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	BA	91	Total	C	N	O	0	0
			449	267	91	91		

- 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 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L3	3373	Total	C	N	O	P	0	0
			72412	32273	13268	23498	3373		

- Molecule 4 is a RNA chain called 5S rRNA.

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

- Molecule 5 is a protein called 60S ribosomal protein L11.

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

- Molecule 6 is a protein called 60S ribosomal protein L13.

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

- Molecule 7 is a protein called 60S ribosomal protein L13a.

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

- Molecule 8 is a protein called 60S ribosomal protein L14.

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

- Molecule 9 is a protein called 60S ribosomal protein L15.

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

- Molecule 10 is a protein called 60S ribosomal protein L17.

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

- Molecule 11 is a protein called 60S ribosomal protein L18.

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

- Molecule 12 is a protein called 60S ribosomal protein L18a.

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

- Molecule 13 is a protein called 60S ribosomal protein L19.

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

- Molecule 14 is a protein called 60S ribosomal protein L21.

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

- Molecule 15 is a protein called 60S ribosomal protein L22.

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

- Molecule 16 is a protein called 60S ribosomal protein L23.

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

- Molecule 17 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LH	117	Total	C	N	O	S	0	0
			958	612	179	166	1		

- Molecule 18 is a protein called 60S ribosomal protein L26.

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

- Molecule 19 is a protein called 60S ribosomal protein L27.

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

- Molecule 20 is a protein called 60S ribosomal protein L27a.

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

- Molecule 21 is a protein called 60S ribosomal protein L28.

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

- Molecule 22 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LM	85	Total	C	N	O	S	0	0
			699	437	152	107	3		

- Molecule 23 is a protein called 60S ribosomal protein L3.

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

- Molecule 24 is a protein called 60S ribosomal protein L30.

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

- Molecule 25 is a protein called 60S ribosomal protein L31.

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

- Molecule 26 is a protein called 60S ribosomal protein L32.

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

- Molecule 27 is a protein called 60S ribosomal protein L34.

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

- Molecule 28 is a protein called 60S ribosomal protein L35.

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

- Molecule 29 is a protein called 60S ribosomal protein L35a.

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

- Molecule 30 is a protein called 60S ribosomal protein L36.

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

- Molecule 31 is a protein called 60S ribosomal protein L36a.

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

- Molecule 32 is a protein called 60S ribosomal protein L37.

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

- Molecule 33 is a protein called 60S ribosomal protein L37a.

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

- Molecule 34 is a protein called 60S ribosomal protein L38.

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

- Molecule 35 is a protein called 60S ribosomal protein L39.

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

- Molecule 36 is a protein called Protein LLP homolog.

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

- Molecule 37 is a protein called Zinc finger protein 593.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	NP	104	Total	C	N	O	S	0	0
			847	520	178	145	4		

- Molecule 38 is a protein called Translation machinery-associated protein 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	NR	152	Total	C	N	O	P	S	
			1299	809	249	235	1	5	0

- Molecule 39 is a protein called 60S ribosomal protein L4.

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

- Molecule 40 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	SB	275	Total	C	N	O	S	0	0
			2243	1419	406	404	14		

- Molecule 41 is a protein called 60S ribosomal protein L6.

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

- Molecule 42 is a protein called 60S ribosomal protein L7.

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

- Molecule 43 is a protein called 60S ribosomal protein L7a.

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

- Molecule 44 is a protein called 60S ribosomal protein L8.

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

- Molecule 45 is a protein called 60S ribosomal protein L9.

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

- Molecule 46 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	SK	244	Total	C	N	O	S	0	0
			1852	1149	318	372	13		

- Molecule 47 is a protein called mRNA turnover protein 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	SQ	127	Total	C	N	O		0	0
			650	388	132	130			

- Molecule 48 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SR	601	Total	C	N	O	S	0	0
			4932	3105	899	902	26		

- Molecule 49 is a protein called Probable ribosome biogenesis protein RLP24.

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

- Molecule 50 is a protein called Leydig cell tumor 10 kDa protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	VB	58	Total	C	N	O	S	0	0
			455	285	95	74	1		

- Molecule 51 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
51	L1	3	Total	Mg	0
			3	3	
51	L3	74	Total	Mg	0
			74	74	
51	L4	3	Total	Mg	0
			3	3	
51	LG	1	Total	Mg	0
			1	1	
51	LN	1	Total	Mg	0
			1	1	
51	LQ	1	Total	Mg	0
			1	1	
51	LR	1	Total	Mg	0
			1	1	
51	LT	1	Total	Mg	0
			1	1	
51	LW	1	Total	Mg	0
			1	1	
51	SF	1	Total	Mg	0
			1	1	
51	SR	1	Total	Mg	0
			1	1	

- Molecule 52 is ZINC ION (CCD ID: ZN) (formula: Zn).

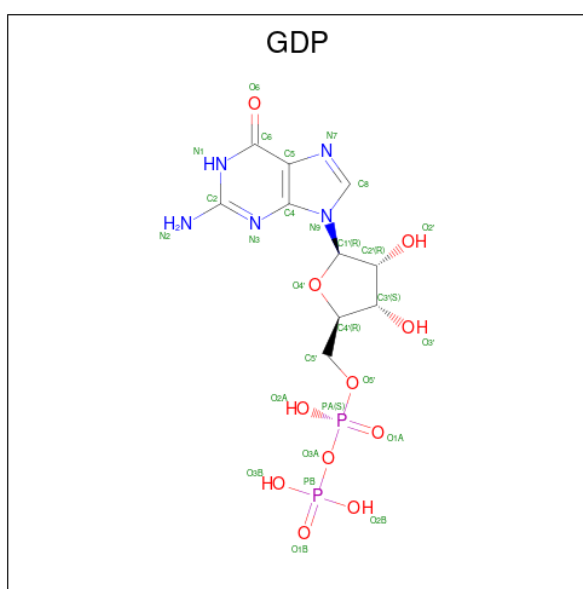
Mol	Chain	Residues	Atoms		AltConf
52	LR	1	Total	Zn	0
			1	1	
52	LV	1	Total	Zn	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
52	LW	1	Total	Zn	0
			1	1	
52	LX	1	Total	Zn	0
			1	1	
52	NP	1	Total	Zn	0
			1	1	
52	SV	1	Total	Zn	0
			1	1	

- Molecule 53 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
53	SR	1	Total	C	N	O	P	0
			28	10	5	11	2	

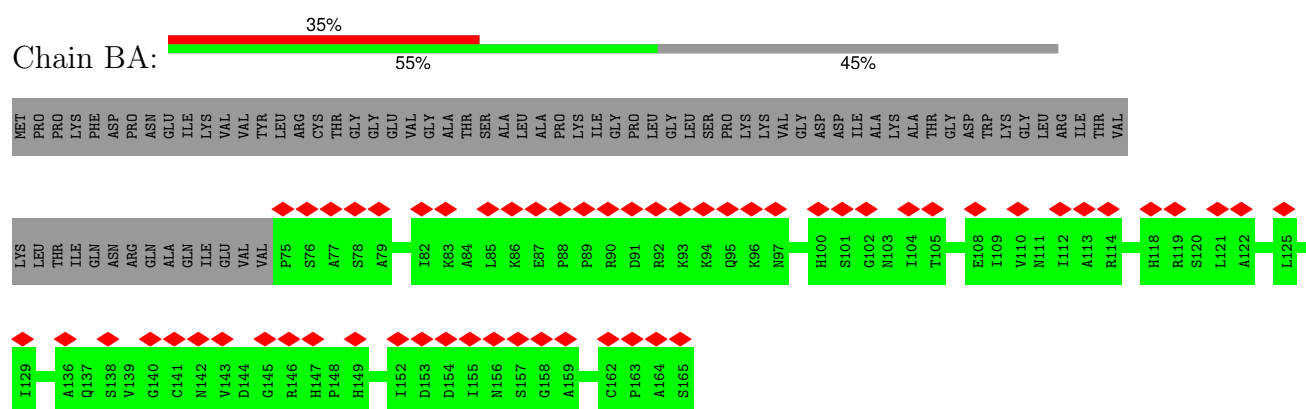
- Molecule 54 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
54	SR	1	Total	K	0
			1	1	

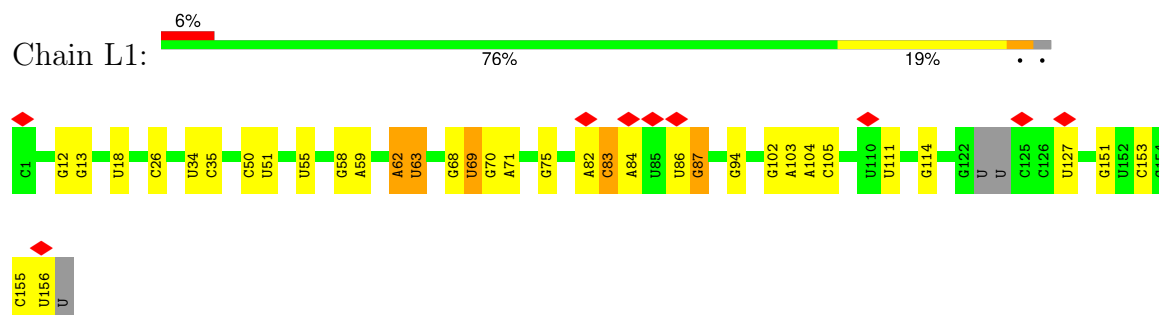
3 Residue-property plots [i](#)

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.

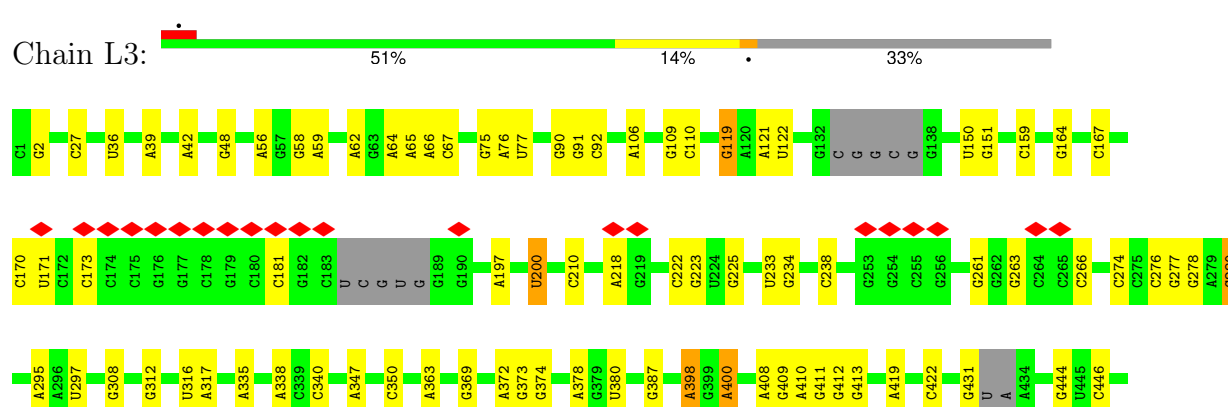
• Molecule 1: 60S ribosomal protein L12



• Molecule 2: 5.8S rRNA



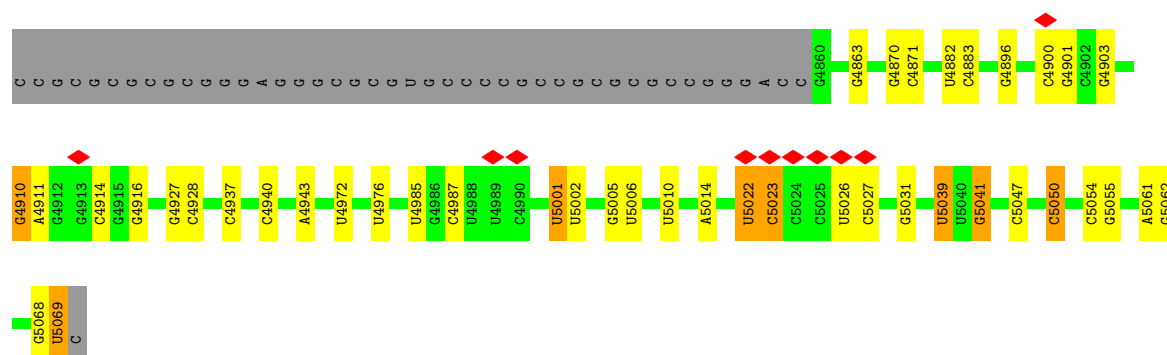
• Molecule 3: 28S rRNA



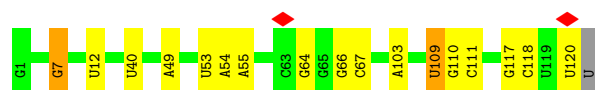
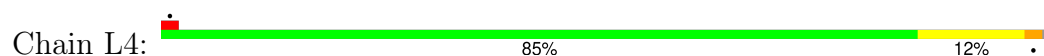




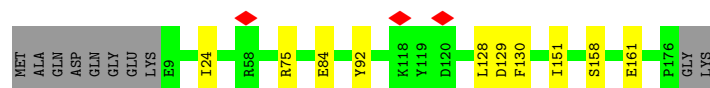
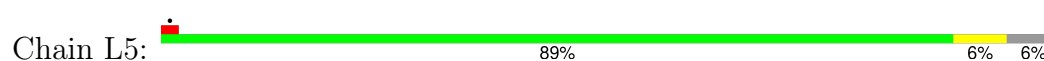




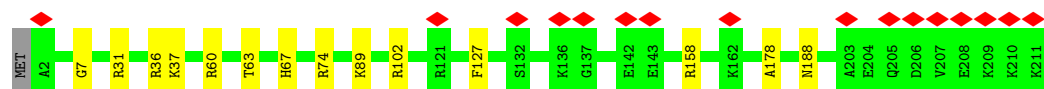
• Molecule 4: 5S rRNA



• Molecule 5: 60S ribosomal protein L11



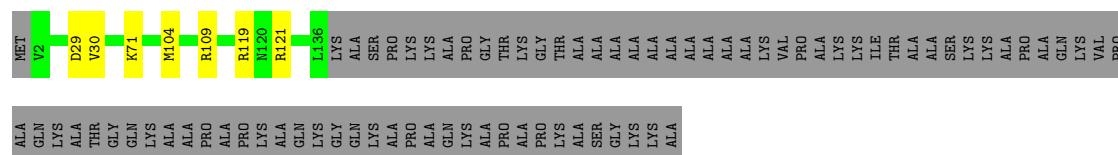
• Molecule 6: 60S ribosomal protein L13



• Molecule 7: 60S ribosomal protein L13a

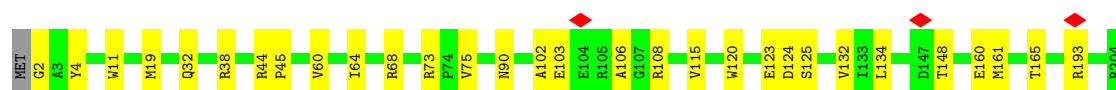


• Molecule 8: 60S ribosomal protein L14



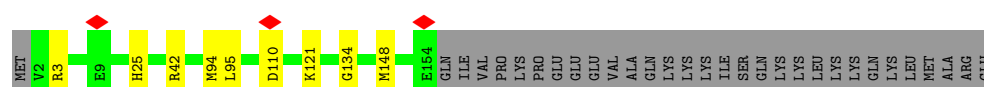
- Molecule 9: 60S ribosomal protein L15

Chain L9:  85% 15%

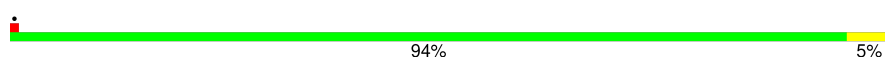


- Molecule 10: 60S ribosomal protein L17

Chain LA:  78% 5% 17%

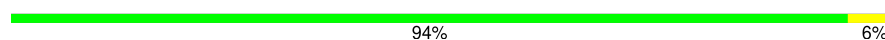


- Molecule 11: 60S ribosomal protein L18

Chain LB:  94% 5%



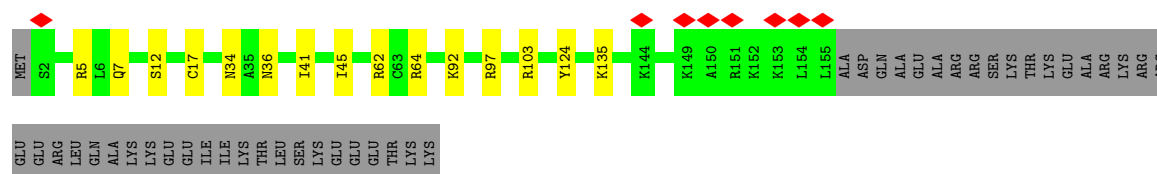
- Molecule 12: 60S ribosomal protein L18a

Chain LC:  94% 6%

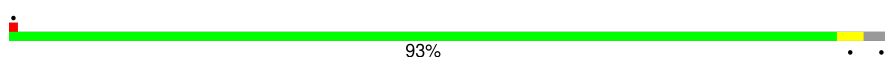


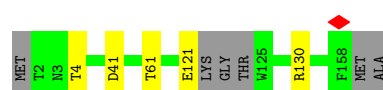
- Molecule 13: 60S ribosomal protein L19

Chain LD:  71% 8% 21%



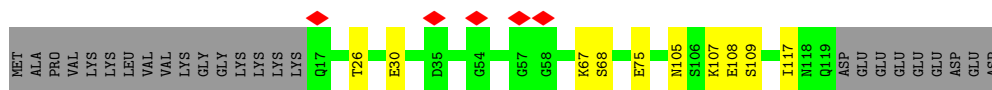
- Molecule 14: 60S ribosomal protein L21

Chain LE:  93%



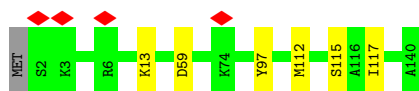
- Molecule 15: 60S ribosomal protein L22

Chain LF:  73% 8% 20%



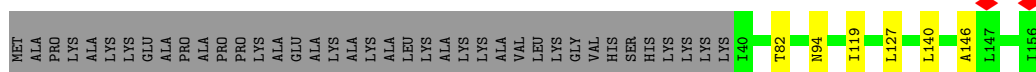
- Molecule 16: 60S ribosomal protein L23

Chain LG: 95%



- Molecule 17: 60S ribosomal protein L23a

Chain LH: 71% 25%



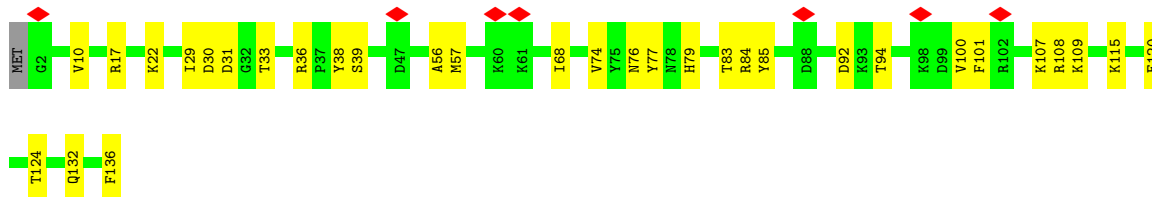
- Molecule 18: 60S ribosomal protein L26

Chain LI: 7% 81% 12% 8%



- Molecule 19: 60S ribosomal protein L27

Chain LJ: 5% 76% 24%



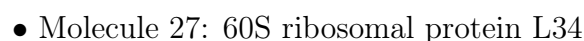
- Molecule 20: 60S ribosomal protein L27a

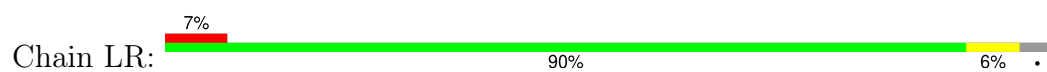
Chain LK: 94% 5%



- Molecule 21: 60S ribosomal protein L28

Chain LL: 6% 88% 9%





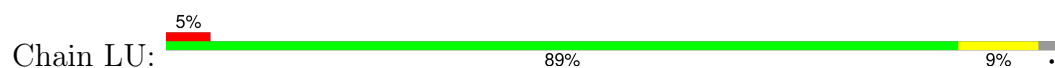
- Molecule 28: 60S ribosomal protein L35



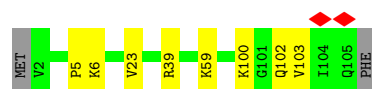
- Molecule 29: 60S ribosomal protein L35a



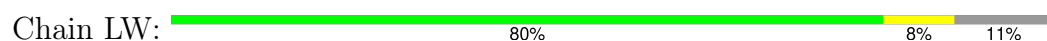
- Molecule 30: 60S ribosomal protein L36



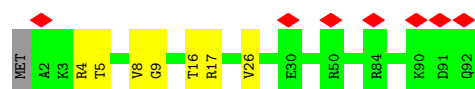
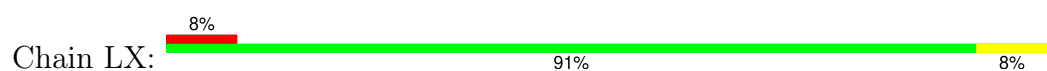
- Molecule 31: 60S ribosomal protein L36a



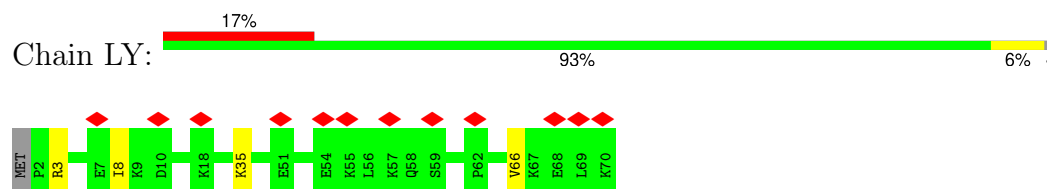
- Molecule 32: 60S ribosomal protein L37



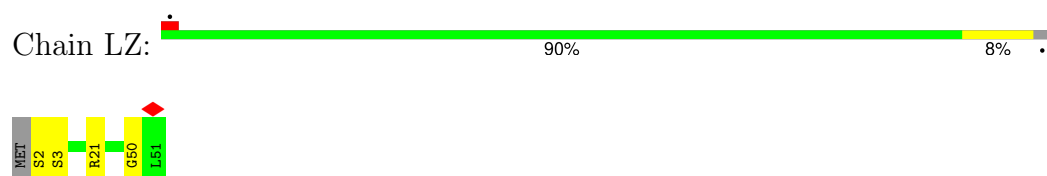
- Molecule 33: 60S ribosomal protein L37a



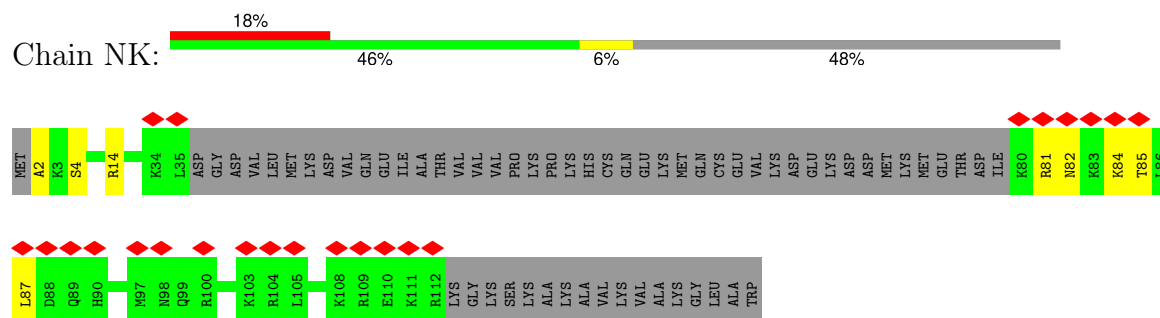
- Molecule 34: 60S ribosomal protein L38



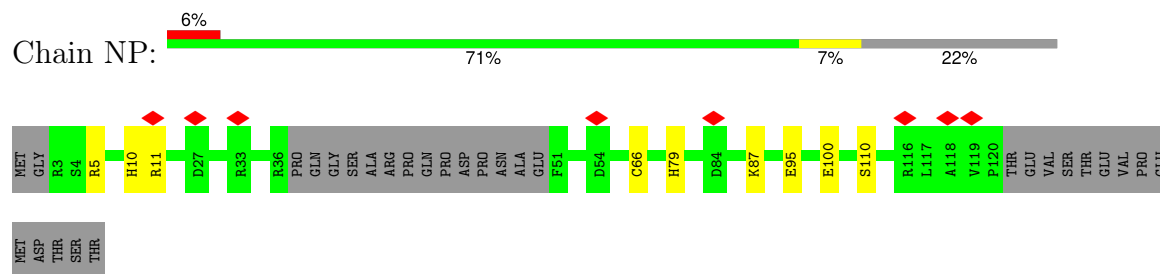
- Molecule 35: 60S ribosomal protein L39



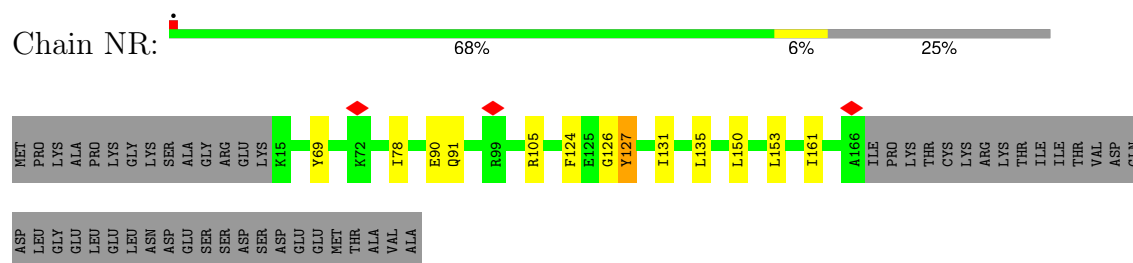
- Molecule 36: Protein LLP homolog



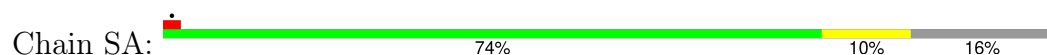
- Molecule 37: Zinc finger protein 593

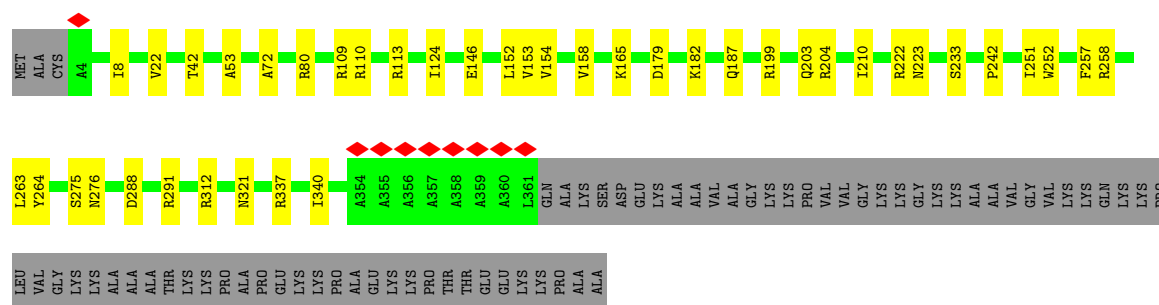


- Molecule 38: Translation machinery-associated protein 16

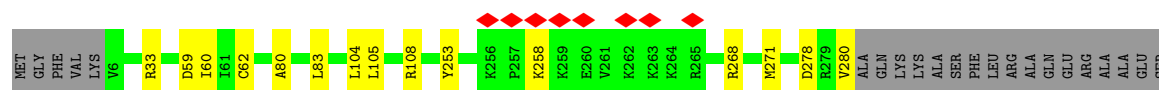


- Molecule 39: 60S ribosomal protein L4

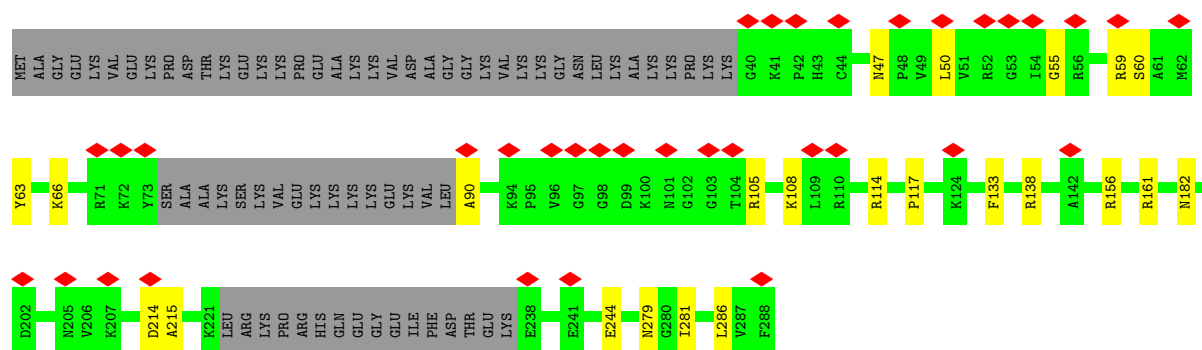




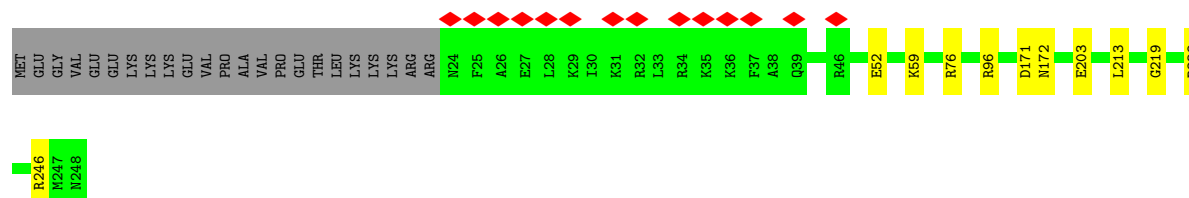
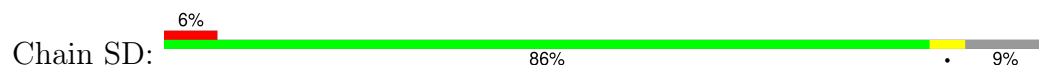
- Molecule 40: 60S ribosomal protein L5



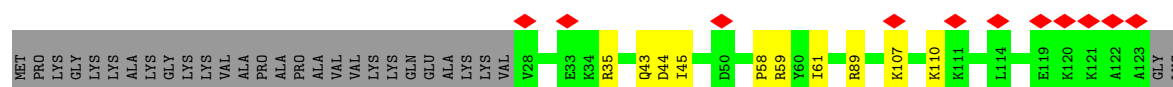
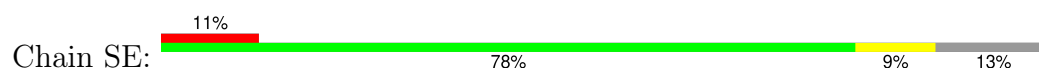
- Molecule 41: 60S ribosomal protein L6



- Molecule 42: 60S ribosomal protein L7



- Molecule 43: 60S ribosomal protein L7a





- Molecule 44: 60S ribosomal protein L8

Chain SF: 89% 7% 5%



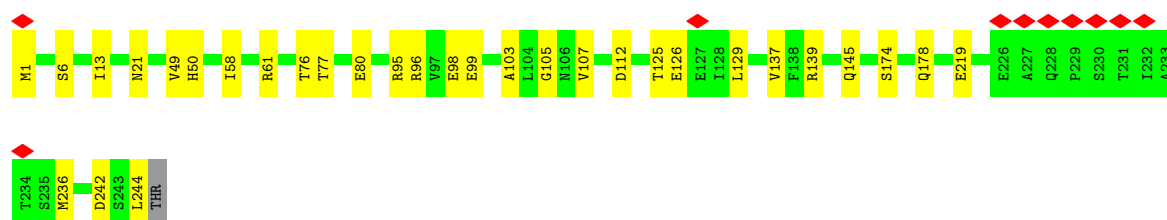
- Molecule 45: 60S ribosomal protein L9

Chain SG: 87% 12% .



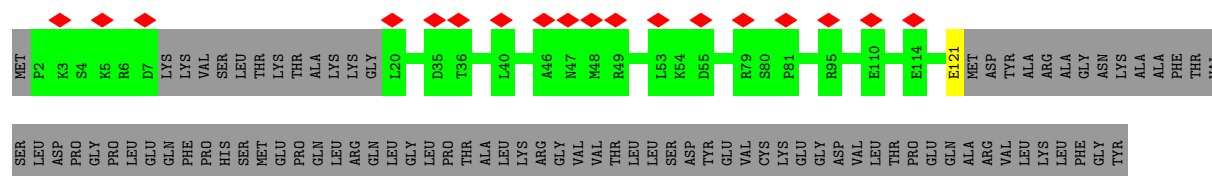
- Molecule 46: Eukaryotic translation initiation factor 6

Chain SK: 87% 13%



- Molecule 47: mRNA turnover protein 4 homolog

Chain SQ: 9% 52% 47%

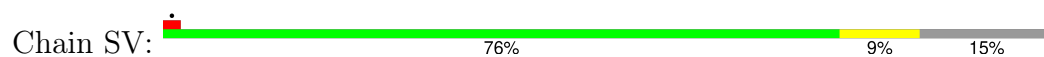


- Molecule 48: GTP-binding protein 4

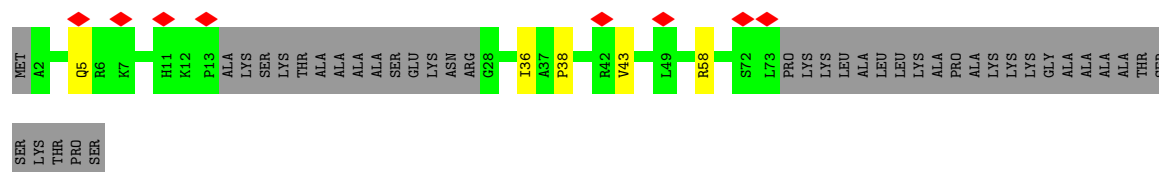
Chain SR: 7% 89% 6% 5%



- Molecule 49: Probable ribosome biogenesis protein RLP24



- Molecule 50: Leydig cell tumor 10 kDa protein homolog



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	20809	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	10.151	Depositor
Minimum map value	-1.391	Depositor
Average map value	0.052	Depositor
Map value standard deviation	0.177	Depositor
Recommended contour level	0.85	Depositor
Map size (Å)	514.56, 514.56, 514.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: PTR, OMU, A2M, OMC, UR3, K, 6MZ, MG, HIC, OMG, PSU, ZN, GDP, 1MA

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	BA	0.09	0/448	0.25	0/622
2	L1	0.10	0/3589	0.23	0/5589
3	L3	0.14	0/78513	0.26	0/122457
4	L4	0.14	0/2861	0.26	0/4459
5	L5	0.13	0/1372	0.31	0/1836
6	L6	0.12	0/1732	0.28	0/2315
7	L7	0.13	0/1682	0.29	0/2250
8	L8	0.13	0/1133	0.26	0/1516
9	L9	0.11	0/1746	0.25	0/2338
10	LA	0.12	0/1268	0.29	0/1701
11	LB	0.11	0/1536	0.28	0/2052
12	LC	0.14	0/1501	0.29	0/2013
13	LD	0.10	0/1305	0.25	0/1727
14	LE	0.14	0/1291	0.34	0/1724
15	LF	0.14	0/856	0.30	0/1149
16	LG	0.13	0/1048	0.33	0/1402
17	LH	0.10	0/975	0.26	0/1312
18	LI	0.11	0/1132	0.26	0/1504
19	LJ	0.11	0/1130	0.27	0/1507
20	LK	0.12	0/1191	0.28	0/1591
21	LL	0.09	0/1017	0.26	0/1364
22	LM	0.13	0/710	0.29	0/935
23	LN	0.11	0/3294	0.28	0/4406
24	LO	0.12	0/748	0.28	0/1004
25	LP	0.12	0/894	0.27	0/1204
26	LQ	0.11	0/1071	0.29	0/1429
27	LR	0.10	0/898	0.27	0/1197
28	LS	0.09	0/1023	0.23	0/1351
29	LT	0.11	0/895	0.28	0/1198
30	LU	0.10	0/843	0.23	0/1115
31	LV	0.13	0/864	0.29	0/1140
32	LW	0.11	0/720	0.30	0/952

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	LX	0.10	0/718	0.27	0/953
34	LY	0.10	0/575	0.27	0/761
35	LZ	0.11	0/454	0.25	0/599
36	NK	0.20	0/587	0.36	0/767
37	NP	0.12	0/864	0.27	0/1154
38	NR	0.11	0/1306	0.27	0/1740
39	SA	0.12	0/2907	0.28	0/3905
40	SB	0.13	0/2287	0.29	0/3065
41	SC	0.12	0/1781	0.28	0/2388
42	SD	0.11	0/1905	0.27	0/2539
43	SE	0.11	0/1903	0.28	0/2559
44	SF	0.13	0/1914	0.31	0/2567
45	SG	0.13	0/1537	0.27	0/2066
46	SK	0.12	0/1877	0.31	0/2554
47	SQ	0.09	0/648	0.25	0/894
48	SR	0.11	0/5014	0.26	0/6727
49	SV	0.12	0/1207	0.27	0/1600
50	VB	0.09	0/459	0.24	0/605
All	All	0.13	0/147229	0.27	0/215802

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BA	449	0	207	0	0
2	L1	3278	0	1665	19	0
3	L3	72412	0	36680	349	0
4	L4	2561	0	1295	7	0
5	L5	1349	0	1383	7	0
6	L6	1701	0	1818	13	0
7	L7	1650	0	1794	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	L8	1111	0	1174	5	0
9	L9	1701	0	1749	23	0
10	LA	1242	0	1269	8	0
11	LB	1512	0	1628	9	0
12	LC	1461	0	1502	11	0
13	LD	1289	0	1429	13	0
14	LE	1264	0	1328	4	0
15	LF	842	0	864	7	0
16	LG	1034	0	1097	4	0
17	LH	958	0	1027	4	0
18	LI	1115	0	1205	12	0
19	LJ	1107	0	1182	22	0
20	LK	1162	0	1213	7	0
21	LL	1002	0	1068	5	0
22	LM	699	0	758	7	0
23	LN	3239	0	3377	32	0
24	LO	738	0	774	3	0
25	LP	879	0	924	6	0
26	LQ	1053	0	1147	12	0
27	LR	888	0	977	6	0
28	LS	1015	0	1148	8	0
29	LT	876	0	912	6	0
30	LU	832	0	917	7	0
31	LV	851	0	920	6	0
32	LW	705	0	737	7	0
33	LX	708	0	756	6	0
34	LY	569	0	637	5	0
35	LZ	444	0	483	4	0
36	NK	581	0	656	9	0
37	NP	847	0	854	8	0
38	NR	1299	0	1318	8	0
39	SA	2853	0	3028	32	0
40	SB	2243	0	2268	11	0
41	SC	1747	0	1897	20	0
42	SD	1870	0	1996	9	0
43	SE	1869	0	2014	18	0
44	SF	1876	0	1970	15	0
45	SG	1518	0	1601	15	0
46	SK	1852	0	1828	19	0
47	SQ	650	0	308	1	0
48	SR	4932	0	5072	30	0
49	SV	1184	0	1248	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	VB	455	0	504	4	0
51	L1	3	0	0	0	0
51	L3	74	0	0	0	0
51	L4	3	0	0	0	0
51	LG	1	0	0	0	0
51	LN	1	0	0	0	0
51	LQ	1	0	0	0	0
51	LR	1	0	0	0	0
51	LT	1	0	0	0	0
51	LW	1	0	0	0	0
51	SF	1	0	0	0	0
51	SR	1	0	0	0	0
52	LR	1	0	0	0	0
52	LV	1	0	0	0	0
52	LW	1	0	0	0	0
52	LX	1	0	0	0	0
52	NP	1	0	0	0	0
52	SV	1	0	0	0	0
53	SR	28	0	12	0	0
54	SR	1	0	0	0	0
All	All	139595	0	103618	643	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 3.

All (643) 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)
36:NK:81:ARG:NH2	36:NK:85:THR:OG1	2.02	0.93
9:L9:64:ILE:HD11	9:L9:106:ALA:HB2	1.49	0.93
3:L3:4903:G:OP1	36:NK:82:ASN:ND2	2.04	0.90
6:L6:60:ARG:NH2	6:L6:67:HIS:O	2.10	0.85
3:L3:2520:C:O2	3:L3:2640:G:N2	2.11	0.83
37:NP:66:CYS:SG	37:NP:79:HIS:CE1	2.69	0.82
4:L4:40:U:O2	5:L5:75:ARG:NH1	2.13	0.81
3:L3:1280:C:O2'	39:SA:321:ASN:OD1	1.99	0.80
3:L3:308:G:OP2	3:L3:308:G:N2	2.11	0.80
19:LJ:92:ASP:OD2	19:LJ:94:THR:OG1	1.98	0.80
2:L1:62:A:OP1	28:LS:52:LYS:NZ	2.15	0.80
3:L3:3641:U:OP2	3:L3:3646:A:N6	2.14	0.79
3:L3:3928:A:OP1	9:L9:90:ASN:ND2	2.16	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L3:1480:C:O2'	3:L3:1482:G:OP2	1.98	0.79
3:L3:1853:G:O2'	3:L3:1854:G:OP2	2.00	0.78
3:L3:1883:G:OP1	26:LQ:47:ARG:NH2	2.16	0.78
3:L3:3748:A:HO2'	44:SF:223:SER:HG	1.28	0.78
15:LF:105:ASN:OD1	15:LF:109:SER:OG	2.02	0.78
3:L3:2553:A:OP2	3:L3:2574:G:O2'	2.01	0.77
27:LR:82:MET:HE1	27:LR:90:ARG:HE	1.50	0.77
2:L1:12:G:OP1	10:LA:3:ARG:NH1	2.18	0.77
2:L1:63:U:OP1	28:LS:48:ARG:NH2	2.18	0.77
3:L3:4688:C:O2'	45:SG:155:SER:OG	1.99	0.77
29:LT:14:TYR:OH	29:LT:92:LEU:O	2.03	0.77
3:L3:277:G:OP2	30:LU:29:ARG:NH2	2.18	0.77
3:L3:1397:A:HO2'	3:L3:1467:C:HO2'	1.32	0.77
3:L3:2407:G:N2	3:L3:2407:G:OP2	2.17	0.76
3:L3:4128:A:O2'	43:SE:35:ARG:NH1	2.19	0.76
39:SA:109:ARG:CG	39:SA:109:ARG:O	2.33	0.76
3:L3:422:C:O2'	10:LA:121:LYS:NZ	2.18	0.76
3:L3:4314:C:O2'	22:LM:36:ASP:OD1	2.04	0.76
2:L1:51:U:OP2	35:LZ:21:ARG:NH2	2.19	0.76
41:SC:161:ARG:O	41:SC:182:ASN:ND2	2.17	0.76
3:L3:4768:G:OP1	7:L7:168:TYR:OH	2.04	0.76
3:L3:695:G:O2'	3:L3:697:G:OP2	2.04	0.75
9:L9:32:GLN:O	43:SE:59:ARG:NH2	2.20	0.75
48:SR:244:LEU:O	48:SR:282:LYS:NZ	2.19	0.75
13:LD:12:SER:OG	13:LD:17:CYS:O	2.03	0.74
3:L3:4120:U:O2'	3:L3:4121:G:OP1	2.04	0.74
3:L3:1185:G:O2'	40:SB:278:ASP:OD1	2.04	0.74
28:LS:10:ARG:NH2	28:LS:63:GLN:OE1	2.20	0.74
2:L1:75:OMG:OP2	18:LI:74:TYR:OH	2.05	0.74
3:L3:2448:G:O2'	44:SF:21:LYS:NZ	2.17	0.74
3:L3:4541:G:N2	3:L3:4544:A:OP2	2.19	0.74
3:L3:1397:A:O2'	3:L3:1467:C:O2'	2.03	0.74
3:L3:67:C:OP2	3:L3:312:G:N2	2.20	0.74
3:L3:110:C:OP1	6:L6:89:LYS:NZ	2.20	0.74
3:L3:1508:A:OP1	39:SA:110:ARG:NH2	2.21	0.74
3:L3:1931:C:N4	3:L3:2039:G:OP2	2.20	0.74
3:L3:295:A:OP2	31:LV:39:ARG:NH1	2.21	0.73
3:L3:122:U:O4	43:SE:107:LYS:NZ	2.19	0.73
3:L3:4717:A:OP2	23:LN:30:LYS:NZ	2.21	0.72
2:L1:153:C:OP1	43:SE:185:LYS:NZ	2.23	0.72
3:L3:62:A:N3	3:L3:77:U:O2'	2.20	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L3:1573:G:OP1	13:LD:92:LYS:NZ	2.23	0.72
48:SR:600:MET:HE1	48:SR:608:GLU:HA	1.71	0.72
5:L5:158:SER:OG	5:L5:161:GLU:OE1	2.02	0.71
3:L3:2545:U:O2'	3:L3:2547:G:N7	2.21	0.71
3:L3:2848:G:O2'	3:L3:3838:U:O4	2.04	0.71
3:L3:502:C:O2'	3:L3:503:C:OP1	2.04	0.71
4:L4:7:G:OP1	40:SB:33:ARG:NH1	2.23	0.71
5:L5:84:GLU:OE2	5:L5:92:TYR:OH	2.09	0.71
46:SK:98:GLU:OE2	49:SV:74:ARG:NH2	2.24	0.71
3:L3:2841:G:OP1	37:NP:10:HIS:NE2	2.24	0.71
3:L3:1177:U:O2'	40:SB:280:VAL:O	2.08	0.71
3:L3:1314:C:O2'	26:LQ:24:GLN:NE2	2.25	0.70
3:L3:75:G:OP2	6:L6:102:ARG:NH1	2.25	0.70
3:L3:369:G:N2	3:L3:372:A:OP2	2.23	0.70
3:L3:2856:C:O2	23:LN:242:ARG:NH2	2.25	0.70
3:L3:1323:A:O2'	3:L3:1325:C:OP2	2.10	0.69
3:L3:2588:C:OP1	3:L3:2768:C:O2'	2.09	0.69
7:L7:202:LEU:O	7:L7:202:LEU:HD23	1.92	0.69
3:L3:1322:1MA:O2'	3:L3:1323:A:O4'	2.11	0.69
3:L3:1646:A:O2'	32:LW:49:TRP:O	2.10	0.69
3:L3:5002:U:OP2	23:LN:385:LYS:NZ	2.24	0.69
39:SA:337:ARG:NH1	41:SC:55:GLY:O	2.26	0.69
3:L3:979:C:OP2	41:SC:66:LYS:NZ	2.18	0.69
3:L3:4476:C:O2'	45:SG:173:ARG:NH2	2.26	0.69
3:L3:1814:C:O2'	22:LM:42:ASN:OD1	2.10	0.69
32:LW:48:ASN:OD1	32:LW:54:LYS:NZ	2.20	0.69
3:L3:1433:A:N6	3:L3:1451:G:O2'	2.26	0.68
39:SA:179:ASP:OD1	39:SA:204:ARG:NH2	2.27	0.68
3:L3:200:U:O4	18:LI:103:LYS:NZ	2.22	0.68
3:L3:1802:A:N3	14:LE:130:ARG:NH2	2.41	0.68
3:L3:408:A:O2'	3:L3:411:G:OP2	2.11	0.68
3:L3:3908:A:O2'	3:L3:4531:U:OP1	2.10	0.68
12:LC:84:TYR:CE1	12:LC:93:MET:HE3	2.28	0.68
3:L3:3734:PSU:H2'	3:L3:3735:G:O4'	1.94	0.67
47:SQ:121:GLU:O	47:SQ:200:PHE:N	2.26	0.67
3:L3:5039:U:O2'	49:SV:115:ASN:OD1	2.11	0.67
3:L3:4765:G:OP1	45:SG:23:ARG:NE	2.28	0.66
16:LG:13:LYS:NZ	16:LG:59:ASP:OD1	2.29	0.65
36:NK:81:ARG:NH1	36:NK:82:ASN:O	2.30	0.65
36:NK:81:ARG:NE	36:NK:87:LEU:O	2.29	0.65
3:L3:1366:G:N2	3:L3:1371:A:OP2	2.29	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:SR:530:ASP:O	48:SR:531:MET:HE2	1.96	0.65
28:LS:35:LYS:O	48:SR:572:ARG:NH1	2.30	0.65
4:L4:117:G:OP1	40:SB:253:TYR:OH	2.11	0.65
2:L1:50:C:O2'	48:SR:578:SER:OG	2.14	0.65
3:L3:151:G:OP2	9:L9:4:TYR:OH	2.14	0.64
3:L3:2556:G:O2'	19:LJ:109:LYS:NZ	2.30	0.64
3:L3:419:A:N3	3:L3:1332:C:O2'	2.27	0.64
3:L3:3620:G:OP1	3:L3:3622:C:N4	2.30	0.64
3:L3:1255:A:OP1	3:L3:1257:A:N6	2.31	0.64
3:L3:1895:G:OP1	42:SD:96:ARG:NH2	2.30	0.64
3:L3:2427:G:OP1	13:LD:5:ARG:NH2	2.31	0.63
3:L3:2543:A:O2'	3:L3:2545:U:OP1	2.09	0.63
29:LT:33:VAL:HG23	29:LT:38:GLU:HB2	1.80	0.63
3:L3:3681:G:N1	44:SF:118:GLU:OE2	2.30	0.63
3:L3:3938:G:N2	3:L3:4171:C:OP2	2.32	0.63
3:L3:1355:G:OP1	11:LB:108:ARG:NH1	2.31	0.63
43:SE:58:PRO:HD2	43:SE:61:ILE:HD12	1.80	0.63
3:L3:1548:G:O2'	3:L3:2812:A:N3	2.30	0.63
9:L9:2:GLY:N	43:SE:141:ASN:OD1	2.32	0.63
38:NR:131:ILE:HG21	38:NR:161:ILE:HD12	1.79	0.63
12:LC:173:ASN:ND2	12:LC:175:PHE:O	2.32	0.63
2:L1:87:G:OP2	28:LS:5:LYS:NZ	2.31	0.63
3:L3:280:G:OP2	9:L9:44:ARG:NH2	2.32	0.63
24:LO:47:ILE:HD12	24:LO:94:LEU:HD11	1.79	0.63
3:L3:2696:A:H62	34:LY:35:LYS:HZ2	1.45	0.62
3:L3:4449:A:OP1	48:SR:118:LYS:NZ	2.31	0.62
3:L3:1214:C:N4	22:LM:90:SER:O	2.31	0.62
16:LG:115:SER:OG	46:SK:145:GLN:OE1	2.13	0.62
3:L3:4124:G:N2	43:SE:43:GLN:O	2.32	0.62
3:L3:4500:PSU:H2'	3:L3:4501:U:C6	2.34	0.62
3:L3:3776:G:OP2	3:L3:3776:G:N2	2.30	0.62
3:L3:1369:C:OP2	3:L3:1370:G:O2'	2.08	0.62
46:SK:242:ASP:OD1	48:SR:169:ARG:NH2	2.32	0.62
3:L3:4122:G:O2'	19:LJ:136:PHE:OXT	2.18	0.62
3:L3:4220:6MZ:OP2	3:L3:4220:6MZ:H8	1.99	0.62
23:LN:357:ARG:NE	48:SR:407:ASP:OD1	2.31	0.62
3:L3:1881:C:O2'	3:L3:1882:U:OP2	2.18	0.62
3:L3:737:C:OP2	8:L8:71:LYS:NZ	2.31	0.61
3:L3:276:C:OP2	30:LU:34:THR:HG21	2.01	0.61
7:L7:189:ILE:HD11	8:L8:119:ARG:HG2	1.82	0.61
3:L3:453:G:O2'	3:L3:705:G:OP1	2.17	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L3:1943:A:C2	50:VB:36:ILE:HD12	2.35	0.61
4:L4:55:A:O2'	5:L5:151:ILE:O	2.13	0.61
3:L3:4529:G:O2'	3:L3:4530:UR3:H5'	2.01	0.61
49:SV:53:LYS:NZ	49:SV:62:GLU:OE2	2.34	0.61
3:L3:489:C:O2'	3:L3:667:A:N6	2.34	0.60
3:L3:2407:G:O6	35:LZ:2:SER:N	2.34	0.60
3:L3:4987:C:N4	23:LN:121:ASN:OD1	2.34	0.60
9:L9:108:ARG:CZ	9:L9:161:MET:HE1	2.30	0.60
3:L3:121:A:OP1	43:SE:110:LYS:NZ	2.33	0.60
39:SA:109:ARG:O	39:SA:109:ARG:HG2	2.00	0.60
3:L3:2262:G:OP1	21:LL:94:ARG:NH1	2.35	0.60
8:L8:104:MET:HE3	8:L8:109:ARG:HG2	1.83	0.60
39:SA:340:ILE:HG21	41:SC:50:LEU:HD13	1.84	0.60
3:L3:4928:C:O4'	8:L8:121:ARG:NH1	2.34	0.60
3:L3:4435:U:OP2	3:L3:4436:U:O2'	2.15	0.60
3:L3:690:C:OP1	21:LL:87:ARG:NH1	2.35	0.60
3:L3:4670:C:O2'	3:L3:4672:A:OP2	2.20	0.60
3:L3:2811:G:N2	3:L3:2814:C:OP2	2.30	0.60
3:L3:454:U:O2	26:LQ:5:ARG:NH2	2.36	0.59
3:L3:1957:U:OP2	38:NR:105:ARG:NH2	2.35	0.59
3:L3:3924:C:O2'	3:L3:3925:OMU:H5''	2.02	0.59
12:LC:84:TYR:HE1	12:LC:93:MET:HE3	1.67	0.59
39:SA:288:ASP:OD2	39:SA:291:ARG:NH1	2.35	0.59
48:SR:176:TYR:CE1	48:SR:271:LEU:HD22	2.36	0.59
3:L3:3748:A:O2'	44:SF:223:SER:OG	2.07	0.59
4:L4:12:U:O3'	4:L4:109:U:O2'	2.17	0.59
48:SR:269:LEU:HD22	48:SR:306:ILE:HG23	1.84	0.59
3:L3:3717:A:OP2	3:L3:3735:G:N2	2.34	0.59
3:L3:2258:C:N3	41:SC:90:ALA:N	2.52	0.58
3:L3:2318:G:N2	3:L3:2321:G:OP2	2.23	0.58
3:L3:4645:C:OP2	13:LD:62:ARG:NH1	2.36	0.58
3:L3:2562:G:O2'	3:L3:2565:A:N6	2.36	0.58
3:L3:76:A:OP2	6:L6:74:ARG:NH1	2.36	0.58
3:L3:2876:OMG:HM22	3:L3:2877:G:H5'	1.86	0.58
50:VB:5:GLN:OE1	50:VB:5:GLN:N	2.36	0.58
3:L3:1521:C:O2'	3:L3:1522:OMG:H5'	2.03	0.58
3:L3:222:C:OP2	39:SA:165:LYS:NZ	2.27	0.58
3:L3:1577:G:C2	3:L3:3637:PSU:H1'	2.39	0.58
3:L3:2695:A:OP1	34:LY:35:LYS:NZ	2.34	0.58
3:L3:347:A:OP2	18:LI:8:THR:OG1	2.21	0.58
3:L3:4371:G:OP1	31:LV:59:LYS:NZ	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:LB:122:THR:OG1	11:LB:124:ASP:OD1	2.18	0.58
45:SG:128:MET:HE1	45:SG:161:ILE:HD11	1.86	0.58
48:SR:396:LYS:NZ	48:SR:404:GLU:OE1	2.26	0.58
3:L3:2350:U:O5'	3:L3:2351:OMC:H5'	2.04	0.57
3:L3:2902:G:O6	3:L3:3596:A:O2'	2.10	0.57
23:LN:213:GLN:NE2	23:LN:285:TYR:O	2.35	0.57
3:L3:1677:PSU:H4'	3:L3:1680:G:C2	2.39	0.57
3:L3:36:U:OP1	3:L3:1651:G:N2	2.37	0.57
3:L3:4299:PSU:OP1	22:LM:33:LYS:NZ	2.36	0.57
43:SE:44:ASP:OD1	43:SE:45:ILE:N	2.38	0.57
46:SK:99:GLU:OE1	46:SK:125:THR:OG1	2.17	0.57
3:L3:2626:U:OP2	48:SR:501:LYS:NZ	2.37	0.57
20:LK:38:LEU:O	20:LK:42:ARG:NH1	2.37	0.57
3:L3:1364:U:OP2	6:L6:36:ARG:NH2	2.37	0.57
19:LJ:56:ALA:O	19:LJ:57:MET:HE2	2.05	0.57
38:NR:90:GLU:OE2	38:NR:91:GLN:NE2	2.37	0.57
3:L3:1880:G:OP1	3:L3:1882:U:O2'	2.15	0.57
3:L3:2580:U:O2'	19:LJ:79:HIS:ND1	2.37	0.57
3:L3:1366:G:N7	6:L6:37:LYS:NZ	2.40	0.56
3:L3:4371:G:O2'	3:L3:4372:U:OP2	2.20	0.56
3:L3:4546:A:N7	44:SF:215:ASN:ND2	2.53	0.56
46:SK:236:MET:HE3	48:SR:214:TYR:CE2	2.40	0.56
3:L3:978:G:OP1	41:SC:47:ASN:ND2	2.38	0.56
23:LN:219:VAL:HG11	23:LN:337:VAL:CG2	2.35	0.56
37:NP:100:GLU:N	37:NP:100:GLU:OE1	2.38	0.56
42:SD:171:ASP:OD1	42:SD:172:ASN:N	2.39	0.56
3:L3:2578:G:N7	19:LJ:17:ARG:NH2	2.51	0.56
2:L1:127:U:N3	3:L3:2544:G:OP1	2.37	0.56
27:LR:44:SER:OG	27:LR:46:CYS:SG	2.56	0.56
43:SE:218:LEU:O	43:SE:222:ILE:HD12	2.05	0.56
3:L3:2725:A:OP2	13:LD:97:ARG:NH2	2.39	0.56
39:SA:153:VAL:HG12	39:SA:252:TRP:HB2	1.88	0.56
3:L3:27:C:OP2	9:L9:193:ARG:NH1	2.38	0.56
3:L3:1670:G:OP2	3:L3:1670:G:N2	2.35	0.56
13:LD:7:GLN:N	13:LD:7:GLN:OE1	2.39	0.56
41:SC:281:ILE:CG2	41:SC:286:LEU:HD11	2.35	0.55
3:L3:4311:A:O2'	3:L3:4312:PSU:H5''	2.05	0.55
19:LJ:22:LYS:NZ	19:LJ:132:GLN:O	2.33	0.55
3:L3:4087:G:OP2	44:SF:37:ARG:NH2	2.40	0.55
3:L3:1238:A:O2'	42:SD:52:GLU:OE2	2.25	0.55
3:L3:4391:G:O2'	3:L3:4392:OMG:H5'	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LP:103:TYR:HE2	25:LP:105:LEU:HD21	1.72	0.55
48:SR:233:ARG:HB2	48:SR:238:MET:HE3	1.89	0.55
3:L3:90:G:OP2	3:L3:92:C:N4	2.39	0.55
3:L3:1378:C:O2	6:L6:158:ARG:NE	2.39	0.55
3:L3:2772:C:OP1	34:LY:3:ARG:NH2	2.40	0.55
3:L3:5068:G:N2	3:L3:5069:U:O4	2.27	0.55
3:L3:2306:G:O2'	3:L3:2307:A:OP2	2.24	0.55
3:L3:2414:G:O2'	3:L3:2415:OMU:H5''	2.07	0.55
3:L3:350:C:OP2	39:SA:199:ARG:NH2	2.40	0.54
23:LN:222:VAL:O	23:LN:343:ARG:NH1	2.40	0.54
3:L3:2363:A2M:H2'	3:L3:2364:OMG:O4'	2.07	0.54
3:L3:2633:U:OP1	13:LD:64:ARG:NH2	2.41	0.54
3:L3:4084:G:O6	44:SF:72:ARG:NH2	2.40	0.54
3:L3:3722:G:OP2	30:LU:68:ARG:NH2	2.41	0.54
23:LN:74:GLU:OE1	23:LN:285:TYR:OH	2.21	0.54
3:L3:1693:U:O4	11:LB:14:ARG:NH2	2.39	0.54
44:SF:142:GLU:OE1	44:SF:143:THR:HG23	2.07	0.54
3:L3:730:G:OP2	42:SD:76:ARG:NE	2.41	0.54
3:L3:4635:A:H3'	3:L3:4636:PSU:H4'	1.90	0.54
13:LD:41:ILE:O	13:LD:45:ILE:HD12	2.08	0.54
3:L3:4987:C:OP2	23:LN:116:ARG:NH2	2.41	0.54
10:LA:94:MET:HG2	10:LA:148:MET:HE2	1.88	0.54
3:L3:2716:C:O3'	15:LF:107:LYS:NZ	2.41	0.54
9:L9:45:PRO:HG2	43:SE:166:LEU:HD21	1.90	0.54
3:L3:4724:A:O2'	23:LN:104:THR:HG22	2.08	0.53
3:L3:497:G:O2'	3:L3:499:G:OP2	2.25	0.53
3:L3:2459:G:N2	3:L3:2462:C:OP2	2.38	0.53
3:L3:4587:G:OP1	7:L7:61:ARG:NH1	2.41	0.53
46:SK:6:SER:HA	46:SK:13:ILE:HD11	1.91	0.53
3:L3:374:G:OP2	32:LW:56:ARG:NH2	2.41	0.53
9:L9:115:VAL:HG22	9:L9:134:LEU:CD2	2.39	0.53
39:SA:8:ILE:HD11	39:SA:257:PHE:CE2	2.43	0.53
3:L3:119:G:O4'	43:SE:132:ARG:NH1	2.42	0.53
3:L3:2469:C:O2'	3:L3:2470:C:OP1	2.26	0.53
3:L3:2844:A:N6	3:L3:3839:G:O2'	2.41	0.53
3:L3:5001:PSU:H2'	3:L3:5002:U:O4'	2.08	0.53
31:LV:100:LYS:O	31:LV:102:GLN:NE2	2.42	0.53
3:L3:1464:C:H5''	22:LM:32:LEU:HD12	1.90	0.53
19:LJ:120:GLU:O	19:LJ:124:THR:HG23	2.09	0.53
3:L3:1340:OMC:H2'	3:L3:1341:U:C6	2.44	0.52
3:L3:4673:PSU:H2'	3:L3:4674:C:C6	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:68:G:O2'	2:L1:69:PSU:H5''	2.09	0.52
3:L3:1676:C:OP2	3:L3:1677:PSU:N1	2.40	0.52
3:L3:2898:G:OP2	13:LD:135:LYS:NZ	2.24	0.52
3:L3:4593:C:OP2	36:NK:2:ALA:N	2.43	0.52
3:L3:2300:A:OP1	26:LQ:83:LYS:NZ	2.41	0.52
45:SG:92:MET:HE1	45:SG:161:ILE:HB	1.92	0.52
2:L1:69:PSU:H2'	2:L1:70:G:O4'	2.09	0.52
3:L3:691:C:OP1	41:SC:114:ARG:NH1	2.41	0.52
3:L3:2402:G:O2'	27:LR:10:ARG:O	2.28	0.52
9:L9:124:ASP:OD1	9:L9:125:SER:N	2.40	0.52
17:LH:82:THR:O	17:LH:82:THR:HG22	2.10	0.52
43:SE:208:ASN:OD1	43:SE:209:SER:N	2.42	0.52
3:L3:952:G:OP1	29:LT:73:LYS:NZ	2.42	0.52
3:L3:1326:A2M:H2'	3:L3:1327:C:C6	2.45	0.52
6:L6:7:GLY:O	20:LK:49:HIS:NE2	2.36	0.52
40:SB:62:CYS:HB3	40:SB:105:LEU:HD22	1.91	0.52
45:SG:103:VAL:HG11	45:SG:144:LEU:HD21	1.92	0.52
3:L3:1523:A:O2'	3:L3:1524:A2M:H5'	2.10	0.52
3:L3:4637:OMG:H2'	3:L3:4638:U:C6	2.45	0.52
3:L3:4457:PSU:O4	23:LN:252:ALA:HB3	2.10	0.51
4:L4:12:U:OP2	4:L4:67:C:O2'	2.28	0.51
9:L9:148:THR:HG22	9:L9:148:THR:O	2.10	0.51
42:SD:203:GLU:N	42:SD:203:GLU:OE1	2.43	0.51
3:L3:4296:PSU:H2'	3:L3:4297:G:O4'	2.10	0.51
6:L6:178:ALA:N	20:LK:134:GLU:OE2	2.43	0.51
9:L9:11:TRP:HA	9:L9:19:MET:HE2	1.91	0.51
14:LE:121:GLU:OE1	14:LE:121:GLU:N	2.43	0.51
18:LI:91:ASN:OD1	18:LI:93:THR:HG22	2.11	0.51
43:SE:231:ASP:OD1	43:SE:232:GLU:N	2.43	0.51
48:SR:524:MET:HE1	48:SR:531:MET:HE3	1.91	0.51
3:L3:1590:C:O2'	37:NP:5:ARG:NH2	2.43	0.51
3:L3:4515:G:OP1	48:SR:49:ARG:NH1	2.43	0.51
3:L3:4524:G:C2	23:LN:252:ALA:HB1	2.45	0.51
16:LG:97:TYR:OH	49:SV:37:HIS:NE2	2.40	0.51
39:SA:109:ARG:O	39:SA:109:ARG:HG3	2.08	0.51
48:SR:233:ARG:CB	48:SR:238:MET:HE3	2.41	0.51
3:L3:1321:G:O2'	3:L3:1322:1MA:H5'	2.09	0.51
23:LN:298:LEU:HD11	23:LN:300:LYS:HE3	1.93	0.51
3:L3:469:C:N3	41:SC:105:ARG:NH2	2.55	0.51
3:L3:2519:U:O2'	3:L3:2530:U:O2	2.27	0.51
11:LB:17:GLU:N	11:LB:17:GLU:OE1	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:NK:84:LYS:HD3	36:NK:85:THR:HG23	1.93	0.51
19:LJ:68:ILE:O	19:LJ:115:LYS:NZ	2.37	0.51
40:SB:268:ARG:NH2	40:SB:271:MET:SD	2.82	0.51
45:SG:52:LYS:O	45:SG:54:ARG:NH1	2.44	0.51
3:L3:3715:PSU:H2'	3:L3:3716:C:O4'	2.11	0.51
3:L3:3723:A:H2'	3:L3:3724:A2M:H8	1.93	0.51
10:LA:95:LEU:HA	10:LA:148:MET:HE1	1.92	0.51
41:SC:281:ILE:HG23	41:SC:286:LEU:HD11	1.93	0.51
3:L3:431:G:N2	3:L3:3889:G:OP2	2.44	0.50
3:L3:1889:U:OP1	29:LT:19:ARG:NH1	2.44	0.50
3:L3:2296:G:O2'	39:SA:242:PRO:O	2.29	0.50
3:L3:4678:G:OP2	36:NK:14:ARG:NH1	2.44	0.50
14:LE:41:ASP:OD1	14:LE:61:THR:OG1	2.20	0.50
19:LJ:76:ASN:OD1	19:LJ:77:TYR:N	2.44	0.50
3:L3:3718:A2M:H2	3:L3:3934:G:O4'	2.12	0.50
19:LJ:10:VAL:HG23	19:LJ:83:THR:OG1	2.11	0.50
23:LN:67:VAL:O	23:LN:67:VAL:HG22	2.11	0.50
3:L3:4219:A:O2'	3:L3:4220:6MZ:O5'	2.21	0.50
23:LN:205:VAL:HG13	23:LN:205:VAL:O	2.12	0.50
13:LD:34:ASN:O	13:LD:36:ASN:ND2	2.43	0.50
44:SF:27:ALA:O	44:SF:128:ARG:NH1	2.44	0.50
6:L6:63:THR:HG21	20:LK:66:ASN:HB3	1.93	0.50
25:LP:57:MET:SD	25:LP:90:ARG:NH1	2.85	0.50
3:L3:5047:C:O2'	3:L3:5050:C:OP2	2.23	0.49
18:LI:30:MET:HE1	18:LI:75:ARG:HG2	1.93	0.49
21:LL:20:ARG:NH1	26:LQ:78:LEU:O	2.45	0.49
23:LN:95:THR:OG1	23:LN:98:GLY:O	2.27	0.49
23:LN:108:GLU:OE2	23:LN:138:GLN:NE2	2.42	0.49
2:L1:71:A:N6	2:L1:83:C:O4'	2.45	0.49
3:L3:3614:G:O6	37:NP:87:LYS:NZ	2.42	0.49
3:L3:223:G:N3	39:SA:223:ASN:ND2	2.56	0.49
3:L3:2411:C:HO2'	3:L3:2526:C:HO2'	1.56	0.49
9:L9:44:ARG:NH1	9:L9:120:TRP:O	2.45	0.49
34:LY:66:VAL:HG13	34:LY:66:VAL:O	2.12	0.49
7:L7:190:ASP:OD1	7:L7:191:LYS:N	2.46	0.49
33:LX:5:THR:HG21	33:LX:8:VAL:HG22	1.94	0.49
46:SK:244:LEU:O	48:SR:352:LYS:NZ	2.30	0.49
3:L3:2368:A:N6	3:L3:2827:G:O2'	2.46	0.49
3:L3:4122:G:O3'	27:LR:90:ARG:NH1	2.45	0.49
40:SB:104:LEU:HD21	40:SB:108:ARG:NH2	2.27	0.49
15:LF:26:THR:O	15:LF:30:GLU:OE1	2.31	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:NR:150:LEU:HD13	38:NR:153:LEU:HD11	1.94	0.49
3:L3:1931:C:N4	3:L3:2041:A:OP1	2.46	0.49
3:L3:1910:G:O2'	3:L3:1917:A:N1	2.43	0.49
3:L3:2667:C:OP2	13:LD:103:ARG:NH1	2.43	0.49
45:SG:118:LEU:HD11	45:SG:167:VAL:HG22	1.95	0.49
30:LU:28:ARG:O	30:LU:32:ARG:NH1	2.45	0.49
3:L3:1340:OMC:H2'	3:L3:1341:U:H6	1.78	0.48
40:SB:104:LEU:HD21	40:SB:108:ARG:CZ	2.43	0.48
3:L3:197:A:N1	3:L3:225:G:O2'	2.46	0.48
26:LQ:26:ASP:OD1	26:LQ:27:ARG:N	2.46	0.48
3:L3:3622:C:OP1	37:NP:11:ARG:NH1	2.46	0.48
3:L3:3867:A2M:HM'3	3:L3:3867:A2M:H1'	1.65	0.48
3:L3:4863:G:OP1	45:SG:21:LYS:NZ	2.43	0.48
9:L9:115:VAL:HA	9:L9:134:LEU:HD23	1.94	0.48
23:LN:219:VAL:HG11	23:LN:337:VAL:HG21	1.95	0.48
41:SC:244:GLU:OE1	41:SC:244:GLU:N	2.44	0.48
3:L3:2666:U:OP2	13:LD:124:TYR:OH	2.22	0.48
3:L3:4620:OMU:OP2	3:L3:4670:C:N4	2.39	0.48
37:NP:110:SER:OG	49:SV:70:GLU:OE2	2.28	0.48
46:SK:21:ASN:ND2	46:SK:112:ASP:OD2	2.45	0.48
46:SK:76:THR:O	46:SK:96:ARG:NH1	2.45	0.48
46:SK:174:SER:O	46:SK:178:GLN:N	2.43	0.48
3:L3:4691:A:OP1	45:SG:75:SER:OG	2.19	0.48
3:L3:508:G:O2'	3:L3:510:U:OP2	2.29	0.48
9:L9:160:GLU:OE1	9:L9:160:GLU:N	2.44	0.48
18:LI:19:PHE:O	18:LI:26:ARG:NH2	2.46	0.48
3:L3:4075:U:OP1	43:SE:249:ARG:NH2	2.47	0.47
3:L3:4536:OMC:H2'	3:L3:4537:C:H6	1.79	0.47
18:LI:109:LEU:HD11	18:LI:115:ARG:HH11	1.79	0.47
24:LO:59:GLU:OE1	27:LR:92:LYS:NZ	2.47	0.47
41:SC:214:ASP:OD1	41:SC:215:ALA:N	2.47	0.47
49:SV:19:MET:SD	49:SV:19:MET:N	2.87	0.47
3:L3:150:U:O4	43:SE:187:LYS:NZ	2.38	0.47
31:LV:6:LYS:C	31:LV:23:VAL:HG12	2.39	0.47
40:SB:59:ASP:OD1	40:SB:60:ILE:N	2.46	0.47
3:L3:3730:PSU:H2'	3:L3:3731:C:C6	2.48	0.47
39:SA:146:GLU:N	39:SA:146:GLU:OE1	2.48	0.47
3:L3:2340:C:H4'	39:SA:42:THR:HG23	1.97	0.47
48:SR:176:TYR:CD1	48:SR:271:LEU:HD22	2.50	0.47
23:LN:370:THR:O	23:LN:370:THR:HG22	2.15	0.47
30:LU:88:GLU:OE2	30:LU:92:ASN:ND2	2.46	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:SV:111:ARG:O	49:SV:114:LYS:NZ	2.48	0.47
3:L3:1238:A:OP2	41:SC:60:SER:OG	2.21	0.47
3:L3:2835:A:O2'	23:LN:228:TYR:O	2.33	0.47
3:L3:3724:A2M:HM'3	3:L3:3724:A2M:H1'	1.58	0.47
3:L3:2843:U:O2'	3:L3:4632:U:OP1	2.32	0.47
3:L3:4288:C:O2'	3:L3:4321:U:OP1	2.33	0.47
15:LF:108:GLU:N	15:LF:108:GLU:OE1	2.48	0.47
22:LM:35:VAL:HB	22:LM:40:LEU:HD11	1.96	0.47
43:SE:200:THR:HG22	43:SE:201:THR:HG23	1.97	0.47
3:L3:1302:U:OP1	26:LQ:18:LYS:NZ	2.48	0.47
3:L3:1314:C:HO2'	26:LQ:24:GLN:NE2	2.13	0.47
3:L3:1952:G:OP1	12:LC:139:ARG:NE	2.48	0.47
3:L3:3822:PSU:H3'	3:L3:3823:G:H21	1.80	0.47
3:L3:1983:A:O2'	3:L3:2011:C:OP1	2.32	0.46
3:L3:2424:OMG:HM23	3:L3:2424:OMG:H1'	1.63	0.46
3:L3:2630:U:H2'	3:L3:2632:PSU:H1'	1.95	0.46
3:L3:4457:PSU:H1'	23:LN:252:ALA:HB3	1.95	0.46
19:LJ:84:ARG:NH2	19:LJ:85:TYR:OH	2.48	0.46
38:NR:69:TYR:O	38:NR:135:LEU:HD13	2.14	0.46
3:L3:4623:OMG:HM23	3:L3:4623:OMG:H1'	1.76	0.46
3:L3:4985:U:O2	23:LN:174:ARG:NH1	2.49	0.46
6:L6:127:PHE:O	28:LS:117:ARG:NH2	2.45	0.46
3:L3:338:A:OP1	6:L6:31:ARG:NH2	2.48	0.46
3:L3:1554:A:OP2	33:LX:4:ARG:NH2	2.49	0.46
3:L3:4673:PSU:H2'	3:L3:4674:C:H6	1.79	0.46
3:L3:4227:OMU:HM23	3:L3:4227:OMU:H1'	1.70	0.46
39:SA:124:ILE:HG21	39:SA:264:TYR:OH	2.15	0.46
49:SV:85:LEU:O	49:SV:89:THR:HG23	2.15	0.46
2:L1:13:G:O2'	10:LA:121:LYS:O	2.34	0.46
3:L3:106:A:O2'	3:L3:335:A:N3	2.48	0.46
21:LL:86:ALA:HB3	41:SC:114:ARG:HH21	1.81	0.46
3:L3:2562:G:N2	3:L3:2565:A:OP2	2.42	0.46
3:L3:4220:6MZ:H2'	3:L3:4222:G:H5''	1.97	0.46
19:LJ:33:THR:HG23	19:LJ:36:ARG:H	1.81	0.46
39:SA:187:GLN:NE2	39:SA:203:GLN:OE1	2.47	0.46
46:SK:58:ILE:O	46:SK:58:ILE:HG13	2.15	0.46
3:L3:2436:U:C2'	17:LH:127:LEU:HD11	2.46	0.46
3:L3:4571:A2M:HM'3	3:L3:4571:A2M:H1'	1.60	0.46
38:NR:150:LEU:CD1	38:NR:153:LEU:HD11	2.46	0.46
3:L3:4352:U:O2'	3:L3:4353:PSU:H5''	2.16	0.46
3:L3:4376:A:O2'	20:LK:42:ARG:NH1	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:LN:220:ILE:HG12	23:LN:278:THR:HG23	1.98	0.46
3:L3:3841:OMC:HM23	3:L3:3841:OMC:H1'	1.50	0.46
3:L3:4663:G:OP1	49:SV:34:SER:OG	2.26	0.46
5:L5:128:LEU:HD23	5:L5:129:ASP:N	2.30	0.46
19:LJ:100:VAL:HG13	19:LJ:107:LYS:HA	1.99	0.46
48:SR:576:ASP:OD1	48:SR:577:VAL:N	2.49	0.46
46:SK:49:VAL:HG12	46:SK:50:HIS:O	2.16	0.45
3:L3:1284:G:O2'	3:L3:1285:U:OP2	2.32	0.45
3:L3:2837:OMU:HM23	3:L3:2837:OMU:H1'	1.67	0.45
3:L3:4591:U:OP1	36:NK:4:SER:OG	2.16	0.45
46:SK:126:GLU:OE1	46:SK:139:ARG:NH2	2.49	0.45
3:L3:1368:A:N3	18:LI:1:MET:HE3	2.32	0.45
8:L8:29:ASP:OD1	8:L8:30:VAL:N	2.47	0.45
23:LN:248:LEU:HD23	23:LN:248:LEU:H	1.81	0.45
39:SA:210:ILE:HG21	39:SA:252:TRP:CZ3	2.51	0.45
3:L3:2823:G:O2'	3:L3:2824:OMC:H5''	2.17	0.45
3:L3:4208:U:OP2	14:LE:4:THR:HG23	2.16	0.45
48:SR:255:MET:HE3	48:SR:268:GLN:HB3	1.99	0.45
3:L3:2555:G:O2'	19:LJ:108:ARG:NH1	2.49	0.45
3:L3:2590:G:O2'	3:L3:2755:A:N6	2.46	0.45
3:L3:2641:A:OP1	27:LR:21:ARG:NH2	2.49	0.45
3:L3:4120:U:HO2'	3:L3:4121:G:P	2.37	0.45
3:L3:4551:U:O2'	3:L3:4552:PSU:H5''	2.16	0.45
9:L9:64:ILE:HD12	9:L9:132:VAL:HG21	1.99	0.45
19:LJ:10:VAL:O	19:LJ:83:THR:OG1	2.25	0.45
32:LW:25:LYS:NZ	35:LZ:50:GLY:O	2.23	0.45
3:L3:2580:U:OP1	19:LJ:36:ARG:NH1	2.45	0.45
5:L5:128:LEU:HD22	5:L5:130:PHE:HE1	1.81	0.45
3:L3:278:G:OP2	30:LU:30:ARG:NH2	2.49	0.45
3:L3:1524:A2M:H2	3:L3:1651:G:O6	2.17	0.45
3:L3:2422:OMC:H1'	3:L3:2422:OMC:HM23	1.45	0.45
3:L3:3687:A:O2'	44:SF:236:GLY:N	2.50	0.45
12:LC:9:GLU:OE2	12:LC:31:ARG:NH1	2.49	0.45
12:LC:84:TYR:OH	12:LC:93:MET:HE3	2.16	0.45
21:LL:112:ARG:NH1	41:SC:117:PRO:O	2.47	0.45
2:L1:155:C:OP2	43:SE:89:ARG:NH1	2.49	0.45
3:L3:2394:G:O4'	3:L3:2397:G:N2	2.48	0.45
3:L3:4208:U:OP1	3:L3:4334:U:O2'	2.30	0.45
9:L9:103:GLU:OE1	9:L9:165:THR:HG21	2.17	0.45
48:SR:292:ASP:OD1	48:SR:292:ASP:N	2.50	0.45
2:L1:26:C:O2'	39:SA:53:ALA:O	2.34	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:LQ:89:LEU:HD13	26:LQ:118:LEU:HD22	1.99	0.45
49:SV:117:GLU:OE1	49:SV:117:GLU:N	2.49	0.45
3:L3:1353:G:N7	11:LB:104:ARG:NH2	2.65	0.45
3:L3:2299:G:OP1	39:SA:182:LYS:NZ	2.35	0.45
3:L3:3744:OMG:HM22	3:L3:3744:OMG:H1'	1.62	0.45
3:L3:4940:C:OP1	41:SC:156:ARG:NH1	2.42	0.45
30:LU:63:VAL:O	30:LU:63:VAL:HG22	2.17	0.45
39:SA:22:VAL:HG22	39:SA:258:ARG:NH2	2.31	0.45
3:L3:2869:U:O2'	3:L3:2881:A:N7	2.36	0.44
20:LK:76:ASP:OD1	20:LK:77:LYS:N	2.50	0.44
3:L3:1352:C:O2'	3:L3:1356:U:OP1	2.34	0.44
3:L3:2351:OMC:H1'	3:L3:2351:OMC:HM23	1.50	0.44
3:L3:3868:G:O2'	3:L3:3869:OMC:H5''	2.16	0.44
44:SF:136:VAL:HG12	44:SF:148:VAL:HG12	1.98	0.44
3:L3:3661:G:N7	44:SF:152:SER:OG	2.48	0.44
3:L3:3859:G:OP2	10:LA:25:HIS:NE2	2.47	0.44
3:L3:4237:C:OP1	3:L3:4327:C:O2'	2.30	0.44
7:L7:186:GLU:HA	7:L7:189:ILE:HG22	1.99	0.44
23:LN:369:ASP:OD2	23:LN:373:LYS:NZ	2.50	0.44
39:SA:275:SER:OG	39:SA:276:ASN:N	2.50	0.44
3:L3:225:G:OP1	39:SA:222:ARG:NE	2.50	0.44
3:L3:1646:A:OP2	39:SA:80:ARG:NH1	2.51	0.44
3:L3:4910:G:N2	7:L7:106:ASP:O	2.47	0.44
9:L9:64:ILE:HD12	9:L9:132:VAL:CG2	2.48	0.44
11:LB:88:ASP:OD1	11:LB:89:ASP:N	2.50	0.44
3:L3:1326:A2M:HM'3	3:L3:1326:A2M:H1'	1.58	0.44
3:L3:2861:OMC:HM23	3:L3:2861:OMC:H1'	1.48	0.44
4:L4:118:C:H41	40:SB:258:LYS:NZ	2.16	0.44
19:LJ:29:ILE:O	19:LJ:31:ASP:N	2.48	0.44
19:LJ:74:VAL:HG23	19:LJ:101:PHE:CZ	2.53	0.44
42:SD:238:ASP:OD1	42:SD:238:ASP:N	2.46	0.44
3:L3:1655:C:OP1	3:L3:1679:A:O2'	2.31	0.44
26:LQ:84:GLU:O	26:LQ:87:VAL:HG22	2.18	0.44
39:SA:72:ALA:HB1	48:SR:622:LEU:HD22	2.00	0.44
40:SB:80:ALA:HA	40:SB:83:LEU:HD13	1.99	0.44
3:L3:373:G:OP2	32:LW:36:LYS:NZ	2.46	0.44
3:L3:2087:C:OP2	11:LB:37:ARG:NE	2.43	0.44
3:L3:4306:OMU:HM23	3:L3:4306:OMU:H1'	1.54	0.44
18:LI:50:ARG:NH1	18:LI:51:LYS:O	2.51	0.44
3:L3:1438:U:O2'	3:L3:1439:C:OP1	2.34	0.43
3:L3:1515:A:OP1	20:LK:33:GLY:N	2.50	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L3:1595:G:N2	48:SR:634:ARG:OXT	2.50	0.43
3:L3:3919:C:O2'	3:L3:3920:PSU:H5''	2.18	0.43
25:LP:27:ILE:HD12	25:LP:86:VAL:HG21	2.00	0.43
3:L3:4552:PSU:H2'	3:L3:4553:A:C8	2.53	0.43
31:LV:103:VAL:O	31:LV:103:VAL:HG13	2.18	0.43
39:SA:152:LEU:HD22	39:SA:251:ILE:HG23	2.00	0.43
39:SA:233:SER:HA	39:SA:263:LEU:HD21	2.00	0.43
3:L3:2824:OMC:HM23	3:L3:2824:OMC:H1'	1.54	0.43
3:L3:4139:G:H21	3:L3:4140:C:N4	2.15	0.43
9:L9:64:ILE:HD13	9:L9:102:ALA:O	2.18	0.43
13:LD:45:ILE:HD12	13:LD:45:ILE:H	1.83	0.43
45:SG:12:ILE:HG12	45:SG:18:ILE:HD12	1.99	0.43
46:SK:77:THR:HG23	46:SK:80:GLU:H	1.84	0.43
3:L3:2422:OMC:H2'	3:L3:2423:A:C8	2.54	0.43
3:L3:3890:A:N6	3:L3:4570:G:O2'	2.48	0.43
28:LS:87:LYS:N	32:LW:80:GLU:OE2	2.47	0.43
3:L3:2052:G:O2'	3:L3:2057:A:N1	2.46	0.43
3:L3:3744:OMG:H2'	3:L3:3745:U:O4'	2.19	0.43
25:LP:103:TYR:CE2	25:LP:105:LEU:HD21	2.54	0.43
37:NP:95:GLU:O	49:SV:47:ARG:NH1	2.46	0.43
3:L3:1683:PSU:H2'	3:L3:1684:A:C8	2.54	0.43
3:L3:3924:C:C2'	3:L3:3925:OMU:H5''	2.49	0.43
17:LH:94:ASN:OD1	17:LH:146:ALA:N	2.49	0.43
3:L3:3718:A2M:H2'	3:L3:3719:A:O4'	2.18	0.43
3:L3:4713:G:OP1	7:L7:148:LYS:NZ	2.40	0.43
12:LC:84:TYR:CZ	12:LC:93:MET:HE3	2.54	0.43
15:LF:117:ILE:HG23	48:SR:543:ALA:HB2	2.01	0.43
48:SR:258:SER:OG	48:SR:293:VAL:HG11	2.18	0.43
3:L3:1912:G:N2	7:L7:87:MET:HE2	2.34	0.42
3:L3:2437:C:OP2	3:L3:2528:G:O2'	2.37	0.42
3:L3:2781:G:O2'	35:LZ:3:SER:O	2.36	0.42
3:L3:3886:G:H2'	3:L3:3887:OMC:H5'	2.00	0.42
3:L3:4755:G:N7	41:SC:279:ASN:ND2	2.67	0.42
23:LN:313:SER:OG	23:LN:314:ILE:N	2.52	0.42
33:LX:26:VAL:HG21	44:SF:180:LEU:HD11	2.00	0.42
44:SF:104:VAL:HG13	44:SF:136:VAL:HG11	2.01	0.42
3:L3:4201:G:O2'	3:L3:4202:U:OP2	2.33	0.42
3:L3:5005:G:H22	3:L3:5041:G:H1'	1.84	0.42
18:LI:51:LYS:NZ	18:LI:71:VAL:O	2.47	0.42
41:SC:59:ARG:O	41:SC:63:TYR:N	2.46	0.42
42:SD:219:GLY:O	42:SD:246:ARG:NH2	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L3:1552:G:O2'	3:L3:1574:G:N2	2.44	0.42
3:L3:2097:U:O3'	3:L3:2098:G:H4'	2.19	0.42
3:L3:2876:OMG:C8	33:LX:16:THR:HG22	2.55	0.42
3:L3:3663:A:N6	3:L3:4168:G:O2'	2.53	0.42
3:L3:4440:G:N2	48:SR:66:LEU:O	2.50	0.42
3:L3:4896:G:N2	3:L3:4927:G:O6	2.52	0.42
5:L5:24:ILE:HD11	5:L5:128:LEU:HD12	2.02	0.42
28:LS:37:THR:O	28:LS:37:THR:HG22	2.19	0.42
3:L3:1283:G:O6	39:SA:312:ARG:NH2	2.53	0.42
3:L3:2347:A:C4	26:LQ:31:ILE:HD11	2.55	0.42
3:L3:3899:OMG:HM23	3:L3:3899:OMG:H1'	1.56	0.42
3:L3:4590:A2M:HM'3	3:L3:4590:A2M:H1'	1.88	0.42
12:LC:45:TRP:HZ3	12:LC:54:MET:HE2	1.85	0.42
18:LI:53:ASP:O	18:LI:70:VAL:HG23	2.19	0.42
41:SC:133:PHE:O	41:SC:138:ARG:NH2	2.51	0.42
3:L3:363:A:N7	3:L3:378:A:N6	2.67	0.42
3:L3:1427:A:C2	11:LB:138:LEU:HD23	2.55	0.42
3:L3:2378:G:N2	3:L3:2381:A:OP2	2.50	0.42
3:L3:2794:C:N4	10:LA:134:GLY:O	2.53	0.42
10:LA:42:ARG:NH2	10:LA:110:ASP:OD1	2.46	0.42
23:LN:240:LEU:HB3	23:LN:241:PRO:HD2	2.01	0.42
45:SG:113:GLU:OE1	45:SG:125:ARG:NE	2.53	0.42
3:L3:4498:OMU:HM23	3:L3:4498:OMU:H1'	1.65	0.42
9:L9:73:ARG:HG2	9:L9:75:VAL:HG13	2.02	0.42
46:SK:61:ARG:O	46:SK:105:GLY:N	2.50	0.42
2:L1:58:G:O6	32:LW:63:ARG:NH1	2.52	0.42
9:L9:68:ARG:NH2	9:L9:123:GLU:OE2	2.52	0.42
15:LF:67:LYS:O	15:LF:68:SER:OG	2.27	0.42
39:SA:110:ARG:O	39:SA:113:ARG:NH1	2.45	0.42
3:L3:2072:C:O2'	42:SD:213:LEU:O	2.38	0.42
45:SG:105:ILE:HD12	45:SG:136:VAL:HG13	2.01	0.42
45:SG:128:MET:SD	45:SG:146:LEU:HD21	2.60	0.42
48:SR:128:GLN:OE1	50:VB:58:ARG:NE	2.52	0.42
2:L1:18:U:O2	3:L3:2309:G:O2'	2.38	0.42
3:L3:380:U:H5''	3:L3:413:G:H21	1.84	0.42
3:L3:2364:OMG:H1'	3:L3:2364:OMG:HM23	1.46	0.42
3:L3:4739:C:H4'	36:NK:87:LEU:HD13	2.00	0.42
45:SG:41:ILE:HG22	45:SG:43:VAL:HG13	2.02	0.42
2:L1:102:G:OP2	2:L1:104:A:O2'	2.28	0.41
3:L3:4636:PSU:N1	25:LP:79:ASN:OD1	2.53	0.41
12:LC:27:LEU:HD12	38:NR:127:PTR:O1P	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:NR:78:ILE:HG21	38:NR:124:PHE:CE1	2.55	0.41
2:L1:75:OMG:HM23	2:L1:75:OMG:H1'	1.48	0.41
3:L3:1683:PSU:H2'	3:L3:1684:A:H8	1.85	0.41
3:L3:3730:PSU:H2'	3:L3:3731:C:H6	1.84	0.41
19:LJ:36:ARG:NH1	19:LJ:38:TYR:OH	2.47	0.41
24:LO:35:LEU:HA	24:LO:38:ILE:HG22	2.02	0.41
25:LP:68:LEU:CD2	25:LP:106:VAL:HG12	2.50	0.41
3:L3:400:A2M:HM'3	3:L3:400:A2M:H1'	1.81	0.41
3:L3:5022:U:O2'	3:L3:5023:C:OP2	2.29	0.41
18:LI:109:LEU:HD11	18:LI:115:ARG:NH1	2.35	0.41
26:LQ:9:LYS:NZ	26:LQ:71:PRO:O	2.54	0.41
12:LC:15:ARG:HB3	12:LC:27:LEU:HD23	2.01	0.41
19:LJ:30:ASP:O	19:LJ:39:SER:OG	2.22	0.41
3:L3:1553:A:O2'	33:LX:9:GLY:O	2.37	0.41
3:L3:398:A2M:HM'3	3:L3:398:A2M:H1'	1.71	0.41
3:L3:1998:A:N3	3:L3:2019:C:O2'	2.50	0.41
3:L3:4570:G:H2'	3:L3:4571:A2M:H8	2.02	0.41
29:LT:78:HIS:N	29:LT:83:MET:O	2.51	0.41
3:L3:1213:G:OP1	42:SD:59:LYS:NZ	2.40	0.41
3:L3:1577:G:OP1	33:LX:17:ARG:NH2	2.47	0.41
3:L3:1888:A:O2'	3:L3:3883:U:O2'	2.35	0.41
3:L3:2084:C:H42	11:LB:14:ARG:HB2	1.85	0.41
3:L3:3744:OMG:H2'	3:L3:3745:U:C6	2.56	0.41
3:L3:4530:UR3:H6	3:L3:4530:UR3:O5'	2.20	0.41
16:LG:112:MET:HE1	16:LG:117:ILE:CG1	2.50	0.41
23:LN:309:LEU:HD12	48:SR:438:ILE:HD11	2.01	0.41
29:LT:33:VAL:O	29:LT:33:VAL:HG13	2.20	0.41
3:L3:317:A:C2	3:L3:4361:PSU:H1'	2.56	0.41
3:L3:496:G:O2'	3:L3:497:G:OP1	2.29	0.41
15:LF:75:GLU:OE1	15:LF:75:GLU:N	2.54	0.41
48:SR:577:VAL:HG12	48:SR:577:VAL:O	2.20	0.41
3:L3:1250:C:N4	3:L3:1261:G:O6	2.54	0.40
23:LN:215:GLU:OE2	23:LN:349:LYS:NZ	2.54	0.40
44:SF:178:PRO:HB2	44:SF:180:LEU:HD12	2.03	0.40
46:SK:1:MET:N	46:SK:219:GLU:OE2	2.44	0.40
3:L3:4618:OMG:HM23	3:L3:4618:OMG:H1'	1.87	0.40
19:LJ:74:VAL:HG23	19:LJ:101:PHE:CE2	2.56	0.40
39:SA:154:VAL:HG11	39:SA:158:VAL:HG21	2.03	0.40
46:SK:129:LEU:HD22	46:SK:137:VAL:HG22	2.04	0.40
3:L3:2259:G:O4'	41:SC:108:LYS:NZ	2.48	0.40
3:L3:2845:A:H61	3:L3:3843:C:H42	1.68	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:LH:119:ILE:HD12	17:LH:140:LEU:HD22	2.04	0.40
23:LN:71:GLU:OE2	23:LN:366:LYS:NZ	2.48	0.40
34:LY:8:ILE:H	34:LY:8:ILE:HD12	1.87	0.40
46:SK:103:ALA:O	46:SK:107:VAL:HG23	2.21	0.40
50:VB:38:PRO:HB2	50:VB:43:VAL:HG23	2.04	0.40
3:L3:1268:G:N7	22:LM:111:ARG:NH2	2.70	0.40
3:L3:1482:G:N7	6:L6:188:ASN:ND2	2.69	0.40
23:LN:80:GLU:OE1	23:LN:323:TYR:OH	2.25	0.40
31:LV:5:PRO:O	31:LV:23:VAL:HG11	2.20	0.40
46:SK:95:ARG:NH2	49:SV:77:GLU:OE2	2.54	0.40
3:L3:1633:G:O6	3:L3:3918:G:O2'	2.39	0.40
3:L3:1952:G:H4'	12:LC:93:MET:HB2	2.03	0.40
3:L3:4456:OMC:HM23	3:L3:4456:OMC:H1'	1.63	0.40
3:L3:4637:OMG:HM23	3:L3:4637:OMG:H1'	1.50	0.40
9:L9:38:ARG:NE	9:L9:60:VAL:HG23	2.36	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	BA	89/165 (54%)	89 (100%)	0	0	100	100
5	L5	166/178 (93%)	164 (99%)	2 (1%)	0	100	100
6	L6	208/211 (99%)	204 (98%)	4 (2%)	0	100	100
7	L7	199/203 (98%)	195 (98%)	4 (2%)	0	100	100
8	L8	133/215 (62%)	132 (99%)	1 (1%)	0	100	100
9	L9	201/204 (98%)	199 (99%)	2 (1%)	0	100	100
10	LA	151/184 (82%)	148 (98%)	3 (2%)	0	100	100
11	LB	185/188 (98%)	183 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	LC	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
13	LD	152/196 (78%)	152 (100%)	0	0	100	100
14	LE	150/160 (94%)	146 (97%)	4 (3%)	0	100	100
15	LF	101/128 (79%)	99 (98%)	2 (2%)	0	100	100
16	LG	137/140 (98%)	134 (98%)	3 (2%)	0	100	100
17	LH	115/156 (74%)	114 (99%)	1 (1%)	0	100	100
18	LI	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
19	LJ	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
20	LK	145/148 (98%)	143 (99%)	2 (1%)	0	100	100
21	LL	123/137 (90%)	122 (99%)	1 (1%)	0	100	100
22	LM	81/159 (51%)	80 (99%)	1 (1%)	0	100	100
23	LN	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
24	LO	93/115 (81%)	92 (99%)	1 (1%)	0	100	100
25	LP	104/125 (83%)	104 (100%)	0	0	100	100
26	LQ	126/135 (93%)	124 (98%)	2 (2%)	0	100	100
27	LR	110/117 (94%)	108 (98%)	2 (2%)	0	100	100
28	LS	120/123 (98%)	120 (100%)	0	0	100	100
29	LT	107/110 (97%)	107 (100%)	0	0	100	100
30	LU	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
31	LV	102/106 (96%)	101 (99%)	1 (1%)	0	100	100
32	LW	84/97 (87%)	83 (99%)	1 (1%)	0	100	100
33	LX	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
34	LY	67/70 (96%)	67 (100%)	0	0	100	100
35	LZ	48/51 (94%)	48 (100%)	0	0	100	100
36	NK	63/129 (49%)	61 (97%)	2 (3%)	0	100	100
37	NP	100/134 (75%)	100 (100%)	0	0	100	100
38	NR	150/203 (74%)	147 (98%)	2 (1%)	1 (1%)	18	34
39	SA	356/427 (83%)	349 (98%)	7 (2%)	0	100	100
40	SB	273/297 (92%)	265 (97%)	8 (3%)	0	100	100
41	SC	211/288 (73%)	204 (97%)	7 (3%)	0	100	100
42	SD	223/248 (90%)	219 (98%)	4 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	SE	228/266 (86%)	227 (100%)	1 (0%)	0	100	100
44	SF	243/257 (95%)	236 (97%)	7 (3%)	0	100	100
45	SG	188/192 (98%)	186 (99%)	2 (1%)	0	100	100
46	SK	242/245 (99%)	235 (97%)	7 (3%)	0	100	100
47	SQ	121/239 (51%)	121 (100%)	0	0	100	100
48	SR	595/634 (94%)	589 (99%)	5 (1%)	1 (0%)	43	64
49	SV	137/163 (84%)	137 (100%)	0	0	100	100
50	VB	54/99 (54%)	54 (100%)	0	0	100	100
All	All	7508/8699 (86%)	7397 (98%)	109 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
38	NR	126	GLY
48	SR	88	ASP

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	
5	L5	142/149 (95%)	142 (100%)	0	100	100
6	L6	176/177 (99%)	176 (100%)	0	100	100
7	L7	173/174 (99%)	173 (100%)	0	100	100
8	L8	115/161 (71%)	115 (100%)	0	100	100
9	L9	171/172 (99%)	171 (100%)	0	100	100
10	LA	134/163 (82%)	134 (100%)	0	100	100
11	LB	164/165 (99%)	164 (100%)	0	100	100
12	LC	157/157 (100%)	157 (100%)	0	100	100
13	LD	138/175 (79%)	138 (100%)	0	100	100
14	LE	136/140 (97%)	136 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	LF	93/115 (81%)	93 (100%)	0	100	100
16	LG	106/107 (99%)	106 (100%)	0	100	100
17	LH	105/133 (79%)	105 (100%)	0	100	100
18	LI	124/135 (92%)	124 (100%)	0	100	100
19	LJ	117/118 (99%)	117 (100%)	0	100	100
20	LK	120/121 (99%)	120 (100%)	0	100	100
21	LL	109/121 (90%)	109 (100%)	0	100	100
22	LM	71/126 (56%)	71 (100%)	0	100	100
23	LN	347/348 (100%)	347 (100%)	0	100	100
24	LO	80/97 (82%)	80 (100%)	0	100	100
25	LP	97/110 (88%)	97 (100%)	0	100	100
26	LQ	114/121 (94%)	114 (100%)	0	100	100
27	LR	96/100 (96%)	96 (100%)	0	100	100
28	LS	109/110 (99%)	109 (100%)	0	100	100
29	LT	88/89 (99%)	88 (100%)	0	100	100
30	LU	86/89 (97%)	86 (100%)	0	100	100
31	LV	92/94 (98%)	92 (100%)	0	100	100
32	LW	73/80 (91%)	73 (100%)	0	100	100
33	LX	74/75 (99%)	74 (100%)	0	100	100
34	LY	64/65 (98%)	64 (100%)	0	100	100
35	LZ	47/48 (98%)	47 (100%)	0	100	100
36	NK	61/115 (53%)	61 (100%)	0	100	100
37	NP	88/114 (77%)	88 (100%)	0	100	100
38	NR	140/183 (76%)	140 (100%)	0	100	100
39	SA	298/348 (86%)	298 (100%)	0	100	100
40	SB	234/250 (94%)	234 (100%)	0	100	100
41	SC	192/252 (76%)	192 (100%)	0	100	100
42	SD	194/215 (90%)	194 (100%)	0	100	100
43	SE	198/223 (89%)	198 (100%)	0	100	100
44	SF	188/199 (94%)	188 (100%)	0	100	100
45	SG	169/171 (99%)	169 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	SK	212/213 (100%)	212 (100%)	0	100	100
47	SQ	6/214 (3%)	6 (100%)	0	100	100
48	SR	545/574 (95%)	545 (100%)	0	100	100
49	SV	128/149 (86%)	128 (100%)	0	100	100
50	VB	48/76 (63%)	48 (100%)	0	100	100
All	All	6419/7331 (88%)	6419 (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 (60) such sidechains are listed below:

Mol	Chain	Res	Type
5	L5	71	HIS
5	L5	112	HIS
6	L6	87	HIS
7	L7	63	ASN
8	L8	20	HIS
8	L8	34	ASN
8	L8	48	GLN
8	L8	69	HIS
9	L9	15	GLN
9	L9	32	GLN
9	L9	86	HIS
9	L9	178	HIS
9	L9	182	HIS
10	LA	56	GLN
10	LA	133	HIS
12	LC	37	HIS
12	LC	122	HIS
12	LC	173	ASN
13	LD	118	HIS
14	LE	58	HIS
14	LE	66	ASN
15	LF	38	ASN
16	LG	27	ASN
16	LG	135	ASN
18	LI	20	ASN
19	LJ	127	ASN
21	LL	95	HIS
23	LN	145	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	LO	72	HIS
25	LP	121	ASN
26	LQ	24	GLN
26	LQ	52	GLN
28	LS	98	HIS
29	LT	56	ASN
31	LV	19	GLN
32	LW	13	ASN
35	LZ	25	GLN
36	NK	90	HIS
38	NR	34	GLN
38	NR	49	ASN
38	NR	102	GLN
39	SA	38	ASN
39	SA	61	GLN
39	SA	198	ASN
41	SC	157	HIS
41	SC	190	HIS
41	SC	211	HIS
42	SD	119	ASN
42	SD	239	GLN
43	SE	141	ASN
44	SF	38	HIS
46	SK	33	ASN
46	SK	157	GLN
48	SR	37	HIS
48	SR	64	GLN
48	SR	153	GLN
48	SR	157	HIS
48	SR	209	HIS
48	SR	218	GLN
49	SV	17	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	L1	152/157 (96%)	17 (11%)	0
3	L3	3344/5070 (65%)	432 (12%)	10 (0%)
4	L4	119/121 (98%)	10 (8%)	1 (0%)
All	All	3615/5348 (67%)	459 (12%)	11 (0%)

All (459) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	L1	34	U
2	L1	35	C
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	87	G
2	L1	94	G
2	L1	103	A
2	L1	105	C
2	L1	111	U
2	L1	114	G
2	L1	151	G
2	L1	156	U
3	L3	2	G
3	L3	39	A
3	L3	42	A
3	L3	48	G
3	L3	56	A
3	L3	58	G
3	L3	59	A
3	L3	64	A
3	L3	65	A
3	L3	66	A
3	L3	91	G
3	L3	109	G
3	L3	119	G
3	L3	159	C
3	L3	164	G
3	L3	167	C
3	L3	170	C
3	L3	171	U
3	L3	173	C
3	L3	181	C
3	L3	200	U
3	L3	210	C
3	L3	218	A
3	L3	233	U
3	L3	234	G
3	L3	238	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L3	261	G
3	L3	263	G
3	L3	266	C
3	L3	274	C
3	L3	280	G
3	L3	297	U
3	L3	316	U
3	L3	340	C
3	L3	387	G
3	L3	409	G
3	L3	410	A
3	L3	412	G
3	L3	444	G
3	L3	446	C
3	L3	450	G
3	L3	452	A
3	L3	453	G
3	L3	454	U
3	L3	464	G
3	L3	467	U
3	L3	469	C
3	L3	473	C
3	L3	479	G
3	L3	492	U
3	L3	493	G
3	L3	496	G
3	L3	497	G
3	L3	499	G
3	L3	501	C
3	L3	502	C
3	L3	503	C
3	L3	504	G
3	L3	509	A
3	L3	510	U
3	L3	511	C
3	L3	657	C
3	L3	658	C
3	L3	660	A
3	L3	667	A
3	L3	668	C
3	L3	669	C
3	L3	686	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L3	697	G
3	L3	704	C
3	L3	730	G
3	L3	731	G
3	L3	739	G
3	L3	741	C
3	L3	742	G
3	L3	746	A
3	L3	757	G
3	L3	913	U
3	L3	915	A
3	L3	916	C
3	L3	917	A
3	L3	926	G
3	L3	932	A
3	L3	933	G
3	L3	943	A
3	L3	944	A
3	L3	945	U
3	L3	956	A
3	L3	959	G
3	L3	960	A
3	L3	971	U
3	L3	972	C
3	L3	1066	G
3	L3	1070	G
3	L3	1072	C
3	L3	1080	C
3	L3	1100	U
3	L3	1169	G
3	L3	1171	G
3	L3	1172	C
3	L3	1173	G
3	L3	1178	G
3	L3	1180	C
3	L3	1181	C
3	L3	1182	C
3	L3	1201	U
3	L3	1203	G
3	L3	1211	G
3	L3	1214	C
3	L3	1215	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L3	1216	C
3	L3	1253	G
3	L3	1254	A
3	L3	1255	A
3	L3	1256	G
3	L3	1266	G
3	L3	1269	G
3	L3	1270	A
3	L3	1272	C
3	L3	1273	G
3	L3	1280	C
3	L3	1284	G
3	L3	1287	G
3	L3	1294	A
3	L3	1295	C
3	L3	1301	C
3	L3	1314	C
3	L3	1315	C
3	L3	1319	U
3	L3	1320	U
3	L3	1323	A
3	L3	1325	C
3	L3	1326	A2M
3	L3	1354	A
3	L3	1358	G
3	L3	1359	G
3	L3	1365	C
3	L3	1366	G
3	L3	1379	C
3	L3	1397	A
3	L3	1420	A
3	L3	1439	C
3	L3	1443	A
3	L3	1489	G
3	L3	1498	G
3	L3	1502	G
3	L3	1523	A
3	L3	1534	A2M
3	L3	1547	A
3	L3	1578	U
3	L3	1581	G
3	L3	1596	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L3	1597	G
3	L3	1613	A
3	L3	1624	G
3	L3	1625	OMG
3	L3	1631	A
3	L3	1633	G
3	L3	1634	A
3	L3	1654	G
3	L3	1661	C
3	L3	1676	C
3	L3	1677	PSU
3	L3	1678	C
3	L3	1691	G
3	L3	1721	G
3	L3	1726	U
3	L3	1734	G
3	L3	1791	U
3	L3	1804	A
3	L3	1811	G
3	L3	1815	G
3	L3	1821	G
3	L3	1822	U
3	L3	1836	G
3	L3	1837	A
3	L3	1842	G
3	L3	1850	A
3	L3	1854	G
3	L3	1855	G
3	L3	1866	U
3	L3	1869	G
3	L3	1880	G
3	L3	1881	C
3	L3	1882	U
3	L3	1883	G
3	L3	1887	G
3	L3	1891	A
3	L3	1897	A
3	L3	1910	G
3	L3	1919	G
3	L3	1921	C
3	L3	1922	G
3	L3	1925	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L3	1936	C
3	L3	1960	A
3	L3	1974	U
3	L3	1984	A
3	L3	1997	U
3	L3	2002	A
3	L3	2011	C
3	L3	2016	C
3	L3	2021	G
3	L3	2026	A
3	L3	2046	G
3	L3	2055	G
3	L3	2056	G
3	L3	2069	A
3	L3	2084	C
3	L3	2085	G
3	L3	2092	G
3	L3	2093	A
3	L3	2095	A
3	L3	2096	G
3	L3	2097	U
3	L3	2098	G
3	L3	2099	G
3	L3	2109	G
3	L3	2110	C
3	L3	2111	G
3	L3	2289	C
3	L3	2300	A
3	L3	2301	G
3	L3	2306	G
3	L3	2313	A
3	L3	2348	G
3	L3	2351	OMC
3	L3	2395	A
3	L3	2401	A2M
3	L3	2417	A
3	L3	2422	OMC
3	L3	2425	U
3	L3	2429	A
3	L3	2437	C
3	L3	2450	G
3	L3	2453	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L3	2470	C
3	L3	2474	G
3	L3	2475	G
3	L3	2476	G
3	L3	2477	A
3	L3	2478	C
3	L3	2479	G
3	L3	2480	G
3	L3	2484	A
3	L3	2498	C
3	L3	2506	G
3	L3	2507	A
3	L3	2512	A
3	L3	2513	A
3	L3	2519	U
3	L3	2544	G
3	L3	2545	U
3	L3	2548	C
3	L3	2554	U
3	L3	2556	G
3	L3	2567	G
3	L3	2587	A
3	L3	2589	C
3	L3	2627	C
3	L3	2653	C
3	L3	2669	C
3	L3	2687	U
3	L3	2694	G
3	L3	2695	A
3	L3	2696	A
3	L3	2711	G
3	L3	2743	A
3	L3	2759	G
3	L3	2760	G
3	L3	2764	A
3	L3	2769	U
3	L3	2771	G
3	L3	2787	A2M
3	L3	2788	U
3	L3	2790	U
3	L3	2814	C
3	L3	2826	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L3	2827	G
3	L3	2829	U
3	L3	2855	G
3	L3	2877	G
3	L3	2902	G
3	L3	3585	G
3	L3	3593	C
3	L3	3595	U
3	L3	3617	G
3	L3	3626	G
3	L3	3635	A
3	L3	3653	A
3	L3	3662	A
3	L3	3673	C
3	L3	3696	C
3	L3	3697	U
3	L3	3838	U
3	L3	3840	U
3	L3	3868	G
3	L3	3872	A
3	L3	3875	G
3	L3	3876	A
3	L3	3877	A
3	L3	3887	OMC
3	L3	3905	A
3	L3	3915	U
3	L3	4069	U
3	L3	4076	G
3	L3	4084	G
3	L3	4085	A
3	L3	4119	C
3	L3	4121	G
3	L3	4122	G
3	L3	4133	C
3	L3	4139	G
3	L3	4140	C
3	L3	4142	C
3	L3	4143	G
3	L3	4144	C
3	L3	4145	C
3	L3	4147	G
3	L3	4150	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L3	4162	C
3	L3	4163	U
3	L3	4164	C
3	L3	4170	A
3	L3	4183	G
3	L3	4184	G
3	L3	4191	G
3	L3	4202	U
3	L3	4205	A
3	L3	4220	6MZ
3	L3	4225	G
3	L3	4228	OMG
3	L3	4229	U
3	L3	4233	A
3	L3	4251	A
3	L3	4254	G
3	L3	4258	C
3	L3	4266	G
3	L3	4268	A
3	L3	4273	A
3	L3	4281	A
3	L3	4291	G
3	L3	4305	G
3	L3	4306	OMU
3	L3	4314	C
3	L3	4329	G
3	L3	4330	G
3	L3	4332	C
3	L3	4339	A
3	L3	4373	G
3	L3	4377	G
3	L3	4378	A
3	L3	4387	C
3	L3	4415	A
3	L3	4418	G
3	L3	4437	U
3	L3	4438	U
3	L3	4439	U
3	L3	4453	C
3	L3	4464	A
3	L3	4466	C
3	L3	4475	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L3	4491	G
3	L3	4498	OMU
3	L3	4512	U
3	L3	4513	A
3	L3	4518	A
3	L3	4519	C
3	L3	4523	A2M
3	L3	4524	G
3	L3	4532	PSU
3	L3	4545	G
3	L3	4548	A
3	L3	4549	G
3	L3	4556	U
3	L3	4558	U
3	L3	4560	C
3	L3	4567	G
3	L3	4573	G
3	L3	4584	A
3	L3	4590	A2M
3	L3	4608	G
3	L3	4618	OMG
3	L3	4636	PSU
3	L3	4637	OMG
3	L3	4656	A
3	L3	4670	C
3	L3	4672	A
3	L3	4678	G
3	L3	4701	A
3	L3	4708	A
3	L3	4709	U
3	L3	4719	G
3	L3	4740	G
3	L3	4741	C
3	L3	4742	G
3	L3	4750	G
3	L3	4751	G
3	L3	4754	G
3	L3	4757	C
3	L3	4759	C
3	L3	4765	G
3	L3	4772	C
3	L3	4773	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L3	4870	G
3	L3	4871	C
3	L3	4882	U
3	L3	4883	C
3	L3	4900	C
3	L3	4901	G
3	L3	4910	G
3	L3	4911	A
3	L3	4914	C
3	L3	4916	G
3	L3	4937	C
3	L3	4943	A
3	L3	4976	U
3	L3	5006	U
3	L3	5014	A
3	L3	5022	U
3	L3	5023	C
3	L3	5026	U
3	L3	5027	C
3	L3	5031	G
3	L3	5039	U
3	L3	5041	G
3	L3	5050	C
3	L3	5054	C
3	L3	5055	G
3	L3	5061	A
3	L3	5062	G
3	L3	5069	U
4	L4	7	G
4	L4	49	A
4	L4	53	U
4	L4	54	A
4	L4	64	G
4	L4	66	G
4	L4	103	A
4	L4	110	G
4	L4	111	C
4	L4	120	U

All (11) RNA pucker outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
-----	-------	-----	------

Mol	Chain	Res	Type
3	L3	496	G
3	L3	502	C
3	L3	503	C
3	L3	1324	A
3	L3	1633	G
3	L3	1853	G
3	L3	2095	A
3	L3	2469	C
3	L3	2477	A
3	L3	3616	U
4	L4	109	U

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

109 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
3	A2M	L3	4571	3	22,25,26	0.85	0	30,36,39	2.04	7 (23%)
3	A2M	L3	2787	3	22,25,26	0.86	0	30,36,39	2.11	7 (23%)
3	PSU	L3	4636	3	18,21,22	1.12	1 (5%)	21,30,33	2.00	5 (23%)
3	PSU	L3	1582	3	18,21,22	1.06	1 (5%)	21,30,33	1.92	4 (19%)
3	OMG	L3	2424	3	23,26,27	0.47	0	32,38,41	0.46	0
3	A2M	L3	3825	3	22,25,26	0.84	0	30,36,39	2.08	7 (23%)
3	OMG	L3	2876	3	23,26,27	0.45	0	32,38,41	0.46	0
3	A2M	L3	2815	3	22,25,26	0.86	0	30,36,39	2.13	8 (26%)
3	PSU	L3	3851	3	18,21,22	1.14	1 (5%)	21,30,33	1.95	6 (28%)
3	A2M	L3	3867	3	22,25,26	0.85	0	30,36,39	2.12	8 (26%)
3	OMG	L3	2364	3	23,26,27	0.46	0	32,38,41	0.46	0
3	OMU	L3	2837	3	19,22,23	2.07	7 (36%)	25,31,34	1.80	5 (20%)
3	OMG	L3	1316	3	23,26,27	0.47	0	32,38,41	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMG	L3	3627	3	23,26,27	0.46	0	32,38,41	0.53	0
3	OMC	L3	3869	3	19,22,23	0.50	0	25,31,34	0.65	0
3	OMC	L3	4536	3	19,22,23	0.51	0	25,31,34	0.66	0
3	OMU	L3	4620	3	19,22,23	2.03	6 (31%)	25,31,34	1.68	4 (16%)
3	PSU	L3	2632	3	18,21,22	1.12	1 (5%)	21,30,33	1.85	4 (19%)
3	OMC	L3	2365	3	19,22,23	0.51	0	25,31,34	0.70	0
3	OMC	L3	4456	3	19,22,23	0.51	0	25,31,34	0.65	0
3	OMU	L3	4227	3	19,22,23	2.05	7 (36%)	25,31,34	1.85	4 (16%)
3	PSU	L3	4312	3	18,21,22	1.07	1 (5%)	21,30,33	1.99	5 (23%)
2	PSU	L1	55	2	18,21,22	1.10	1 (5%)	21,30,33	1.96	5 (23%)
3	OMG	L3	3899	3	23,26,27	0.46	0	32,38,41	0.54	0
3	OMC	L3	2422	51,3	19,22,23	0.50	0	25,31,34	0.78	1 (4%)
3	PSU	L3	4500	3	18,21,22	1.08	1 (5%)	21,30,33	1.91	4 (19%)
3	6MZ	L3	4220	3	22,25,26	1.14	1 (4%)	29,36,39	2.17	9 (31%)
3	PSU	L3	5010	3	18,21,22	1.13	1 (5%)	21,30,33	1.93	5 (23%)
3	OMG	L3	1625	3	23,26,27	0.47	0	32,38,41	0.45	0
3	PSU	L3	4471	3	18,21,22	1.13	1 (5%)	21,30,33	1.95	5 (23%)
3	OMC	L3	2351	51,3	19,22,23	0.52	0	25,31,34	0.70	0
3	OMC	L3	2861	3	19,22,23	0.48	0	25,31,34	0.68	0
3	PSU	L3	3822	3	18,21,22	1.13	1 (5%)	21,30,33	1.95	5 (23%)
3	PSU	L3	1536	3	18,21,22	1.10	1 (5%)	21,30,33	1.96	5 (23%)
3	PSU	L3	3884	3	18,21,22	1.09	1 (5%)	21,30,33	1.91	4 (19%)
3	PSU	L3	2839	3	18,21,22	1.11	1 (5%)	21,30,33	1.96	5 (23%)
3	PSU	L3	4972	3	18,21,22	1.09	1 (5%)	21,30,33	1.94	5 (23%)
3	OMG	L3	1522	3	23,26,27	0.46	0	32,38,41	0.47	0
3	A2M	L3	3724	3	22,25,26	0.86	0	30,36,39	2.05	7 (23%)
3	PSU	L3	1860	3	18,21,22	1.11	1 (5%)	21,30,33	1.93	5 (23%)
3	PSU	L3	5001	3	18,21,22	1.14	1 (5%)	21,30,33	1.94	6 (28%)
23	HIC	LN	245	23	10,11,12	1.53	1 (10%)	9,14,16	1.21	1 (11%)
3	PSU	L3	1677	3	18,21,22	1.07	1 (5%)	21,30,33	1.90	5 (23%)
3	OMU	L3	2415	3	19,22,23	2.07	7 (36%)	25,31,34	1.80	5 (20%)
3	A2M	L3	2363	51,3	22,25,26	0.88	0	30,36,39	2.09	7 (23%)
3	1MA	L3	1322	3	21,25,26	0.47	0	30,37,40	0.84	1 (3%)
3	PSU	L3	4299	3	18,21,22	1.07	1 (5%)	21,30,33	2.00	5 (23%)
3	PSU	L3	1683	3	18,21,22	1.11	1 (5%)	21,30,33	1.93	5 (23%)
3	PSU	L3	4293	3	18,21,22	1.05	1 (5%)	21,30,33	1.87	4 (19%)
3	PSU	L3	4403	3	18,21,22	1.10	1 (5%)	21,30,33	1.97	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMG	L3	4494	3	23,26,27	0.48	0	32,38,41	0.51	0
3	PSU	L3	4296	3	18,21,22	1.08	1 (5%)	21,30,33	1.99	5 (23%)
3	A2M	L3	3718	3	22,25,26	0.85	0	30,36,39	2.11	8 (26%)
3	OMC	L3	3841	3	19,22,23	0.49	0	25,31,34	0.63	0
3	OMG	L3	4392	3	23,26,27	0.46	0	32,38,41	0.48	0
3	OMU	L3	4306	3	19,22,23	2.04	6 (31%)	25,31,34	1.79	5 (20%)
2	PSU	L1	69	2	18,21,22	1.13	1 (5%)	21,30,33	1.95	5 (23%)
3	PSU	L3	4552	3	18,21,22	1.10	1 (5%)	21,30,33	1.92	5 (23%)
3	A2M	L3	400	3	22,25,26	0.85	0	30,36,39	2.09	8 (26%)
3	OMU	L3	4498	3	19,22,23	2.10	7 (36%)	25,31,34	1.79	5 (20%)
3	PSU	L3	4576	3	18,21,22	1.12	1 (5%)	21,30,33	1.93	6 (28%)
3	PSU	L3	4431	3	18,21,22	1.14	1 (5%)	21,30,33	1.95	5 (23%)
3	OMC	L3	3701	3	19,22,23	0.47	0	25,31,34	0.66	0
3	OMC	L3	3887	3	19,22,23	0.51	0	25,31,34	0.68	0
3	PSU	L3	3920	51,3	18,21,22	1.06	1 (5%)	21,30,33	1.94	6 (28%)
3	PSU	L3	3695	3	18,21,22	1.13	1 (5%)	21,30,33	1.96	5 (23%)
3	OMC	L3	2824	3	19,22,23	0.49	0	25,31,34	0.62	0
3	PSU	L3	1792	3	18,21,22	1.11	1 (5%)	21,30,33	1.91	5 (23%)
3	OMG	L3	4370	3	23,26,27	0.49	0	32,38,41	0.53	0
3	OMG	L3	4499	3	23,26,27	0.44	0	32,38,41	0.47	0
3	PSU	L3	4353	3	18,21,22	1.10	1 (5%)	21,30,33	1.99	5 (23%)
3	PSU	L3	3734	3	18,21,22	1.13	1 (5%)	21,30,33	1.91	5 (23%)
3	PSU	L3	1862	3	18,21,22	1.12	1 (5%)	21,30,33	1.99	6 (28%)
3	PSU	L3	3844	3	18,21,22	1.12	1 (5%)	21,30,33	1.95	5 (23%)
3	A2M	L3	1534	51,3	22,25,26	0.83	0	30,36,39	2.18	8 (26%)
3	A2M	L3	1524	3	22,25,26	0.86	0	30,36,39	2.11	8 (26%)
3	A2M	L3	4523	3	22,25,26	0.85	0	30,36,39	2.12	8 (26%)
3	OMG	L3	4623	3	23,26,27	0.48	0	32,38,41	0.53	0
3	A2M	L3	3830	3	22,25,26	0.83	0	30,36,39	2.08	7 (23%)
3	A2M	L3	2401	3	22,25,26	0.85	0	30,36,39	2.13	8 (26%)
3	OMC	L3	2804	3	19,22,23	0.51	0	25,31,34	0.70	0
3	A2M	L3	1871	3	22,25,26	0.84	0	30,36,39	2.17	8 (26%)
3	A2M	L3	1326	3	22,25,26	0.86	0	30,36,39	2.08	7 (23%)
3	A2M	L3	4590	3	22,25,26	0.87	0	30,36,39	2.05	8 (26%)
3	OMG	L3	4618	3	23,26,27	0.48	0	32,38,41	0.51	0
3	PSU	L3	3853	3	18,21,22	1.10	1 (5%)	21,30,33	1.86	4 (19%)
3	PSU	L3	3637	3	18,21,22	1.11	1 (5%)	21,30,33	2.12	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L3	3639	3	18,21,22	1.11	1 (5%)	21,30,33	1.95	5 (23%)
3	OMG	L3	3744	3	23,26,27	0.44	0	32,38,41	0.48	0
3	PSU	L3	4579	3	18,21,22	1.10	1 (5%)	21,30,33	1.93	4 (19%)
3	OMG	L3	4637	3	23,26,27	0.46	0	32,38,41	0.46	0
3	A2M	L3	398	3	22,25,26	0.83	0	30,36,39	2.13	8 (26%)
3	OMU	L3	3925	3	19,22,23	2.06	7 (36%)	25,31,34	1.79	5 (20%)
3	PSU	L3	3715	3	18,21,22	1.13	1 (5%)	21,30,33	1.94	6 (28%)
3	UR3	L3	4530	3	19,22,23	1.07	3 (15%)	26,32,35	1.52	2 (7%)
3	PSU	L3	4628	3	18,21,22	1.03	1 (5%)	21,30,33	1.92	6 (28%)
38	PTR	NR	127	38	15,16,17	1.28	1 (6%)	17,22,24	0.65	0
3	PSU	L3	4532	3	18,21,22	1.11	1 (5%)	21,30,33	1.97	5 (23%)
3	PSU	L3	4689	3	18,21,22	1.08	1 (5%)	21,30,33	1.96	5 (23%)
3	OMC	L3	1340	3	19,22,23	0.52	0	25,31,34	0.64	0
2	OMG	L1	75	2	23,26,27	0.45	0	32,38,41	0.46	0
3	PSU	L3	4673	3	18,21,22	1.10	1 (5%)	21,30,33	1.94	5 (23%)
3	PSU	L3	3730	3	18,21,22	1.08	1 (5%)	21,30,33	1.95	5 (23%)
3	PSU	L3	4457	3	18,21,22	1.09	1 (5%)	21,30,33	1.91	4 (19%)
3	PSU	L3	2508	3	18,21,22	1.12	1 (5%)	21,30,33	1.91	5 (23%)
3	PSU	L3	4521	3	18,21,22	1.10	1 (5%)	21,30,33	1.91	5 (23%)
3	OMG	L3	4228	3	23,26,27	0.48	0	32,38,41	0.54	0
3	PSU	L3	4361	3	18,21,22	1.06	1 (5%)	21,30,33	1.96	5 (23%)
3	PSU	L3	4493	3	18,21,22	1.09	1 (5%)	21,30,33	1.95	5 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	L3	4571	3	-	1/9/27/28	0/3/3/3
3	A2M	L3	2787	3	-	5/9/27/28	0/3/3/3
3	PSU	L3	4636	3	-	2/7/25/26	0/2/2/2
3	PSU	L3	1582	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	2424	3	-	1/9/27/28	0/3/3/3
3	A2M	L3	3825	3	-	1/9/27/28	0/3/3/3
3	OMG	L3	2876	3	-	3/9/27/28	0/3/3/3
3	A2M	L3	2815	3	-	1/9/27/28	0/3/3/3
3	PSU	L3	3851	3	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	L3	3867	3	-	2/9/27/28	0/3/3/3
3	OMG	L3	2364	3	-	1/9/27/28	0/3/3/3
3	OMU	L3	2837	3	-	1/9/27/28	0/2/2/2
3	OMG	L3	1316	3	-	1/9/27/28	0/3/3/3
3	OMG	L3	3627	3	-	1/9/27/28	0/3/3/3
3	OMC	L3	3869	3	-	0/9/27/28	0/2/2/2
3	OMC	L3	4536	3	-	1/9/27/28	0/2/2/2
3	OMU	L3	4620	3	-	0/9/27/28	0/2/2/2
3	PSU	L3	2632	3	-	0/7/25/26	0/2/2/2
3	OMC	L3	2365	3	-	0/9/27/28	0/2/2/2
3	OMC	L3	4456	3	-	1/9/27/28	0/2/2/2
3	OMU	L3	4227	3	-	1/9/27/28	0/2/2/2
3	PSU	L3	4312	3	-	0/7/25/26	0/2/2/2
2	PSU	L1	55	2	-	0/7/25/26	0/2/2/2
3	OMG	L3	3899	3	-	1/9/27/28	0/3/3/3
3	OMC	L3	2422	51,3	-	2/9/27/28	0/2/2/2
3	PSU	L3	4500	3	-	0/7/25/26	0/2/2/2
3	6MZ	L3	4220	3	-	3/9/27/28	0/3/3/3
3	PSU	L3	5010	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	1625	3	-	2/9/27/28	0/3/3/3
3	PSU	L3	4471	3	-	0/7/25/26	0/2/2/2
3	OMC	L3	2351	51,3	-	3/9/27/28	0/2/2/2
3	OMC	L3	2861	3	-	1/9/27/28	0/2/2/2
3	PSU	L3	3822	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	1536	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	3884	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	2839	3	-	1/7/25/26	0/2/2/2
3	PSU	L3	4972	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	1522	3	-	0/9/27/28	0/3/3/3
3	A2M	L3	3724	3	-	1/9/27/28	0/3/3/3
3	PSU	L3	1860	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	5001	3	-	0/7/25/26	0/2/2/2
23	HIC	LN	245	23	-	2/5/6/8	0/1/1/1
3	PSU	L3	1677	3	-	4/7/25/26	0/2/2/2
3	OMU	L3	2415	3	-	2/9/27/28	0/2/2/2
3	A2M	L3	2363	51,3	-	0/9/27/28	0/3/3/3
3	1MA	L3	1322	3	-	0/7/25/26	0/3/3/3
3	PSU	L3	4299	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	1683	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	4293	3	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L3	4403	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	4494	3	-	0/9/27/28	0/3/3/3
3	PSU	L3	4296	3	-	0/7/25/26	0/2/2/2
3	A2M	L3	3718	3	-	1/9/27/28	0/3/3/3
3	OMC	L3	3841	3	-	1/9/27/28	0/2/2/2
3	OMG	L3	4392	3	-	1/9/27/28	0/3/3/3
3	OMU	L3	4306	3	-	1/9/27/28	0/2/2/2
2	PSU	L1	69	2	-	0/7/25/26	0/2/2/2
3	PSU	L3	4552	3	-	0/7/25/26	0/2/2/2
3	A2M	L3	400	3	-	1/9/27/28	0/3/3/3
3	OMU	L3	4498	3	-	4/9/27/28	0/2/2/2
3	PSU	L3	4576	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	4431	3	-	0/7/25/26	0/2/2/2
3	OMC	L3	3701	3	-	7/9/27/28	0/2/2/2
3	OMC	L3	3887	3	-	2/9/27/28	0/2/2/2
3	PSU	L3	3920	51,3	-	0/7/25/26	0/2/2/2
3	PSU	L3	3695	3	-	0/7/25/26	0/2/2/2
3	OMC	L3	2824	3	-	1/9/27/28	0/2/2/2
3	PSU	L3	1792	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	4370	3	-	0/9/27/28	0/3/3/3
3	OMG	L3	4499	3	-	0/9/27/28	0/3/3/3
3	PSU	L3	4353	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	3734	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	1862	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	3844	3	-	1/7/25/26	0/2/2/2
3	A2M	L3	1534	51,3	-	2/9/27/28	0/3/3/3
3	A2M	L3	1524	3	-	2/9/27/28	0/3/3/3
3	A2M	L3	4523	3	-	2/9/27/28	0/3/3/3
3	OMG	L3	4623	3	-	1/9/27/28	0/3/3/3
3	A2M	L3	3830	3	-	1/9/27/28	0/3/3/3
3	A2M	L3	2401	3	-	2/9/27/28	0/3/3/3
3	OMC	L3	2804	3	-	1/9/27/28	0/2/2/2
3	A2M	L3	1871	3	-	0/9/27/28	0/3/3/3
3	A2M	L3	1326	3	-	4/9/27/28	0/3/3/3
3	A2M	L3	4590	3	-	4/9/27/28	0/3/3/3
3	OMG	L3	4618	3	-	2/9/27/28	0/3/3/3
3	PSU	L3	3853	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	3637	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	3639	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	3744	3	-	1/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L3	4579	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	4637	3	-	3/9/27/28	0/3/3/3
3	A2M	L3	398	3	-	1/9/27/28	0/3/3/3
3	OMU	L3	3925	3	-	2/9/27/28	0/2/2/2
3	PSU	L3	3715	3	-	0/7/25/26	0/2/2/2
3	UR3	L3	4530	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	4628	3	-	0/7/25/26	0/2/2/2
38	PTR	NR	127	38	-	0/10/11/13	0/1/1/1
3	PSU	L3	4532	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	4689	3	-	0/7/25/26	0/2/2/2
3	OMC	L3	1340	3	-	1/9/27/28	0/2/2/2
2	OMG	L1	75	2	-	1/9/27/28	0/3/3/3
3	PSU	L3	4673	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	3730	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	4457	3	-	1/7/25/26	0/2/2/2
3	PSU	L3	2508	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	4521	3	-	2/7/25/26	0/2/2/2
3	OMG	L3	4228	3	-	3/9/27/28	0/3/3/3
3	PSU	L3	4361	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	4493	3	-	0/7/25/26	0/2/2/2

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L3	4498	OMU	C6-N1	4.87	1.49	1.38
3	L3	2837	OMU	C6-N1	4.77	1.49	1.38
3	L3	2415	OMU	C6-N1	4.76	1.49	1.38
3	L3	4620	OMU	C6-N1	4.75	1.49	1.38
3	L3	3925	OMU	C6-N1	4.73	1.49	1.38
3	L3	4227	OMU	C6-N1	4.71	1.49	1.38
3	L3	4306	OMU	C6-N1	4.69	1.49	1.38
38	NR	127	PTR	OH-CZ	-4.66	1.30	1.40
3	L3	4498	OMU	C2-N1	4.41	1.45	1.38
3	L3	2837	OMU	C2-N1	4.25	1.45	1.38
3	L3	4227	OMU	C2-N1	4.23	1.45	1.38
3	L3	3925	OMU	C2-N1	4.23	1.45	1.38
3	L3	4620	OMU	C2-N1	4.21	1.45	1.38
3	L3	2415	OMU	C2-N1	4.18	1.45	1.38
3	L3	4498	OMU	C5-C4	4.14	1.52	1.43
3	L3	4306	OMU	C2-N1	4.11	1.44	1.38
3	L3	2415	OMU	C5-C4	4.10	1.52	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L3	2837	OMU	C5-C4	4.07	1.52	1.43
3	L3	4227	OMU	C5-C4	4.06	1.52	1.43
3	L3	4220	6MZ	C6-N6	4.05	1.38	1.34
3	L3	3925	OMU	C5-C4	4.04	1.52	1.43
3	L3	4306	OMU	C5-C4	3.97	1.52	1.43
3	L3	4620	OMU	C5-C4	3.91	1.52	1.43
3	L3	4431	PSU	C6-C5	3.75	1.39	1.35
3	L3	2632	PSU	C6-C5	3.74	1.39	1.35
3	L3	3822	PSU	C6-C5	3.72	1.39	1.35
3	L3	5001	PSU	C6-C5	3.71	1.39	1.35
3	L3	3715	PSU	C6-C5	3.70	1.39	1.35
3	L3	5010	PSU	C6-C5	3.67	1.39	1.35
3	L3	3695	PSU	C6-C5	3.66	1.39	1.35
3	L3	2839	PSU	C6-C5	3.65	1.39	1.35
3	L3	3851	PSU	C6-C5	3.65	1.39	1.35
3	L3	4576	PSU	C6-C5	3.65	1.39	1.35
3	L3	3853	PSU	C6-C5	3.65	1.39	1.35
3	L3	3734	PSU	C6-C5	3.65	1.39	1.35
3	L3	2508	PSU	C6-C5	3.64	1.39	1.35
3	L3	4636	PSU	C6-C5	3.63	1.39	1.35
3	L3	4471	PSU	C6-C5	3.63	1.39	1.35
3	L3	1862	PSU	C6-C5	3.63	1.39	1.35
3	L3	3844	PSU	C6-C5	3.62	1.39	1.35
3	L3	1860	PSU	C6-C5	3.62	1.39	1.35
2	L1	69	PSU	C6-C5	3.61	1.39	1.35
3	L3	4521	PSU	C6-C5	3.60	1.39	1.35
3	L3	4353	PSU	C6-C5	3.59	1.39	1.35
3	L3	4673	PSU	C6-C5	3.58	1.39	1.35
3	L3	1683	PSU	C6-C5	3.58	1.39	1.35
3	L3	4972	PSU	C6-C5	3.57	1.39	1.35
2	L1	55	PSU	C6-C5	3.57	1.39	1.35
3	L3	4403	PSU	C6-C5	3.57	1.39	1.35
3	L3	1792	PSU	C6-C5	3.57	1.39	1.35
3	L3	3639	PSU	C6-C5	3.57	1.39	1.35
3	L3	4532	PSU	C6-C5	3.56	1.39	1.35
3	L3	4493	PSU	C6-C5	3.54	1.39	1.35
3	L3	3884	PSU	C6-C5	3.53	1.39	1.35
3	L3	3637	PSU	C6-C5	3.53	1.39	1.35
3	L3	4500	PSU	C6-C5	3.53	1.39	1.35
3	L3	4579	PSU	C6-C5	3.52	1.39	1.35
3	L3	4552	PSU	C6-C5	3.52	1.39	1.35
3	L3	4457	PSU	C6-C5	3.51	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L3	3730	PSU	C6-C5	3.49	1.39	1.35
3	L3	1536	PSU	C6-C5	3.48	1.39	1.35
3	L3	4689	PSU	C6-C5	3.46	1.39	1.35
3	L3	1582	PSU	C6-C5	3.46	1.39	1.35
3	L3	4312	PSU	C6-C5	3.45	1.39	1.35
3	L3	4296	PSU	C6-C5	3.42	1.39	1.35
3	L3	4361	PSU	C6-C5	3.36	1.39	1.35
3	L3	4299	PSU	C6-C5	3.36	1.39	1.35
3	L3	4293	PSU	C6-C5	3.34	1.39	1.35
3	L3	3920	PSU	C6-C5	3.30	1.38	1.35
3	L3	1677	PSU	C6-C5	3.28	1.38	1.35
3	L3	4628	PSU	C6-C5	3.20	1.38	1.35
23	LN	245	HIC	CD2-CG	3.15	1.41	1.36
3	L3	4306	OMU	O4-C4	-2.81	1.19	1.24
3	L3	4227	OMU	O4-C4	-2.80	1.19	1.24
3	L3	4620	OMU	O4-C4	-2.78	1.19	1.24
3	L3	4530	UR3	C4-N3	-2.77	1.35	1.40
3	L3	4530	UR3	C2-N1	-2.75	1.34	1.38
3	L3	2837	OMU	O4-C4	-2.71	1.19	1.24
3	L3	2415	OMU	O4-C4	-2.68	1.19	1.24
3	L3	3925	OMU	O4-C4	-2.67	1.19	1.24
3	L3	2415	OMU	C2-N3	2.66	1.42	1.38
3	L3	4498	OMU	O4-C4	-2.66	1.19	1.24
3	L3	4498	OMU	C2-N3	2.59	1.42	1.38
3	L3	3925	OMU	C2-N3	2.58	1.42	1.38
3	L3	2837	OMU	C2-N3	2.58	1.42	1.38
3	L3	4306	OMU	C2-N3	2.46	1.42	1.38
3	L3	4306	OMU	O2-C2	-2.36	1.18	1.23
3	L3	4620	OMU	C2-N3	2.34	1.42	1.38
3	L3	4227	OMU	C2-N3	2.33	1.42	1.38
3	L3	4227	OMU	O2-C2	-2.23	1.19	1.23
3	L3	4620	OMU	O2-C2	-2.20	1.19	1.23
3	L3	3925	OMU	O2-C2	-2.18	1.19	1.23
3	L3	2837	OMU	O2-C2	-2.17	1.19	1.23
3	L3	2415	OMU	O2-C2	-2.17	1.19	1.23
3	L3	2837	OMU	C4-N3	2.16	1.42	1.38
3	L3	4530	UR3	C2-N3	-2.14	1.34	1.39
3	L3	4498	OMU	O2-C2	-2.11	1.19	1.23
3	L3	3925	OMU	C4-N3	2.10	1.42	1.38
3	L3	2415	OMU	C4-N3	2.10	1.42	1.38
3	L3	4498	OMU	C4-N3	2.10	1.42	1.38
3	L3	4227	OMU	C4-N3	2.00	1.42	1.38

All (424) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L3	4220	6MZ	C5-C4-N3	-5.81	118.71	126.72
3	L3	1534	A2M	C5-C4-N3	-5.71	118.86	126.72
3	L3	2363	A2M	C5-C4-N3	-5.66	118.93	126.72
3	L3	4571	A2M	C5-C4-N3	-5.62	118.98	126.72
3	L3	4227	OMU	C4-N3-C2	-5.60	119.66	126.61
3	L3	2815	A2M	C5-C4-N3	-5.60	119.00	126.72
3	L3	3867	A2M	C5-C4-N3	-5.57	119.04	126.72
3	L3	1326	A2M	C5-C4-N3	-5.55	119.08	126.72
3	L3	3825	A2M	C5-C4-N3	-5.54	119.08	126.72
3	L3	2787	A2M	C5-C4-N3	-5.53	119.11	126.72
3	L3	2401	A2M	C5-C4-N3	-5.52	119.11	126.72
3	L3	3724	A2M	C5-C4-N3	-5.51	119.13	126.72
3	L3	1524	A2M	C5-C4-N3	-5.46	119.20	126.72
3	L3	400	A2M	C5-C4-N3	-5.45	119.21	126.72
3	L3	4523	A2M	C5-C4-N3	-5.44	119.23	126.72
3	L3	4530	UR3	C4-N3-C2	-5.41	120.22	124.58
3	L3	2837	OMU	C4-N3-C2	-5.41	119.89	126.61
3	L3	398	A2M	C5-C4-N3	-5.40	119.28	126.72
3	L3	3718	A2M	C5-C4-N3	-5.39	119.29	126.72
3	L3	4498	OMU	C4-N3-C2	-5.36	119.96	126.61
3	L3	3830	A2M	C5-C4-N3	-5.35	119.35	126.72
3	L3	2415	OMU	C4-N3-C2	-5.34	119.98	126.61
3	L3	3637	PSU	N1-C2-N3	5.34	120.80	115.17
3	L3	4306	OMU	C4-N3-C2	-5.32	120.01	126.61
3	L3	3925	OMU	C4-N3-C2	-5.31	120.02	126.61
3	L3	1871	A2M	C5-C4-N3	-5.27	119.47	126.72
3	L3	3637	PSU	C4-N3-C2	-5.13	119.31	126.37
3	L3	4312	PSU	N1-C2-N3	5.08	120.53	115.17
3	L3	4299	PSU	N1-C2-N3	5.00	120.44	115.17
3	L3	4353	PSU	N1-C2-N3	5.00	120.44	115.17
3	L3	4299	PSU	C4-N3-C2	-4.99	119.50	126.37
3	L3	4296	PSU	C4-N3-C2	-4.96	119.53	126.37
3	L3	4636	PSU	C4-N3-C2	-4.96	119.54	126.37
3	L3	1582	PSU	C4-N3-C2	-4.95	119.55	126.37
3	L3	4353	PSU	C4-N3-C2	-4.95	119.56	126.37
3	L3	4689	PSU	N1-C2-N3	4.94	120.38	115.17
3	L3	1862	PSU	N1-C2-N3	4.93	120.36	115.17
3	L3	4296	PSU	N1-C2-N3	4.92	120.36	115.17
3	L3	4532	PSU	C4-N3-C2	-4.92	119.60	126.37
3	L3	4636	PSU	N1-C2-N3	4.91	120.35	115.17
3	L3	4590	A2M	C5-C4-N3	-4.90	119.97	126.72
3	L3	1862	PSU	C4-N3-C2	-4.90	119.62	126.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L3	4361	PSU	N1-C2-N3	4.90	120.34	115.17
3	L3	4471	PSU	N1-C2-N3	4.90	120.33	115.17
3	L3	1677	PSU	C4-N3-C2	-4.89	119.63	126.37
3	L3	4493	PSU	C4-N3-C2	-4.89	119.63	126.37
3	L3	2839	PSU	N1-C2-N3	4.89	120.33	115.17
3	L3	4493	PSU	N1-C2-N3	4.88	120.32	115.17
3	L3	4403	PSU	C4-N3-C2	-4.87	119.66	126.37
3	L3	2839	PSU	C4-N3-C2	-4.87	119.67	126.37
3	L3	3851	PSU	C4-N3-C2	-4.86	119.68	126.37
3	L3	1860	PSU	C4-N3-C2	-4.85	119.69	126.37
2	L1	55	PSU	C4-N3-C2	-4.84	119.70	126.37
3	L3	4431	PSU	C4-N3-C2	-4.84	119.70	126.37
3	L3	1536	PSU	C4-N3-C2	-4.84	119.71	126.37
3	L3	5010	PSU	C4-N3-C2	-4.83	119.71	126.37
3	L3	4552	PSU	C4-N3-C2	-4.83	119.72	126.37
3	L3	4312	PSU	C4-N3-C2	-4.83	119.72	126.37
3	L3	4403	PSU	N1-C2-N3	4.83	120.26	115.17
3	L3	4361	PSU	C4-N3-C2	-4.83	119.72	126.37
3	L3	1536	PSU	N1-C2-N3	4.82	120.26	115.17
3	L3	5001	PSU	C4-N3-C2	-4.82	119.73	126.37
3	L3	1683	PSU	N1-C2-N3	4.82	120.25	115.17
3	L3	3730	PSU	C4-N3-C2	-4.82	119.73	126.37
3	L3	4689	PSU	C4-N3-C2	-4.82	119.73	126.37
3	L3	3695	PSU	C4-N3-C2	-4.82	119.73	126.37
3	L3	3844	PSU	C4-N3-C2	-4.81	119.74	126.37
3	L3	4521	PSU	N1-C2-N3	4.81	120.25	115.17
3	L3	3844	PSU	N1-C2-N3	4.81	120.25	115.17
3	L3	3730	PSU	N1-C2-N3	4.81	120.24	115.17
3	L3	3822	PSU	N1-C2-N3	4.81	120.24	115.17
3	L3	4220	6MZ	N3-C4-N9	4.81	135.34	127.17
3	L3	3715	PSU	C4-N3-C2	-4.81	119.75	126.37
3	L3	3639	PSU	N1-C2-N3	4.80	120.23	115.17
3	L3	1792	PSU	N1-C2-N3	4.80	120.23	115.17
3	L3	3884	PSU	N1-C2-N3	4.80	120.23	115.17
3	L3	3695	PSU	N1-C2-N3	4.80	120.23	115.17
3	L3	1582	PSU	N1-C2-N3	4.80	120.23	115.17
3	L3	4431	PSU	N1-C2-N3	4.80	120.23	115.17
3	L3	5001	PSU	N1-C2-N3	4.80	120.23	115.17
3	L3	3822	PSU	C4-N3-C2	-4.80	119.77	126.37
3	L3	4972	PSU	C4-N3-C2	-4.79	119.77	126.37
3	L3	4293	PSU	N1-C2-N3	4.79	120.22	115.17
3	L3	4673	PSU	N1-C2-N3	4.79	120.22	115.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L3	1792	PSU	C4-N3-C2	-4.79	119.78	126.37
3	L3	4576	PSU	N1-C2-N3	4.79	120.22	115.17
3	L3	4673	PSU	C4-N3-C2	-4.79	119.78	126.37
3	L3	3851	PSU	N1-C2-N3	4.79	120.22	115.17
3	L3	4471	PSU	C4-N3-C2	-4.78	119.78	126.37
3	L3	5010	PSU	N1-C2-N3	4.78	120.21	115.17
3	L3	2508	PSU	C4-N3-C2	-4.78	119.78	126.37
3	L3	3639	PSU	C4-N3-C2	-4.78	119.78	126.37
3	L3	4579	PSU	C4-N3-C2	-4.78	119.78	126.37
3	L3	4500	PSU	N1-C2-N3	4.78	120.21	115.17
3	L3	3715	PSU	N1-C2-N3	4.78	120.21	115.17
2	L1	55	PSU	N1-C2-N3	4.78	120.21	115.17
3	L3	4972	PSU	N1-C2-N3	4.78	120.21	115.17
3	L3	1677	PSU	N1-C2-N3	4.77	120.20	115.17
3	L3	4620	OMU	C4-N3-C2	-4.77	120.69	126.61
3	L3	1683	PSU	C4-N3-C2	-4.77	119.80	126.37
3	L3	3920	PSU	C4-N3-C2	-4.77	119.80	126.37
3	L3	4532	PSU	N1-C2-N3	4.77	120.20	115.17
3	L3	3920	PSU	N1-C2-N3	4.77	120.19	115.17
3	L3	4500	PSU	C4-N3-C2	-4.77	119.81	126.37
3	L3	2632	PSU	C4-N3-C2	-4.76	119.81	126.37
3	L3	1860	PSU	N1-C2-N3	4.76	120.19	115.17
3	L3	4457	PSU	N1-C2-N3	4.75	120.18	115.17
3	L3	4457	PSU	C4-N3-C2	-4.75	119.83	126.37
3	L3	4579	PSU	N1-C2-N3	4.75	120.17	115.17
3	L3	4521	PSU	C4-N3-C2	-4.74	119.84	126.37
3	L3	4576	PSU	C4-N3-C2	-4.74	119.84	126.37
2	L1	69	PSU	N1-C2-N3	4.74	120.17	115.17
2	L1	69	PSU	C4-N3-C2	-4.74	119.85	126.37
3	L3	1534	A2M	N3-C4-N9	4.73	135.21	127.17
3	L3	4628	PSU	N1-C2-N3	4.72	120.14	115.17
3	L3	2363	A2M	N3-C4-N9	4.71	135.19	127.17
3	L3	4628	PSU	C4-N3-C2	-4.71	119.88	126.37
3	L3	3734	PSU	C4-N3-C2	-4.71	119.88	126.37
3	L3	3853	PSU	N1-C2-N3	4.70	120.13	115.17
3	L3	4552	PSU	N1-C2-N3	4.70	120.13	115.17
3	L3	3884	PSU	C4-N3-C2	-4.70	119.89	126.37
3	L3	3734	PSU	N1-C2-N3	4.70	120.13	115.17
3	L3	2508	PSU	N1-C2-N3	4.67	120.10	115.17
3	L3	2632	PSU	N1-C2-N3	4.67	120.09	115.17
3	L3	3867	A2M	N3-C4-N9	4.62	135.02	127.17
3	L3	3825	A2M	N3-C4-N9	4.62	135.02	127.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L3	4571	A2M	N3-C4-N9	4.62	135.02	127.17
3	L3	3853	PSU	C4-N3-C2	-4.59	120.05	126.37
3	L3	4523	A2M	N3-C4-N9	4.58	134.96	127.17
3	L3	1326	A2M	N3-C4-N9	4.58	134.95	127.17
3	L3	2815	A2M	N3-C4-N9	4.56	134.92	127.17
3	L3	400	A2M	N3-C4-N9	4.55	134.91	127.17
3	L3	3724	A2M	N3-C4-N9	4.54	134.89	127.17
3	L3	4293	PSU	C4-N3-C2	-4.54	120.12	126.37
3	L3	2401	A2M	N3-C4-N9	4.52	134.86	127.17
3	L3	3718	A2M	N3-C4-N9	4.51	134.84	127.17
3	L3	2787	A2M	N3-C4-N9	4.50	134.83	127.17
3	L3	1524	A2M	N3-C4-N9	4.47	134.77	127.17
3	L3	398	A2M	N3-C4-N9	4.46	134.75	127.17
3	L3	3830	A2M	N3-C4-N9	4.42	134.68	127.17
3	L3	1871	A2M	N3-C4-N9	4.40	134.65	127.17
3	L3	4590	A2M	N3-C2-N1	-4.38	121.95	128.58
3	L3	1871	A2M	N3-C2-N1	-4.17	122.27	128.58
3	L3	3830	A2M	N3-C2-N1	-4.14	122.31	128.58
3	L3	4523	A2M	N3-C2-N1	-4.13	122.32	128.58
3	L3	3825	A2M	N3-C2-N1	-4.12	122.34	128.58
3	L3	2401	A2M	N3-C2-N1	-4.11	122.35	128.58
3	L3	400	A2M	N3-C2-N1	-4.11	122.36	128.58
3	L3	398	A2M	N3-C2-N1	-4.11	122.36	128.58
3	L3	1524	A2M	N3-C2-N1	-4.11	122.37	128.58
3	L3	3724	A2M	N3-C2-N1	-4.10	122.37	128.58
3	L3	2815	A2M	N3-C2-N1	-4.08	122.41	128.58
3	L3	4227	OMU	N3-C2-N1	4.06	120.18	114.89
3	L3	4571	A2M	N3-C2-N1	-4.06	122.44	128.58
3	L3	2415	OMU	N3-C2-N1	4.06	120.17	114.89
3	L3	2787	A2M	N3-C2-N1	-4.05	122.46	128.58
3	L3	1326	A2M	N3-C2-N1	-4.04	122.47	128.58
3	L3	3867	A2M	N3-C2-N1	-4.02	122.49	128.58
3	L3	4498	OMU	N3-C2-N1	4.00	120.10	114.89
3	L3	2837	OMU	N3-C2-N1	4.00	120.10	114.89
3	L3	2363	A2M	N3-C2-N1	-3.98	122.56	128.58
3	L3	4306	OMU	N3-C2-N1	3.96	120.05	114.89
3	L3	3925	OMU	N3-C2-N1	3.96	120.05	114.89
3	L3	4227	OMU	C5-C4-N3	3.96	120.35	114.80
3	L3	1534	A2M	N3-C2-N1	-3.94	122.61	128.58
3	L3	4590	A2M	N3-C4-N9	3.92	133.83	127.17
3	L3	3718	A2M	N3-C2-N1	-3.91	122.66	128.58
3	L3	4220	6MZ	N1-C2-N3	-3.89	122.69	128.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L3	3830	A2M	C5-N7-C8	3.83	109.47	103.45
3	L3	2815	A2M	C5-N7-C8	3.83	109.47	103.45
3	L3	2363	A2M	C5-N7-C8	3.81	109.44	103.45
3	L3	2401	A2M	C5-N7-C8	3.81	109.44	103.45
3	L3	1534	A2M	C5-N7-C8	3.80	109.42	103.45
3	L3	1326	A2M	C5-N7-C8	3.79	109.41	103.45
3	L3	3825	A2M	C5-N7-C8	3.79	109.41	103.45
3	L3	398	A2M	C5-N7-C8	3.79	109.41	103.45
3	L3	2787	A2M	C5-N7-C8	3.79	109.40	103.45
3	L3	4590	A2M	C5-N7-C8	3.78	109.39	103.45
3	L3	4523	A2M	C5-N7-C8	3.78	109.39	103.45
3	L3	3867	A2M	C5-N7-C8	3.76	109.36	103.45
3	L3	4498	OMU	C5-C4-N3	3.75	120.06	114.80
3	L3	1871	A2M	C5-N7-C8	3.75	109.35	103.45
3	L3	400	A2M	C5-N7-C8	3.75	109.34	103.45
3	L3	3724	A2M	C5-N7-C8	3.74	109.33	103.45
3	L3	3718	A2M	C5-N7-C8	3.74	109.33	103.45
3	L3	1524	A2M	C5-N7-C8	3.74	109.33	103.45
3	L3	2837	OMU	C5-C4-N3	3.73	120.02	114.80
3	L3	4220	6MZ	C5-N7-C8	3.72	109.29	103.45
3	L3	4306	OMU	C5-C4-N3	3.71	120.00	114.80
3	L3	3925	OMU	C5-C4-N3	3.71	120.00	114.80
3	L3	4571	A2M	C5-N7-C8	3.68	109.23	103.45
3	L3	4620	OMU	N3-C2-N1	3.67	119.67	114.89
3	L3	2815	A2M	C2-N3-C4	3.65	120.75	111.83
3	L3	3825	A2M	C2-N3-C4	3.65	120.74	111.83
3	L3	2401	A2M	C2-N3-C4	3.64	120.72	111.83
3	L3	1534	A2M	C2-N3-C4	3.64	120.71	111.83
3	L3	4571	A2M	C2-N3-C4	3.63	120.71	111.83
3	L3	1326	A2M	C2-N3-C4	3.63	120.70	111.83
3	L3	4220	6MZ	C2-N3-C4	3.63	120.69	111.83
3	L3	2415	OMU	C5-C4-N3	3.63	119.88	114.80
3	L3	3867	A2M	C2-N3-C4	3.62	120.67	111.83
3	L3	1524	A2M	C2-N3-C4	3.61	120.66	111.83
3	L3	4523	A2M	C2-N3-C4	3.60	120.64	111.83
3	L3	4620	OMU	C5-C4-N3	3.60	119.84	114.80
3	L3	3724	A2M	C2-N3-C4	3.60	120.62	111.83
3	L3	400	A2M	C2-N3-C4	3.60	120.62	111.83
3	L3	2787	A2M	C2-N3-C4	3.59	120.60	111.83
3	L3	398	A2M	C2-N3-C4	3.59	120.59	111.83
3	L3	2363	A2M	C2-N3-C4	3.59	120.59	111.83
3	L3	3830	A2M	C2-N3-C4	3.58	120.57	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L3	1871	A2M	C2-N3-C4	3.55	120.51	111.83
3	L3	4590	A2M	C2-N3-C4	3.52	120.42	111.83
3	L3	3718	A2M	C2-N3-C4	3.50	120.39	111.83
3	L3	1871	A2M	C2'-C1'-N9	-3.44	108.09	113.75
3	L3	4530	UR3	C5-C4-N3	3.29	119.38	115.04
3	L3	3718	A2M	C2'-C1'-N9	-3.21	108.47	113.75
3	L3	4590	A2M	C4-C5-N7	-3.13	107.00	110.58
3	L3	3637	PSU	C6-C5-C4	3.09	120.26	118.17
3	L3	2815	A2M	C4-C5-N7	-3.08	107.06	110.58
3	L3	2401	A2M	C4-C5-N7	-3.04	107.11	110.58
23	LN	245	HIC	NE2-CE1-ND1	-3.03	111.50	112.66
3	L3	1326	A2M	C4-C5-N7	-3.03	107.12	110.58
3	L3	3830	A2M	C4-C5-N7	-3.03	107.12	110.58
3	L3	2363	A2M	C4-C5-N7	-3.02	107.13	110.58
3	L3	3724	A2M	C4-C5-N7	-3.01	107.14	110.58
3	L3	4628	PSU	O2-C2-N1	-3.00	119.69	122.79
3	L3	398	A2M	C4-C5-N7	-3.00	107.15	110.58
3	L3	4571	A2M	C4-C5-N7	-3.00	107.15	110.58
3	L3	2787	A2M	C4-C5-N7	-3.00	107.16	110.58
3	L3	1534	A2M	C4-C5-N7	-2.99	107.16	110.58
3	L3	3825	A2M	C4-C5-N7	-2.99	107.16	110.58
3	L3	3867	A2M	C4-C5-N7	-2.99	107.17	110.58
3	L3	4500	PSU	O2-C2-N1	-2.97	119.73	122.79
3	L3	3925	OMU	O4-C4-C5	-2.96	120.05	125.16
3	L3	1524	A2M	C4-C5-N7	-2.96	107.19	110.58
3	L3	1871	A2M	C4-C5-N7	-2.96	107.20	110.58
3	L3	3718	A2M	C4-C5-N7	-2.96	107.20	110.58
3	L3	2839	PSU	O2-C2-N1	-2.95	119.74	122.79
3	L3	3830	A2M	N9-C8-N7	-2.95	109.76	113.94
3	L3	4227	OMU	O4-C4-C5	-2.94	120.09	125.16
3	L3	400	A2M	C4-C5-N7	-2.93	107.23	110.58
3	L3	4220	6MZ	C4-C5-N7	-2.93	107.23	110.58
2	L1	55	PSU	O2-C2-N1	-2.93	119.77	122.79
3	L3	4523	A2M	C4-C5-N7	-2.92	107.24	110.58
3	L3	3822	PSU	O2-C2-N1	-2.92	119.78	122.79
3	L3	4306	OMU	O4-C4-C5	-2.91	120.14	125.16
3	L3	4576	PSU	O2-C2-N1	-2.90	119.80	122.79
3	L3	2837	OMU	O4-C4-C5	-2.90	120.17	125.16
3	L3	3844	PSU	O2-C2-N1	-2.89	119.80	122.79
3	L3	1536	PSU	O2-C2-N1	-2.89	119.81	122.79
3	L3	2415	OMU	O4-C4-C5	-2.89	120.18	125.16
3	L3	4220	6MZ	C9-N6-C6	-2.89	120.17	122.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L3	3715	PSU	O2-C2-N1	-2.88	119.82	122.79
3	L3	4498	OMU	O4-C4-C5	-2.86	120.23	125.16
3	L3	4523	A2M	N9-C8-N7	-2.86	109.88	113.94
3	L3	4361	PSU	O2-C2-N1	-2.86	119.84	122.79
3	L3	4620	OMU	O4-C4-C5	-2.85	120.24	125.16
3	L3	4457	PSU	O2-C2-N1	-2.85	119.85	122.79
3	L3	398	A2M	N9-C8-N7	-2.85	109.89	113.94
3	L3	4590	A2M	N9-C8-N7	-2.85	109.90	113.94
3	L3	4636	PSU	O2-C2-N1	-2.85	119.85	122.79
3	L3	3639	PSU	O2-C2-N1	-2.84	119.86	122.79
3	L3	1871	A2M	N9-C8-N7	-2.84	109.91	113.94
3	L3	1534	A2M	O4'-C1'-C2'	-2.83	101.72	106.59
3	L3	2815	A2M	N9-C8-N7	-2.83	109.92	113.94
3	L3	4353	PSU	O2-C2-N1	-2.83	119.87	122.79
3	L3	4296	PSU	O2-C2-N1	-2.82	119.88	122.79
3	L3	3734	PSU	O2-C2-N1	-2.82	119.88	122.79
2	L1	69	PSU	O2-C2-N1	-2.81	119.89	122.79
3	L3	3695	PSU	O2-C2-N1	-2.81	119.89	122.79
3	L3	1326	A2M	N9-C8-N7	-2.80	109.96	113.94
3	L3	2401	A2M	N9-C8-N7	-2.80	109.96	113.94
3	L3	3884	PSU	O2-C2-N1	-2.79	119.91	122.79
3	L3	4579	PSU	O2-C2-N1	-2.78	119.92	122.79
3	L3	1524	A2M	N9-C8-N7	-2.78	109.99	113.94
3	L3	1677	PSU	O2-C2-N1	-2.78	119.92	122.79
3	L3	400	A2M	N9-C8-N7	-2.78	110.00	113.94
3	L3	3718	A2M	N9-C8-N7	-2.77	110.00	113.94
3	L3	3825	A2M	N9-C8-N7	-2.77	110.01	113.94
3	L3	3853	PSU	O2-C2-N1	-2.77	119.94	122.79
3	L3	4972	PSU	O2-C2-N1	-2.77	119.94	122.79
3	L3	4673	PSU	O2-C2-N1	-2.75	119.95	122.79
3	L3	3920	PSU	O2-C2-N1	-2.75	119.96	122.79
3	L3	4532	PSU	O2-C2-N1	-2.74	119.96	122.79
3	L3	4431	PSU	O2-C2-N1	-2.74	119.96	122.79
3	L3	1582	PSU	O2-C2-N1	-2.74	119.96	122.79
3	L3	1862	PSU	O2-C2-N1	-2.74	119.96	122.79
3	L3	4403	PSU	O2-C2-N1	-2.74	119.96	122.79
3	L3	5010	PSU	O2-C2-N1	-2.74	119.97	122.79
3	L3	3851	PSU	O2-C2-N1	-2.73	119.97	122.79
3	L3	3730	PSU	O2-C2-N1	-2.73	119.97	122.79
3	L3	2787	A2M	N9-C8-N7	-2.73	110.06	113.94
3	L3	1534	A2M	N9-C8-N7	-2.72	110.07	113.94
3	L3	3867	A2M	N9-C8-N7	-2.72	110.08	113.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L3	2508	PSU	O2-C2-N1	-2.71	119.99	122.79
3	L3	4293	PSU	C6-N1-C2	-2.71	120.17	122.69
3	L3	2363	A2M	N9-C8-N7	-2.71	110.09	113.94
3	L3	4299	PSU	O2-C2-N1	-2.71	120.00	122.79
3	L3	5001	PSU	O2-C2-N1	-2.71	120.00	122.79
3	L3	4312	PSU	C6-N1-C2	-2.70	120.19	122.69
3	L3	3884	PSU	C6-N1-C2	-2.69	120.19	122.69
3	L3	4628	PSU	C6-N1-C2	-2.69	120.19	122.69
3	L3	3724	A2M	N9-C8-N7	-2.69	110.12	113.94
3	L3	4689	PSU	O2-C2-N1	-2.67	120.03	122.79
3	L3	398	A2M	C2'-C1'-N9	-2.67	109.36	113.75
3	L3	4552	PSU	O2-C2-N1	-2.67	120.04	122.79
3	L3	4532	PSU	C6-C5-C4	2.65	119.97	118.17
3	L3	4579	PSU	C6-N1-C2	-2.65	120.23	122.69
3	L3	4493	PSU	O2-C2-N1	-2.64	120.06	122.79
3	L3	2815	A2M	C2'-C1'-N9	-2.64	109.41	113.75
3	L3	4312	PSU	O2-C2-N1	-2.64	120.07	122.79
3	L3	4689	PSU	C6-N1-C2	-2.63	120.25	122.69
3	L3	1860	PSU	O2-C2-N1	-2.63	120.07	122.79
3	L3	4471	PSU	O2-C2-N1	-2.63	120.08	122.79
3	L3	4636	PSU	C6-C5-C4	2.60	119.93	118.17
3	L3	3730	PSU	C6-N1-C2	-2.59	120.29	122.69
3	L3	4521	PSU	O2-C2-N1	-2.58	120.13	122.79
3	L3	3920	PSU	C6-N1-C2	-2.57	120.30	122.69
3	L3	1792	PSU	O2-C2-N1	-2.57	120.14	122.79
3	L3	4571	A2M	N9-C8-N7	-2.57	110.29	113.94
2	L1	69	PSU	C6-N1-C2	-2.55	120.33	122.69
3	L3	3637	PSU	O2-C2-N1	-2.55	120.16	122.79
3	L3	2839	PSU	C6-N1-C2	-2.54	120.33	122.69
3	L3	3853	PSU	C6-N1-C2	-2.54	120.34	122.69
3	L3	4576	PSU	C6-N1-C2	-2.53	120.34	122.69
3	L3	2401	A2M	C2'-C1'-N9	-2.53	109.59	113.75
3	L3	4361	PSU	C6-N1-C2	-2.52	120.35	122.69
3	L3	1862	PSU	C6-C5-C4	2.52	119.87	118.17
3	L3	1683	PSU	C6-N1-C2	-2.51	120.36	122.69
3	L3	3637	PSU	C6-N1-C2	-2.51	120.36	122.69
3	L3	1536	PSU	C6-N1-C2	-2.51	120.36	122.69
3	L3	4521	PSU	C6-N1-C2	-2.51	120.36	122.69
3	L3	4500	PSU	C6-N1-C2	-2.50	120.37	122.69
3	L3	3695	PSU	C6-C5-C4	2.49	119.85	118.17
3	L3	4457	PSU	C6-N1-C2	-2.49	120.38	122.69
3	L3	3639	PSU	C6-N1-C2	-2.48	120.39	122.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L3	5010	PSU	C6-N1-C2	-2.48	120.39	122.69
3	L3	4299	PSU	C6-C5-C4	2.47	119.84	118.17
3	L3	3734	PSU	C6-N1-C2	-2.47	120.40	122.69
3	L3	1683	PSU	O2-C2-N1	-2.47	120.24	122.79
3	L3	4471	PSU	C6-C5-C4	2.47	119.84	118.17
3	L3	3822	PSU	C6-N1-C2	-2.47	120.40	122.69
3	L3	4220	6MZ	N9-C8-N7	-2.46	110.44	113.94
3	L3	5001	PSU	C6-N1-C2	-2.46	120.41	122.69
3	L3	4403	PSU	C6-C5-C4	2.45	119.83	118.17
3	L3	1862	PSU	C6-N1-C2	-2.45	120.42	122.69
3	L3	3844	PSU	C6-N1-C2	-2.45	120.42	122.69
3	L3	4471	PSU	C6-N1-C2	-2.45	120.42	122.69
3	L3	4293	PSU	O2-C2-N1	-2.45	120.26	122.79
3	L3	1792	PSU	C6-N1-C2	-2.45	120.42	122.69
3	L3	3715	PSU	C6-N1-C2	-2.45	120.42	122.69
3	L3	4353	PSU	C6-N1-C2	-2.45	120.42	122.69
3	L3	3851	PSU	C6-N1-C2	-2.44	120.43	122.69
3	L3	4523	A2M	C2'-C1'-N9	-2.44	109.74	113.75
3	L3	4673	PSU	C6-N1-C2	-2.44	120.43	122.69
3	L3	4431	PSU	C6-C5-C4	2.43	119.82	118.17
3	L3	4296	PSU	C6-N1-C2	-2.43	120.44	122.69
3	L3	4299	PSU	C6-N1-C2	-2.43	120.44	122.69
2	L1	55	PSU	C6-N1-C2	-2.42	120.44	122.69
3	L3	3639	PSU	C6-C5-C4	2.42	119.81	118.17
3	L3	1524	A2M	C2'-C1'-N9	-2.42	109.77	113.75
2	L1	69	PSU	O4'-C1'-C2'	2.42	108.50	105.15
3	L3	3695	PSU	C6-N1-C2	-2.42	120.45	122.69
3	L3	4431	PSU	C6-N1-C2	-2.40	120.46	122.69
3	L3	4972	PSU	C6-N1-C2	-2.40	120.46	122.69
3	L3	4312	PSU	C6-C5-C4	2.40	119.79	118.17
3	L3	4552	PSU	C6-N1-C2	-2.39	120.47	122.69
3	L3	2632	PSU	C6-N1-C2	-2.39	120.47	122.69
3	L3	2508	PSU	C6-N1-C2	-2.39	120.48	122.69
3	L3	2632	PSU	O2-C2-N1	-2.37	120.34	122.79
3	L3	4403	PSU	C6-N1-C2	-2.36	120.50	122.69
3	L3	1536	PSU	C6-C5-C4	2.36	119.77	118.17
3	L3	1860	PSU	C6-N1-C2	-2.36	120.50	122.69
3	L3	1677	PSU	C6-C5-C4	2.35	119.76	118.17
3	L3	4636	PSU	C6-N1-C2	-2.34	120.52	122.69
3	L3	3822	PSU	C6-C5-C4	2.34	119.75	118.17
3	L3	1677	PSU	C6-N1-C2	-2.34	120.52	122.69
3	L3	3844	PSU	C6-C5-C4	2.34	119.75	118.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L3	4296	PSU	C6-C5-C4	2.33	119.74	118.17
3	L3	4493	PSU	C6-N1-C2	-2.32	120.54	122.69
3	L3	2415	OMU	O2-C2-N1	-2.31	119.78	122.80
2	L1	55	PSU	C6-C5-C4	2.29	119.72	118.17
3	L3	4493	PSU	C6-C5-C4	2.29	119.72	118.17
3	L3	4972	PSU	C6-C5-C4	2.28	119.71	118.17
3	L3	4361	PSU	C6-C5-C4	2.27	119.71	118.17
3	L3	1322	1MA	N1-C6-N6	2.27	125.42	119.71
3	L3	4673	PSU	C6-C5-C4	2.27	119.70	118.17
3	L3	3867	A2M	C2'-C1'-N9	-2.25	110.04	113.75
3	L3	2837	OMU	O2-C2-N1	-2.23	119.89	122.80
3	L3	3920	PSU	C6-C5-C4	2.23	119.68	118.17
3	L3	4353	PSU	C6-C5-C4	2.22	119.67	118.17
3	L3	4689	PSU	C6-C5-C4	2.20	119.66	118.17
3	L3	4532	PSU	C6-N1-C2	-2.18	120.67	122.69
3	L3	3730	PSU	C6-C5-C4	2.18	119.64	118.17
3	L3	4552	PSU	C6-C5-C4	2.18	119.64	118.17
3	L3	1860	PSU	C6-C5-C4	2.18	119.64	118.17
3	L3	3925	OMU	O2-C2-N1	-2.17	119.97	122.80
3	L3	1582	PSU	C6-N1-C2	-2.16	120.68	122.69
3	L3	3715	PSU	C6-C5-C4	2.15	119.63	118.17
3	L3	5010	PSU	C6-C5-C4	2.15	119.63	118.17
3	L3	2422	OMC	C1'-N1-C2	2.15	123.20	118.44
3	L3	3851	PSU	O4'-C1'-C2'	2.15	108.12	105.15
3	L3	4521	PSU	C6-C5-C4	2.15	119.62	118.17
3	L3	3734	PSU	C6-C5-C4	2.13	119.61	118.17
3	L3	3715	PSU	O4'-C1'-C2'	2.12	108.09	105.15
3	L3	5001	PSU	C6-C5-C4	2.12	119.61	118.17
3	L3	1683	PSU	C6-C5-C4	2.12	119.60	118.17
3	L3	4628	PSU	C6-C5-C4	2.12	119.60	118.17
3	L3	4306	OMU	O2-C2-N1	-2.11	120.05	122.80
3	L3	400	A2M	C2'-C1'-N9	-2.11	110.28	113.75
3	L3	5001	PSU	O4'-C1'-C2'	2.11	108.06	105.15
3	L3	4576	PSU	C6-C5-C4	2.10	119.59	118.17
3	L3	2508	PSU	C6-C5-C4	2.10	119.59	118.17
3	L3	4220	6MZ	C4-C5-C6	2.10	118.52	116.78
3	L3	2839	PSU	C6-C5-C4	2.09	119.59	118.17
3	L3	1792	PSU	C6-C5-C4	2.07	119.57	118.17
3	L3	4590	A2M	C2-N1-C6	2.06	122.12	118.73
3	L3	3851	PSU	C6-C5-C4	2.06	119.56	118.17
3	L3	4498	OMU	O2-C2-N1	-2.05	120.13	122.80
3	L3	4403	PSU	O4'-C1'-C2'	2.05	107.98	105.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L3	4576	PSU	O4'-C1'-C2'	2.03	107.96	105.15
3	L3	1862	PSU	O4'-C1'-C2'	2.03	107.96	105.15
3	L3	3920	PSU	O4'-C1'-C2'	2.02	107.95	105.15
3	L3	4628	PSU	O4'-C1'-C2'	2.01	107.93	105.15

There are no chirality outliers.

All (101) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L1	75	OMG	C1'-C2'-O2'-CM2
3	L3	398	A2M	C1'-C2'-O2'-CM'
3	L3	400	A2M	C1'-C2'-O2'-CM'
3	L3	1316	OMG	C1'-C2'-O2'-CM2
3	L3	1326	A2M	O4'-C4'-C5'-O5'
3	L3	1326	A2M	C3'-C4'-C5'-O5'
3	L3	1326	A2M	C1'-C2'-O2'-CM'
3	L3	1340	OMC	C1'-C2'-O2'-CM2
3	L3	2351	OMC	C1'-C2'-O2'-CM2
3	L3	2364	OMG	C1'-C2'-O2'-CM2
3	L3	2422	OMC	C1'-C2'-O2'-CM2
3	L3	2424	OMG	C1'-C2'-O2'-CM2
3	L3	2804	OMC	C1'-C2'-O2'-CM2
3	L3	2815	A2M	C1'-C2'-O2'-CM'
3	L3	2824	OMC	C1'-C2'-O2'-CM2
3	L3	2837	OMU	C1'-C2'-O2'-CM2
3	L3	2861	OMC	C1'-C2'-O2'-CM2
3	L3	3627	OMG	C1'-C2'-O2'-CM2
3	L3	3701	OMC	C2'-C1'-N1-C2
3	L3	3701	OMC	C2'-C1'-N1-C6
3	L3	3718	A2M	C1'-C2'-O2'-CM'
3	L3	3724	A2M	C1'-C2'-O2'-CM'
3	L3	3744	OMG	C1'-C2'-O2'-CM2
3	L3	3825	A2M	C1'-C2'-O2'-CM'
3	L3	3830	A2M	C1'-C2'-O2'-CM'
3	L3	3841	OMC	C1'-C2'-O2'-CM2
3	L3	3867	A2M	C1'-C2'-O2'-CM'
3	L3	3899	OMG	C1'-C2'-O2'-CM2
3	L3	3925	OMU	C1'-C2'-O2'-CM2
3	L3	4227	OMU	C1'-C2'-O2'-CM2
3	L3	4306	OMU	C1'-C2'-O2'-CM2
3	L3	4392	OMG	C1'-C2'-O2'-CM2
3	L3	4456	OMC	C1'-C2'-O2'-CM2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	L3	4498	OMU	C1'-C2'-O2'-CM2
3	L3	4498	OMU	O4'-C4'-C5'-O5'
3	L3	4498	OMU	C4'-C5'-O5'-P
3	L3	4523	A2M	O4'-C4'-C5'-O5'
3	L3	4536	OMC	C1'-C2'-O2'-CM2
3	L3	4571	A2M	C1'-C2'-O2'-CM'
3	L3	4590	A2M	C1'-C2'-O2'-CM'
3	L3	4618	OMG	O4'-C4'-C5'-O5'
3	L3	4623	OMG	C1'-C2'-O2'-CM2
3	L3	4637	OMG	C1'-C2'-O2'-CM2
3	L3	2401	A2M	O4'-C4'-C5'-O5'
3	L3	2401	A2M	C3'-C4'-C5'-O5'
3	L3	2787	A2M	C3'-C4'-C5'-O5'
3	L3	2876	OMG	O4'-C4'-C5'-O5'
3	L3	2876	OMG	C3'-C4'-C5'-O5'
3	L3	3887	OMC	C3'-C4'-C5'-O5'
3	L3	3887	OMC	O4'-C4'-C5'-O5'
3	L3	4220	6MZ	O4'-C4'-C5'-O5'
3	L3	4498	OMU	C3'-C4'-C5'-O5'
3	L3	4590	A2M	C3'-C4'-C5'-O5'
3	L3	1534	A2M	O4'-C4'-C5'-O5'
3	L3	1625	OMG	C3'-C4'-C5'-O5'
3	L3	1677	PSU	C3'-C4'-C5'-O5'
3	L3	1677	PSU	O4'-C4'-C5'-O5'
3	L3	4228	OMG	C3'-C4'-C5'-O5'
3	L3	4523	A2M	C3'-C4'-C5'-O5'
3	L3	4590	A2M	O4'-C4'-C5'-O5'
3	L3	4637	OMG	O4'-C4'-C5'-O5'
23	LN	245	HIC	CA-CB-CG-ND1
3	L3	1534	A2M	C3'-C4'-C5'-O5'
3	L3	4228	OMG	O4'-C4'-C5'-O5'
3	L3	4590	A2M	C4'-C5'-O5'-P
3	L3	2787	A2M	O4'-C4'-C5'-O5'
3	L3	4220	6MZ	C3'-C4'-C5'-O5'
3	L3	4618	OMG	C3'-C4'-C5'-O5'
3	L3	3701	OMC	O4'-C4'-C5'-O5'
3	L3	2787	A2M	C2'-C1'-N9-C8
23	LN	245	HIC	CA-CB-CG-CD2
3	L3	1625	OMG	O4'-C4'-C5'-O5'
3	L3	2415	OMU	O4'-C4'-C5'-O5'
3	L3	4637	OMG	C3'-C4'-C5'-O5'
3	L3	3701	OMC	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	L3	3844	PSU	C4'-C5'-O5'-P
3	L3	1677	PSU	O4'-C1'-C5-C4
3	L3	2839	PSU	O4'-C1'-C5-C4
3	L3	4457	PSU	O4'-C1'-C5-C4
3	L3	4521	PSU	O4'-C1'-C5-C4
3	L3	4636	PSU	O4'-C1'-C5-C4
3	L3	2787	A2M	C2'-C1'-N9-C4
3	L3	2422	OMC	O4'-C4'-C5'-O5'
3	L3	1524	A2M	O4'-C1'-N9-C4
3	L3	4220	6MZ	C4'-C5'-O5'-P
3	L3	1524	A2M	O4'-C1'-N9-C8
3	L3	3701	OMC	O4'-C1'-N1-C6
3	L3	3867	A2M	C3'-C2'-O2'-CM'
3	L3	4636	PSU	C4'-C5'-O5'-P
3	L3	1677	PSU	O4'-C1'-C5-C6
3	L3	4521	PSU	O4'-C1'-C5-C6
3	L3	2787	A2M	O4'-C1'-N9-C8
3	L3	2351	OMC	C2'-C1'-N1-C6
3	L3	2876	OMG	C3'-C2'-O2'-CM2
3	L3	3925	OMU	C3'-C2'-O2'-CM2
3	L3	4228	OMG	C3'-C2'-O2'-CM2
3	L3	3701	OMC	C4'-C5'-O5'-P
3	L3	2415	OMU	C3'-C4'-C5'-O5'
3	L3	3701	OMC	O4'-C1'-N1-C2
3	L3	1326	A2M	C4'-C5'-O5'-P
3	L3	2351	OMC	C2'-C1'-N1-C2

There are no ring outliers.

63 monomers are involved in 90 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L3	4571	A2M	2	0
3	L3	4636	PSU	2	0
3	L3	2424	OMG	1	0
3	L3	2876	OMG	2	0
3	L3	3867	A2M	1	0
3	L3	2364	OMG	2	0
3	L3	2837	OMU	1	0
3	L3	3869	OMC	1	0
3	L3	4536	OMC	1	0
3	L3	4620	OMU	1	0
3	L3	2632	PSU	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L3	4456	OMC	1	0
3	L3	4227	OMU	1	0
3	L3	4312	PSU	1	0
3	L3	3899	OMG	1	0
3	L3	2422	OMC	2	0
3	L3	4500	PSU	1	0
3	L3	4220	6MZ	3	0
3	L3	2351	OMC	2	0
3	L3	2861	OMC	1	0
3	L3	3822	PSU	1	0
3	L3	1522	OMG	1	0
3	L3	3724	A2M	2	0
3	L3	5001	PSU	1	0
3	L3	1677	PSU	2	0
3	L3	2415	OMU	1	0
3	L3	2363	A2M	1	0
3	L3	1322	1MA	2	0
3	L3	4299	PSU	1	0
3	L3	1683	PSU	2	0
3	L3	4296	PSU	1	0
3	L3	3718	A2M	2	0
3	L3	3841	OMC	1	0
3	L3	4392	OMG	1	0
3	L3	4306	OMU	1	0
2	L1	69	PSU	2	0
3	L3	4552	PSU	2	0
3	L3	400	A2M	1	0
3	L3	4498	OMU	1	0
3	L3	3887	OMC	1	0
3	L3	3920	PSU	1	0
3	L3	2824	OMC	2	0
3	L3	4353	PSU	1	0
3	L3	3734	PSU	1	0
3	L3	1524	A2M	2	0
3	L3	4623	OMG	1	0
3	L3	1326	A2M	2	0
3	L3	4590	A2M	1	0
3	L3	4618	OMG	1	0
3	L3	3637	PSU	1	0
3	L3	3744	OMG	3	0
3	L3	4637	OMG	2	0
3	L3	398	A2M	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L3	3925	OMU	2	0
3	L3	3715	PSU	1	0
3	L3	4530	UR3	2	0
38	NR	127	PTR	1	0
3	L3	1340	OMC	2	0
2	L1	75	OMG	2	0
3	L3	4673	PSU	2	0
3	L3	3730	PSU	2	0
3	L3	4457	PSU	2	0
3	L3	4361	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 96 ligands modelled in this entry, 95 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
53	GDP	SR	1001	51,54	29,30,30	3.03	12 (41%)	45,47,47	2.69	16 (35%)

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
53	GDP	SR	1001	51,54	-	0/16/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	SR	1001	GDP	O6-C6	8.81	1.40	1.23
53	SR	1001	GDP	C5-N7	6.54	1.52	1.39
53	SR	1001	GDP	PA-O3A	5.20	1.65	1.59
53	SR	1001	GDP	C2-N2	4.80	1.45	1.34
53	SR	1001	GDP	C8-N9	-3.96	1.28	1.37
53	SR	1001	GDP	C4-N9	-3.79	1.28	1.38
53	SR	1001	GDP	C5-C4	3.78	1.49	1.38
53	SR	1001	GDP	C4-N3	2.83	1.40	1.34
53	SR	1001	GDP	PB-O2B	-2.28	1.46	1.54
53	SR	1001	GDP	O4'-C1'	2.27	1.47	1.42
53	SR	1001	GDP	PB-O3B	-2.25	1.46	1.54
53	SR	1001	GDP	C2'-C3'	-2.07	1.47	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	SR	1001	GDP	C8-N9-C4	7.70	120.47	106.03
53	SR	1001	GDP	C5-C4-N3	-6.71	117.71	128.39
53	SR	1001	GDP	N9-C4-N3	6.62	139.19	125.95
53	SR	1001	GDP	C2-N3-C4	5.38	121.56	112.30
53	SR	1001	GDP	C6-C5-N7	4.84	139.11	130.29
53	SR	1001	GDP	C4-C5-N7	-4.64	103.33	110.67
53	SR	1001	GDP	C3'-C2'-C1'	3.09	107.31	101.46
53	SR	1001	GDP	N9-C8-N7	-3.00	107.83	113.40
53	SR	1001	GDP	C2-N1-C6	-2.98	119.71	125.11
53	SR	1001	GDP	C1'-N9-C4	-2.92	117.86	126.49
53	SR	1001	GDP	O2B-PB-O3A	2.85	114.19	104.64
53	SR	1001	GDP	O3B-PB-O3A	2.82	114.11	104.64
53	SR	1001	GDP	C2'-C3'-C4'	2.75	107.93	102.61
53	SR	1001	GDP	C5-C6-N1	2.61	119.90	113.25
53	SR	1001	GDP	O6-C6-C5	-2.44	120.08	126.53
53	SR	1001	GDP	O2A-PA-O1A	-2.40	101.29	112.44

There are no chirality outliers.

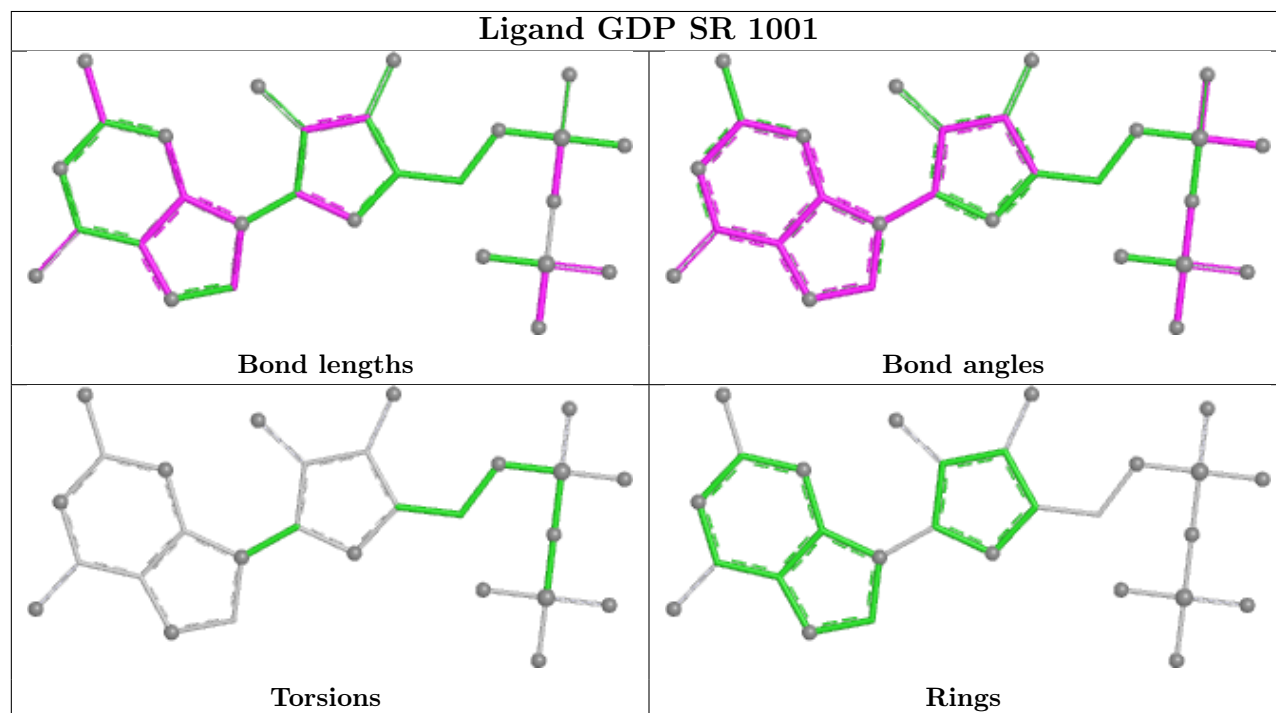
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

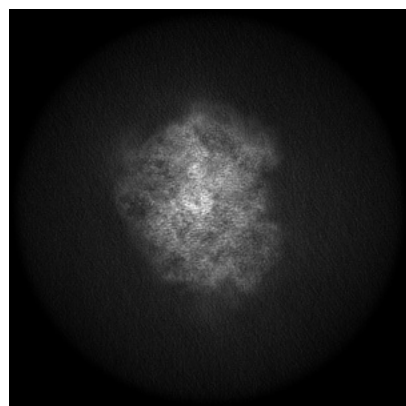
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29274. These allow visual inspection of the internal detail of the map and identification of artifacts.

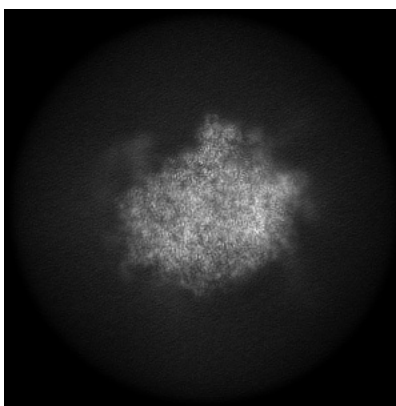
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

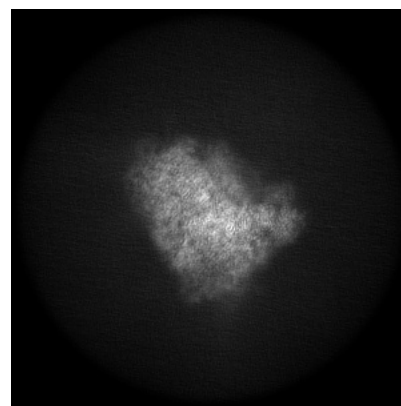
6.1.1 Primary map



X

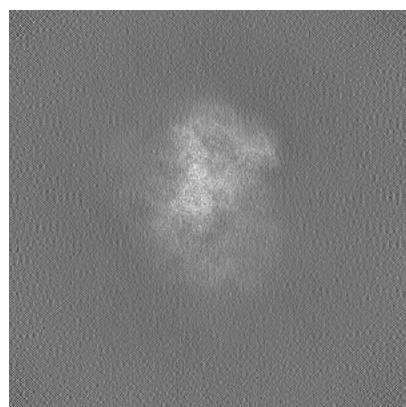


Y

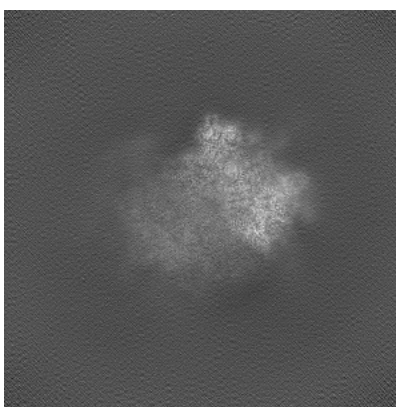


Z

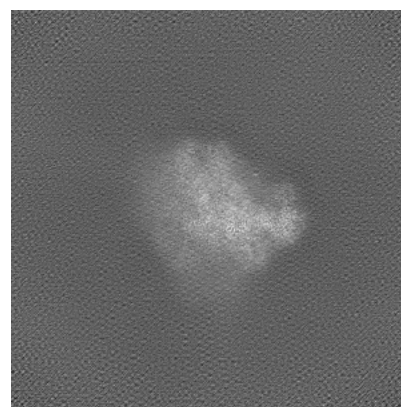
6.1.2 Raw map



X



Y

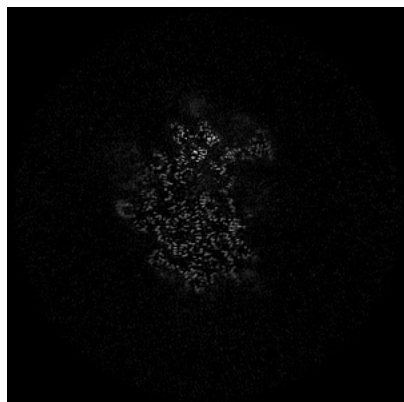


Z

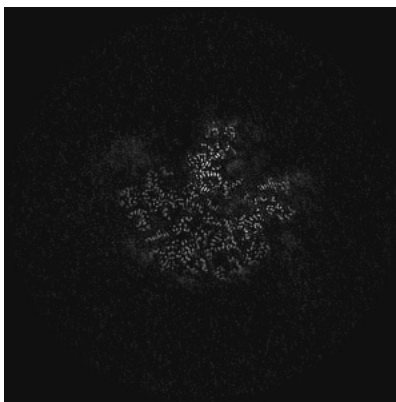
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

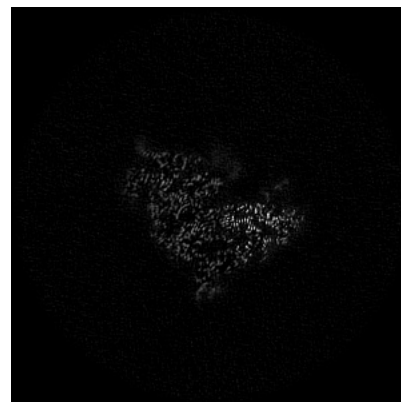
6.2.1 Primary map



X Index: 240

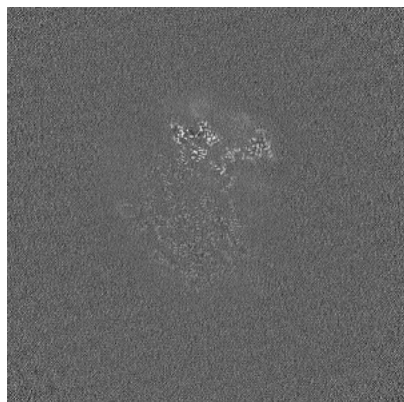


Y Index: 240

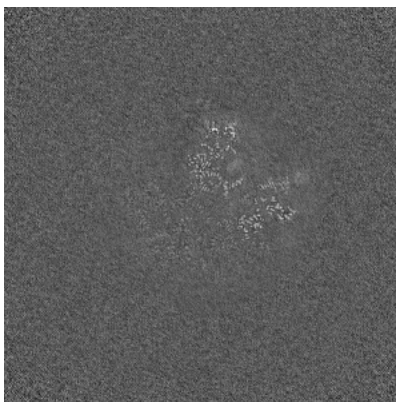


Z Index: 240

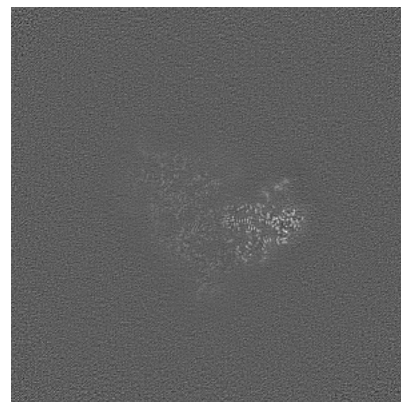
6.2.2 Raw map



X Index: 240



Y Index: 240

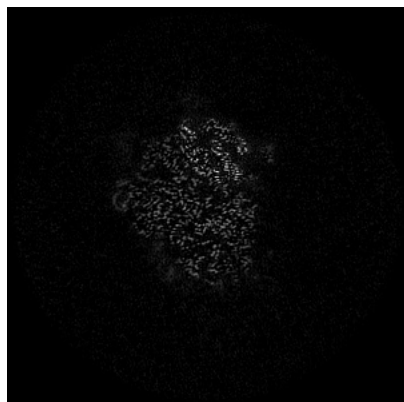


Z Index: 240

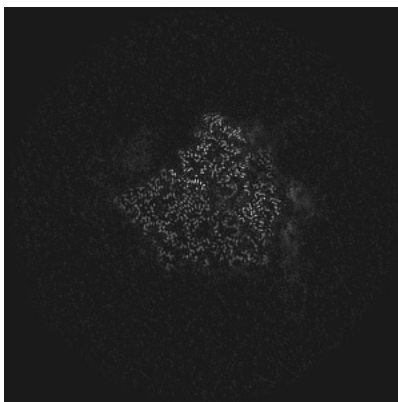
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

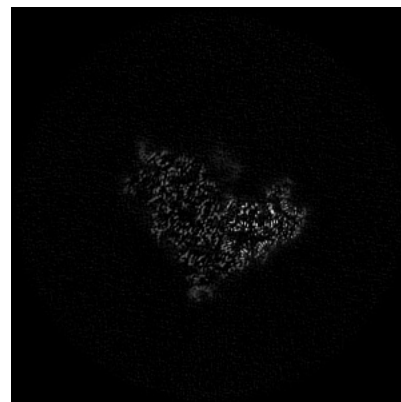
6.3.1 Primary map



X Index: 226

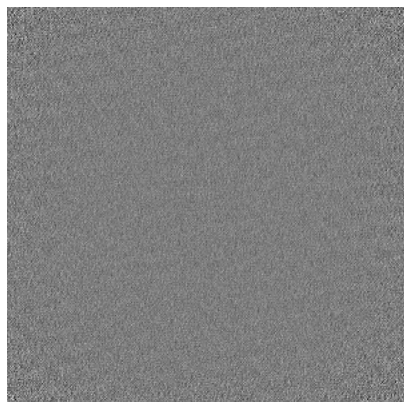


Y Index: 227

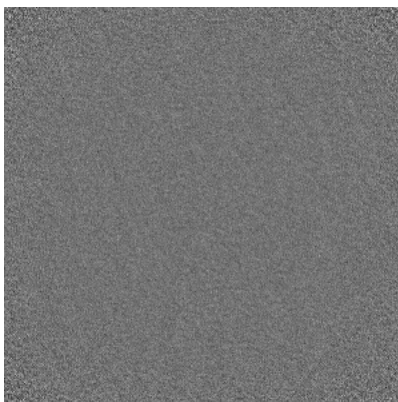


Z Index: 245

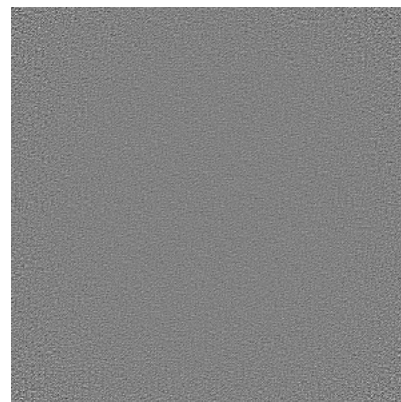
6.3.2 Raw map



X Index: 0



Y Index: 0

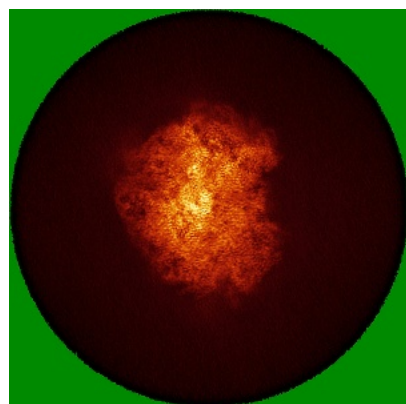


Z Index: 0

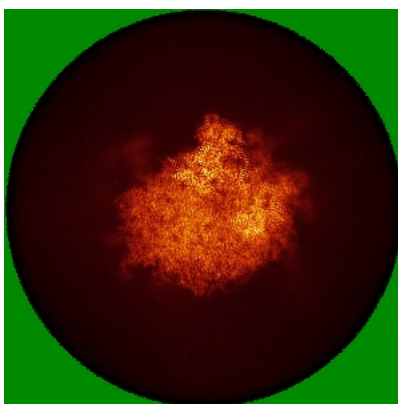
The images above show the largest variance slices of the map in three orthogonal directions.

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

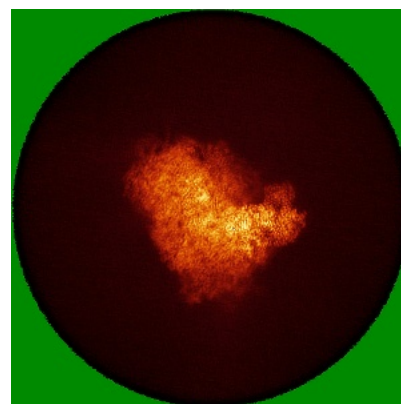
6.4.1 Primary map



X

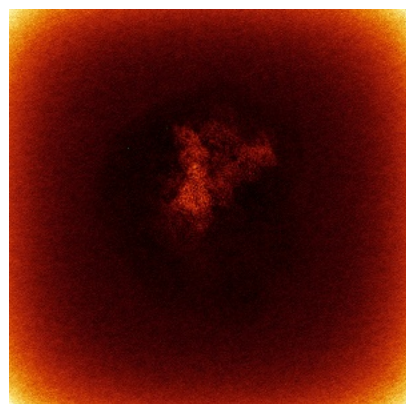


Y

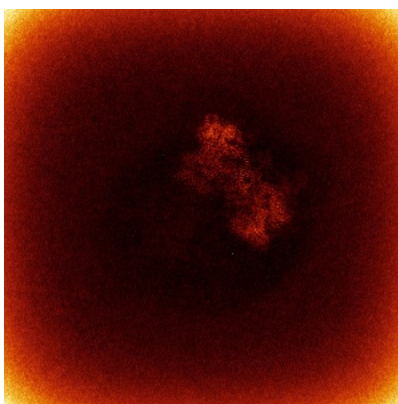


Z

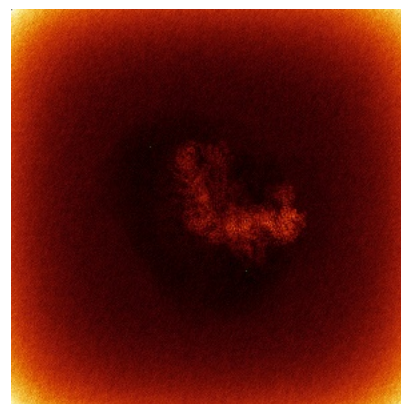
6.4.2 Raw map



X



Y

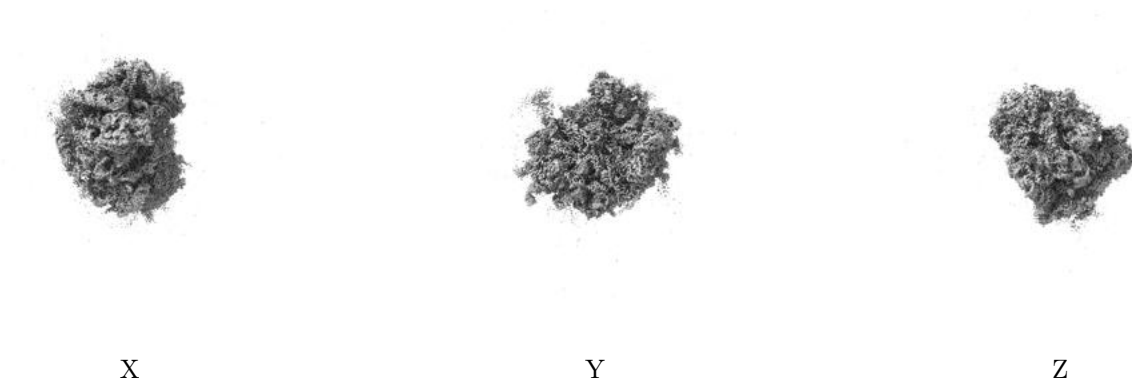


Z

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

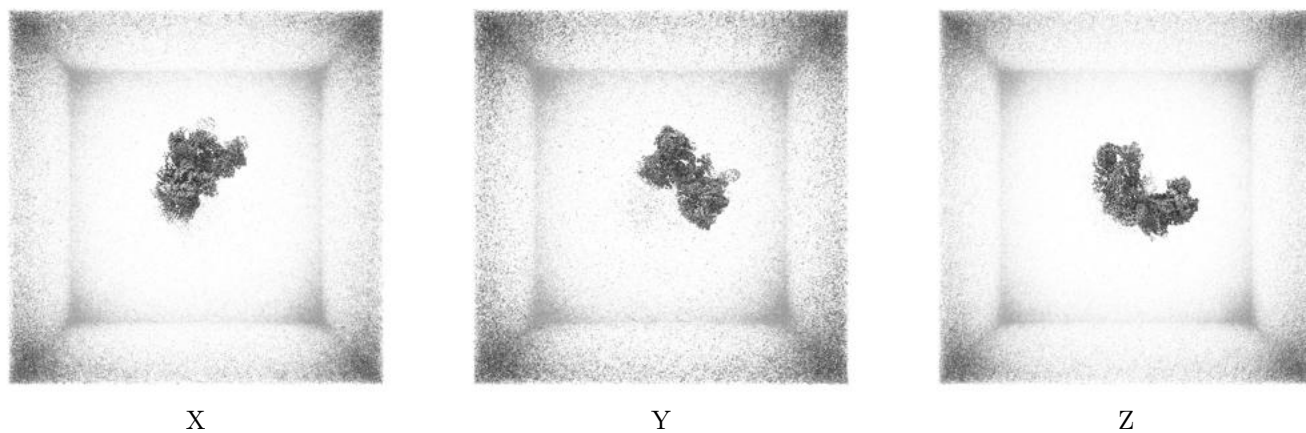
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.85. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

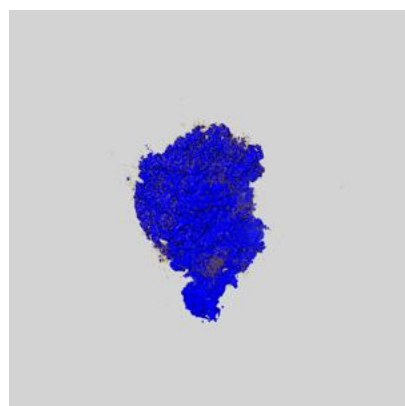
6.6 Mask visualisation [i](#)

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

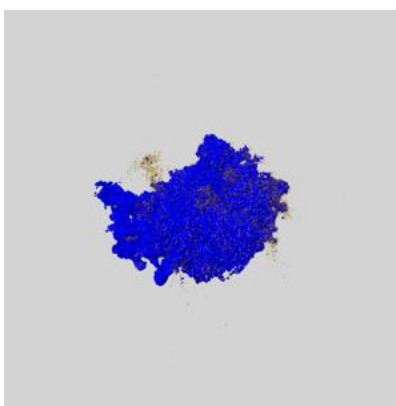
A mask typically either:

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

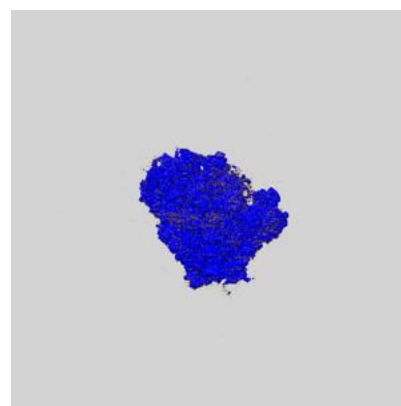
6.6.1 emd_29274_msk_1.map [i](#)



X



Y

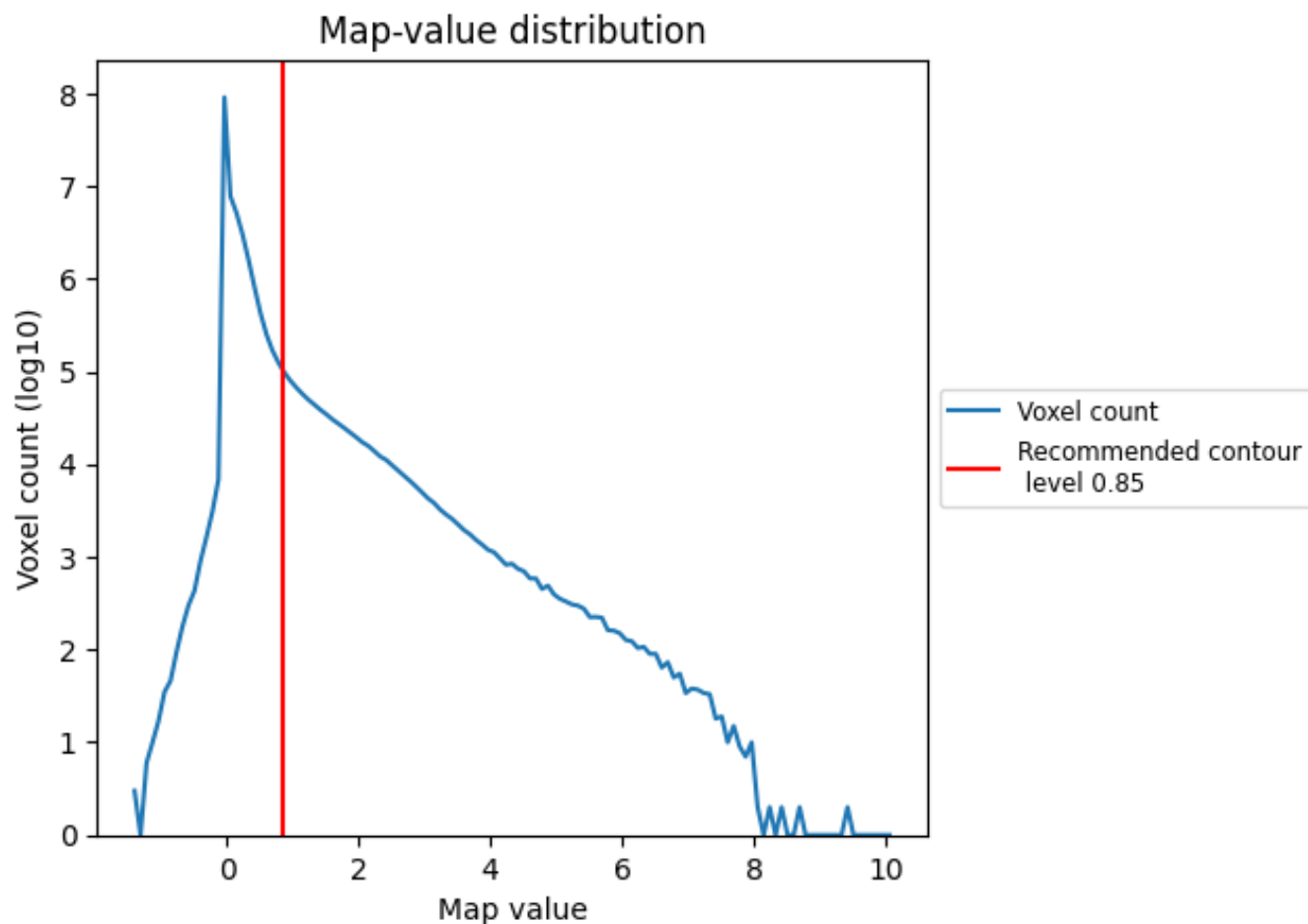


Z

7 Map analysis [i](#)

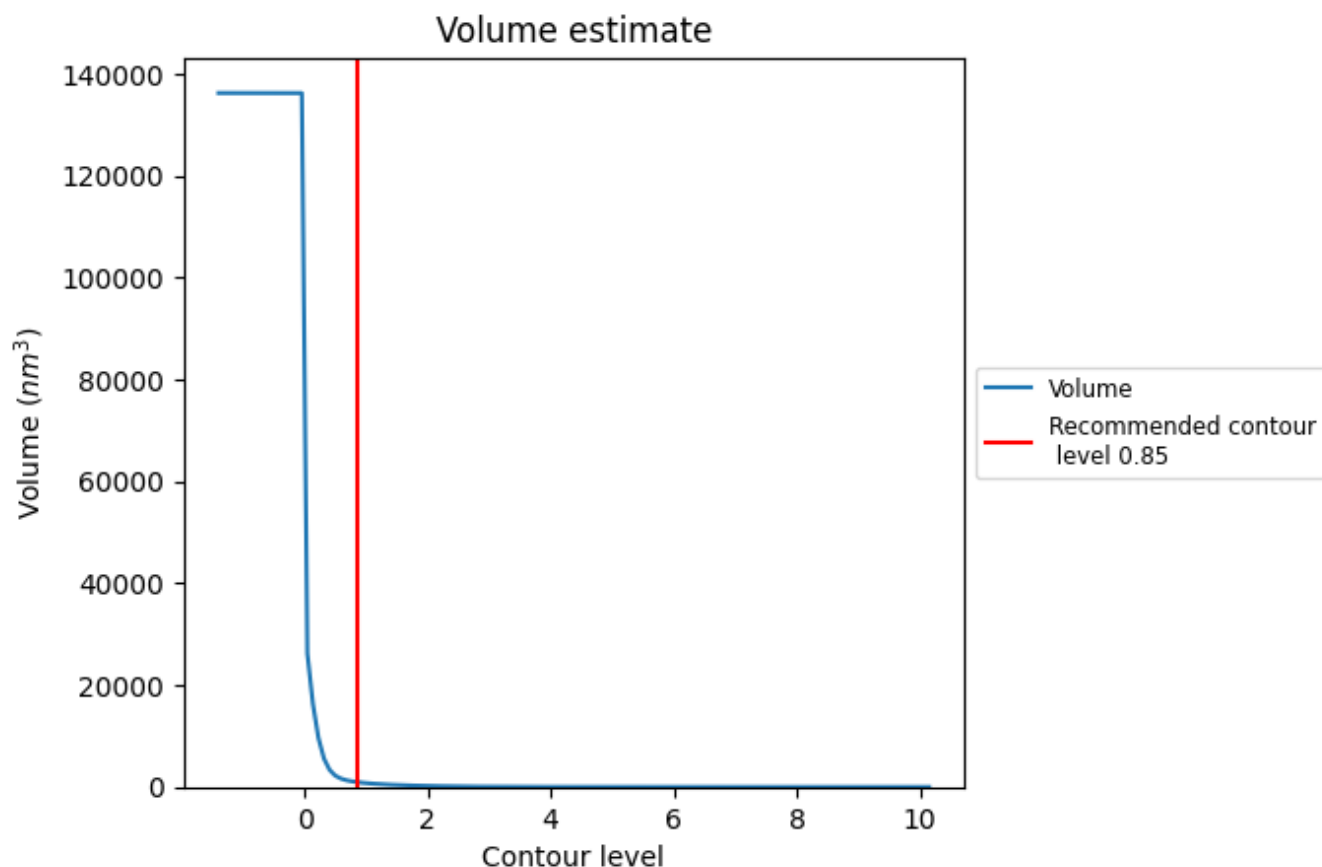
This section contains the results of statistical analysis of the map.

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.

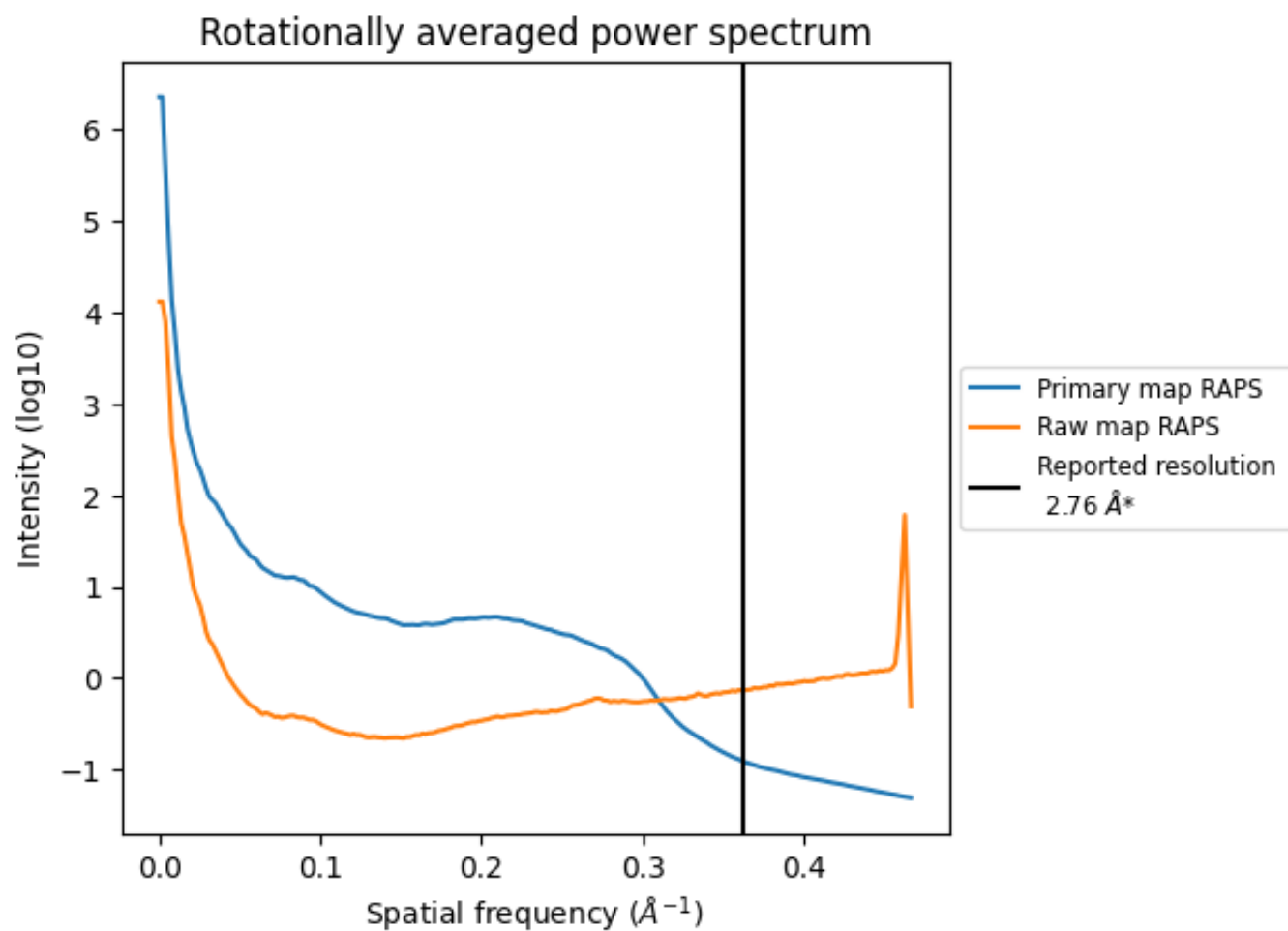
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 966 nm^3 ; this corresponds to an approximate mass of 873 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 ⓘ

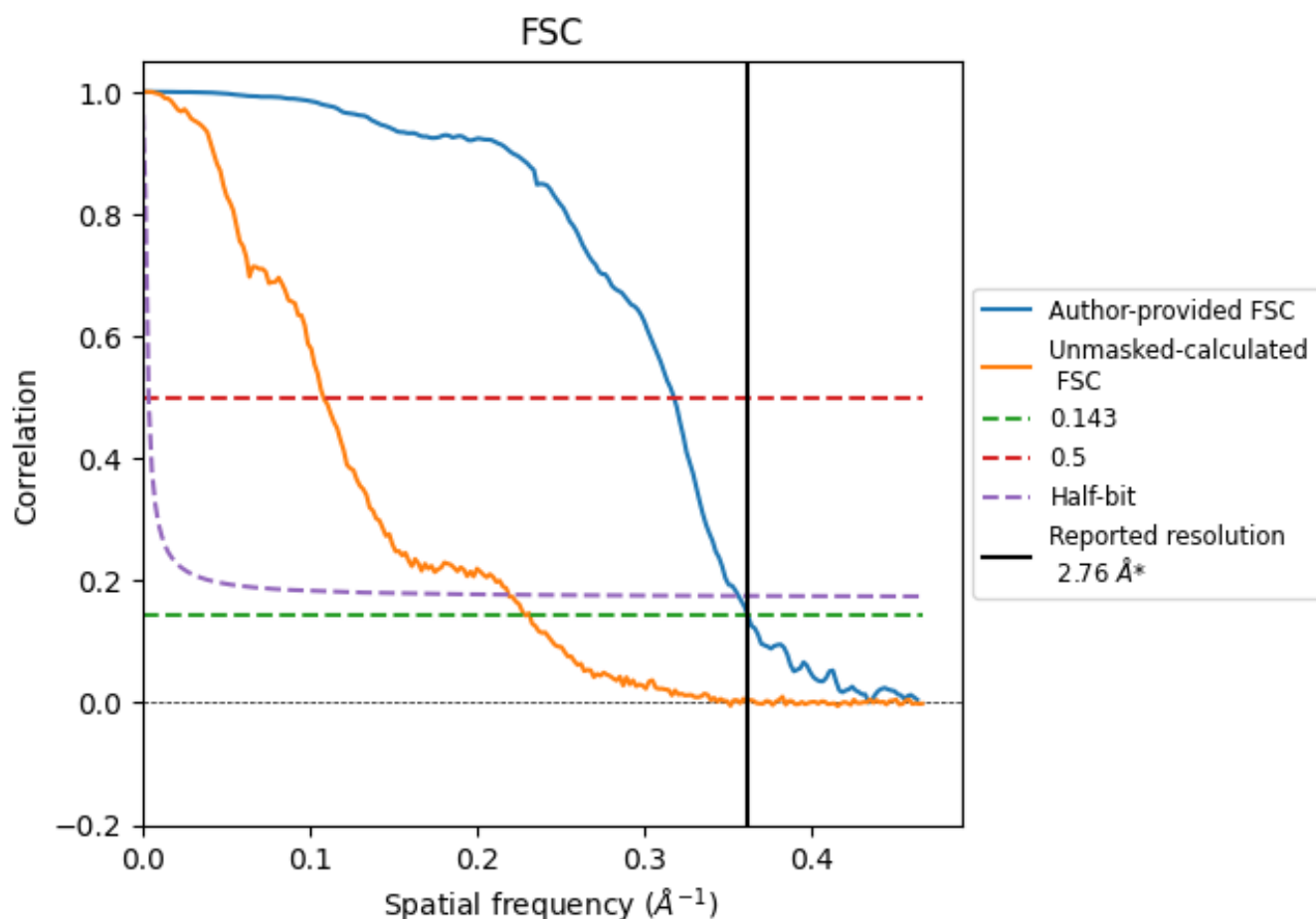


*Reported resolution corresponds to spatial frequency of 0.362 Å⁻¹

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 0.362 Å⁻¹

8.2 Resolution estimates [i](#)

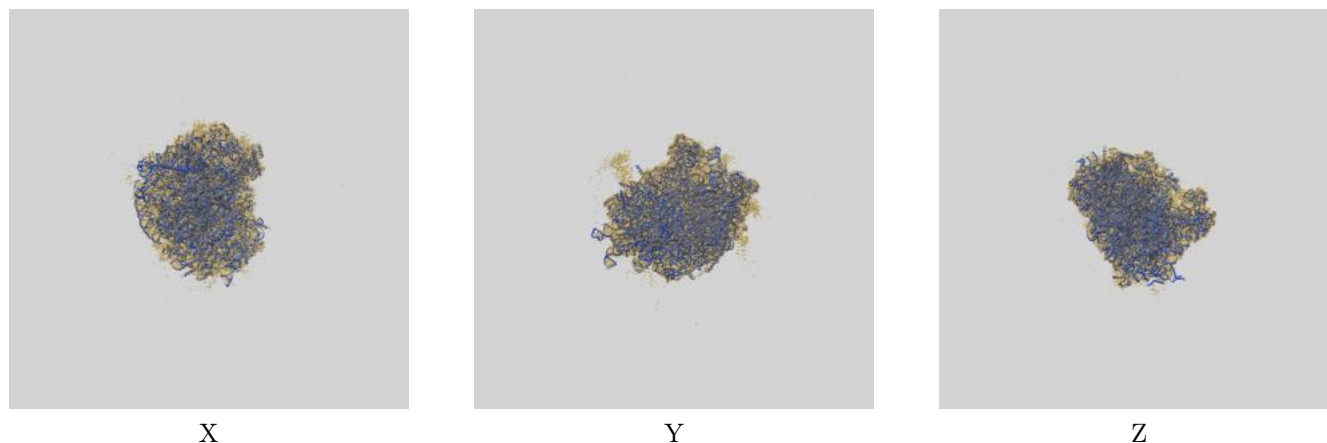
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.76	-	-
Author-provided FSC curve	2.76	3.14	2.80
Unmasked-calculated*	4.36	9.23	4.56

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.36 differs from the reported value 2.76 by more than 10 %

9 Map-model fit [i](#)

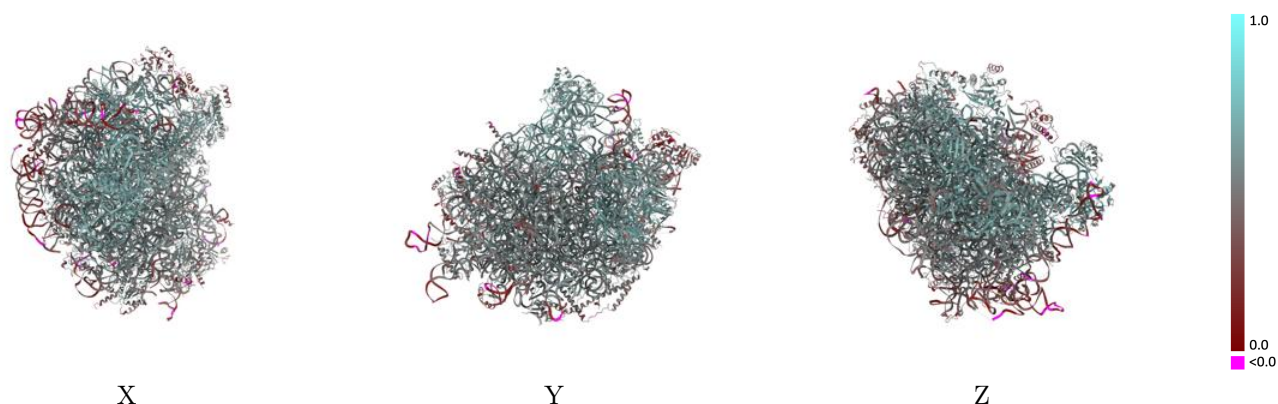
This section contains information regarding the fit between EMDB map EMD-29274 and PDB model 8FLC. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



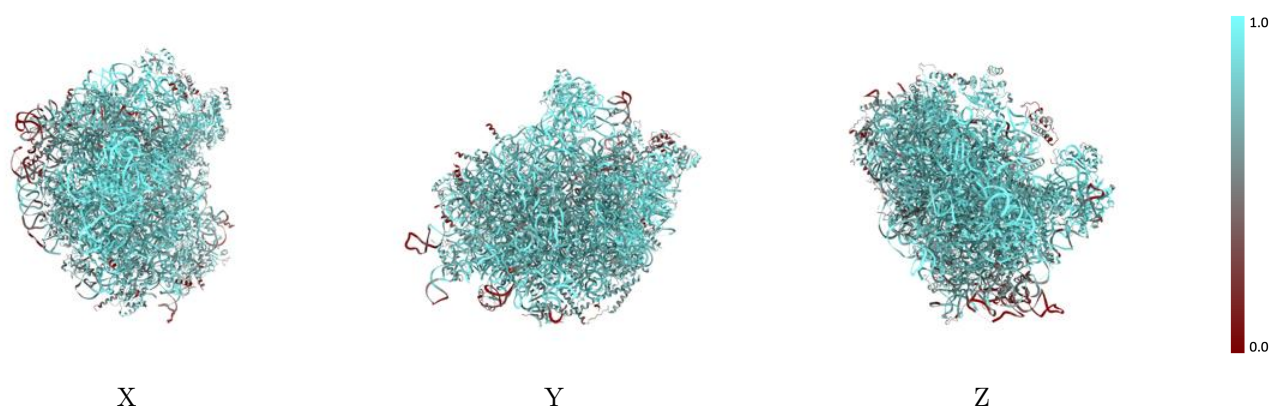
The images above show the 3D surface view of the map at the recommended contour level 0.85 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



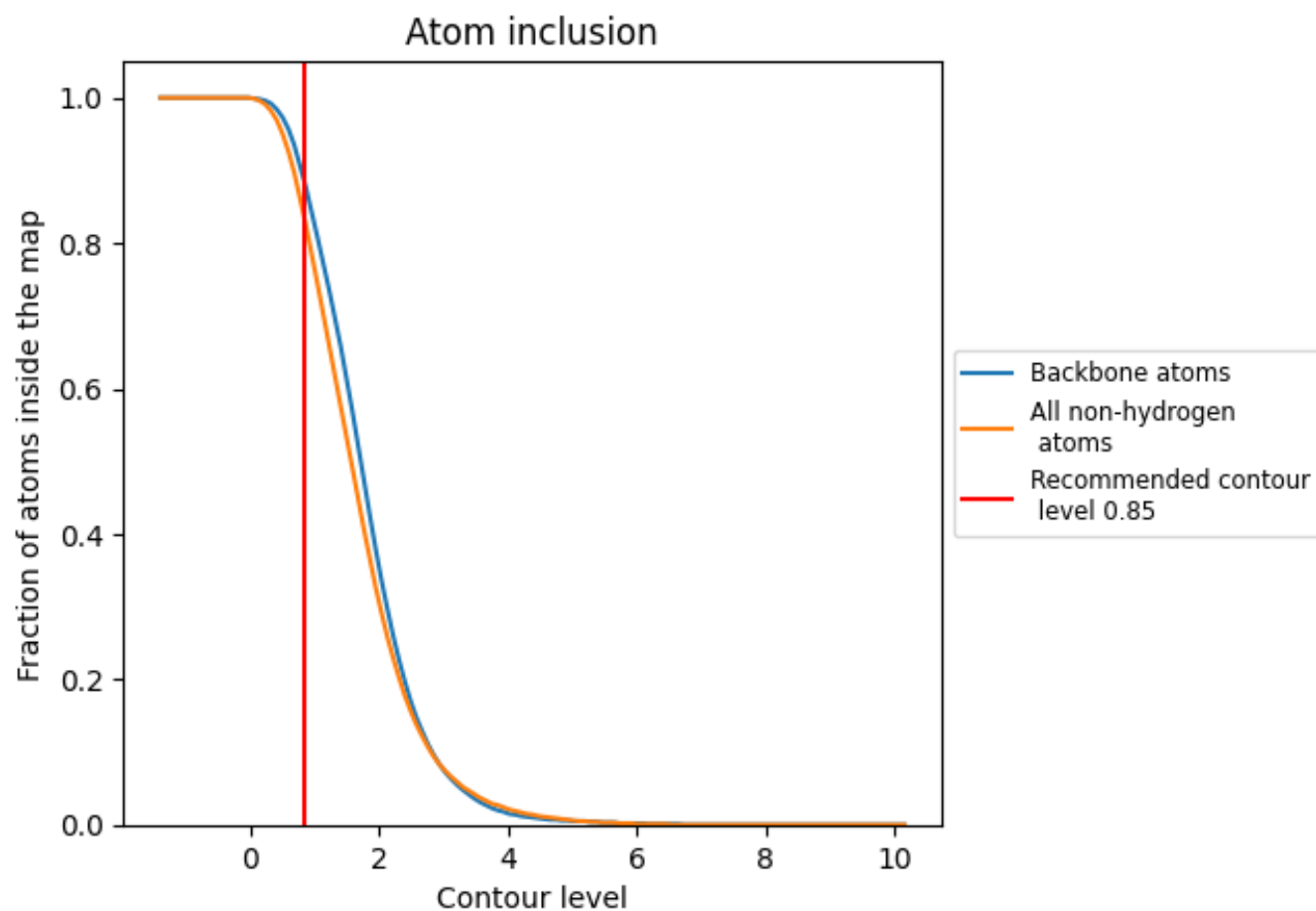
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.85).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 83% 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 (0.85) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8300	 0.5090
BA	 0.3790	 0.2720
L1	 0.8720	 0.5000
L3	 0.8560	 0.4900
L4	 0.9820	 0.6130
L5	 0.8410	 0.5550
L6	 0.7570	 0.5030
L7	 0.8900	 0.6050
L8	 0.8970	 0.5880
L9	 0.8550	 0.5550
LA	 0.7840	 0.5220
LB	 0.8400	 0.5570
LC	 0.9650	 0.6500
LD	 0.7530	 0.4990
LE	 0.9070	 0.5930
LF	 0.7200	 0.4790
LG	 0.8700	 0.5890
LH	 0.7600	 0.5050
LI	 0.7560	 0.5010
LJ	 0.7070	 0.4770
LK	 0.8560	 0.5630
LL	 0.7580	 0.5000
LM	 0.6970	 0.5030
LN	 0.8310	 0.5500
LO	 0.6860	 0.4460
LP	 0.7380	 0.5090
LQ	 0.7740	 0.5360
LR	 0.7430	 0.5010
LS	 0.7440	 0.4920
LT	 0.8280	 0.5480
LU	 0.7290	 0.4960
LV	 0.8910	 0.6010
LW	 0.8460	 0.5490
LX	 0.7320	 0.4910
LY	 0.6410	 0.4340



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
LZ	 0.8370	 0.5480
NK	 0.5990	 0.4310
NP	 0.7180	 0.4880
NR	 0.7440	 0.5330
SA	 0.7880	 0.5240
SB	 0.8970	 0.5930
SC	 0.6260	 0.4410
SD	 0.8140	 0.5350
SE	 0.6760	 0.4500
SF	 0.8090	 0.5320
SG	 0.9180	 0.6090
SK	 0.8260	 0.5500
SQ	 0.7150	 0.3740
SR	 0.7680	 0.5160
SV	 0.7590	 0.5010
VB	 0.6670	 0.5280