



Full wwPDB EM Validation Report ⓘ

Jun 19, 2026 – 07:18 am BST

PDB ID : 7R4X / pdb_00007r4x
EMDB ID : EMD-14317
Title : Cryo-EM reconstruction of the human 40S ribosomal subunit - Full map
Authors : Pellegrino, S.; Dent, K.C.; Spikes, T.; Warren, A.J.
Deposited on : 2022-02-09
Resolution : 2.15 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:

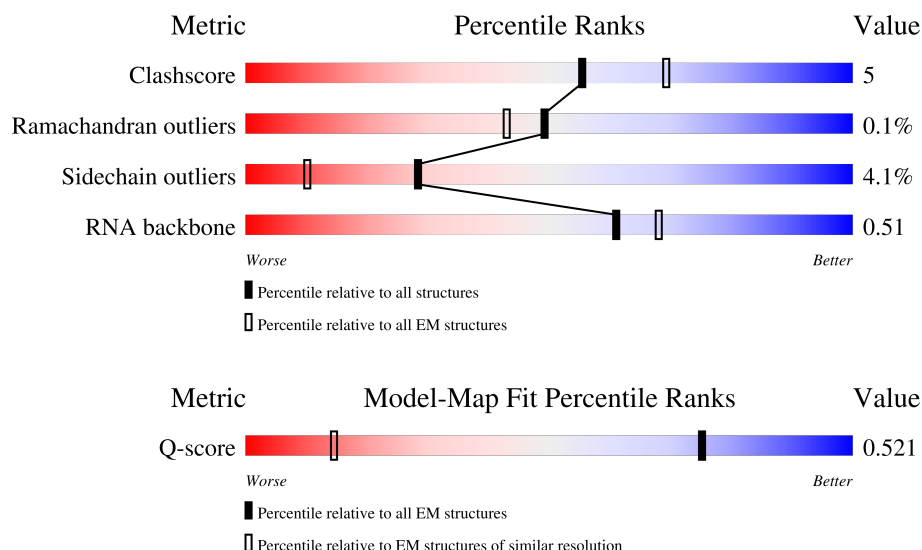
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.15 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	2551 (1.66 - 2.65)

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	n	25	
2	2	1868	
3	B	264	

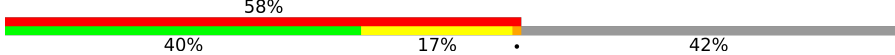
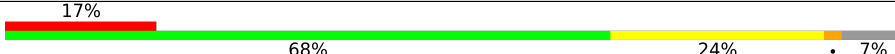
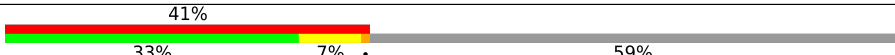
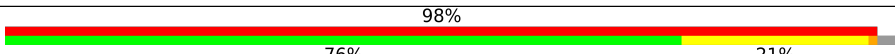
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	243	
5	E	263	
6	F	204	
7	H	194	
8	I	208	
9	K	165	
10	L	158	
11	P	145	
12	Q	146	
13	R	135	
14	S	152	
15	T	145	
16	U	119	
17	V	83	
18	X	143	
19	a	115	
20	c	69	
21	d	56	
22	C	293	
23	G	249	
24	J	194	
25	M	132	
26	N	151	
27	O	151	
28	W	130	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	Y	133	
30	Z	125	
31	b	84	
32	e	59	
33	f	156	
34	g	317	
35	A	295	

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 77936 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	n	20	Total	C	N	O	S	0	0
			193	119	51	20	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1646	Total	C	N	O	P	7	0
			35347	15805	6355	11535	1652		

- Molecule 3 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	210	Total	C	N	O	S	0	0
			1711	1086	306	305	14		

- Molecule 4 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	224	Total	C	N	O	S	0	0
			1745	1112	314	312	7		

- Molecule 5 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	257	Total	C	N	O	S	0	0
			2041	1305	379	349	8		

- Molecule 6 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	182	Total	C	N	O	S	0	0
			1445	906	271	261	7		

- Molecule 7 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	184	Total	C	N	O	S	0	0
			1477	942	271	263	1		

- Molecule 8 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	205	Total	C	N	O	S	0	0
			1682	1056	331	290	5		

- Molecule 9 is a protein called 40S ribosomal protein S10.

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

- Molecule 10 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	141	Total	C	N	O	S	0	0
			1157	737	217	197	6		

- Molecule 11 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	123	Total	C	N	O	S	0	0
			1005	638	188	172	7		

- Molecule 12 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Q	139	Total	C	N	O	S	0	0
			1105	704	207	191	3		

- Molecule 13 is a protein called 40S ribosomal protein S17.

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

- Molecule 14 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S	143	Total	C	N	O	S	1	0
			1192	751	240	200	1		

- Molecule 15 is a protein called 40S ribosomal protein S19.

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

- Molecule 16 is a protein called 40S ribosomal protein S20.

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

- Molecule 17 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	V	83	Total	C	N	O	S	0	0
			639	395	117	122	5		

- Molecule 18 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	140	Total	C	N	O	S	0	0
			1088	687	215	183	3		

- Molecule 19 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	a	99	Total	C	N	O	S	0	0
			792	492	165	130	5		

- Molecule 20 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	c	59	Total	C	N	O	S	0	0
			464	281	93	88	2		

- Molecule 21 is a protein called 40S ribosomal protein S29.

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

- Molecule 22 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	C	219	Total	C	N	O	S	1	0
			1708	1105	295	298	10		

- Molecule 23 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	G	227	Total	C	N	O	S	0	0
			1840	1149	367	317	7		

- Molecule 24 is a protein called 40S ribosomal protein S9.

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

- Molecule 25 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	M	104	Total	C	N	O	S	0	0
			790	494	138	151	7		

- Molecule 26 is a protein called 40S ribosomal protein S13.

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

- Molecule 27 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	O	127	Total	C	N	O	S	0	0
			957	585	189	177	6		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 28 is a protein called 40S ribosomal protein S15a.

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

- Molecule 29 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	122	Total	C	N	O	S	0	0
			1002	635	196	166	5		

- Molecule 30 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	72	Total	C	N	O	S	0	0
			570	366	104	99	1		

- Molecule 31 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	82	Total	C	N	O	S	0	0
			640	402	118	113	7		

- Molecule 32 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	55	Total	C	N	O	S	0	0
			438	271	95	71	1		

- Molecule 33 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	64	Total	C	N	O	S	0	0
			522	329	99	87	7		

- Molecule 34 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	312	Total	C	N	O	S	0	0
			2429	1531	423	463	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	A	206	Total	C	N	O	S	1	0
			1628	1042	287	291	8		

- Molecule 36 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
36	2	76	Total	K	0
			76	76	
36	E	1	Total	K	0
			1	1	
36	L	1	Total	K	0
			1	1	
36	S	1	Total	K	0
			1	1	
36	U	1	Total	K	0
			1	1	
36	d	1	Total	K	0
			1	1	
36	O	1	Total	K	0
			1	1	

- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	2	88	Total	Mg	0
			88	88	

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

Mol	Chain	Residues	Atoms		AltConf
38	a	1	Total	Zn	0
			1	1	
38	d	1	Total	Zn	0
			1	1	
38	f	1	Total	Zn	0
			1	1	

- Molecule 39 is water.

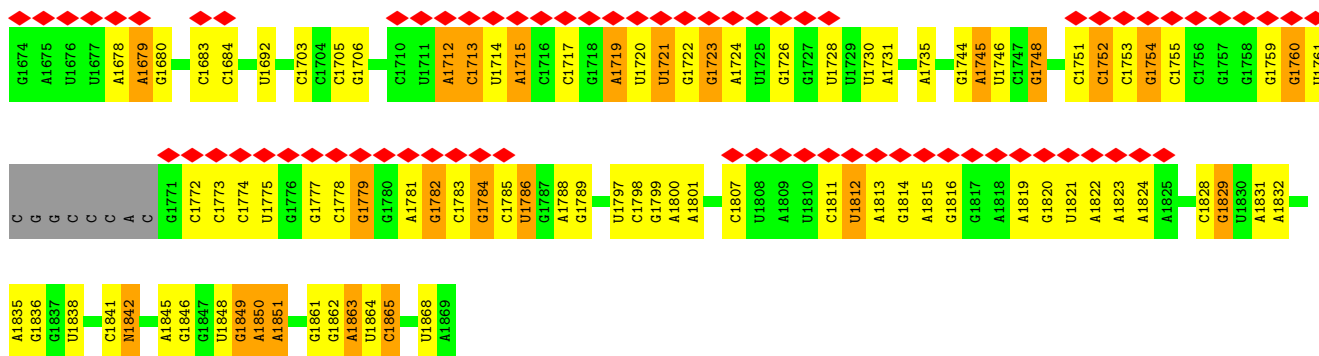
Mol	Chain	Residues	Atoms		AltConf
39	n	10	Total 10	O 10	0
39	2	3102	Total 3102	O 3102	0
39	B	30	Total 30	O 30	0
39	D	24	Total 24	O 24	0
39	E	79	Total 79	O 79	0
39	F	34	Total 34	O 34	0
39	H	8	Total 8	O 8	0
39	I	45	Total 45	O 45	0
39	K	20	Total 20	O 20	0
39	L	62	Total 62	O 62	0
39	P	32	Total 32	O 32	0
39	Q	46	Total 46	O 46	0
39	R	13	Total 13	O 13	0
39	S	30	Total 30	O 30	0
39	T	51	Total 51	O 51	0
39	U	25	Total 25	O 25	0
39	V	19	Total 19	O 19	0
39	X	47	Total 47	O 47	0
39	a	30	Total 30	O 30	0
39	c	6	Total 6	O 6	0
39	d	26	Total 26	O 26	0

Continued on next page...

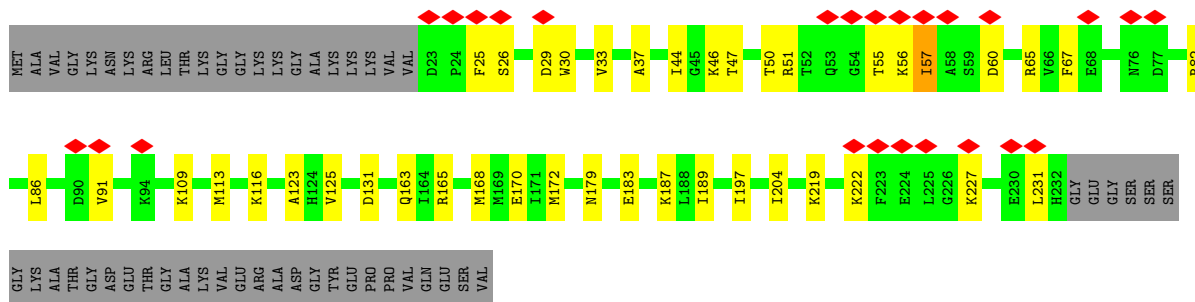
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
39	C	56	Total 56	O 56	0
39	G	18	Total 18	O 18	0
39	J	85	Total 85	O 85	0
39	N	30	Total 30	O 30	0
39	O	28	Total 28	O 28	0
39	W	63	Total 63	O 63	0
39	Y	25	Total 25	O 25	0
39	Z	2	Total 2	O 2	0
39	b	12	Total 12	O 12	0
39	e	13	Total 13	O 13	0
39	g	16	Total 16	O 16	0
39	A	30	Total 30	O 30	0

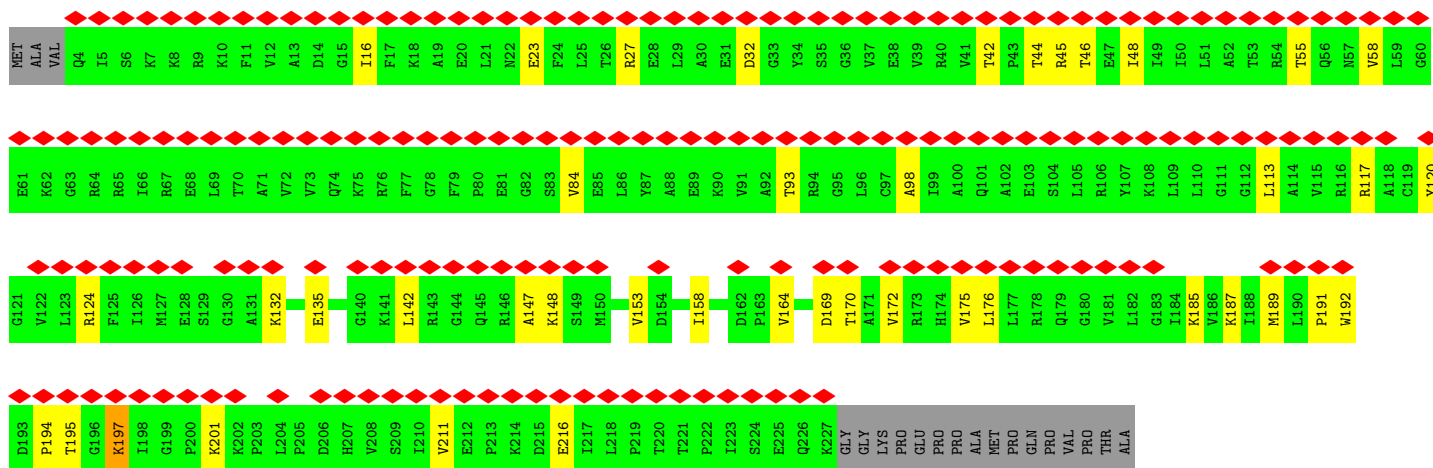
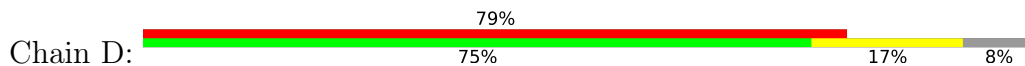




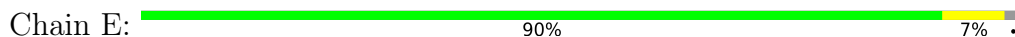
• Molecule 3: 40S ribosomal protein S3a



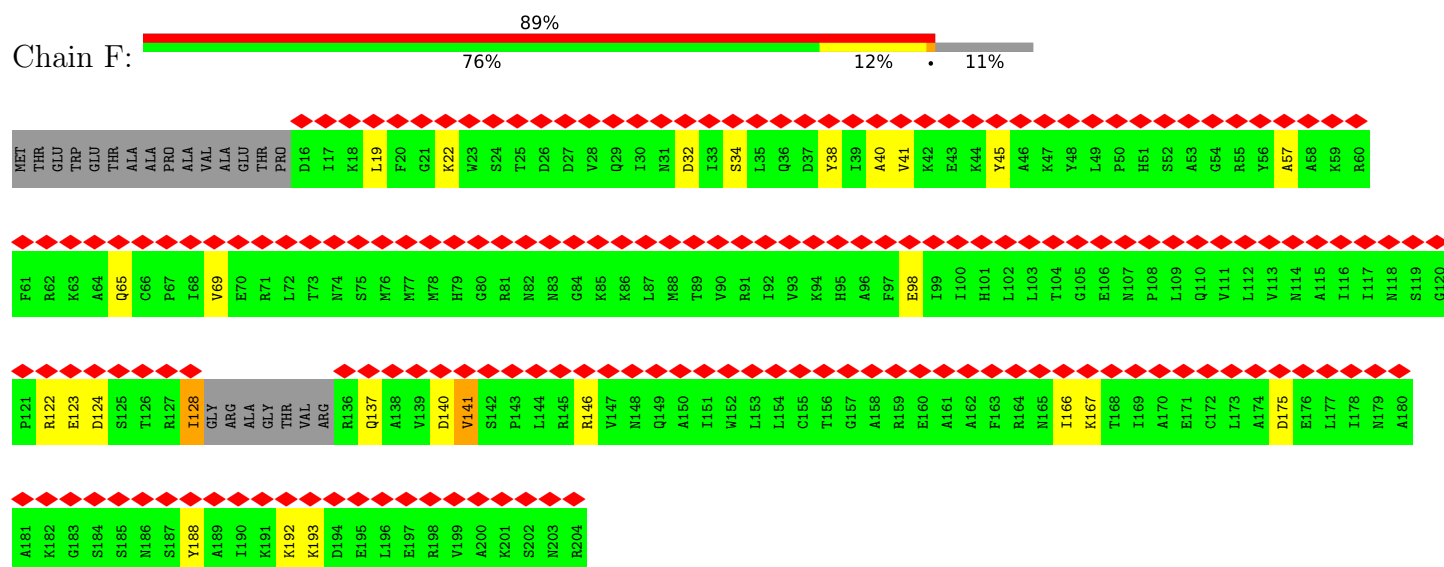
• Molecule 4: 40S ribosomal protein S3



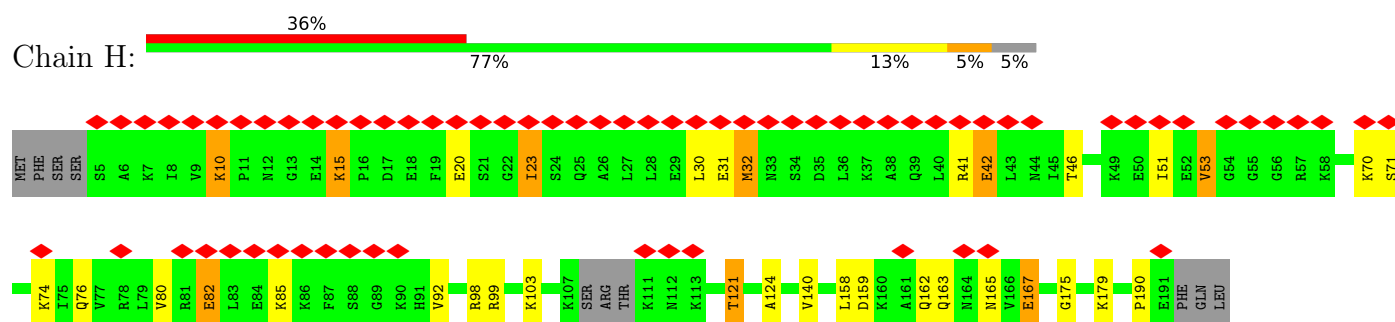
• Molecule 5: 40S ribosomal protein S4, X isoform



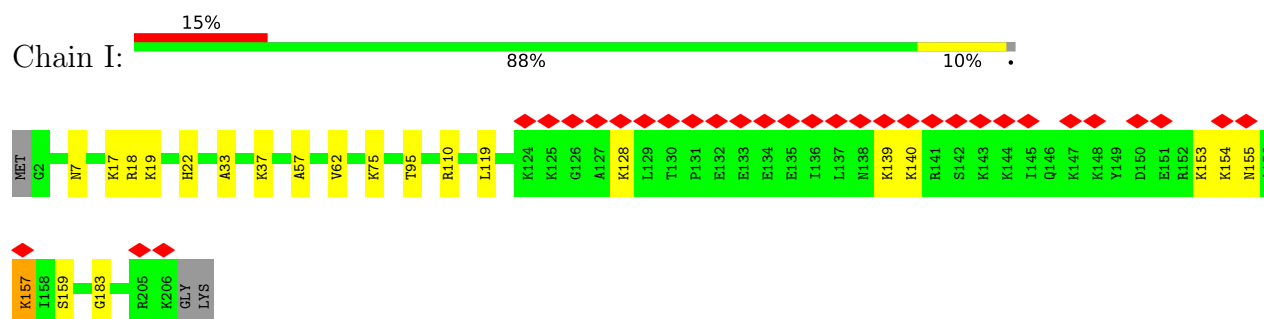
- Molecule 6: 40S ribosomal protein S5



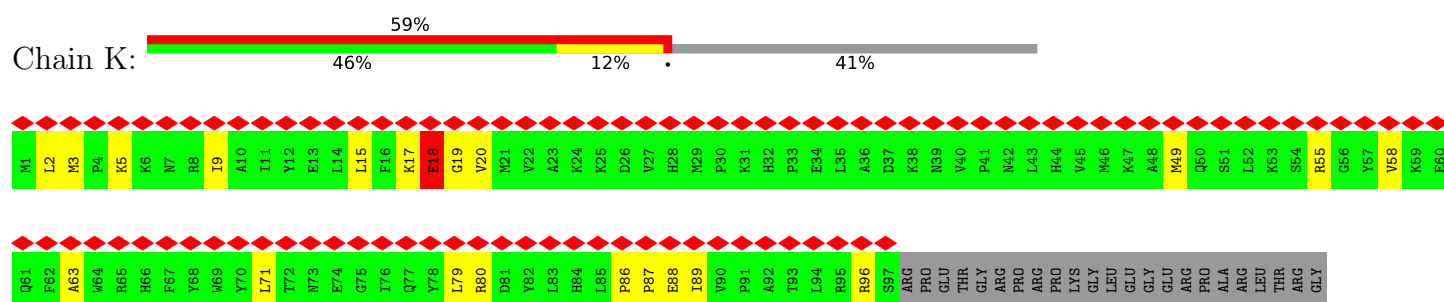
- Molecule 7: 40S ribosomal protein S7



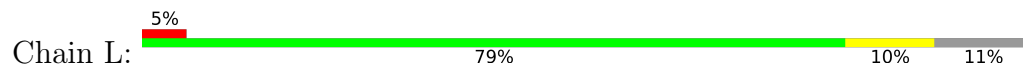
- Molecule 8: 40S ribosomal protein S8



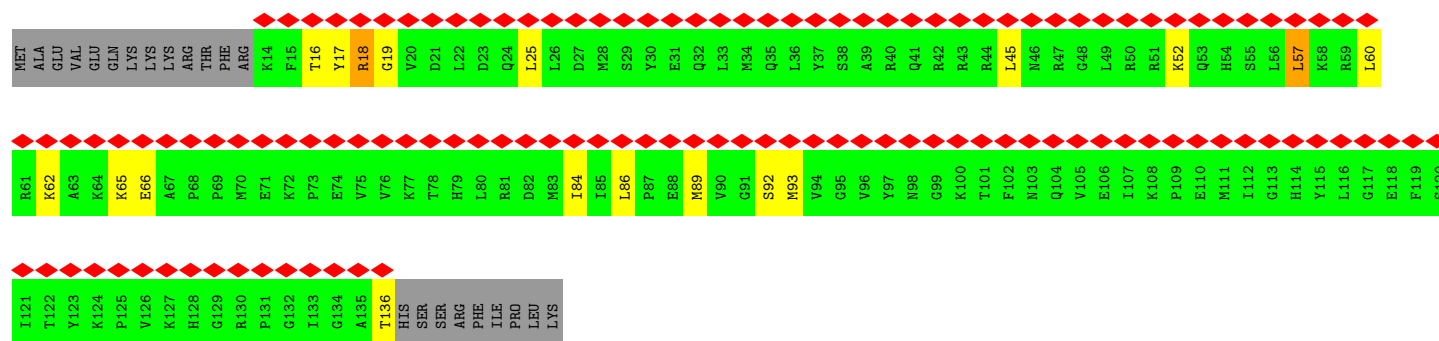
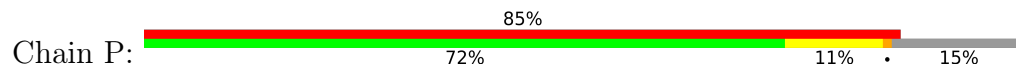
- Molecule 9: 40S ribosomal protein S10



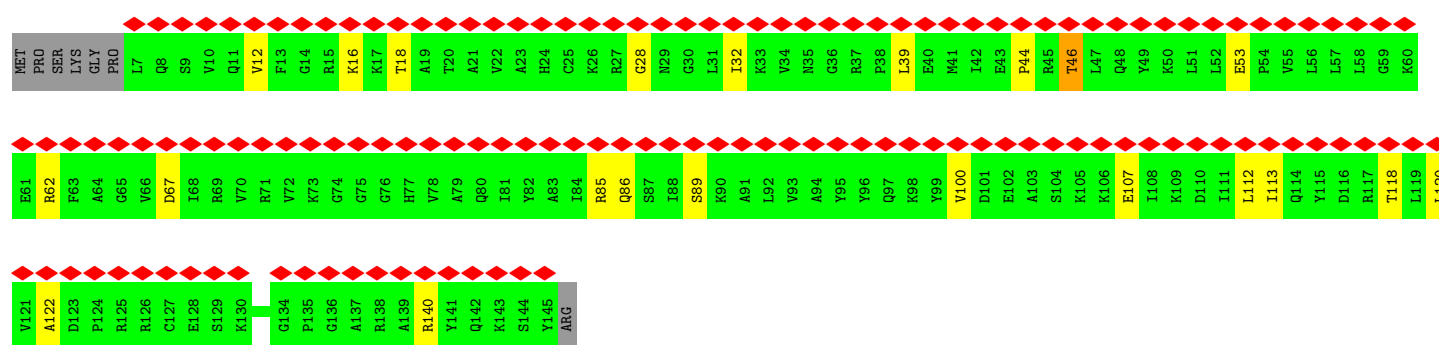
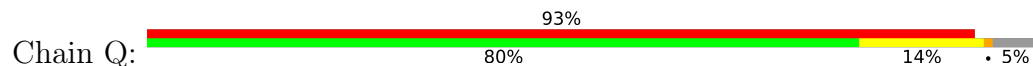
- Molecule 10: 40S ribosomal protein S11



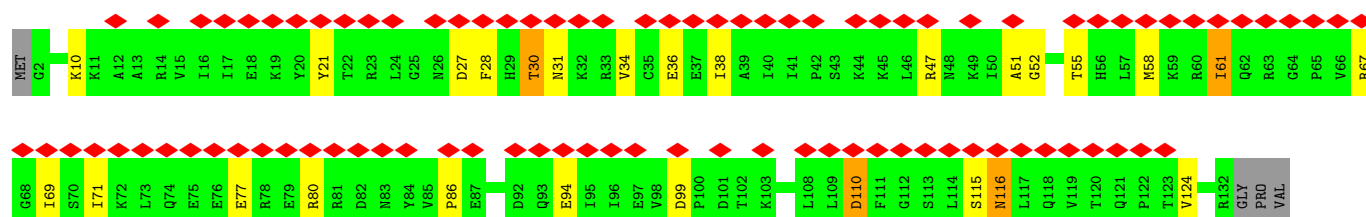
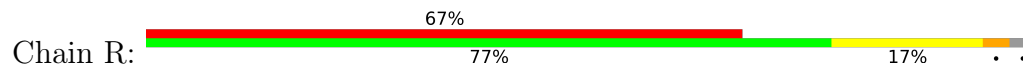
- Molecule 11: 40S ribosomal protein S15



- Molecule 12: 40S ribosomal protein S16

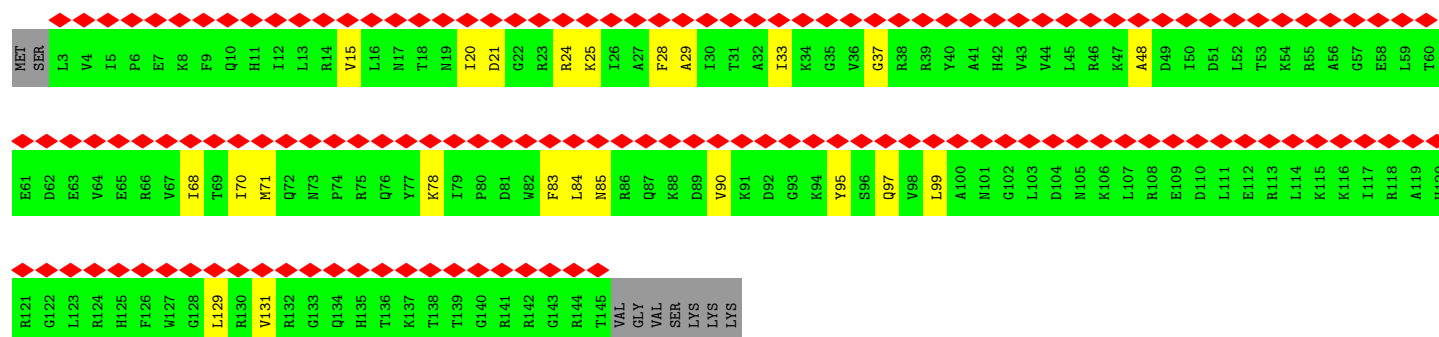


- Molecule 13: 40S ribosomal protein S17

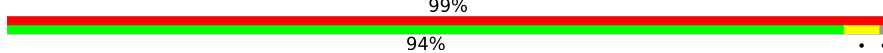


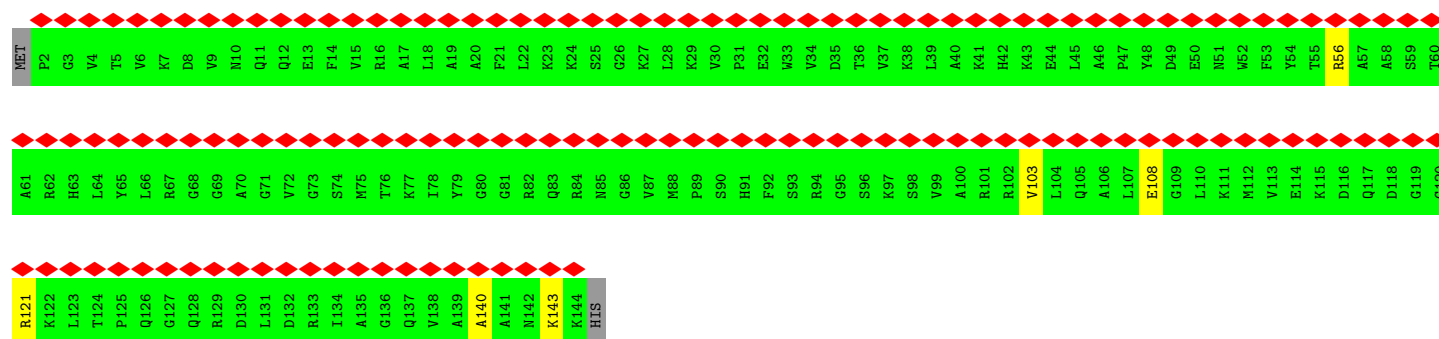
- Molecule 14: 40S ribosomal protein S18

Chain S: 



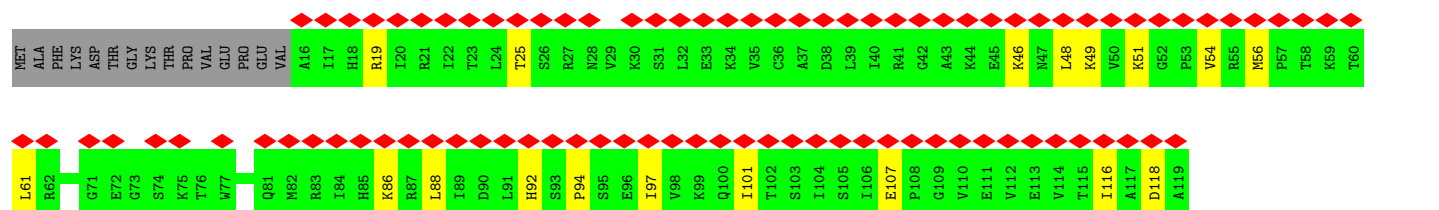
- Molecule 15: 40S ribosomal protein S19

Chain T: 



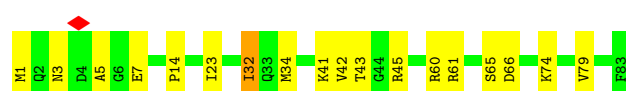
- Molecule 16: 40S ribosomal protein S20

Chain U: 



- Molecule 17: 40S ribosomal protein S21

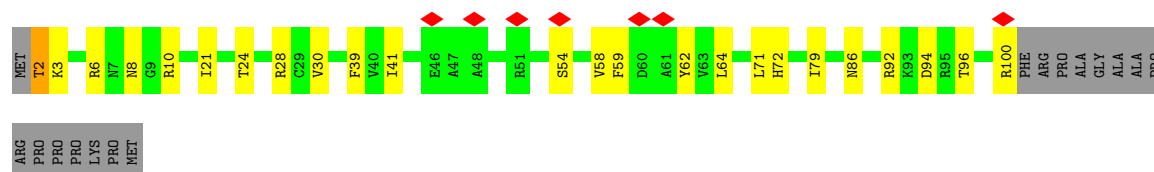
Chain V: 

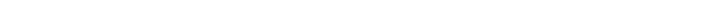


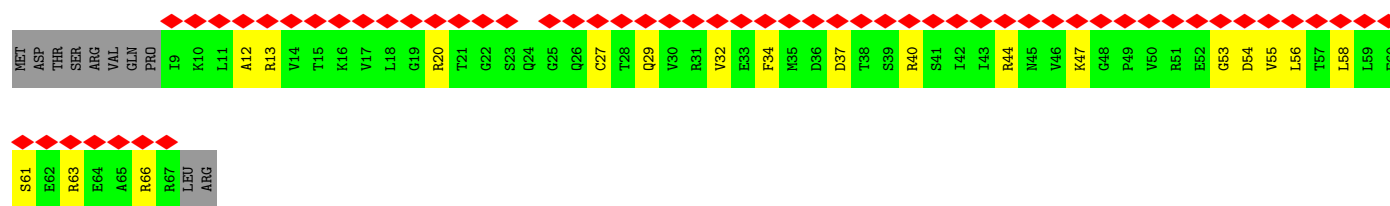
- Molecule 18: 40S ribosomal protein S23

[illegible]

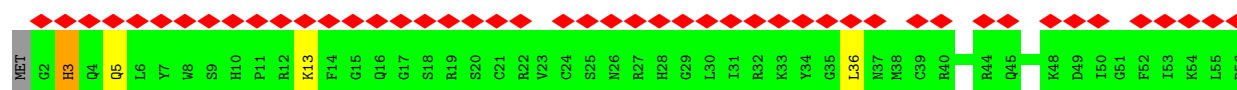
- Chain a: 6% 65% 20% 9%

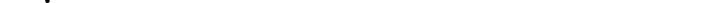


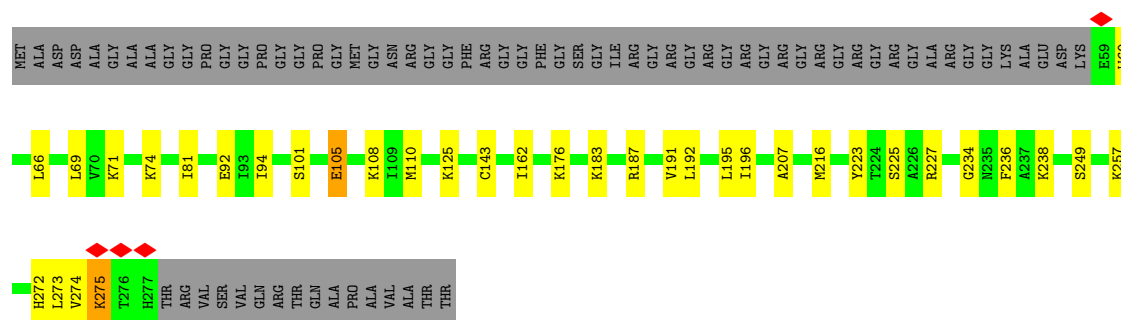
- Chain c:  84% 28% 14%



- Chain d:  84% 91% 5% . .

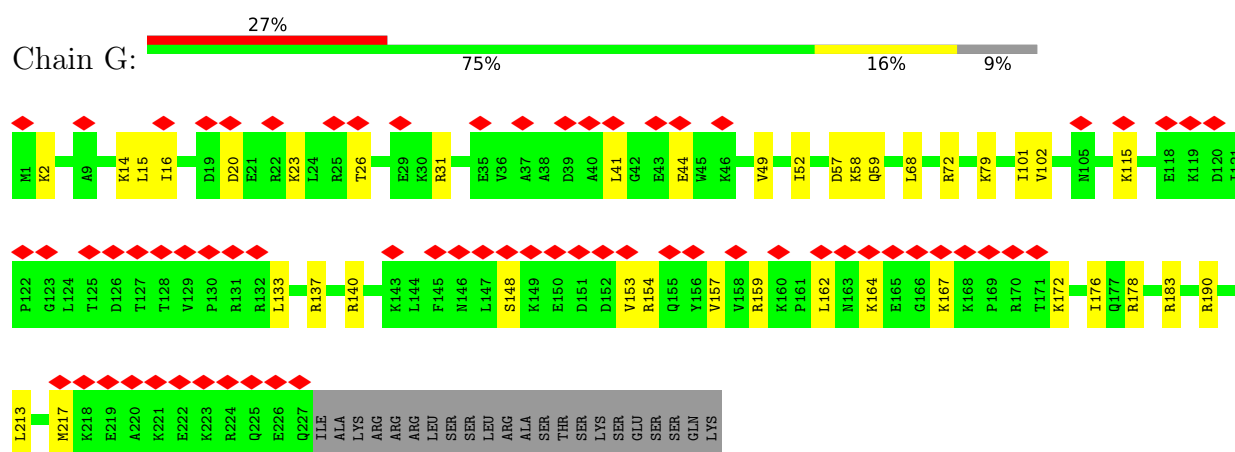


- Chain C:  62% 12% 25%

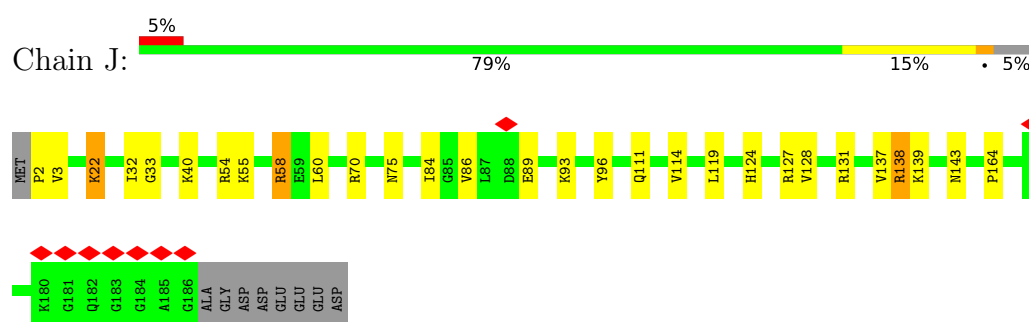


- WORLDWIDE

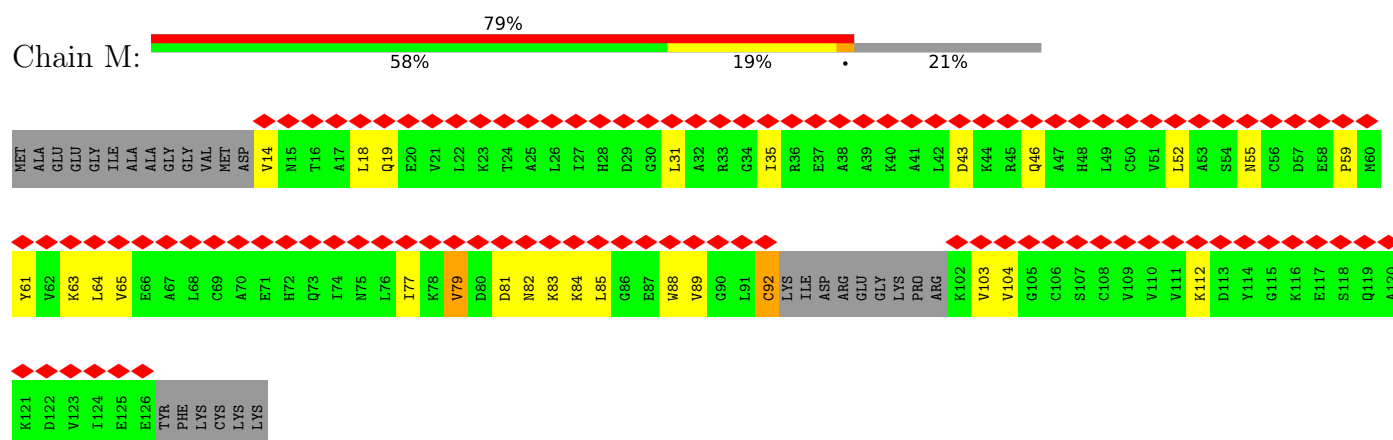
PROTEIN DATA BANK



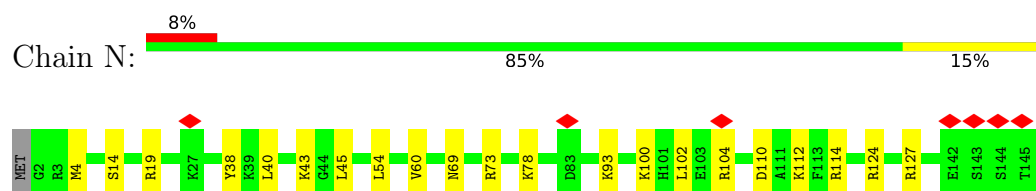
• Molecule 24: 40S ribosomal protein S9



• Molecule 25: 40S ribosomal protein S12

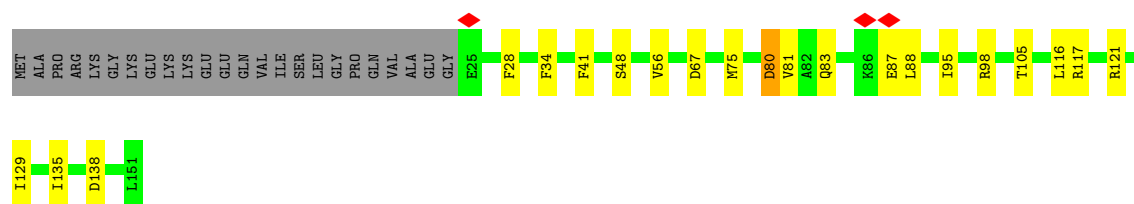


• Molecule 26: 40S ribosomal protein S13



• Molecule 27: 40S ribosomal protein S14





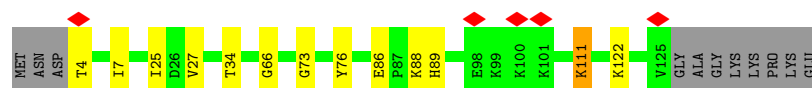
- Molecule 28: 40S ribosomal protein S15a

Chain W: 90% 9%



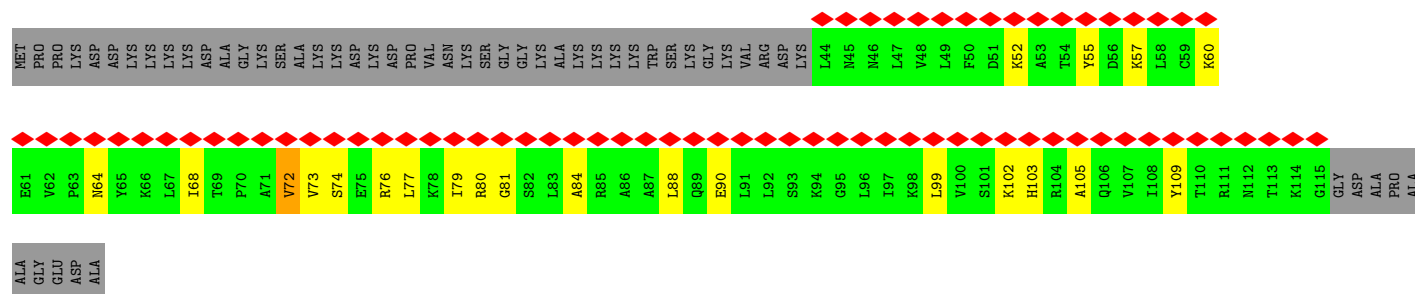
- Molecule 29: 40S ribosomal protein S24

Chain Y: 82% 9% 8%



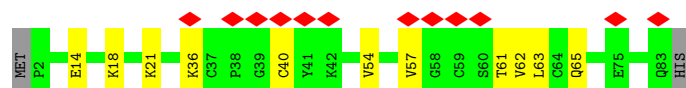
- Molecule 30: 40S ribosomal protein S25

Chain Z: 58% 40% 17% 42%



- Molecule 31: 40S ribosomal protein S27

Chain b: 14% 85% 13%

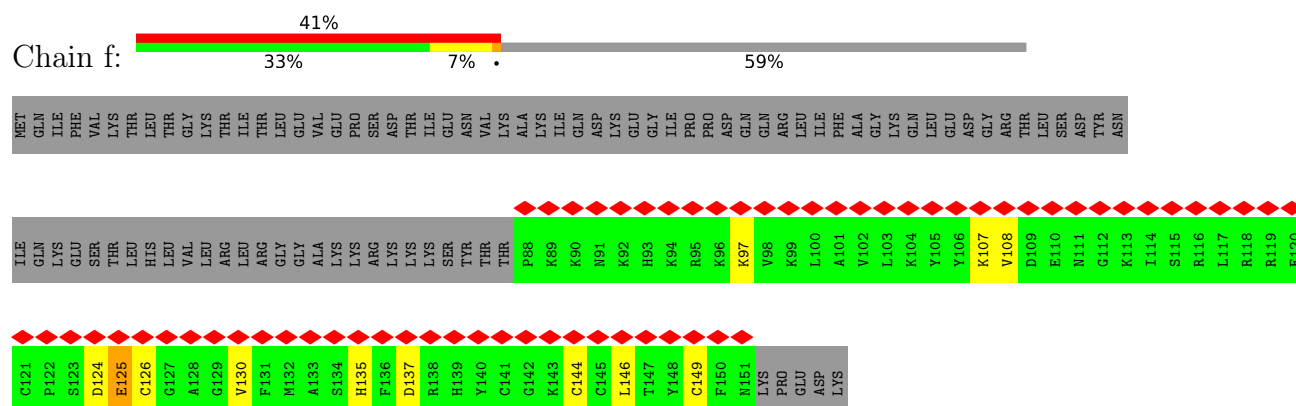


- Molecule 32: 40S ribosomal protein S30

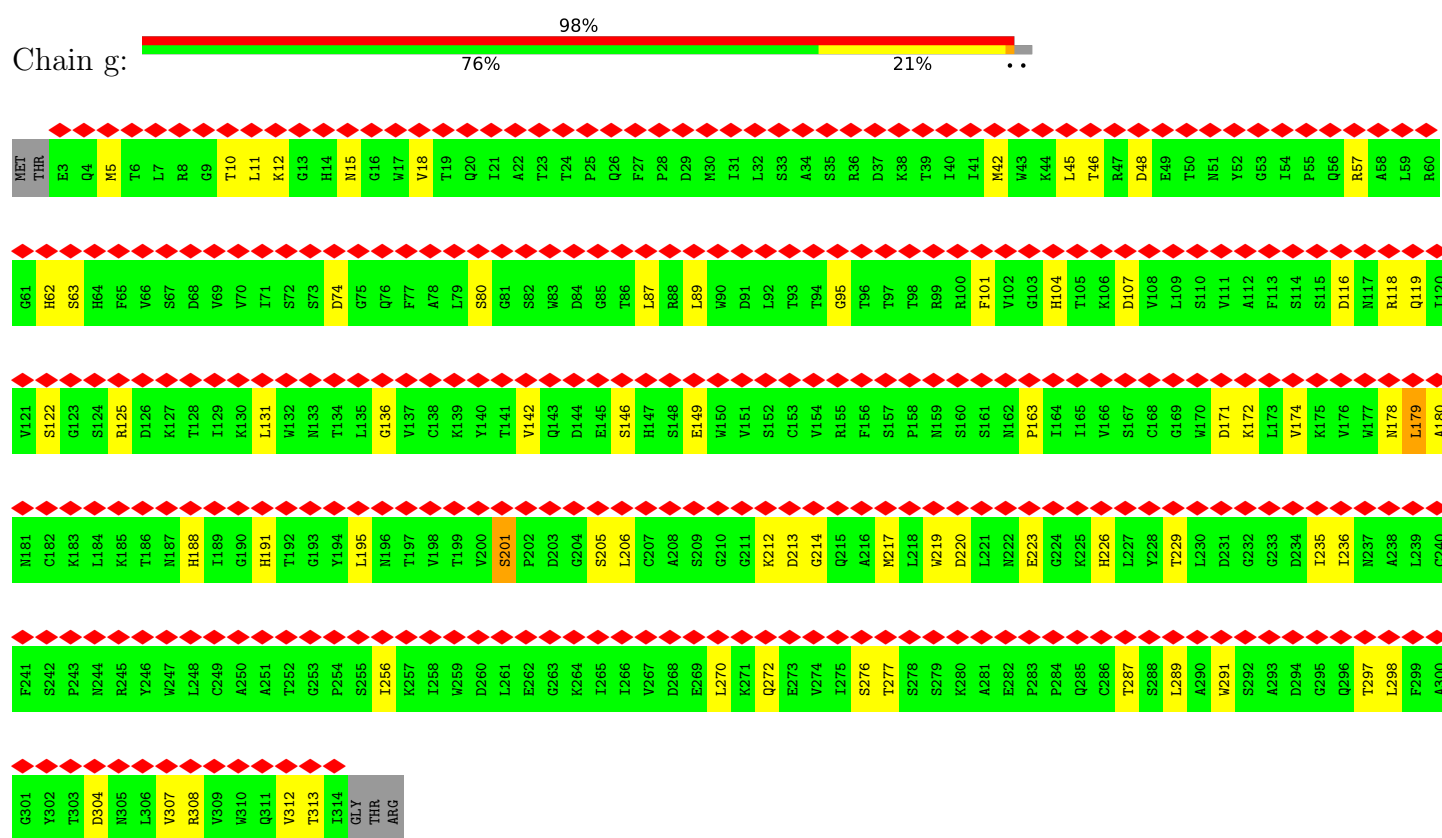
Chain e: 17% 68% 24% 7%



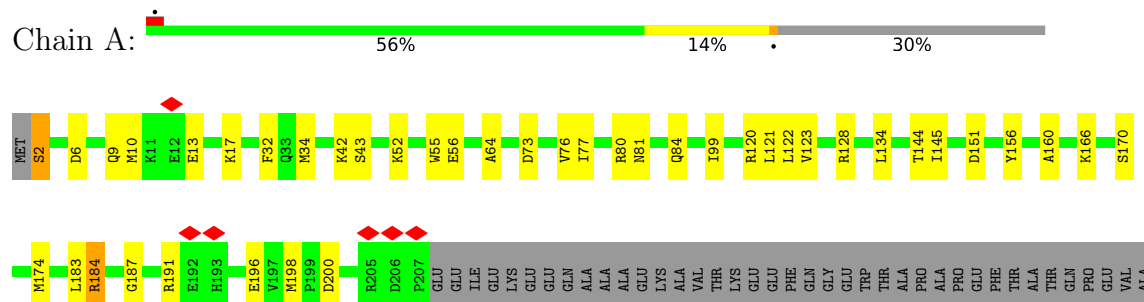
• Molecule 33: Ubiquitin-40S ribosomal protein S27a



• Molecule 34: Receptor of activated protein C kinase 1



• Molecule 35: 40S ribosomal protein SA



ASP	TRP	SER	GLU	GLY	VAL	GLN	VAL	PRO	SER	VAL	PRO	ILE	GLN	PHE	PRO	THR	GLU	ASP	TRP	SER	ALA	GLN	PRO	ALA	THR	GLU	ASP	TRP	SER	ALA	ALA	PRO	THR	ALA	GLN	ALA	THR	GLU	TRP	VAL	GLY	ALA	THR	THR	ASP	TRP	SER
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	474276	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 ($e^-/\text{\AA}^2$)	40.56	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.283	Depositor
Minimum map value	-0.102	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.025	Depositor
Map size ($\text{\AA}$)	423.2704, 423.2704, 423.2704	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.8267, 0.8267, 0.8267	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SAC, PSU, 7MG, HY3, MG, B8N, MA6, A2M, K, 4AC, AME, OMG, OMC, 6MZ, IAS, OMU, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	n	0.50	0/194	0.78	0/246
2	2	0.55	2/37770 (0.0%)	0.54	2/58857 (0.0%)
3	B	0.40	0/1738	0.49	0/2325
4	D	0.49	0/1773	0.64	0/2387
5	E	0.41	0/2083	0.53	0/2805
6	F	0.46	0/1465	0.65	0/1969
7	H	0.30	0/1498	0.55	0/2005
8	I	0.51	0/1711	0.67	0/2282
9	K	0.48	0/840	0.67	3/1133 (0.3%)
10	L	0.44	0/1177	0.53	0/1574
11	P	0.34	0/1024	0.52	0/1369
12	Q	0.40	0/1122	0.59	2/1503 (0.1%)
13	R	0.42	0/1078	0.59	2/1447 (0.1%)
14	S	0.39	0/1214	0.59	0/1626
15	T	0.41	0/1131	0.52	0/1515
16	U	0.37	0/831	0.57	0/1115
17	V	0.44	0/635	0.54	0/850
18	X	0.48	0/1096	0.61	0/1461
19	a	0.58	0/805	0.67	0/1079
20	c	0.52	0/465	0.70	0/621
21	d	0.39	0/470	0.51	0/623
22	C	0.54	0/1748	0.62	0/2361
23	G	0.34	0/1863	0.52	0/2481
24	J	0.52	0/1550	0.71	0/2069
25	M	0.26	0/796	0.48	0/1072
26	N	0.37	0/1232	0.55	0/1656
27	O	0.54	0/960	0.66	0/1284
28	W	0.52	0/1051	0.64	0/1406
29	Y	0.41	0/1019	0.49	0/1354
30	Z	0.29	0/576	0.59	0/774
31	b	0.36	0/653	0.49	0/876
32	e	0.39	0/443	0.56	0/582

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	f	0.56	0/533	0.80	0/706
34	g	0.40	0/2486	0.59	1/3384 (0.0%)
35	A	0.46	0/1659	0.53	0/2254
All	All	0.49	2/76689 (0.0%)	0.56	10/111051 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	H	0	2
14	S	0	1
16	U	0	1
24	J	0	1
35	A	0	1
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1622	U	O3'-P	-13.48	1.41	1.61
2	2	99	A2M	O3'-P	5.80	1.62	1.56

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	R	86	PRO	N-CD-CG	-7.13	92.51	103.20
2	2	1622	U	P-O3'-C3'	6.93	130.59	120.20
9	K	18	GLU	N-CA-C	-6.08	97.38	108.02
9	K	63	ALA	CA-C-N	5.88	132.78	121.54
9	K	63	ALA	C-N-CA	5.88	132.78	121.54
34	g	118	ARG	N-CA-C	-5.86	106.75	114.31
13	R	86	PRO	CA-N-CD	-5.77	103.92	112.00
12	Q	16	LYS	CA-C-N	5.61	132.26	121.54
12	Q	16	LYS	C-N-CA	5.61	132.26	121.54
2	2	1520	G	C2'-C3'-O3'	-5.04	106.14	113.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
35	A	2	SAC	Mainchain
7	H	15	LYS	Peptide
7	H	42	GLU	Peptide
24	J	137	VAL	Peptide
14	S	99	LEU	Peptide
16	U	107	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	n	193	0	237	3	0
2	2	35347	0	17896	284	0
3	B	1711	0	1782	23	0
4	D	1745	0	1839	19	0
5	E	2041	0	2143	12	0
6	F	1445	0	1495	13	0
7	H	1477	0	1573	24	0
8	I	1682	0	1769	11	0
9	K	816	0	841	10	0
10	L	1157	0	1222	9	0
11	P	1005	0	1053	13	0
12	Q	1105	0	1172	10	0
13	R	1064	0	1118	17	0
14	S	1192	0	1253	15	0
15	T	1112	0	1146	3	0
16	U	821	0	883	11	0
17	V	639	0	638	14	0
18	X	1088	0	1149	10	0
19	a	792	0	841	16	0
20	c	464	0	488	10	0
21	d	459	0	448	4	0
22	C	1708	0	1797	25	0
23	G	1840	0	1989	26	0
24	J	1525	0	1640	18	0
25	M	790	0	808	12	0
26	N	1208	0	1293	13	0
27	O	957	0	981	9	0
28	W	1034	0	1080	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	Y	1002	0	1075	8	0
30	Z	570	0	626	11	0
31	b	640	0	665	5	0
32	e	438	0	484	8	0
33	f	522	0	529	8	0
34	g	2429	0	2386	34	0
35	A	1628	0	1649	28	0
36	2	76	0	0	0	0
36	E	1	0	0	0	0
36	L	1	0	0	0	0
36	O	1	0	0	0	0
36	S	1	0	0	0	0
36	U	1	0	0	0	0
36	d	1	0	0	0	0
37	2	88	0	0	0	0
38	a	1	0	0	0	0
38	d	1	0	0	0	0
38	f	1	0	0	0	0
39	2	3102	0	0	16	0
39	A	30	0	0	1	0
39	B	30	0	0	1	0
39	C	56	0	0	3	0
39	D	24	0	0	0	0
39	E	79	0	0	0	0
39	F	34	0	0	0	0
39	G	18	0	0	0	0
39	H	8	0	0	0	0
39	I	45	0	0	0	0
39	J	85	0	0	0	0
39	K	20	0	0	0	0
39	L	62	0	0	0	0
39	N	30	0	0	1	0
39	O	28	0	0	0	0
39	P	32	0	0	0	0
39	Q	46	0	0	0	0
39	R	13	0	0	0	0
39	S	30	0	0	0	0
39	T	51	0	0	0	0
39	U	25	0	0	0	0
39	V	19	0	0	0	0
39	W	63	0	0	1	0
39	X	47	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	Y	25	0	0	0	0
39	Z	2	0	0	0	0
39	a	30	0	0	2	0
39	b	12	0	0	0	0
39	c	6	0	0	1	0
39	d	26	0	0	0	0
39	e	13	0	0	1	0
39	g	16	0	0	0	0
39	n	10	0	0	0	0
All	All	77936	0	57988	651	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 5.

All (651) 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)
24:J:54:ARG:O	24:J:58:ARG:HG3	1.65	0.95
26:N:73:ARG:HD2	39:N:201:HOH:O	1.67	0.95
2:2:925:G:H1	2:2:1017:U:H3	1.18	0.88
2:2:928:G:H1	2:2:1013:U:H3	1.21	0.86
39:2:4896:HOH:O	14:S:28[B]:PHE:HE1	1.60	0.85
33:f:126:CYS:HB3	33:f:130:VAL:HG21	1.60	0.81
11:P:86:LEU:H	11:P:89:MET:HE3	1.51	0.76
2:2:730:C:H2'	2:2:731:G:H4'	1.67	0.74
2:2:417:C:H3'	39:2:2481:HOH:O	1.88	0.74
2:2:1868:U:O2'	19:a:100:ARG:NH1	2.20	0.74
2:2:913:A:N6	7:H:98:ARG:O	2.23	0.71
2:2:678:U:OP1	26:N:127:ARG:NH2	2.24	0.71
39:2:4896:HOH:O	14:S:28[B]:PHE:CE1	2.37	0.70
17:V:41:LYS:H	17:V:41:LYS:HD2	1.56	0.69
2:2:1719:A:N6	2:2:1814:G:O2'	2.25	0.69
2:2:616:A:H1'	32:e:12:VAL:HG13	1.74	0.68
2:2:1228:A:H2'	2:2:1229:G:C8	2.29	0.68
13:R:28:PHE:HA	13:R:55:THR:HG21	1.75	0.68
2:2:1381:G:N7	39:2:2127:HOH:O	2.28	0.67
3:B:47:THR:OG1	3:B:65:ARG:NH1	2.28	0.66
2:2:1373:C:O2'	13:R:10:LYS:NZ	2.28	0.66
4:D:170:THR:HG23	4:D:187:LYS:HG3	1.76	0.66
34:g:174:VAL:HB	34:g:188:HIS:HB2	1.78	0.66
7:H:121:THR:HG22	7:H:124:ALA:H	1.60	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:57:LEU:HD11	11:P:89:MET:HE2	1.78	0.65
2:2:65:C:H4'	23:G:172:LYS:HD3	1.78	0.65
2:2:1751:C:H42	2:2:1782:G:H21	1.45	0.65
2:2:405:G:N7	39:2:2129:HOH:O	2.28	0.65
4:D:194:PRO:O	4:D:201:LYS:NZ	2.29	0.65
2:2:319:C:O2	2:2:332:G:N2	2.23	0.65
2:2:1473:G:N7	39:2:2140:HOH:O	2.30	0.65
2:2:1037:G:N7	39:2:2141:HOH:O	2.30	0.64
7:H:71:SER:HA	7:H:74:LYS:HE2	1.78	0.64
2:2:76:U:O2'	23:G:159:ARG:NH1	2.31	0.64
2:2:650:A:N6	39:2:2139:HOH:O	2.30	0.64
2:2:1307:U:O2'	33:f:135:HIS:ND1	2.21	0.64
16:U:56:MET:HG3	16:U:86:LYS:HE3	1.79	0.64
2:2:736:C:H2'	2:2:737:G:C8	2.33	0.63
2:2:1277:C:H5''	9:K:55:ARG:HD2	1.79	0.63
32:e:50:GLY:O	32:e:53:LYS:NZ	2.31	0.63
11:P:17:TYR:O	11:P:19:GLY:N	2.31	0.63
2:2:981:A:H2'	2:2:982:G:C8	2.34	0.63
2:2:1754:G:N2	2:2:1779:G:O2'	2.31	0.62
2:2:1639:7MG:H2'	2:2:1640:A:C8	2.35	0.62
9:K:15:LEU:HD22	9:K:49:MET:HE1	1.80	0.62
2:2:1091:C:HO2'	28:W:2:VAL:N	1.98	0.62
16:U:49:LYS:HE2	16:U:92:HIS:CD2	2.35	0.62
2:2:605:A:OP1	24:J:22:LYS:NZ	2.34	0.61
7:H:162:GLN:OE1	7:H:165:ASN:ND2	2.30	0.61
16:U:116:ILE:HG22	16:U:118:ASP:H	1.64	0.61
3:B:26:SER:O	3:B:51:ARG:NH2	2.33	0.60
34:g:11:LEU:HB2	34:g:307:VAL:HB	1.84	0.60
34:g:10:THR:HG22	34:g:308:ARG:HG2	1.84	0.60
7:H:51:ILE:HG21	7:H:179:LYS:HG2	1.82	0.60
17:V:66:ASP:OD1	35:A:160:ALA:N	2.32	0.60
3:B:57:ILE:HB	3:B:60:ASP:HB2	1.83	0.60
2:2:921:G:H5'	31:b:21:LYS:HE3	1.83	0.60
28:W:80:ASP:OD1	28:W:124:LYS:NZ	2.33	0.60
2:2:697:G:OP2	2:2:733:C:N4	2.35	0.60
20:c:13:ARG:NH1	20:c:53:GLY:O	2.35	0.60
22:C:105:GLU:HB2	22:C:216:MET:HE1	1.84	0.60
24:J:124:HIS:ND1	32:e:31:ARG:HD2	2.17	0.59
35:A:81:ASN:HA	35:A:84:GLN:HE21	1.68	0.59
2:2:70:G:OP2	23:G:167:LYS:NZ	2.35	0.59
30:Z:68:ILE:HB	30:Z:109:TYR:HB2	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:3:LYS:NZ	19:a:8:ASN:OD1	2.27	0.59
20:c:29:GLN:NE2	20:c:66:ARG:O	2.34	0.59
7:H:159:ASP:N	7:H:159:ASP:OD1	2.34	0.58
26:N:40:LEU:HB3	26:N:45:LEU:HD12	1.85	0.58
7:H:53:VAL:HG12	7:H:175:GLY:HA3	1.83	0.58
1:n:2:ARG:HH22	2:2:1842:4AC:HM72	1.69	0.58
2:2:943:U:O2'	27:O:135:ILE:O	2.20	0.58
39:2:2610:HOH:O	8:I:19:LYS:HD2	2.03	0.58
2:2:77:A:H1'	23:G:176:ILE:HG13	1.85	0.58
2:2:386:C:H2'	2:2:387:C:C6	2.39	0.57
13:R:51:ALA:O	13:R:55:THR:HG23	2.03	0.57
35:A:10:MET:HE2	35:A:55:TRP:HB2	1.87	0.57
2:2:1868:U:HO2'	19:a:100:ARG:HH12	1.52	0.57
6:F:45:TYR:OH	6:F:65:GLN:OE1	2.22	0.57
2:2:68:A:OP2	23:G:164:LYS:NZ	2.37	0.57
2:2:689:U:OP1	7:H:103:LYS:NZ	2.35	0.57
2:2:1603:G:H5''	14:S:28[B]:PHE:CE1	2.39	0.57
25:M:55:ASN:HD21	25:M:82:ASN:H	1.51	0.57
2:2:1723:G:H2'	2:2:1724:A:C8	2.39	0.57
13:R:77:GLU:HA	13:R:80:ARG:HG2	1.87	0.56
34:g:256:ILE:HD13	34:g:289:LEU:HD21	1.87	0.56
2:2:1088:U:H4'	2:2:1089:G:OP2	2.04	0.56
4:D:192:TRP:NE1	4:D:201:LYS:O	2.27	0.56
25:M:64:LEU:HA	33:f:108:VAL:HG21	1.87	0.56
35:A:128:ARG:NH2	35:A:151:ASP:O	2.38	0.56
2:2:913:A:OP1	7:H:99:ARG:NE	2.32	0.56
2:2:1630:A:H5''	14:S:37:GLY:H	1.70	0.56
4:D:135:GLU:HG3	4:D:153:VAL:HG12	1.86	0.56
25:M:81:ASP:HB3	25:M:84:LYS:HB2	1.87	0.56
2:2:1748:G:H1	2:2:1786:U:H3	1.52	0.56
34:g:18:VAL:O	34:g:287:THR:OG1	2.20	0.56
13:R:27:ASP:OD2	13:R:30:THR:OG1	2.24	0.56
3:B:33:VAL:HG12	3:B:44:ILE:HD12	1.88	0.56
2:2:640:A:H2'	2:2:641:A:C8	2.40	0.55
2:2:617:G:O5'	18:X:88:ASP:HA	2.06	0.55
3:B:37:ALA:N	3:B:231:LEU:O	2.39	0.55
34:g:104:HIS:NE2	34:g:122:SER:OG	2.30	0.55
2:2:1536:G:H2'	2:2:1537:A:C8	2.42	0.55
14:S:33:ILE:HD13	14:S:71:MET:HE1	1.88	0.55
2:2:1190:A:N3	2:2:1714:U:O2'	2.37	0.55
31:b:36:LYS:HE3	31:b:40:CYS:O	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:140:C:H42	2:2:313:A:H61	1.55	0.55
2:2:1705:C:H2'	2:2:1706:G:C8	2.41	0.55
19:a:10:ARG:NH1	39:a:302:HOH:O	2.39	0.55
23:G:57:ASP:OD1	23:G:58:LYS:N	2.39	0.55
7:H:140:VAL:HG12	26:N:19:ARG:HD2	1.89	0.55
16:U:49:LYS:HB3	16:U:92:HIS:HD2	1.71	0.55
24:J:54:ARG:O	24:J:58:ARG:CG	2.47	0.55
2:2:693:A:N6	2:2:737:G:N7	2.55	0.55
2:2:1288:OMU:OP2	33:f:97:LYS:NZ	2.38	0.55
2:2:1101:U:H2'	2:2:1102:G:C8	2.42	0.54
2:2:1550:G:H3'	2:2:1579:A:H61	1.72	0.54
35:A:196:GLU:CD	35:A:196:GLU:H	2.14	0.54
9:K:80:ARG:NH1	9:K:89:ILE:O	2.40	0.54
16:U:94:PRO:HD2	16:U:97:ILE:HD11	1.89	0.54
19:a:59:PHE:HB2	19:a:62:TYR:HB2	1.88	0.54
25:M:79:VAL:HG21	25:M:85:LEU:HD13	1.89	0.54
2:2:857:U:H2'	2:2:858:A:C8	2.41	0.54
2:2:1723:G:N2	2:2:1812:U:O2	2.40	0.54
3:B:179:ASN:OD1	3:B:187:LYS:NZ	2.41	0.54
33:f:144:CYS:SG	33:f:146:LEU:HB2	2.48	0.54
7:H:163:GLN:HG2	7:H:167:GLU:HG3	1.90	0.54
2:2:56:G:OP1	29:Y:111:LYS:NZ	2.40	0.53
2:2:641:A:O2'	2:2:645:C:OP1	2.26	0.53
2:2:1098:C:H2'	2:2:1099:G:C8	2.43	0.53
2:2:145:G:O6	23:G:178:ARG:NH2	2.40	0.53
2:2:874:G:H2'	2:2:875:A:H8	1.73	0.53
17:V:14:PRO:HG2	17:V:23:ILE:HD12	1.91	0.53
22:C:125:LYS:HG2	22:C:143:CYS:HB2	1.90	0.53
35:A:77:ILE:HG12	35:A:99:ILE:HB	1.89	0.53
35:A:80:ARG:NH2	39:A:304:HOH:O	2.41	0.53
12:Q:89:SER:HB3	12:Q:112:LEU:HD13	1.91	0.53
13:R:21:TYR:CE1	13:R:58:MET:HE1	2.44	0.53
35:A:81:ASN:HA	35:A:84:GLN:HG3	1.89	0.53
2:2:60:A:N3	2:2:316:G:O2'	2.37	0.53
8:I:128:LYS:H	8:I:128:LYS:HD2	1.74	0.53
30:Z:60:LYS:O	30:Z:64:ASN:ND2	2.41	0.53
2:2:996:A:H2'	2:2:997:A:C8	2.44	0.52
15:T:108:GLU:OE2	15:T:121:ARG:NE	2.42	0.52
2:2:1752:C:N4	2:2:1754:G:O6	2.42	0.52
29:Y:76:TYR:OH	29:Y:86:GLU:OE2	2.25	0.52
2:2:1714:U:H2'	2:2:1715:A:C8	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:C:94:ILE:HG21	22:C:162:ILE:HD12	1.90	0.52
2:2:1058:A:H2'	2:2:1059:G:C8	2.44	0.52
2:2:1521:C:OP1	14:S:129:LEU:HD13	2.08	0.52
19:a:21:ILE:HD13	19:a:72:HIS:HB3	1.91	0.52
26:N:4:MET:HE2	26:N:124:ARG:NH2	2.25	0.52
16:U:19:ARG:HD2	16:U:92:HIS:CE1	2.45	0.52
2:2:463:C:O2'	2:2:466:G:O6	2.25	0.52
2:2:1759:G:N2	2:2:1760:G:O6	2.42	0.52
18:X:41:PHE:O	18:X:76:LYS:NZ	2.40	0.52
20:c:32:VAL:HG11	20:c:56:LEU:HD12	1.91	0.52
23:G:59:GLN:OE1	23:G:72:ARG:NH1	2.37	0.52
2:2:367:U:H4'	2:2:371:A:C8	2.45	0.52
35:A:13:GLU:HG3	35:A:17:LYS:HZ1	1.75	0.52
2:2:683:OMG:N1	2:2:1022:U:OP2	2.36	0.52
2:2:1499:U:H4'	4:D:176:LEU:HD13	1.91	0.52
3:B:168:MET:HG2	3:B:197:ILE:HG21	1.92	0.52
4:D:120:TYR:O	4:D:124:ARG:HG2	2.10	0.52
23:G:52:ILE:HD13	23:G:102:VAL:HG21	1.92	0.52
23:G:137:ARG:HB3	23:G:140:ARG:HG3	1.92	0.52
30:Z:72:VAL:HG13	30:Z:76:ARG:HH22	1.75	0.52
2:2:67:C:C5	23:G:162:LEU:HB3	2.46	0.51
2:2:656:G:H5'	2:2:662:G:N2	2.25	0.51
2:2:1037:G:H4'	2:2:1845:A:H4'	1.92	0.51
2:2:160:U:O2'	2:2:162:C:OP2	2.29	0.51
26:N:38:TYR:CZ	26:N:78:LYS:HG3	2.46	0.51
34:g:107:ASP:OD2	34:g:125:ARG:NH1	2.42	0.51
8:I:57:ALA:HB2	8:I:183:GLY:HA2	1.92	0.51
12:Q:62:ARG:NH2	12:Q:107:GLU:OE2	2.42	0.51
24:J:32:ILE:HD11	24:J:40:LYS:HD3	1.93	0.51
7:H:10:LYS:HD3	7:H:20:GLU:HG3	1.92	0.51
2:2:535:G:O2'	2:2:536:A:N7	2.43	0.51
12:Q:53:GLU:OE1	12:Q:85:ARG:NH2	2.33	0.51
11:P:62:LYS:NZ	11:P:66:GLU:OE1	2.38	0.51
2:2:1174:PSU:H2'	2:2:1175:G:C8	2.45	0.51
2:2:1406:G:H2'	2:2:1407:U:C6	2.45	0.51
2:2:821:G:N7	39:2:2174:HOH:O	2.35	0.51
17:V:61:ARG:NH1	35:A:156:TYR:OH	2.43	0.51
7:H:20:GLU:HA	7:H:23:ILE:HD12	1.92	0.50
24:J:93:LYS:HD3	24:J:96:TYR:HE2	1.76	0.50
32:e:12:VAL:HA	32:e:15:GLN:HB2	1.93	0.50
34:g:57:ARG:HD3	34:g:95:GLY:HA3	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:29:ASP:OD1	3:B:51:ARG:NH1	2.44	0.50
2:2:952:G:OP1	3:B:56:LYS:NZ	2.42	0.50
2:2:587:A:H5'	2:2:592:C:H41	1.76	0.50
34:g:191:HIS:CG	34:g:195:LEU:HD21	2.46	0.50
2:2:545:A:H2'	2:2:546:G:C8	2.46	0.50
2:2:1588:A:H2'	2:2:1589:A:C8	2.47	0.50
2:2:531:A:H2'	2:2:532:C:C6	2.46	0.50
2:2:1520:G:N3	2:2:1520:G:H2'	2.25	0.50
3:B:179:ASN:ND2	3:B:183:GLU:OE2	2.44	0.50
9:K:15:LEU:HD23	9:K:79:LEU:HD11	1.94	0.50
19:a:94:ASP:OD1	19:a:96:THR:HG22	2.12	0.50
23:G:14:LYS:HD2	23:G:16:ILE:HG12	1.94	0.50
2:2:385:G:H3'	10:L:136:LYS:HB2	1.94	0.50
2:2:1217:A:H2'	2:2:1218:C:C6	2.47	0.50
22:C:110:MET:HE1	39:C:345:HOH:O	2.11	0.50
2:2:562:U:H2'	2:2:563:G:C8	2.47	0.50
34:g:214:GLY:HA2	34:g:236:ILE:HG13	1.93	0.50
34:g:220:ASP:OD2	34:g:223:GLU:N	2.31	0.50
35:A:134:LEU:HD22	35:A:144:THR:HG21	1.94	0.50
8:I:139:LYS:NZ	8:I:140:LYS:O	2.44	0.50
22:C:187:ARG:NH1	22:C:187:ARG:HB3	2.27	0.50
2:2:528:A:H2'	2:2:529:A:H8	1.77	0.49
2:2:1723:G:H2'	2:2:1724:A:H8	1.77	0.49
4:D:132:LYS:HG3	4:D:191:PRO:HA	1.94	0.49
7:H:30:LEU:HD13	7:H:82:GLU:HB3	1.94	0.49
2:2:115:U:H2'	2:2:116:OMU:C6	2.42	0.49
12:Q:113:ILE:HG12	12:Q:120:LEU:HD12	1.94	0.49
34:g:42:MET:HE2	34:g:57:ARG:HB3	1.94	0.49
2:2:15:U:H2'	2:2:16:G:O4'	2.13	0.49
2:2:913:A:N7	7:H:99:ARG:HB2	2.27	0.49
2:2:1745:A:H4'	23:G:31:ARG:HH22	1.76	0.49
34:g:5:MET:HB2	34:g:270:LEU:HD21	1.93	0.49
2:2:940:U:H2'	2:2:941:C:C6	2.47	0.49
2:2:1214:A:H2'	2:2:1217:A:N7	2.28	0.49
16:U:19:ARG:HD2	16:U:92:HIS:HE1	1.77	0.49
22:C:108:LYS:HD3	22:C:110:MET:HB2	1.93	0.49
2:2:107:A:H2'	2:2:108:G:C8	2.48	0.49
3:B:29:ASP:OD2	3:B:51:ARG:HG2	2.12	0.49
24:J:84:ILE:HG13	24:J:86:VAL:HG13	1.94	0.49
2:2:1453:C:O2'	13:R:52:GLY:HA3	2.12	0.49
4:D:142:LEU:HD12	4:D:148:LYS:HG3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:d:3:HIS:CE1	21:d:5:GLN:HB2	2.47	0.49
28:W:83:LEU:HD11	28:W:120:HIS:HA	1.94	0.49
17:V:41:LYS:HD2	17:V:41:LYS:N	2.27	0.49
2:2:379:C:H5'	8:I:33:ALA:HA	1.94	0.49
4:D:195:THR:OG1	4:D:197:LYS:HG3	2.12	0.49
13:R:99:ASP:CG	35:A:42:LYS:HD3	2.38	0.49
25:M:92:CYS:HB2	25:M:103:VAL:HG22	1.95	0.49
2:2:528:A:H2'	2:2:529:A:C8	2.48	0.49
2:2:942:G:H2'	2:2:943:U:C6	2.48	0.49
2:2:1201:U:H2'	2:2:1202:U:C6	2.48	0.49
2:2:1845:A:H2'	2:2:1846:G:C8	2.48	0.49
22:C:60:TRP:CD1	22:C:92:GLU:HG2	2.48	0.49
22:C:227[B]:ARG:NH1	39:C:302:HOH:O	2.46	0.49
2:2:1203:G:H2'	2:2:1204:A:C8	2.48	0.48
6:F:22:LYS:HB3	6:F:22:LYS:HE2	1.51	0.48
33:f:137:ASP:OD1	33:f:137:ASP:N	2.46	0.48
5:E:238:LEU:HB2	5:E:242:LYS:HD2	1.94	0.48
25:M:31:LEU:HD11	25:M:89:VAL:HG23	1.93	0.48
27:O:34:PHE:HB3	27:O:41:PHE:HB2	1.95	0.48
2:2:436:OMG:HM22	2:2:437:G:H5'	1.94	0.48
2:2:1113:A:H2'	2:2:1114:U:C6	2.48	0.48
2:2:1811:C:H2'	2:2:1812:U:C6	2.48	0.48
2:2:102:A:H4'	2:2:104:A:C8	2.47	0.48
2:2:319:C:H2'	2:2:320:G:O4'	2.13	0.48
2:2:382:C:H2'	2:2:383:G:H8	1.79	0.48
34:g:142:VAL:HG12	34:g:146:SER:HB2	1.95	0.48
2:2:303:C:H5''	8:I:75:LYS:HE3	1.94	0.48
2:2:953:C:H2'	2:2:954:U:O4'	2.13	0.48
2:2:1531:A:H2'	2:2:1532:C:C6	2.48	0.48
2:2:1628:C:H2'	2:2:1629:C:C6	2.48	0.48
2:2:1865:C:O2	19:a:92:ARG:HB3	2.13	0.48
13:R:31:ASN:OD1	13:R:55:THR:HG22	2.12	0.48
34:g:163:PRO:HB2	34:g:179:LEU:HB2	1.96	0.48
2:2:65:C:C2	23:G:133:LEU:HD22	2.48	0.48
2:2:1220:A:H2'	2:2:1221:G:O4'	2.14	0.48
2:2:952:G:H2'	2:2:953:C:C6	2.48	0.48
2:2:1052:A:H2'	2:2:1053:C:O4'	2.14	0.48
24:J:93:LYS:HD3	24:J:96:TYR:CE2	2.49	0.48
2:2:804:U:H2'	2:2:805:U:C6	2.49	0.47
2:2:1667:U:H2'	2:2:1668:U:C6	2.48	0.47
2:2:1797:U:H2'	2:2:1798:C:C6	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:455:A:O2'	2:2:1735:A:N3	2.41	0.47
11:P:17:TYR:HB2	11:P:25:LEU:HD11	1.96	0.47
2:2:433:A:H5''	8:I:22:HIS:HB3	1.96	0.47
3:B:179:ASN:HB3	3:B:183:GLU:HB3	1.96	0.47
3:B:219:LYS:HB3	3:B:219:LYS:HE3	1.60	0.47
2:2:416:U:H2'	2:2:417:C:O4'	2.13	0.47
17:V:42:VAL:HG23	17:V:43:THR:HG23	1.96	0.47
23:G:31:ARG:HH21	23:G:68:LEU:HD21	1.79	0.47
30:Z:99:LEU:HD11	30:Z:102:LYS:HB2	1.96	0.47
2:2:461:U:H2'	2:2:462:OMC:C6	2.50	0.47
2:2:29:G:H2'	2:2:30:C:C6	2.49	0.47
2:2:1330:G:H4'	2:2:1331:C:H3'	1.97	0.47
2:2:1374:C:H2'	2:2:1375:G:O4'	2.14	0.47
4:D:23:GLU:OE1	4:D:27:ARG:NE	2.48	0.47
4:D:158:ILE:HG12	4:D:189:MET:SD	2.54	0.47
6:F:167:LYS:NZ	6:F:175:ASP:OD2	2.33	0.47
17:V:32:ILE:HG12	17:V:60:ARG:HD2	1.96	0.47
2:2:321:C:H2'	2:2:322:C:C6	2.49	0.47
2:2:420:G:H1'	2:2:661:U:O2	2.15	0.47
2:2:874:G:H2'	2:2:875:A:C8	2.50	0.47
2:2:1232:PSU:H2'	2:2:1233:G:C8	2.50	0.47
2:2:1643:PSU:H2'	2:2:1644:C:C6	2.49	0.47
2:2:1672:U:OP1	12:Q:18:THR:OG1	2.24	0.47
2:2:1720:U:P	2:2:1721:U:H5''	2.55	0.47
3:B:30:TRP:HB3	3:B:46:LYS:HE2	1.95	0.47
6:F:22:LYS:NZ	6:F:98:GLU:OE2	2.38	0.47
6:F:141:VAL:HG22	6:F:146:ARG:HG3	1.97	0.47
19:a:39:PHE:CE2	19:a:41:ILE:HD11	2.49	0.47
2:2:573:U:O2	2:2:576:A2M:H8	2.15	0.47
2:2:1863:A:H1'	19:a:79:ILE:HD13	1.96	0.47
9:K:71:LEU:HD11	9:K:79:LEU:HD12	1.96	0.47
34:g:217:MET:HG2	34:g:229:THR:HG23	1.96	0.47
2:2:59:U:H5''	2:2:503:C:N4	2.29	0.47
2:2:1828:C:H2'	2:2:1829:G:O4'	2.14	0.47
13:R:110:ASP:N	13:R:110:ASP:OD1	2.47	0.47
14:S:78:LYS:HE2	14:S:78:LYS:HB2	1.79	0.47
13:R:116:ASN:OD1	13:R:116:ASN:N	2.47	0.47
29:Y:25:ILE:HD11	29:Y:73:GLY:HA3	1.97	0.47
2:2:317:C:OP2	23:G:183:ARG:NH1	2.45	0.46
22:C:272:HIS:HA	22:C:275:LYS:HD3	1.97	0.46
2:2:929:G:H2'	2:2:930:C:O4'	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1597:C:H4'	2:2:1603:G:C6	2.50	0.46
26:N:100:LYS:HE2	26:N:104:ARG:HH12	1.80	0.46
34:g:5:MET:HE3	34:g:312:VAL:HB	1.96	0.46
2:2:674:C:H2'	2:2:675:U:C6	2.50	0.46
2:2:1439:A:H2'	2:2:1440:C:O4'	2.15	0.46
2:2:1536:G:H2'	2:2:1537:A:H8	1.79	0.46
8:I:37:LYS:NZ	8:I:95:THR:OG1	2.48	0.46
24:J:60:LEU:O	24:J:70:ARG:HD2	2.15	0.46
35:A:6:ASP:HA	35:A:9:GLN:HG2	1.96	0.46
2:2:294:U:OP1	10:L:36:TYR:OH	2.33	0.46
2:2:1255:G:OP1	2:2:1256:G:O2'	2.28	0.46
2:2:1511:U:H2'	2:2:1512:C:C6	2.51	0.46
24:J:55:LYS:HB2	24:J:55:LYS:HE2	1.62	0.46
30:Z:73:VAL:HG21	30:Z:88:LEU:HD21	1.97	0.46
35:A:184:ARG:HD2	35:A:191:ARG:HG2	1.97	0.46
22:C:191:VAL:HG11	22:C:236:PHE:HA	1.98	0.46
8:I:110:ARG:HG3	8:I:110:ARG:HH11	1.81	0.46
2:2:1016:U:H5''	26:N:14:SER:HB3	1.98	0.46
2:2:1035:A:H2'	2:2:1036:A:O4'	2.16	0.46
3:B:25:PHE:CD2	27:O:88:LEU:HD21	2.51	0.46
5:E:20:LEU:HD21	5:E:46:ILE:HD12	1.98	0.46
21:d:3:HIS:HE1	21:d:5:GLN:HB2	1.80	0.46
30:Z:57:LYS:HD3	30:Z:77:LEU:HD22	1.96	0.46
34:g:46:THR:HB	34:g:48:ASP:OD1	2.16	0.46
2:2:334:C:H41	23:G:190:ARG:HD3	1.80	0.46
2:2:495:U:H2'	2:2:496:C:O4'	2.16	0.46
2:2:574:A:H5''	29:Y:89:HIS:CD2	2.50	0.46
2:2:847:A:OP1	5:E:108:ARG:NH1	2.48	0.46
16:U:46:LYS:HE2	16:U:48:LEU:HD11	1.97	0.46
2:2:116:OMU:H6	2:2:116:OMU:O5'	2.16	0.46
2:2:667:U:H5''	2:2:1087:A:C5	2.51	0.46
24:J:111:GLN:NE2	24:J:127:ARG:HB2	2.31	0.46
2:2:550:C:H2'	2:2:551:U:C6	2.51	0.46
5:E:44:LEU:HD13	5:E:72:ILE:HD11	1.98	0.46
28:W:14:ILE:HG13	28:W:27:ILE:HD11	1.97	0.46
30:Z:103:HIS:HD1	30:Z:105:ALA:H	1.62	0.46
2:2:116:OMU:HM23	2:2:116:OMU:H1'	1.73	0.45
2:2:1406:G:H2'	2:2:1407:U:H6	1.81	0.45
18:X:41:PHE:CZ	18:X:102:VAL:HG23	2.51	0.45
18:X:52:LEU:HD11	18:X:73:GLN:HB2	1.97	0.45
24:J:164:PRO:HB3	24:J:170:PRO:HA	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:581:U:H4'	29:Y:66:GLY:HA2	1.98	0.45
2:2:1841:C:C4	2:2:1842:4AC:HM73	2.51	0.45
23:G:20:ASP:HB3	23:G:23:LYS:HG3	1.99	0.45
31:b:14:GLU:OE1	31:b:18:LYS:NZ	2.37	0.45
2:2:928:G:H2'	2:2:929:G:C8	2.50	0.45
2:2:1277:C:H2'	2:2:1278:A:H8	1.80	0.45
2:2:1407:U:H2'	2:2:1408:U:C6	2.52	0.45
6:F:188:TYR:CZ	6:F:192:LYS:HE2	2.52	0.45
17:V:74:LYS:HG2	17:V:79:VAL:HB	1.99	0.45
20:c:12:ALA:HB1	20:c:32:VAL:HB	1.97	0.45
29:Y:7:ILE:HG22	29:Y:27:VAL:HG13	1.99	0.45
7:H:76:GLN:O	7:H:80:VAL:HG23	2.17	0.45
22:C:234:GLY:O	22:C:238:LYS:HG3	2.15	0.45
2:2:461:U:H2'	2:2:462:OMC:H6	1.80	0.45
2:2:494:C:N4	2:2:509:OMG:HN22	2.15	0.45
2:2:1030:A:H2'	2:2:1031:A2M:H8	1.98	0.45
14:S:15:VAL:HG22	14:S:68:ILE:HD11	1.99	0.45
19:a:58:VAL:HG21	27:O:28:PHE:HZ	1.82	0.45
30:Z:81:GLY:HA2	30:Z:84:ALA:HB3	1.99	0.45
15:T:140:ALA:HA	15:T:143:LYS:HE3	1.98	0.45
22:C:227[A]:ARG:HD3	39:C:347:HOH:O	2.17	0.45
23:G:49:VAL:HB	23:G:115:LYS:HB2	1.98	0.45
35:A:77:ILE:HD12	35:A:122:LEU:HD11	1.97	0.45
2:2:536:A:H3'	2:2:537:C:H5''	1.99	0.45
2:2:733:C:H3'	2:2:734:C:O4'	2.16	0.45
20:c:20:ARG:NH1	39:c:102:HOH:O	2.46	0.45
28:W:30:CYS:SG	28:W:31:SER:N	2.90	0.45
34:g:149:GLU:HG2	34:g:171:ASP:HB3	1.99	0.45
2:2:1368:U:O2'	2:2:1370:A:N7	2.41	0.45
2:2:615:C:OP2	18:X:64:SER:OG	2.28	0.45
7:H:41:ARG:HG3	7:H:42:GLU:H	1.82	0.45
23:G:2:LYS:HB3	23:G:15:LEU:HD11	1.99	0.45
27:O:83:GLN:O	27:O:87:GLU:HG3	2.17	0.45
34:g:191:HIS:CD2	34:g:195:LEU:HD11	2.52	0.45
2:2:1139:C:H2'	2:2:1140:G:O4'	2.16	0.45
7:H:85:LYS:HB2	7:H:85:LYS:HE3	1.74	0.45
34:g:212:LYS:HZ2	34:g:235:ILE:HD11	1.81	0.45
2:2:145:G:H2'	2:2:146:G:C8	2.52	0.44
2:2:320:G:H2'	2:2:321:C:C6	2.52	0.44
20:c:37:ASP:OD1	20:c:37:ASP:N	2.50	0.44
2:2:563:G:O2'	2:2:564:A:H5''	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1253:A:OP1	39:2:2101:HOH:O	2.21	0.44
6:F:34:SER:HA	20:c:55:VAL:HB	1.98	0.44
22:C:69:LEU:HD21	22:C:273:LEU:HG	1.98	0.44
27:O:95:ILE:HB	27:O:129:ILE:HG12	1.99	0.44
35:A:121[B]:LEU:HD11	35:A:145:ILE:HD12	1.98	0.44
2:2:5:U:H2'	2:2:6:G:H8	1.82	0.44
2:2:1277:C:H2'	2:2:1278:A:C8	2.52	0.44
2:2:1784:G:H2'	2:2:1785:C:C6	2.52	0.44
2:2:1798:C:H2'	2:2:1799:G:O4'	2.17	0.44
4:D:197:LYS:HE2	4:D:197:LYS:HB2	1.70	0.44
6:F:128:ILE:HD12	6:F:137:GLN:HG2	2.00	0.44
2:2:77:A:C8	23:G:154:ARG:HG2	2.52	0.44
2:2:551:U:H2'	2:2:552:G:C8	2.53	0.44
2:2:606:G:H1'	32:e:58:ASN:OD1	2.17	0.44
16:U:54:VAL:HB	16:U:88:LEU:HB2	1.98	0.44
10:L:88:ILE:HD11	10:L:109:MET:HE2	1.99	0.44
12:Q:86:GLN:HE22	12:Q:122:ALA:HA	1.83	0.44
17:V:45:ARG:HD2	35:A:187:GLY:HA2	2.00	0.44
2:2:484:A2M:H8	2:2:484:A2M:O5'	2.16	0.44
2:2:639:C:H2'	2:2:640:A:C8	2.53	0.44
4:D:16:ILE:HD11	21:d:36:LEU:HD23	1.98	0.44
4:D:172:VAL:HG22	4:D:185:LYS:HG2	1.99	0.44
11:P:60:LEU:HD22	11:P:92:SER:HB3	1.99	0.44
21:d:13:LYS:HE2	21:d:13:LYS:HB2	1.68	0.44
23:G:44:GLU:H	23:G:44:GLU:CD	2.25	0.44
2:2:1375:G:H5'	13:R:67:ARG:HH21	1.83	0.44
10:L:4:ILE:HD12	10:L:56:ILE:HG12	1.99	0.44
15:T:56:ARG:HG3	15:T:103:VAL:HG21	1.99	0.44
20:c:34:PHE:HE2	20:c:61:SER:HB3	1.83	0.44
34:g:89:LEU:HB2	34:g:101:PHE:HE1	1.83	0.44
35:A:13:GLU:HG3	35:A:17:LYS:NZ	2.32	0.44
35:A:52:LYS:HE2	35:A:56:GLU:HG2	1.99	0.44
2:2:1382:A:H2'	2:2:1383:A2M:H8	1.99	0.44
23:G:213:LEU:O	23:G:217:MET:HG2	2.17	0.44
25:M:82:ASN:OD1	25:M:83:LYS:N	2.51	0.44
26:N:54:LEU:HB3	26:N:60:VAL:HB	2.00	0.44
35:A:198:MET:HG2	35:A:200:ASP:H	1.81	0.44
2:2:570:C:O2'	29:Y:34:THR:O	2.28	0.44
6:F:40:ALA:HB1	6:F:45:TYR:CG	2.52	0.44
35:A:73:ASP:HB3	35:A:120:ARG:HB2	2.00	0.44
2:2:1748:G:O6	2:2:1786:U:O4	2.35	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Q:44:PRO:HB2	12:Q:46:THR:HG22	2.00	0.43
2:2:945:U:H2'	2:2:946:U:C6	2.53	0.43
2:2:1550:G:O2'	2:2:1558:C:O2	2.34	0.43
10:L:124:ASP:OD2	10:L:147:LYS:NZ	2.40	0.43
17:V:3:ASN:C	17:V:5:ALA:H	2.26	0.43
2:2:912:C:C2	2:2:914:U:H1'	2.53	0.43
2:2:1398:G:H1'	34:g:63:SER:HB3	1.99	0.43
3:B:123:ALA:HB2	3:B:165:ARG:HG3	2.00	0.43
3:B:125:VAL:HG12	3:B:172:MET:HE3	2.00	0.43
11:P:18:ARG:H	11:P:18:ARG:HG2	1.59	0.43
13:R:34:VAL:O	13:R:38:ILE:HG13	2.18	0.43
26:N:110:ASP:O	26:N:114:ARG:HG2	2.18	0.43
33:f:107:LYS:HA	33:f:107:LYS:HD2	1.78	0.43
2:2:980:A:H2'	2:2:981:A:C8	2.53	0.43
11:P:52:LYS:HE3	11:P:52:LYS:HB2	1.58	0.43
2:2:320:G:H2'	2:2:321:C:H6	1.83	0.43
2:2:1356:G:H2'	2:2:1357:A:C8	2.53	0.43
10:L:49:GLU:CD	10:L:49:GLU:H	2.25	0.43
11:P:18:ARG:HD3	14:S:90:VAL:HA	2.00	0.43
22:C:273:LEU:HA	22:C:273:LEU:HD23	1.89	0.43
32:e:13:ARG:NH1	39:e:102:HOH:O	2.44	0.43
34:g:201:SER:HB2	34:g:206:LEU:HB2	2.00	0.43
1:n:11:ARG:NH2	2:2:1184:G:OP1	2.50	0.43
2:2:51:U:H2'	2:2:52:G:C8	2.54	0.43
2:2:118:C:H1'	2:2:445:A:C5	2.53	0.43
2:2:1199:A:OP1	19:a:2:THR:N	2.51	0.43
2:2:1463:U:C6	39:2:2302:HOH:O	2.57	0.43
2:2:1472:C:O3'	34:g:15:ASN:ND2	2.32	0.43
14:S:21:ASP:OD2	14:S:24:ARG:HG3	2.18	0.43
16:U:46:LYS:HB2	16:U:48:LEU:HD11	2.01	0.43
34:g:101:PHE:CD2	34:g:136:GLY:HA2	2.54	0.43
1:n:2:ARG:HH22	2:2:1842:4AC:CM7	2.29	0.43
2:2:159:A2M:H2	2:2:468:A2M:O4'	2.17	0.43
2:2:1001:A:N3	39:2:2183:HOH:O	2.36	0.43
3:B:222:LYS:HE3	3:B:222:LYS:HB2	1.71	0.43
18:X:68:LYS:HB3	18:X:91:LEU:HD13	2.00	0.43
20:c:44:ARG:HD2	20:c:44:ARG:HA	1.83	0.43
23:G:164:LYS:HD3	23:G:167:LYS:HD2	2.01	0.43
17:V:23:ILE:HG21	22:C:249:SER:HA	2.00	0.43
22:C:60:TRP:O	22:C:71:LYS:NZ	2.45	0.43
23:G:79:LYS:HE2	23:G:79:LYS:HB3	1.77	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:695:C:H41	2:2:737:G:H1'	1.83	0.43
2:2:1174:PSU:H2'	2:2:1175:G:H8	1.83	0.43
2:2:1683:C:H2'	2:2:1684:C:H6	1.83	0.43
34:g:62:HIS:NE2	34:g:80:SER:OG	2.39	0.43
2:2:1097:G:H4'	35:A:32:PHE:CD1	2.54	0.43
3:B:82:ARG:NH1	3:B:189:ILE:O	2.52	0.43
14:S:20:ILE:HD11	14:S:33:ILE:HD11	2.00	0.43
22:C:60:TRP:CG	22:C:92:GLU:HG2	2.54	0.43
22:C:74:LYS:HA	22:C:74:LYS:HD3	1.74	0.43
26:N:104:ARG:H	26:N:104:ARG:HG2	1.65	0.43
29:Y:88:LYS:HA	29:Y:88:LYS:HD3	1.87	0.43
2:2:4:C:H4'	22:C:207:ALA:HB2	2.00	0.42
24:J:33:GLY:HA3	32:e:38:TYR:CG	2.54	0.42
2:2:1101:U:H2'	2:2:1102:G:H8	1.82	0.42
2:2:1285:G:H5'	25:M:35:ILE:HG22	2.01	0.42
39:2:4829:HOH:O	19:a:86:ASN:HB3	2.19	0.42
5:E:124:CYS:HB3	5:E:141:THR:HB	1.99	0.42
6:F:19:LEU:HD21	6:F:69:VAL:HG11	2.00	0.42
10:L:91:ASP:HB3	10:L:104:LYS:HE2	2.01	0.42
28:W:87:GLU:HG2	39:W:207:HOH:O	2.19	0.42
2:2:634:A:H2'	2:2:635:G:C8	2.53	0.42
2:2:829:C:OP1	5:E:21:ASP:HB2	2.19	0.42
2:2:912:C:H3'	2:2:913:A:H5''	2.01	0.42
2:2:1568:C:H2'	2:2:1569:A:C8	2.55	0.42
2:2:1712:A:H2'	2:2:1713:C:C6	2.54	0.42
4:D:98:ALA:N	4:D:169:ASP:OD2	2.45	0.42
11:P:45:LEU:HD21	11:P:84:ILE:HD11	2.00	0.42
22:C:183:LYS:HA	22:C:195:LEU:O	2.19	0.42
24:J:169:ARG:HA	24:J:170:PRO:HD2	1.87	0.42
25:M:112:LYS:HB2	25:M:112:LYS:HE3	1.71	0.42
27:O:75:MET:HG3	27:O:121:ARG:HH22	1.85	0.42
35:A:166:LYS:HB2	35:A:166:LYS:HE3	1.82	0.42
35:A:183:LEU:HD23	35:A:183:LEU:HA	1.82	0.42
2:2:558:G:H2'	2:2:559:G:C8	2.54	0.42
2:2:1616:U:H2'	2:2:1617:G:O4'	2.20	0.42
11:P:93:MET:HE3	11:P:93:MET:HB3	1.83	0.42
22:C:66:LEU:HD11	22:C:81:ILE:HG12	2.01	0.42
22:C:257:LYS:HB2	22:C:257:LYS:NZ	2.34	0.42
2:2:5:U:H2'	2:2:6:G:C8	2.55	0.42
2:2:1228:A:H2'	2:2:1229:G:H8	1.78	0.42
14:S:84:LEU:HD12	14:S:95:TYR:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:3:ASN:HD21	17:V:7:GLU:HB2	1.85	0.42
27:O:56:VAL:HG21	27:O:80:ASP:HB3	2.00	0.42
30:Z:74:SER:OG	30:Z:79:ILE:O	2.29	0.42
2:2:502:C:O4'	5:E:66:MET:HG3	2.20	0.42
2:2:575:A:H2'	2:2:576:A2M:O4'	2.19	0.42
5:E:11:ARG:HA	5:E:28:ALA:HB2	2.01	0.42
7:H:70:LYS:HD3	7:H:70:LYS:HA	1.89	0.42
34:g:178:ASN:ND2	34:g:180:ALA:O	2.53	0.42
2:2:27:A2M:H1'	2:2:27:A2M:HM'3	1.73	0.42
2:2:1046:PSU:H2'	2:2:1047:C:O4'	2.20	0.42
7:H:158:LEU:O	7:H:190:PRO:HD2	2.19	0.42
26:N:102:LEU:HD11	26:N:112:LYS:HA	2.01	0.42
35:A:76:VAL:HG12	35:A:123:VAL:HB	2.02	0.42
35:A:170:SER:O	35:A:174:MET:HG2	2.20	0.42
2:2:582:C:H2'	2:2:583:C:H5''	2.01	0.42
2:2:1644:C:H4'	12:Q:140:ARG:HB2	2.01	0.42
4:D:192:TRP:CH2	4:D:194:PRO:HG3	2.54	0.42
7:H:179:LYS:HD2	7:H:179:LYS:HA	1.88	0.42
25:M:61:TYR:O	25:M:65:VAL:HG12	2.20	0.42
34:g:219:TRP:CZ3	34:g:226:HIS:HB2	2.55	0.42
2:2:591:U:H5''	2:2:593:C:O4'	2.20	0.42
2:2:614:C:O2'	2:2:626[B]:G:N2	2.53	0.42
2:2:862:A:C8	28:W:107:SER:HA	2.54	0.42
2:2:1148:A:H4'	2:2:1149:A:O4'	2.20	0.42
2:2:1788:A:H2'	2:2:1789:G:O4'	2.19	0.42
13:R:21:TYR:CE1	13:R:61:ILE:HD11	2.54	0.42
17:V:34:MET:HE2	35:A:64:ALA:HB1	2.02	0.42
2:2:301:A:H2'	2:2:302:A:O4'	2.20	0.42
2:2:1402:A:H5'	16:U:51:LYS:HE2	2.02	0.42
12:Q:28:GLY:HA3	12:Q:67:ASP:OD2	2.20	0.42
24:J:139:LYS:HA	24:J:139:LYS:HD3	1.86	0.42
2:2:1154:U:H2'	22:C:192:LEU:HD11	2.01	0.41
5:E:45:ILE:HA	5:E:61:VAL:HG11	2.01	0.41
9:K:3:MET:HB2	9:K:3:MET:HE3	1.75	0.41
9:K:18:GLU:C	9:K:20:VAL:H	2.28	0.41
34:g:191:HIS:ND1	34:g:195:LEU:HD21	2.35	0.41
2:2:614:C:H5''	2:2:615:C:C5	2.55	0.41
2:2:1597:C:H4'	2:2:1603:G:O6	2.20	0.41
2:2:1679:A:N6	6:F:57:ALA:O	2.53	0.41
2:2:1849:G:H3'	2:2:1850:MA6:H8	2.02	0.41
4:D:113:LEU:HD11	4:D:117:ARG:NH2	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:45:ILE:HG13	5:E:61:VAL:HG21	2.02	0.41
34:g:11:LEU:N	34:g:307:VAL:O	2.49	0.41
2:2:1618:C:H2'	2:2:1619:A:C8	2.55	0.41
2:2:1842:4AC:H6	2:2:1842:4AC:O5'	2.20	0.41
2:2:1848:U:H2'	2:2:1850:MA6:OP2	2.20	0.41
7:H:41:ARG:H	7:H:41:ARG:HG2	1.66	0.41
18:X:93:PHE:O	18:X:140:ARG:NH1	2.49	0.41
19:a:24:THR:HG21	19:a:71:LEU:HD22	2.01	0.41
2:2:114:G:O6	2:2:351:G:H1'	2.20	0.41
2:2:383:G:H4'	10:L:132:ARG:HD2	2.03	0.41
2:2:668:A2M:HM'3	2:2:668:A2M:H1'	1.85	0.41
2:2:1538:C:H2'	2:2:1539:U:C6	2.55	0.41
2:2:1559:C:H2'	2:2:1560:U:O4'	2.20	0.41
7:H:31:GLU:O	7:H:32:MET:HB3	2.20	0.41
14:S:25:LYS:O	14:S:29:ALA:N	2.52	0.41
22:C:196:ILE:HB	22:C:223:TYR:HB2	2.02	0.41
24:J:114:VAL:HG13	24:J:119:LEU:HB2	2.02	0.41
25:M:19:GLN:HG2	25:M:88:TRP:CD2	2.56	0.41
2:2:158:A:H2'	2:2:159:A2M:O4'	2.20	0.41
5:E:107:GLY:HA2	5:E:189:LEU:HG	2.01	0.41
9:K:5:LYS:O	9:K:9:ILE:HG12	2.20	0.41
19:a:28:ARG:NH2	39:a:306:HOH:O	2.53	0.41
31:b:54:VAL:HG12	31:b:63:LEU:HD12	2.02	0.41
34:g:291:TRP:CE2	34:g:298:LEU:HD13	2.54	0.41
2:2:53:C:O2'	2:2:507:G:N7	2.44	0.41
2:2:296:PSU:H2'	2:2:297:A:O4'	2.20	0.41
2:2:1491:G:H2'	2:2:1492:U:C6	2.55	0.41
7:H:15:LYS:HA	7:H:15:LYS:HD2	1.88	0.41
9:K:17:LYS:HE2	9:K:18:GLU:HG2	2.02	0.41
30:Z:55:TYR:OH	30:Z:90:GLU:OE2	2.29	0.41
2:2:1395:C:H1'	2:2:1474:A:C4	2.56	0.41
2:2:1397:U:O4'	2:2:1442:OMU:H5''	2.20	0.41
2:2:1823:A:H3'	2:2:1824:A:H2	1.86	0.41
9:K:86:PRO:HA	9:K:87:PRO:HD3	1.96	0.41
12:Q:32:ILE:HG21	12:Q:39:LEU:HD22	2.03	0.41
13:R:36:GLU:HB3	13:R:47:ARG:HD2	2.03	0.41
35:A:34:MET:HE3	35:A:34:MET:HB3	1.67	0.41
2:2:693:A:C2	2:2:737:G:H2'	2.56	0.41
2:2:1232:PSU:H2'	2:2:1233:G:H8	1.86	0.41
2:2:1259:A:H1'	2:2:1264:C:N4	2.35	0.41
2:2:1820:G:H2'	2:2:1821:U:O4'	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:139:LYS:HE2	8:I:139:LYS:HB2	1.78	0.41
22:C:176:LYS:HA	22:C:176:LYS:HD3	1.78	0.41
33:f:125:GLU:H	33:f:125:GLU:HG3	1.59	0.41
2:2:560:A:H5'	24:J:174:LYS:HB2	2.03	0.41
2:2:1335:G:H2'	2:2:1336:C:O4'	2.21	0.41
2:2:1448:A:H2'	2:2:1449:G:O4'	2.21	0.41
2:2:1653:U:H2'	2:2:1654:G:C8	2.56	0.41
11:P:17:TYR:HD1	11:P:17:TYR:HA	1.80	0.41
11:P:65:LYS:HE3	11:P:65:LYS:HB3	1.67	0.41
18:X:140:ARG:HA	18:X:141:PRO:HD3	1.92	0.41
24:J:131:ARG:HD2	24:J:143:ASN:O	2.20	0.41
34:g:272:GLN:NE2	34:g:272:GLN:H	2.19	0.41
2:2:347:G:N7	39:2:2202:HOH:O	2.37	0.41
2:2:733:C:N4	39:2:2206:HOH:O	2.37	0.41
2:2:1598:G:H3'	30:Z:80:ARG:HD3	2.02	0.41
2:2:1629:C:H2'	2:2:1630:A:O4'	2.20	0.41
2:2:1865:C:H5	19:a:6:ARG:H	1.65	0.41
14:S:48:ALA:HB2	14:S:70:ILE:HD12	2.03	0.41
14:S:85:ASN:HB2	14:S:97:GLN:CD	2.46	0.41
2:2:344:U:H2'	2:2:345:U:C6	2.56	0.40
2:2:455:A:H2'	2:2:456:C:C6	2.56	0.40
2:2:847:A:O2'	5:E:106:LYS:NZ	2.55	0.40
2:2:1293:A:H2'	2:2:1294:G:C8	2.57	0.40
2:2:1589:A:H2'	2:2:1590:C:O4'	2.21	0.40
2:2:1650:A:H2'	2:2:1651:A:O4'	2.21	0.40
2:2:1752:C:H2'	2:2:1779:G:H1	1.86	0.40
13:R:69:ILE:HG22	13:R:71:ILE:HG13	2.03	0.40
25:M:59:PRO:O	25:M:63:LYS:HB2	2.22	0.40
2:2:71:G:H2'	2:2:72:C:O4'	2.21	0.40
2:2:926:A:H2'	2:2:927:C:O4'	2.21	0.40
3:B:67:PHE:CE2	27:O:48:SER:HB3	2.56	0.40
3:B:163:GLN:HB3	3:B:204:ILE:HD13	2.03	0.40
10:L:82:MET:HB3	10:L:85:THR:HB	2.03	0.40
26:N:100:LYS:HG2	26:N:104:ARG:NH1	2.37	0.40
31:b:62:VAL:HG11	31:b:65:GLN:HE21	1.86	0.40
2:2:1193:U:H5'	2:2:1822:A:H5''	2.03	0.40
2:2:1730:U:H2'	2:2:1731:A:O4'	2.22	0.40
3:B:116:LYS:NZ	39:B:302:HOH:O	2.52	0.40
4:D:216:GLU:OE2	34:g:172:LYS:NZ	2.51	0.40
6:F:38:TYR:OH	20:c:54:ASP:OD1	2.32	0.40
6:F:193:LYS:HB3	6:F:193:LYS:HE2	1.78	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:157:LYS:HD2	8:I:157:LYS:HA	1.90	0.40
18:X:41:PHE:HZ	18:X:102:VAL:HG23	1.85	0.40
23:G:31:ARG:HG2	23:G:101:ILE:HG12	2.03	0.40
32:e:36:MET:HG2	32:e:40:ARG:NH1	2.37	0.40
2:2:1323:U:H2'	2:2:1324:G:C8	2.57	0.40
2:2:1405:A:H2'	2:2:1406:G:O4'	2.21	0.40
13:R:31:ASN:HD22	13:R:31:ASN:HA	1.63	0.40
17:V:60:ARG:HG2	17:V:65:SER:HB2	2.03	0.40
2:2:174:OMC:HM23	2:2:174:OMC:H1'	1.81	0.40
2:2:1333:U:H4'	4:D:147:ALA:HB2	2.04	0.40
3:B:109:LYS:HE3	3:B:113:MET:SD	2.62	0.40
18:X:93:PHE:O	18:X:140:ARG:HD2	2.22	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	n	18/25 (72%)	17 (94%)	1 (6%)	0	100	100
3	B	208/264 (79%)	202 (97%)	6 (3%)	0	100	100
4	D	222/243 (91%)	218 (98%)	4 (2%)	0	100	100
5	E	255/263 (97%)	251 (98%)	4 (2%)	0	100	100
6	F	178/204 (87%)	171 (96%)	7 (4%)	0	100	100
7	H	180/194 (93%)	156 (87%)	24 (13%)	0	100	100
8	I	203/208 (98%)	199 (98%)	4 (2%)	0	100	100
9	K	95/165 (58%)	86 (90%)	8 (8%)	1 (1%)	11	7
10	L	137/158 (87%)	131 (96%)	6 (4%)	0	100	100
11	P	121/145 (83%)	118 (98%)	2 (2%)	1 (1%)	16	10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	Q	137/146 (94%)	131 (96%)	6 (4%)	0	100	100
13	R	129/135 (96%)	121 (94%)	8 (6%)	0	100	100
14	S	142/152 (93%)	138 (97%)	4 (3%)	0	100	100
15	T	141/145 (97%)	139 (99%)	2 (1%)	0	100	100
16	U	102/119 (86%)	98 (96%)	4 (4%)	0	100	100
17	V	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
18	X	137/143 (96%)	135 (98%)	2 (2%)	0	100	100
19	a	97/115 (84%)	95 (98%)	2 (2%)	0	100	100
20	c	57/69 (83%)	53 (93%)	4 (7%)	0	100	100
21	d	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
22	C	218/293 (74%)	212 (97%)	6 (3%)	0	100	100
23	G	225/249 (90%)	221 (98%)	4 (2%)	0	100	100
24	J	183/194 (94%)	177 (97%)	5 (3%)	1 (0%)	24	20
25	M	100/132 (76%)	92 (92%)	8 (8%)	0	100	100
26	N	148/151 (98%)	144 (97%)	4 (3%)	0	100	100
27	O	123/151 (82%)	120 (98%)	3 (2%)	0	100	100
28	W	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
29	Y	120/133 (90%)	118 (98%)	2 (2%)	0	100	100
30	Z	70/125 (56%)	68 (97%)	2 (3%)	0	100	100
31	b	80/84 (95%)	77 (96%)	3 (4%)	0	100	100
32	e	53/59 (90%)	48 (91%)	5 (9%)	0	100	100
33	f	62/156 (40%)	56 (90%)	6 (10%)	0	100	100
34	g	310/317 (98%)	286 (92%)	24 (8%)	0	100	100
35	A	205/295 (70%)	200 (98%)	5 (2%)	0	100	100
All	All	4717/5501 (86%)	4535 (96%)	179 (4%)	3 (0%)	49	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	K	19	GLY
24	J	138	ARG
11	P	18	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	n	19/24 (79%)	19 (100%)	0	100	100
3	B	192/231 (83%)	184 (96%)	8 (4%)	26	25
4	D	188/202 (93%)	174 (93%)	14 (7%)	13	8
5	E	220/225 (98%)	218 (99%)	2 (1%)	70	77
6	F	155/170 (91%)	146 (94%)	9 (6%)	18	14
7	H	164/174 (94%)	155 (94%)	9 (6%)	19	15
8	I	178/180 (99%)	168 (94%)	10 (6%)	19	15
9	K	88/136 (65%)	83 (94%)	5 (6%)	18	14
10	L	128/142 (90%)	126 (98%)	2 (2%)	55	61
11	P	109/130 (84%)	106 (97%)	3 (3%)	38	40
12	Q	115/121 (95%)	111 (96%)	4 (4%)	32	32
13	R	119/122 (98%)	112 (94%)	7 (6%)	18	13
14	S	125/132 (95%)	123 (98%)	2 (2%)	55	61
15	T	113/115 (98%)	113 (100%)	0	100	100
16	U	94/107 (88%)	91 (97%)	3 (3%)	34	36
17	V	66/66 (100%)	65 (98%)	1 (2%)	57	64
18	X	111/114 (97%)	107 (96%)	4 (4%)	31	31
19	a	86/98 (88%)	82 (95%)	4 (5%)	23	21
20	c	52/62 (84%)	47 (90%)	5 (10%)	8	4
21	d	48/49 (98%)	47 (98%)	1 (2%)	47	52
22	C	186/225 (83%)	181 (97%)	5 (3%)	39	41
23	G	198/218 (91%)	191 (96%)	7 (4%)	32	32
24	J	161/168 (96%)	153 (95%)	8 (5%)	22	18
25	M	86/108 (80%)	77 (90%)	9 (10%)	6	3
26	N	130/131 (99%)	126 (97%)	4 (3%)	35	37
27	O	99/118 (84%)	92 (93%)	7 (7%)	13	8

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	W	112/113 (99%)	111 (99%)	1 (1%)	70	77
29	Y	107/115 (93%)	104 (97%)	3 (3%)	38	40
30	Z	63/103 (61%)	61 (97%)	2 (3%)	34	36
31	b	74/76 (97%)	72 (97%)	2 (3%)	39	41
32	e	45/48 (94%)	39 (87%)	6 (13%)	4	1
33	f	57/140 (41%)	54 (95%)	3 (5%)	20	17
34	g	271/275 (98%)	255 (94%)	16 (6%)	18	13
35	A	172/242 (71%)	170 (99%)	2 (1%)	63	70
All	All	4131/4680 (88%)	3963 (96%)	168 (4%)	28	26

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	50	THR
3	B	55	THR
3	B	57	ILE
3	B	86	LEU
3	B	91	VAL
3	B	131	ASP
3	B	170	GLU
3	B	227	LYS
4	D	32	ASP
4	D	42	THR
4	D	44	THR
4	D	45	ARG
4	D	46	THR
4	D	48	ILE
4	D	55	THR
4	D	58	VAL
4	D	84	VAL
4	D	93	THR
4	D	164	VAL
4	D	175	VAL
4	D	197	LYS
4	D	211	VAL
5	E	108	ARG
5	E	236	ILE
6	F	32	ASP
6	F	41	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	122	ARG
6	F	123	GLU
6	F	124	ASP
6	F	128	ILE
6	F	140	ASP
6	F	141	VAL
6	F	166	ILE
7	H	10	LYS
7	H	23	ILE
7	H	32	MET
7	H	46	THR
7	H	53	VAL
7	H	82	GLU
7	H	92	VAL
7	H	121	THR
7	H	167	GLU
8	I	7	ASN
8	I	17	LYS
8	I	18	ARG
8	I	62	VAL
8	I	119	LEU
8	I	153	LYS
8	I	154	LYS
8	I	155	ASN
8	I	157	LYS
8	I	159	SER
9	K	2	LEU
9	K	18	GLU
9	K	58	VAL
9	K	88	GLU
9	K	96	ARG
10	L	20	LYS
10	L	74	SER
11	P	16	THR
11	P	57	LEU
11	P	136	THR
12	Q	12	VAL
12	Q	46	THR
12	Q	100	VAL
12	Q	118	THR
13	R	30	THR
13	R	61	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	R	94	GLU
13	R	110	ASP
13	R	115	SER
13	R	116	ASN
13	R	124	VAL
14	S	83	PHE
14	S	131	VAL
16	U	25	THR
16	U	61	LEU
16	U	101	ILE
17	V	32	ILE
18	X	7	LEU
18	X	61	GLN
18	X	72	VAL
18	X	119	ARG
19	a	2	THR
19	a	30	VAL
19	a	54	SER
19	a	64	LEU
20	c	27	CYS
20	c	40	ARG
20	c	47	LYS
20	c	58	LEU
20	c	63	ARG
21	d	3	HIS
22	C	101	SER
22	C	105	GLU
22	C	225	SER
22	C	274	VAL
22	C	275	LYS
23	G	26	THR
23	G	41	LEU
23	G	148	SER
23	G	153	VAL
23	G	157	VAL
23	G	200	LYS
23	G	203	LYS
24	J	2	PRO
24	J	3	VAL
24	J	22	LYS
24	J	58	ARG
24	J	75	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	J	89	GLU
24	J	128	VAL
24	J	138	ARG
25	M	14	VAL
25	M	18	LEU
25	M	43	ASP
25	M	46	GLN
25	M	52	LEU
25	M	77	ILE
25	M	79	VAL
25	M	92	CYS
25	M	104	VAL
26	N	43	LYS
26	N	69	ASN
26	N	93	LYS
26	N	149	LEU
27	O	67	ASP
27	O	80	ASP
27	O	81	VAL
27	O	98	ARG
27	O	105	THR
27	O	116	LEU
27	O	117	ARG
28	W	71	LYS
29	Y	4	THR
29	Y	111	LYS
29	Y	122	LYS
30	Z	52	LYS
30	Z	72	VAL
31	b	57	VAL
31	b	61	THR
32	e	5	SER
32	e	12	VAL
32	e	43	VAL
32	e	46	VAL
32	e	48	THR
32	e	51	LYS
33	f	124	ASP
33	f	125	GLU
33	f	149	CYS
34	g	12	LYS
34	g	45	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	g	74	ASP
34	g	87	LEU
34	g	116	ASP
34	g	119	GLN
34	g	131	LEU
34	g	179	LEU
34	g	201	SER
34	g	205	SER
34	g	213	ASP
34	g	276	SER
34	g	277	THR
34	g	297	THR
34	g	304	ASP
34	g	313	THR
35	A	43	SER
35	A	184	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
3	B	101	HIS
6	F	83	ASN
6	F	179	ASN
7	H	12	ASN
7	H	168	HIS
8	I	7	ASN
8	I	155	ASN
9	K	50	GLN
9	K	77	GLN
9	K	84	HIS
10	L	108	ASN
12	Q	8	GLN
13	R	121	GLN
14	S	10	GLN
14	S	73	ASN
15	T	83	GLN
16	U	92	HIS
18	X	26	GLN
19	a	25	ASN
28	W	15	ASN
28	W	70	ASN
28	W	82	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	Y	112	ASN
33	f	151	ASN
34	g	76	GLN
34	g	178	ASN
34	g	272	GLN
35	A	9	GLN
35	A	111	GLN
35	A	141	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	2	1628/1868 (87%)	263 (16%)	7 (0%)

All (263) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	2	4	C
2	2	17	C
2	2	33	G
2	2	46	A
2	2	56	G
2	2	59	U
2	2	65	C
2	2	67	C
2	2	68	A
2	2	72	C
2	2	74	G
2	2	75	G
2	2	82	G
2	2	99	A2M
2	2	103	A
2	2	113	G
2	2	115	U
2	2	126	G
2	2	130	G
2	2	143	U
2	2	155	G
2	2	160	U
2	2	178	C
2	2	184	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	191	A
2	2	192	C
2	2	205	G
2	2	211	G
2	2	212	C
2	2	302	A
2	2	306	C
2	2	309	G
2	2	319	C
2	2	320	G
2	2	330	G
2	2	332	G
2	2	333	G
2	2	335	G
2	2	339	A
2	2	340	C
2	2	347	G
2	2	362	C
2	2	364	A
2	2	368	U
2	2	370	G
2	2	385	G
2	2	386	C
2	2	409	C
2	2	438	G
2	2	448	A
2	2	449	A
2	2	450	C
2	2	464	A
2	2	470	G
2	2	471	G
2	2	472	C
2	2	474	G
2	2	482	G
2	2	487	U
2	2	492	C
2	2	516	A
2	2	532	C
2	2	533	A
2	2	535	G
2	2	536	A
2	2	537	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	538	U
2	2	540	U
2	2	541	U
2	2	542	U
2	2	543	C
2	2	544	G
2	2	546	G
2	2	547	G
2	2	548	C
2	2	549	C
2	2	550	C
2	2	554	A
2	2	555	A
2	2	563	G
2	2	583	C
2	2	587	A
2	2	589	G
2	2	591	U
2	2	614	C
2	2	617	G
2	2	628	A
2	2	629	A
2	2	632	C
2	2	643	A
2	2	655	A
2	2	668	A2M
2	2	669	A
2	2	671	A
2	2	672	A
2	2	688	U
2	2	690	G
2	2	692	G
2	2	693	A
2	2	695	C
2	2	696	G
2	2	697	G
2	2	698	G
2	2	731	G
2	2	732	U
2	2	733	C
2	2	735	C
2	2	736	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	738	C
2	2	739	C
2	2	801	U
2	2	821	G
2	2	822	PSU
2	2	847	A
2	2	859	G
2	2	869	A
2	2	870	A
2	2	871	U
2	2	877	C
2	2	913	A
2	2	920	A
2	2	922	A
2	2	933	G
2	2	943	U
2	2	955	A
2	2	971	G
2	2	990	A
2	2	992	A
2	2	1017	U
2	2	1023	A
2	2	1060	A
2	2	1061	U
2	2	1062	A
2	2	1078	C
2	2	1083	A
2	2	1085	C
2	2	1087	A
2	2	1109	C
2	2	1115	U
2	2	1116	C
2	2	1117	C
2	2	1119	A
2	2	1121	G
2	2	1133	A
2	2	1138	C
2	2	1144	A
2	2	1153	C
2	2	1154	U
2	2	1171	G
2	2	1195	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	1207	G
2	2	1215	C
2	2	1221	G
2	2	1242	U
2	2	1243	U
2	2	1248	B8N
2	2	1251	A
2	2	1253	A
2	2	1256	G
2	2	1257	G
2	2	1259	A
2	2	1274	G
2	2	1275	G
2	2	1294	G
2	2	1295	A
2	2	1301	A
2	2	1302	G
2	2	1303	C
2	2	1308	U
2	2	1320	G
2	2	1322	G
2	2	1342	U
2	2	1344	A
2	2	1348	G
2	2	1371	U
2	2	1372	U
2	2	1378	A
2	2	1382	A
2	2	1397	U
2	2	1404	U
2	2	1406	G
2	2	1423	C
2	2	1435	C
2	2	1436	C
2	2	1449	G
2	2	1454	A
2	2	1461	G
2	2	1462	U
2	2	1463	U
2	2	1488	C
2	2	1489	A
2	2	1490	OMG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	1497	G
2	2	1498	A
2	2	1508	A
2	2	1520	G
2	2	1521	C
2	2	1533	A
2	2	1548	G
2	2	1553	C
2	2	1579	A
2	2	1580	A
2	2	1588	A
2	2	1601	A
2	2	1621	U
2	2	1639	7MG
2	2	1654	G
2	2	1664	A
2	2	1665	G
2	2	1671	G
2	2	1680	G
2	2	1712	A
2	2	1713	C
2	2	1715	A
2	2	1717	C
2	2	1719	A
2	2	1721	U
2	2	1722	G
2	2	1723	G
2	2	1726	G
2	2	1728	U
2	2	1744	G
2	2	1745	A
2	2	1746	U
2	2	1748	G
2	2	1752	C
2	2	1753	C
2	2	1754	G
2	2	1755	C
2	2	1760	G
2	2	1761	U
2	2	1772	C
2	2	1773	C
2	2	1774	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	1775	U
2	2	1777	G
2	2	1778	C
2	2	1779	G
2	2	1781	A
2	2	1782	G
2	2	1783	C
2	2	1784	G
2	2	1786	U
2	2	1800	A
2	2	1801	A
2	2	1807	C
2	2	1812	U
2	2	1813	A
2	2	1815	A
2	2	1816	G
2	2	1819	A
2	2	1829	G
2	2	1831	A
2	2	1835	A
2	2	1836	G
2	2	1838	U
2	2	1849	G
2	2	1851	MA6
2	2	1861	G
2	2	1862	G
2	2	1863	A
2	2	1864	U
2	2	1865	C

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	331	C
2	2	531	A
2	2	912	C
2	2	1165	G
2	2	1434	C
2	2	1520	G
2	2	1679	A

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

77 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$
2	A2M	2	590	2	22,25,26	3.18	9 (40%)	31,36,39	3.21	14 (45%)
2	A2M	2	99	37,2	22,25,26	3.19	9 (40%)	31,36,39	3.05	11 (35%)
2	PSU	2	1692	36,2	18,21,22	3.74	7 (38%)	22,30,33	1.79	4 (18%)
2	OMC	2	1391	2	19,22,23	2.70	8 (42%)	26,31,34	0.91	0
2	OMU	2	354	2	19,22,23	2.88	8 (42%)	26,31,34	1.91	6 (23%)
2	OMG	2	1490	37,2	23,26,27	1.22	3 (13%)	33,38,41	1.95	7 (21%)
2	PSU	2	119	2	18,21,22	3.99	7 (38%)	22,30,33	1.80	5 (22%)
2	A2M	2	166	2	22,25,26	3.28	10 (45%)	31,36,39	3.04	12 (38%)
2	OMU	2	121	2	19,22,23	2.73	8 (42%)	26,31,34	1.75	5 (19%)
2	A2M	2	468	2	22,25,26	3.23	11 (50%)	31,36,39	3.17	11 (35%)
2	PSU	2	572	36,2	18,21,22	4.06	7 (38%)	22,30,33	1.88	4 (18%)
2	4AC	2	1842	2	21,24,25	3.02	10 (47%)	29,34,37	1.51	4 (13%)
2	OMC	2	462	2	19,22,23	2.73	8 (42%)	26,31,34	0.77	0
2	PSU	2	681	2	18,21,22	3.93	8 (44%)	22,30,33	1.83	4 (18%)
2	PSU	2	814	2	18,21,22	3.86	7 (38%)	22,30,33	1.66	3 (13%)
2	PSU	2	296	2	18,21,22	3.97	7 (38%)	22,30,33	1.81	5 (22%)
2	A2M	2	484	2	22,25,26	1.45	4 (18%)	31,36,39	2.03	9 (29%)
2	OMG	2	509	37,2	23,26,27	2.30	8 (34%)	33,38,41	2.12	14 (42%)
2	A2M	2	576	36,2	22,25,26	3.33	11 (50%)	31,36,39	2.98	13 (41%)
2	PSU	2	406	2	18,21,22	3.94	7 (38%)	22,30,33	1.78	4 (18%)
2	A2M	2	1383	2	22,25,26	3.41	11 (50%)	31,36,39	3.02	14 (45%)
2	A2M	2	668	37,2	22,25,26	1.46	5 (22%)	31,36,39	2.11	11 (35%)
2	PSU	2	1244	2	18,21,22	3.98	7 (38%)	22,30,33	2.12	5 (22%)
2	PSU	2	1046	36,2	18,21,22	4.00	7 (38%)	22,30,33	1.78	3 (13%)
2	A2M	2	512	2	22,25,26	3.28	10 (45%)	31,36,39	3.12	14 (45%)
2	B8N	2	1248	2	24,29,30	2.86	7 (29%)	29,42,45	1.91	7 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMU	2	1326	37,2	19,22,23	2.86	8 (42%)	26,31,34	2.02	5 (19%)
2	OMC	2	174	37,2	19,22,23	2.75	8 (42%)	26,31,34	0.93	0
2	PSU	2	1445	2	18,21,22	3.99	7 (38%)	22,30,33	1.78	4 (18%)
2	OMU	2	172	2	19,22,23	2.86	7 (36%)	26,31,34	1.85	6 (23%)
2	PSU	2	1625	2	18,21,22	3.95	7 (38%)	22,30,33	1.92	5 (22%)
35	SAC	A	2	35	7,8,9	1.57	2 (28%)	8,9,11	1.45	2 (25%)
2	PSU	2	105	36,2	18,21,22	3.91	7 (38%)	22,30,33	2.12	5 (22%)
2	A2M	2	1678	2	22,25,26	1.39	4 (18%)	31,36,39	2.15	9 (29%)
2	PSU	2	36	2	18,21,22	1.45	4 (22%)	22,30,33	1.80	4 (18%)
2	PSU	2	649	2	18,21,22	4.06	7 (38%)	22,30,33	1.93	5 (22%)
2	OMU	2	428	37,2	19,22,23	2.86	8 (42%)	26,31,34	1.59	5 (19%)
2	OMU	2	1288	2	19,22,23	2.86	7 (36%)	26,31,34	1.75	4 (15%)
2	PSU	2	93	2	18,21,22	4.01	7 (38%)	22,30,33	1.66	4 (18%)
2	MA6	2	1851	2	23,26,27	1.46	5 (21%)	34,38,41	2.40	14 (41%)
2	OMG	2	601	2	23,26,27	2.26	8 (34%)	33,38,41	2.24	14 (42%)
2	PSU	2	1056	2	18,21,22	3.82	7 (38%)	22,30,33	2.08	5 (22%)
27	IAS	O	138	27	6,7,8	0.99	0	6,8,10	1.97	3 (50%)
2	6MZ	2	1832	36,37,2	22,25,26	3.56	6 (27%)	30,36,39	2.33	10 (33%)
2	OMC	2	1272	2	19,22,23	2.71	8 (42%)	26,31,34	0.68	0
2	7MG	2	1639	2	22,26,27	1.38	3 (13%)	29,39,42	2.53	7 (24%)
2	4AC	2	1337	2	21,24,25	3.37	10 (47%)	29,34,37	1.63	6 (20%)
2	OMG	2	683	2	23,26,27	2.34	8 (34%)	33,38,41	2.16	14 (42%)
2	PSU	2	1081	2	18,21,22	3.99	8 (44%)	22,30,33	1.87	6 (27%)
2	PSU	2	1643	37,2	18,21,22	1.48	4 (22%)	22,30,33	1.89	4 (18%)
2	OMG	2	644	2	23,26,27	2.26	9 (39%)	33,38,41	2.17	12 (36%)
2	PSU	2	109	36,2	18,21,22	4.06	7 (38%)	22,30,33	1.82	4 (18%)
2	PSU	2	1174	36,2	18,21,22	1.41	3 (16%)	22,30,33	1.83	3 (13%)
2	PSU	2	1232	2	18,21,22	3.98	7 (38%)	22,30,33	1.74	4 (18%)
2	OMG	2	1328	36,2	23,26,27	2.33	9 (39%)	33,38,41	2.44	11 (33%)
2	OMC	2	517	2	19,22,23	2.68	8 (42%)	26,31,34	0.79	0
2	MA6	2	1850	2	23,26,27	1.46	3 (13%)	34,38,41	2.52	13 (38%)
2	OMC	2	1703	2	19,22,23	2.67	8 (42%)	26,31,34	0.86	0
2	A2M	2	27	37,2	22,25,26	1.44	4 (18%)	31,36,39	2.31	12 (38%)
17	AME	V	1	17	9,10,11	1.36	1 (11%)	9,11,13	2.01	2 (22%)
2	OMU	2	1442	37,2	19,22,23	2.87	8 (42%)	26,31,34	1.81	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	2	822	2	18,21,22	3.94	8 (44%)	22,30,33	1.77	4 (18%)
2	PSU	2	1177	2	18,21,22	1.36	4 (22%)	22,30,33	1.89	4 (18%)
2	PSU	2	651	2	18,21,22	3.93	8 (44%)	22,30,33	2.29	5 (22%)
2	OMU	2	116	2	19,22,23	2.78	7 (36%)	26,31,34	1.56	5 (19%)
2	A2M	2	1031	2	22,25,26	3.24	11 (50%)	31,36,39	3.16	12 (38%)
2	PSU	2	1238	2	18,21,22	3.92	7 (38%)	22,30,33	1.79	4 (18%)
2	PSU	2	1136	2	18,21,22	3.86	8 (44%)	22,30,33	1.96	4 (18%)
2	OMG	2	1447	2	23,26,27	2.26	9 (39%)	33,38,41	2.28	12 (36%)
18	HY3	X	62	36,18	6,8,9	8.45	4 (66%)	5,10,12	1.18	0
2	PSU	2	1347	2	18,21,22	1.44	3 (16%)	22,30,33	1.90	4 (18%)
2	PSU	2	815	2	18,21,22	4.01	7 (38%)	22,30,33	1.85	4 (18%)
2	PSU	2	686	2	18,21,22	4.08	7 (38%)	22,30,33	1.98	5 (22%)
2	PSU	2	863	2	18,21,22	3.72	7 (38%)	22,30,33	2.05	5 (22%)
2	PSU	2	1045	2	18,21,22	4.14	7 (38%)	22,30,33	1.94	5 (22%)
2	OMG	2	436	2	23,26,27	2.33	8 (34%)	33,38,41	2.15	14 (42%)
2	A2M	2	159	2	22,25,26	3.22	9 (40%)	31,36,39	3.13	14 (45%)

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
2	A2M	2	590	2	-	0/9/27/28	0/3/3/3
2	A2M	2	99	37,2	-	2/9/27/28	0/3/3/3
2	PSU	2	1692	36,2	-	0/7/25/26	0/2/2/2
2	OMC	2	1391	2	-	0/9/27/28	0/2/2/2
2	OMU	2	354	2	-	0/9/27/28	0/2/2/2
2	OMG	2	1490	37,2	-	1/9/27/28	0/3/3/3
2	PSU	2	119	2	-	0/7/25/26	0/2/2/2
2	A2M	2	166	2	-	0/9/27/28	0/3/3/3
2	OMU	2	121	2	-	0/9/27/28	0/2/2/2
2	A2M	2	468	2	-	1/9/27/28	0/3/3/3
2	PSU	2	572	36,2	-	0/7/25/26	0/2/2/2
2	4AC	2	1842	2	-	2/11/29/30	0/2/2/2
2	OMC	2	462	2	-	0/9/27/28	0/2/2/2
2	PSU	2	681	2	-	0/7/25/26	0/2/2/2
2	PSU	2	814	2	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	2	296	2	-	0/7/25/26	0/2/2/2
2	A2M	2	484	2	-	1/9/27/28	0/3/3/3
2	OMG	2	509	37,2	-	0/9/27/28	0/3/3/3
2	A2M	2	576	36,2	-	2/9/27/28	0/3/3/3
2	PSU	2	406	2	-	0/7/25/26	0/2/2/2
2	A2M	2	1383	2	-	0/9/27/28	0/3/3/3
2	A2M	2	668	37,2	-	3/9/27/28	0/3/3/3
2	PSU	2	1244	2	-	0/7/25/26	0/2/2/2
2	PSU	2	1046	36,2	-	0/7/25/26	0/2/2/2
2	A2M	2	512	2	-	0/9/27/28	0/3/3/3
2	B8N	2	1248	2	-	2/16/34/35	0/2/2/2
2	OMU	2	1326	37,2	-	0/9/27/28	0/2/2/2
2	OMC	2	174	37,2	-	1/9/27/28	0/2/2/2
2	PSU	2	1445	2	-	0/7/25/26	0/2/2/2
2	OMU	2	172	2	-	1/9/27/28	0/2/2/2
2	PSU	2	1625	2	-	0/7/25/26	0/2/2/2
35	SAC	A	2	35	-	0/7/8/10	-
2	PSU	2	105	36,2	-	0/7/25/26	0/2/2/2
2	A2M	2	1678	2	-	1/9/27/28	0/3/3/3
2	PSU	2	36	2	-	0/7/25/26	0/2/2/2
2	PSU	2	649	2	-	0/7/25/26	0/2/2/2
2	OMU	2	428	37,2	-	4/9/27/28	0/2/2/2
2	OMU	2	1288	2	-	0/9/27/28	0/2/2/2
2	PSU	2	93	2	-	0/7/25/26	0/2/2/2
2	MA6	2	1851	2	-	6/11/29/30	0/3/3/3
2	OMG	2	601	2	-	0/9/27/28	0/3/3/3
2	PSU	2	1056	2	-	0/7/25/26	0/2/2/2
27	IAS	O	138	27	-	2/7/7/8	-
2	6MZ	2	1832	36,37,2	-	0/9/27/28	0/3/3/3
2	OMC	2	1272	2	-	0/9/27/28	0/2/2/2
2	7MG	2	1639	2	-	0/7/37/38	0/3/3/3
2	4AC	2	1337	2	-	2/11/29/30	0/2/2/2
2	OMG	2	683	2	-	0/9/27/28	0/3/3/3
2	PSU	2	1081	2	-	1/7/25/26	0/2/2/2
2	PSU	2	1643	37,2	-	0/7/25/26	0/2/2/2
2	OMG	2	644	2	-	1/9/27/28	0/3/3/3
2	PSU	2	109	36,2	-	0/7/25/26	0/2/2/2
2	PSU	2	1174	36,2	-	0/7/25/26	0/2/2/2
2	PSU	2	1232	2	-	0/7/25/26	0/2/2/2
2	OMG	2	1328	36,2	-	0/9/27/28	0/3/3/3
2	OMC	2	517	2	-	0/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MA6	2	1850	2	-	2/11/29/30	0/3/3/3
2	OMC	2	1703	2	-	0/9/27/28	0/2/2/2
2	A2M	2	27	37,2	-	1/9/27/28	0/3/3/3
17	AME	V	1	17	-	3/9/10/12	-
2	OMU	2	1442	37,2	-	0/9/27/28	0/2/2/2
2	PSU	2	822	2	-	0/7/25/26	0/2/2/2
2	PSU	2	1177	2	-	0/7/25/26	0/2/2/2
2	PSU	2	651	2	-	0/7/25/26	0/2/2/2
2	OMU	2	116	2	-	1/9/27/28	0/2/2/2
2	A2M	2	1031	2	-	0/9/27/28	0/3/3/3
2	PSU	2	1238	2	-	0/7/25/26	0/2/2/2
2	PSU	2	1136	2	-	0/7/25/26	0/2/2/2
2	OMG	2	1447	2	-	2/9/27/28	0/3/3/3
18	HY3	X	62	36,18	-	1/1/12/14	0/1/1/1
2	PSU	2	1347	2	-	1/7/25/26	0/2/2/2
2	PSU	2	815	2	-	0/7/25/26	0/2/2/2
2	PSU	2	686	2	-	0/7/25/26	0/2/2/2
2	PSU	2	863	2	-	0/7/25/26	0/2/2/2
2	PSU	2	1045	2	-	0/7/25/26	0/2/2/2
2	OMG	2	436	2	-	0/9/27/28	0/3/3/3
2	A2M	2	159	2	-	0/9/27/28	0/3/3/3

All (535) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	X	62	HY3	C3-CA	-19.76	1.35	1.55
2	2	1832	6MZ	C6-N6	14.91	1.50	1.34
2	2	686	PSU	C6-C5	10.90	1.48	1.35
2	2	93	PSU	C6-C5	10.88	1.48	1.35
2	2	815	PSU	C6-C5	10.84	1.47	1.35
2	2	1232	PSU	C6-C5	10.77	1.47	1.35
2	2	109	PSU	C6-C5	10.76	1.47	1.35
2	2	649	PSU	C6-C5	10.73	1.47	1.35
2	2	572	PSU	C6-C5	10.71	1.47	1.35
2	2	651	PSU	C6-C5	10.53	1.47	1.35
2	2	1045	PSU	C6-C5	10.51	1.47	1.35
2	2	1445	PSU	C6-C5	10.50	1.47	1.35
2	2	296	PSU	C6-C5	10.46	1.47	1.35
2	2	1046	PSU	C6-C5	10.46	1.47	1.35
2	2	1136	PSU	C6-C5	10.42	1.47	1.35
2	2	406	PSU	C6-C5	10.39	1.47	1.35
2	2	1625	PSU	C6-C5	10.33	1.47	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	105	PSU	C6-C5	10.24	1.47	1.35
2	2	1081	PSU	C6-C5	10.21	1.47	1.35
2	2	1238	PSU	C6-C5	10.11	1.47	1.35
2	2	119	PSU	C6-C5	10.00	1.47	1.35
2	2	814	PSU	C6-C5	9.96	1.46	1.35
2	2	1692	PSU	C6-C5	9.87	1.46	1.35
2	2	681	PSU	C6-C5	9.81	1.46	1.35
2	2	1244	PSU	C6-C5	9.80	1.46	1.35
2	2	822	PSU	C6-C5	9.76	1.46	1.35
2	2	1056	PSU	C6-C5	9.66	1.46	1.35
2	2	1045	PSU	C2-N1	9.34	1.49	1.36
2	2	863	PSU	C6-C5	9.26	1.46	1.35
2	2	1244	PSU	C2-N1	9.23	1.49	1.36
2	2	166	A2M	C3'-C4'	-9.22	1.29	1.53
2	2	119	PSU	C2-N1	8.99	1.48	1.36
2	2	686	PSU	C2-N1	8.98	1.48	1.36
2	2	109	PSU	C2-N1	8.98	1.48	1.36
2	2	572	PSU	C2-N1	8.98	1.48	1.36
2	2	649	PSU	C2-N1	8.96	1.48	1.36
2	2	822	PSU	C2-N1	8.93	1.48	1.36
2	2	590	A2M	C3'-C4'	-8.91	1.30	1.53
2	2	576	A2M	C3'-C4'	-8.87	1.30	1.53
2	2	468	A2M	C3'-C4'	-8.86	1.30	1.53
2	2	1046	PSU	C2-N1	8.86	1.48	1.36
2	2	681	PSU	C2-N1	8.86	1.48	1.36
2	2	815	PSU	C2-N1	8.84	1.48	1.36
2	2	1238	PSU	C2-N1	8.83	1.48	1.36
2	2	406	PSU	C2-N1	8.82	1.48	1.36
2	2	1081	PSU	C2-N1	8.80	1.48	1.36
2	2	1383	A2M	C3'-C4'	-8.75	1.30	1.53
2	2	159	A2M	C3'-C4'	-8.74	1.30	1.53
2	2	512	A2M	C3'-C4'	-8.74	1.30	1.53
2	2	1445	PSU	C2-N1	8.71	1.48	1.36
2	2	1056	PSU	C2-N1	8.69	1.48	1.36
2	2	1248	B8N	C4-N3	-8.69	1.24	1.40
2	2	99	A2M	C3'-C4'	-8.64	1.30	1.53
2	2	1031	A2M	C3'-C4'	-8.64	1.30	1.53
2	2	1232	PSU	C2-N1	8.60	1.48	1.36
2	2	1136	PSU	C2-N1	8.59	1.48	1.36
2	2	814	PSU	C2-N1	8.53	1.48	1.36
2	2	296	PSU	C2-N1	8.48	1.48	1.36
2	2	1625	PSU	C2-N1	8.45	1.48	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	651	PSU	C2-N1	8.40	1.48	1.36
2	2	93	PSU	C2-N1	8.36	1.48	1.36
2	2	105	PSU	C2-N1	8.16	1.47	1.36
2	2	1383	A2M	O4'-C4'	7.96	1.62	1.45
2	2	863	PSU	C2-N1	7.93	1.47	1.36
2	2	512	A2M	O4'-C4'	7.84	1.62	1.45
2	2	576	A2M	O4'-C4'	7.78	1.62	1.45
2	2	1692	PSU	C2-N1	7.77	1.47	1.36
2	2	159	A2M	O4'-C4'	7.75	1.62	1.45
2	2	166	A2M	O4'-C4'	7.74	1.62	1.45
2	2	99	A2M	O4'-C4'	7.60	1.62	1.45
2	2	1031	A2M	O4'-C4'	7.53	1.61	1.45
2	2	468	A2M	O4'-C4'	7.35	1.61	1.45
2	2	1045	PSU	C2-N3	7.07	1.49	1.37
2	2	1248	B8N	C6-N1	7.05	1.54	1.36
2	2	1625	PSU	C2-N3	6.93	1.49	1.37
2	2	1244	PSU	C2-N3	6.86	1.49	1.37
2	2	590	A2M	O4'-C4'	6.79	1.60	1.45
2	2	105	PSU	C2-N3	6.71	1.49	1.37
2	2	296	PSU	C2-N3	6.71	1.49	1.37
2	2	572	PSU	C2-N3	6.70	1.49	1.37
2	2	686	PSU	C2-N3	6.69	1.49	1.37
2	2	119	PSU	C2-N3	6.63	1.48	1.37
2	2	93	PSU	C2-N3	6.62	1.48	1.37
2	2	681	PSU	C2-N3	6.59	1.48	1.37
2	2	649	PSU	C2-N3	6.59	1.48	1.37
2	2	172	OMU	C2-N3	6.56	1.49	1.38
2	2	863	PSU	C2-N3	6.56	1.48	1.37
2	2	651	PSU	C2-N3	6.52	1.48	1.37
2	2	1445	PSU	C2-N3	6.51	1.48	1.37
2	2	1046	PSU	C2-N3	6.51	1.48	1.37
2	2	172	OMU	C2-N1	6.48	1.48	1.38
2	2	1288	OMU	C2-N1	6.47	1.48	1.38
2	2	354	OMU	C2-N1	6.43	1.48	1.38
2	2	1442	OMU	C2-N1	6.42	1.48	1.38
2	2	1056	PSU	C2-N3	6.34	1.48	1.37
2	2	822	PSU	C2-N3	6.28	1.48	1.37
2	2	1232	PSU	C2-N3	6.28	1.48	1.37
2	2	1326	OMU	C2-N1	6.28	1.48	1.38
2	2	1288	OMU	C2-N3	6.28	1.49	1.38
2	2	1337	4AC	C7-N4	6.22	1.48	1.37
2	2	116	OMU	C2-N3	6.22	1.49	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	406	PSU	C2-N3	6.19	1.48	1.37
2	2	1081	PSU	C2-N3	6.19	1.48	1.37
2	2	428	OMU	C2-N1	6.18	1.48	1.38
2	2	814	PSU	C2-N3	6.17	1.48	1.37
2	2	1326	OMU	C2-N3	6.15	1.48	1.38
2	2	109	PSU	C2-N3	6.14	1.48	1.37
2	2	116	OMU	C2-N1	6.14	1.48	1.38
2	2	1238	PSU	C2-N3	6.11	1.48	1.37
2	2	815	PSU	C2-N3	6.10	1.48	1.37
2	2	428	OMU	C2-N3	6.10	1.48	1.38
2	2	1337	4AC	C6-C5	6.07	1.49	1.35
2	2	174	OMC	C6-C5	6.05	1.49	1.35
2	2	1442	OMU	C2-N3	6.03	1.48	1.38
2	2	1337	4AC	C4-N3	5.97	1.43	1.32
2	2	1692	PSU	C2-N3	5.82	1.47	1.37
2	2	436	OMG	C4-N3	5.79	1.48	1.34
2	2	121	OMU	C2-N3	5.78	1.48	1.38
2	2	462	OMC	C6-C5	5.77	1.48	1.35
2	2	1136	PSU	C2-N3	5.73	1.47	1.37
2	2	354	OMU	C2-N3	5.73	1.48	1.38
2	2	121	OMU	C2-N1	5.70	1.47	1.38
2	2	517	OMC	C6-C5	5.67	1.48	1.35
2	2	354	OMU	C6-C5	5.59	1.48	1.35
2	2	683	OMG	C4-N3	5.58	1.47	1.34
2	2	1842	4AC	C6-C5	5.58	1.48	1.35
2	2	1328	OMG	C4-N3	5.57	1.47	1.34
2	2	1391	OMC	C6-C5	5.54	1.47	1.35
2	2	428	OMU	C6-C5	5.52	1.47	1.35
2	2	121	OMU	C6-C5	5.50	1.47	1.35
2	2	1272	OMC	C6-C5	5.46	1.47	1.35
2	2	1272	OMC	C2-N3	5.43	1.47	1.36
2	2	1447	OMG	C4-N3	5.41	1.47	1.34
2	2	174	OMC	C2-N3	5.37	1.47	1.36
2	2	1391	OMC	C2-N3	5.34	1.47	1.36
2	2	1442	OMU	C6-C5	5.28	1.47	1.35
2	2	462	OMC	C2-N3	5.27	1.47	1.36
2	2	1703	OMC	C6-C5	5.27	1.47	1.35
2	2	1248	B8N	C2-N1	5.23	1.54	1.39
2	2	1288	OMU	C6-C5	5.23	1.47	1.35
2	2	1842	4AC	C4-N3	5.20	1.41	1.32
2	2	644	OMG	C4-N3	5.16	1.46	1.34
2	2	1383	A2M	O4'-C1'	-5.15	1.29	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	509	OMG	C4-N3	5.15	1.46	1.34
2	2	517	OMC	C2-N3	5.13	1.46	1.36
2	2	601	OMG	C4-N3	5.13	1.46	1.34
2	2	116	OMU	C6-C5	5.12	1.46	1.35
2	2	1337	4AC	C4-N4	5.11	1.47	1.39
2	2	590	A2M	O4'-C1'	-5.11	1.29	1.42
2	2	172	OMU	C6-C5	5.08	1.46	1.35
2	2	1703	OMC	C2-N3	5.07	1.46	1.36
2	2	1045	PSU	C6-N1	5.05	1.44	1.36
2	2	1326	OMU	C6-C5	5.01	1.46	1.35
2	2	576	A2M	O4'-C1'	-5.01	1.30	1.42
2	2	468	A2M	O4'-C1'	-5.01	1.30	1.42
2	2	1031	A2M	O4'-C1'	-5.00	1.30	1.42
2	2	119	PSU	C6-N1	4.94	1.44	1.36
2	2	1842	4AC	C7-N4	4.94	1.46	1.37
2	2	1337	4AC	C5-C4	4.92	1.51	1.40
2	2	512	A2M	O4'-C1'	-4.89	1.30	1.42
2	2	1337	4AC	C2-N3	4.86	1.46	1.36
2	2	822	PSU	C6-N1	4.68	1.44	1.36
2	2	109	PSU	C6-N1	4.66	1.44	1.36
2	2	1337	4AC	C2-N1	4.66	1.50	1.40
2	2	1842	4AC	C5-C4	4.61	1.50	1.40
2	2	166	A2M	O4'-C1'	-4.61	1.31	1.42
2	2	815	PSU	C6-N1	4.58	1.43	1.36
2	2	1081	PSU	C6-N1	4.58	1.43	1.36
2	2	1391	OMC	C4-N4	4.57	1.44	1.33
2	2	159	A2M	O4'-C1'	-4.57	1.31	1.42
2	2	99	A2M	O4'-C1'	-4.57	1.31	1.42
2	2	644	OMG	C2-N3	4.54	1.44	1.33
2	2	1046	PSU	C6-N1	4.49	1.43	1.36
2	2	572	PSU	C6-N1	4.49	1.43	1.36
2	2	406	PSU	C6-N1	4.48	1.43	1.36
2	2	296	PSU	C6-N1	4.48	1.43	1.36
2	2	1328	OMG	C2-N3	4.48	1.44	1.33
2	2	93	PSU	C6-N1	4.47	1.43	1.36
2	2	649	PSU	C6-N1	4.46	1.43	1.36
2	2	166	A2M	C6-N6	4.46	1.45	1.34
2	2	1445	PSU	C6-N1	4.45	1.43	1.36
2	2	1447	OMG	C2-N3	4.45	1.43	1.33
2	2	174	OMC	C4-N4	4.43	1.44	1.33
2	2	1703	OMC	O2-C2	-4.43	1.15	1.23
2	2	1842	4AC	O2-C2	-4.43	1.15	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	X	62	HY3	C5-N	-4.40	1.33	1.49
2	2	686	PSU	C6-N1	4.39	1.43	1.36
2	2	436	OMG	C2-N3	4.38	1.43	1.33
2	2	1850	MA6	C5-C4	4.37	1.47	1.39
2	2	814	PSU	C6-N1	4.37	1.43	1.36
2	2	1232	PSU	C6-N1	4.37	1.43	1.36
2	2	462	OMC	C4-N4	4.37	1.44	1.33
2	2	1625	PSU	C6-N1	4.36	1.43	1.36
2	2	1272	OMC	C4-N4	4.34	1.44	1.33
2	2	484	A2M	C5-C4	4.33	1.47	1.39
2	2	576	A2M	C6-N6	4.33	1.45	1.34
2	2	683	OMG	C2-N3	4.32	1.43	1.33
2	2	159	A2M	C6-N6	4.32	1.45	1.34
2	2	1447	OMG	C2-N2	4.31	1.44	1.34
2	2	27	A2M	C5-C4	4.31	1.47	1.39
2	2	1136	PSU	C6-N1	4.29	1.43	1.36
2	2	517	OMC	C4-N4	4.29	1.44	1.33
2	2	1851	MA6	C5-C4	4.29	1.47	1.39
2	2	1328	OMG	C2-N2	4.26	1.44	1.34
2	2	436	OMG	C2-N2	4.22	1.44	1.34
2	2	683	OMG	C2-N2	4.19	1.44	1.34
2	2	1842	4AC	C4-N4	4.19	1.45	1.39
2	2	1238	PSU	C6-N1	4.19	1.43	1.36
2	2	174	OMC	C4-N3	4.18	1.42	1.34
2	2	105	PSU	C6-N1	4.17	1.43	1.36
2	2	462	OMC	C4-N3	4.17	1.42	1.34
2	2	1272	OMC	C4-N3	4.16	1.42	1.34
2	2	509	OMG	C2-N3	4.15	1.43	1.33
2	2	1842	4AC	C2-N1	4.14	1.49	1.40
2	2	1703	OMC	C4-N3	4.14	1.42	1.34
2	2	601	OMG	C2-N3	4.13	1.43	1.33
2	2	1248	B8N	C6-C5	4.13	1.40	1.34
2	2	668	A2M	C5-C4	4.12	1.46	1.39
2	2	468	A2M	C6-N6	4.12	1.44	1.34
2	2	354	OMU	O4-C4	-4.09	1.16	1.24
2	2	1391	OMC	C4-N3	4.08	1.42	1.34
2	2	601	OMG	O6-C6	-4.07	1.15	1.23
2	2	1703	OMC	C4-N4	4.06	1.43	1.33
2	2	863	PSU	C6-N1	4.05	1.42	1.36
2	2	1678	A2M	C5-C4	4.04	1.46	1.39
2	2	99	A2M	C6-N6	4.01	1.44	1.34
2	2	681	PSU	C6-N1	4.00	1.42	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	509	OMG	O6-C6	-3.99	1.16	1.23
2	2	1031	A2M	C6-N6	3.98	1.44	1.34
2	2	1244	PSU	C6-N1	3.95	1.42	1.36
2	2	590	A2M	C6-N6	3.95	1.44	1.34
2	2	512	A2M	C6-N6	3.95	1.44	1.34
2	2	517	OMC	C4-N3	3.91	1.42	1.34
2	2	462	OMC	C2-N1	3.90	1.48	1.40
2	2	1692	PSU	C6-N1	3.89	1.42	1.36
2	2	1288	OMU	C4-N3	3.88	1.45	1.38
2	2	1272	OMC	C2-N1	3.88	1.48	1.40
2	2	509	OMG	C4-N9	-3.87	1.28	1.38
2	2	1326	OMU	C4-N3	3.86	1.45	1.38
2	2	651	PSU	C6-N1	3.86	1.42	1.36
2	2	1326	OMU	O4-C4	-3.85	1.17	1.24
2	2	174	OMC	C2-N1	3.85	1.48	1.40
2	2	1056	PSU	C6-N1	3.84	1.42	1.36
2	2	1692	PSU	O4-C4	-3.84	1.16	1.23
2	2	601	OMG	C2-N2	3.82	1.43	1.34
2	2	1383	A2M	C5-C4	-3.81	1.31	1.39
2	2	1383	A2M	C6-N6	3.80	1.43	1.34
2	2	296	PSU	C4-N3	3.79	1.45	1.38
2	2	644	OMG	C4-N9	-3.78	1.28	1.38
2	2	172	OMU	C4-N3	3.76	1.45	1.38
2	2	681	PSU	O4-C4	-3.74	1.16	1.23
2	2	109	PSU	O4-C4	-3.72	1.16	1.23
2	2	1238	PSU	O4-C4	-3.72	1.16	1.23
2	2	1391	OMC	C2-N1	3.71	1.48	1.40
2	2	517	OMC	C2-N1	3.70	1.48	1.40
2	2	509	OMG	C2-N2	3.69	1.43	1.34
2	2	1442	OMU	O4-C4	-3.69	1.17	1.24
2	2	1328	OMG	O6-C6	-3.66	1.16	1.23
2	2	1045	PSU	C4-N3	3.64	1.45	1.38
2	2	863	PSU	O4-C4	-3.64	1.16	1.23
2	2	644	OMG	C2-N2	3.63	1.42	1.34
2	2	1832	6MZ	C5-N7	-3.61	1.32	1.39
2	2	822	PSU	O4-C4	-3.60	1.16	1.23
2	2	116	OMU	O4-C4	-3.59	1.17	1.24
2	2	1442	OMU	C4-N3	3.57	1.45	1.38
2	2	428	OMU	O4-C4	-3.55	1.17	1.24
2	2	121	OMU	O4-C4	-3.53	1.17	1.24
2	2	1703	OMC	C2-N1	3.52	1.47	1.40
2	2	601	OMG	C5-N7	-3.51	1.32	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1842	4AC	C2-N3	3.49	1.43	1.36
2	2	1244	PSU	C4-N3	3.48	1.45	1.38
2	2	428	OMU	C4-N3	3.47	1.44	1.38
2	2	436	OMG	O6-C6	-3.47	1.17	1.23
2	2	814	PSU	C4-N3	3.46	1.45	1.38
2	2	1383	A2M	C8-N9	-3.45	1.31	1.37
2	2	509	OMG	C5-N7	-3.45	1.32	1.39
2	2	683	OMG	C4-N9	-3.45	1.29	1.38
2	2	462	OMC	O2-C2	-3.44	1.17	1.23
2	2	105	PSU	O2-C2	-3.43	1.16	1.23
2	2	517	OMC	O2-C2	-3.43	1.17	1.23
2	2	683	OMG	O6-C6	-3.41	1.17	1.23
2	2	172	OMU	O4-C4	-3.40	1.17	1.24
2	2	1288	OMU	O4-C4	-3.40	1.17	1.24
2	2	1244	PSU	O4-C4	-3.40	1.17	1.23
2	2	815	PSU	O4-C4	-3.38	1.17	1.23
2	2	1031	A2M	C5-C4	-3.37	1.32	1.39
2	2	406	PSU	O4-C4	-3.37	1.17	1.23
2	2	512	A2M	C5-C4	-3.37	1.32	1.39
2	2	651	PSU	O4-C4	-3.37	1.17	1.23
2	2	1056	PSU	O4-C4	-3.36	1.17	1.23
2	2	1383	A2M	O3'-C3'	3.36	1.50	1.43
2	2	1445	PSU	O4-C4	-3.34	1.17	1.23
2	2	468	A2M	C5-C4	-3.34	1.32	1.39
2	2	1081	PSU	O4-C4	-3.32	1.17	1.23
2	2	1692	PSU	O2-C2	-3.32	1.16	1.23
2	2	1842	4AC	O7-C7	-3.31	1.15	1.23
2	2	93	PSU	O4-C4	-3.30	1.17	1.23
2	2	1832	6MZ	C8-N9	-3.30	1.31	1.37
2	2	601	OMG	C4-N9	-3.29	1.29	1.38
2	2	1046	PSU	O4-C4	-3.29	1.17	1.23
2	2	105	PSU	O4-C4	-3.28	1.17	1.23
2	2	119	PSU	C4-N3	3.28	1.44	1.38
2	2	1046	PSU	O2-C2	-3.27	1.16	1.23
2	2	1337	4AC	C6-N1	3.26	1.45	1.38
2	2	1272	OMC	O2-C2	-3.26	1.17	1.23
2	2	863	PSU	C4-N3	3.26	1.44	1.38
2	2	116	OMU	C4-N3	3.25	1.44	1.38
2	2	174	OMC	O2-C2	-3.24	1.17	1.23
2	2	1136	PSU	O4-C4	-3.24	1.17	1.23
2	2	1625	PSU	C4-N3	3.24	1.44	1.38
2	2	36	PSU	C4-N3	-3.23	1.32	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	105	PSU	C4-N3	3.23	1.44	1.38
2	2	99	A2M	C5-N7	-3.22	1.32	1.39
2	2	166	A2M	C5-C4	-3.22	1.33	1.39
18	X	62	HY3	C4-C5	3.21	1.58	1.53
2	2	686	PSU	O4-C4	-3.21	1.17	1.23
2	2	121	OMU	O2-C2	-3.21	1.17	1.23
2	2	436	OMG	C4-N9	-3.21	1.29	1.38
2	2	590	A2M	C5-C4	-3.21	1.33	1.39
2	2	1391	OMC	O2-C2	-3.20	1.17	1.23
2	2	1445	PSU	C4-N3	3.19	1.44	1.38
2	2	1081	PSU	O2-C2	-3.19	1.16	1.23
2	2	1337	4AC	O2-C2	-3.18	1.17	1.23
2	2	572	PSU	C4-N3	3.18	1.44	1.38
2	2	576	A2M	C8-N9	-3.18	1.31	1.37
2	2	1136	PSU	O2-C2	-3.18	1.16	1.23
2	2	1328	OMG	C5-N7	-3.17	1.32	1.39
2	2	1383	A2M	C5-N7	-3.17	1.33	1.39
2	2	649	PSU	O4-C4	-3.16	1.17	1.23
2	2	1272	OMC	C6-N1	3.16	1.45	1.38
2	2	683	OMG	C5-N7	-3.16	1.33	1.39
2	2	649	PSU	C4-N3	3.16	1.44	1.38
2	2	822	PSU	C4-N3	3.15	1.44	1.38
2	2	436	OMG	C5-N7	-3.14	1.33	1.39
2	2	354	OMU	O2-C2	-3.13	1.17	1.23
2	2	644	OMG	O6-C6	-3.13	1.17	1.23
2	2	649	PSU	O2-C2	-3.13	1.16	1.23
2	2	681	PSU	O2-C2	-3.12	1.16	1.23
2	2	1031	A2M	C5-N7	-3.12	1.33	1.39
2	2	354	OMU	C4-N3	3.12	1.44	1.38
2	2	1832	6MZ	C5-C4	-3.12	1.33	1.39
17	V	1	AME	CT1-N	3.12	1.45	1.34
2	2	1347	PSU	C4-N3	-3.11	1.33	1.38
2	2	1639	7MG	C4-N9	-3.11	1.34	1.37
2	2	681	PSU	C4-N3	3.10	1.44	1.38
2	2	1391	OMC	C6-N1	3.10	1.45	1.38
2	2	1238	PSU	C4-N3	3.10	1.44	1.38
2	2	462	OMC	C6-N1	3.10	1.45	1.38
2	2	1232	PSU	O4-C4	-3.09	1.17	1.23
2	2	1643	PSU	C4-N3	-3.08	1.33	1.38
2	2	572	PSU	O4-C4	-3.08	1.17	1.23
2	2	590	A2M	C5-N7	-3.08	1.33	1.39
2	2	644	OMG	C5-N7	-3.08	1.33	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1832	6MZ	C6-N1	-3.08	1.30	1.35
2	2	1447	OMG	C5-N7	-3.07	1.33	1.39
2	2	119	PSU	O4-C4	-3.07	1.17	1.23
2	2	517	OMC	C6-N1	3.07	1.45	1.38
2	2	576	A2M	C5-C4	-3.06	1.33	1.39
2	2	814	PSU	O4-C4	-3.06	1.17	1.23
2	2	1442	OMU	O2-C2	-3.06	1.17	1.23
2	2	109	PSU	O2-C2	-3.06	1.17	1.23
2	2	1692	PSU	C4-N3	3.05	1.44	1.38
2	2	686	PSU	C4-N3	3.05	1.44	1.38
35	A	2	SAC	C1A-N	3.05	1.44	1.34
2	2	576	A2M	C5-N7	-3.05	1.33	1.39
2	2	863	PSU	O2-C2	-3.04	1.17	1.23
2	2	1232	PSU	C4-N3	3.03	1.44	1.38
2	2	1347	PSU	C6-C5	3.02	1.38	1.35
2	2	1056	PSU	C4-N3	3.01	1.44	1.38
2	2	651	PSU	O2-C2	-3.01	1.17	1.23
2	2	1625	PSU	O4-C4	-3.01	1.17	1.23
2	2	99	A2M	C5-C4	-3.01	1.33	1.39
2	2	121	OMU	C4-N3	3.01	1.43	1.38
2	2	1447	OMG	C4-N9	-3.01	1.30	1.38
2	2	590	A2M	C8-N9	-3.00	1.32	1.37
2	2	814	PSU	O2-C2	-3.00	1.17	1.23
2	2	296	PSU	O4-C4	-3.00	1.17	1.23
2	2	1244	PSU	O2-C2	-3.00	1.17	1.23
2	2	822	PSU	O2-C2	-2.99	1.17	1.23
2	2	815	PSU	C4-N3	2.99	1.44	1.38
2	2	116	OMU	O2-C2	-2.99	1.17	1.23
2	2	1326	OMU	O2-C2	-2.98	1.17	1.23
2	2	1232	PSU	O2-C2	-2.98	1.17	1.23
2	2	159	A2M	C5-N7	-2.98	1.33	1.39
2	2	93	PSU	O2-C2	-2.97	1.17	1.23
2	2	93	PSU	C4-N3	2.97	1.44	1.38
2	2	1081	PSU	C4-N3	2.97	1.44	1.38
2	2	1056	PSU	O2-C2	-2.97	1.17	1.23
2	2	651	PSU	C4-N3	2.97	1.44	1.38
2	2	1625	PSU	O2-C2	-2.96	1.17	1.23
2	2	1238	PSU	O2-C2	-2.96	1.17	1.23
2	2	1031	A2M	C8-N9	-2.96	1.32	1.37
2	2	686	PSU	O2-C2	-2.96	1.17	1.23
2	2	1177	PSU	C4-N3	-2.96	1.33	1.38
2	2	174	OMC	C6-N1	2.96	1.45	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	119	PSU	O2-C2	-2.95	1.17	1.23
2	2	512	A2M	C8-N9	-2.95	1.32	1.37
2	2	576	A2M	O2'-C2'	-2.95	1.35	1.42
2	2	159	A2M	C5-C4	-2.93	1.33	1.39
2	2	1383	A2M	O2'-C2'	-2.92	1.35	1.42
2	2	406	PSU	O2-C2	-2.91	1.17	1.23
2	2	1445	PSU	O2-C2	-2.91	1.17	1.23
2	2	1174	PSU	C6-C5	2.90	1.38	1.35
2	2	1490	OMG	C5-C4	2.89	1.46	1.38
2	2	468	A2M	C5-N7	-2.89	1.33	1.39
2	2	1328	OMG	C4-N9	-2.87	1.30	1.38
2	2	1639	7MG	C5-C4	2.87	1.47	1.38
2	2	512	A2M	C5-N7	-2.87	1.33	1.39
2	2	1643	PSU	C6-C5	2.87	1.38	1.35
2	2	99	A2M	C8-N9	-2.87	1.32	1.37
2	2	406	PSU	C4-N3	2.86	1.44	1.38
2	2	1447	OMG	O6-C6	-2.85	1.18	1.23
2	2	428	OMU	C6-N1	2.84	1.44	1.38
2	2	172	OMU	O2-C2	-2.84	1.17	1.23
2	2	109	PSU	C4-N3	2.83	1.44	1.38
2	2	1174	PSU	C4-N3	-2.83	1.33	1.38
2	2	1046	PSU	C4-N3	2.82	1.44	1.38
2	2	159	A2M	O2'-C2'	-2.80	1.35	1.42
2	2	572	PSU	O2-C2	-2.80	1.17	1.23
2	2	815	PSU	O2-C2	-2.78	1.17	1.23
2	2	468	A2M	C8-N9	-2.77	1.32	1.37
2	2	512	A2M	O3'-C3'	2.77	1.49	1.43
2	2	1703	OMC	C6-N1	2.76	1.44	1.38
2	2	428	OMU	O2-C2	-2.76	1.18	1.23
2	2	99	A2M	O2'-C2'	-2.74	1.35	1.42
2	2	159	A2M	C8-N9	-2.74	1.32	1.37
2	2	354	OMU	C6-N1	2.74	1.44	1.38
2	2	1045	PSU	O4-C4	-2.73	1.18	1.23
2	2	1326	OMU	C6-N1	2.73	1.44	1.38
2	2	512	A2M	O2'-C2'	-2.72	1.35	1.42
2	2	1288	OMU	O2-C2	-2.72	1.18	1.23
2	2	1851	MA6	C5-C6	2.69	1.48	1.41
2	2	1031	A2M	O2'-C2'	-2.69	1.35	1.42
2	2	1842	4AC	C6-N1	2.69	1.44	1.38
2	2	590	A2M	O2'-C2'	-2.68	1.35	1.42
2	2	166	A2M	C5-N7	-2.67	1.34	1.39
2	2	1337	4AC	O7-C7	-2.67	1.17	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	166	A2M	C8-N9	-2.66	1.32	1.37
2	2	36	PSU	C6-C5	2.64	1.38	1.35
2	2	468	A2M	O3'-C3'	2.63	1.49	1.43
2	2	121	OMU	C6-N1	2.62	1.44	1.38
2	2	484	A2M	C5-N7	-2.60	1.34	1.39
2	2	1288	OMU	C6-N1	2.60	1.44	1.38
2	2	1851	MA6	C8-N7	2.57	1.36	1.31
2	2	166	A2M	O2'-C2'	-2.56	1.36	1.42
2	2	1177	PSU	C6-C5	2.56	1.38	1.35
2	2	1639	7MG	C6-N1	-2.55	1.34	1.38
2	2	668	A2M	C5-C6	2.55	1.48	1.41
2	2	576	A2M	O3'-C3'	2.54	1.49	1.43
2	2	296	PSU	O2-C2	-2.54	1.18	1.23
2	2	468	A2M	O2'-C2'	-2.53	1.36	1.42
2	2	1490	OMG	C6-N1	-2.53	1.34	1.38
2	2	1045	PSU	O2-C2	-2.52	1.18	1.23
2	2	166	A2M	O3'-C3'	2.51	1.48	1.43
2	2	27	A2M	C5-C6	2.50	1.48	1.41
2	2	668	A2M	C4-N9	-2.47	1.32	1.37
2	2	1383	A2M	C4-N9	-2.47	1.32	1.37
2	2	27	A2M	C5-N7	-2.44	1.34	1.39
2	2	484	A2M	C5-C6	2.44	1.47	1.41
2	2	159	A2M	O3'-C3'	2.44	1.48	1.43
2	2	1248	B8N	O2-C2	-2.44	1.18	1.22
2	2	1447	OMG	C2-N1	2.43	1.43	1.37
2	2	1678	A2M	C5-C6	2.42	1.47	1.41
2	2	1328	OMG	C2-N1	2.41	1.43	1.37
2	2	1081	PSU	O4'-C1'	-2.41	1.40	1.43
2	2	668	A2M	C5-N7	-2.41	1.34	1.39
2	2	517	OMC	C5-C4	2.41	1.48	1.42
2	2	1248	B8N	O4-C4	-2.41	1.18	1.23
2	2	428	OMU	C5-C4	2.40	1.48	1.43
2	2	1442	OMU	C6-N1	2.40	1.43	1.38
2	2	354	OMU	C5-C4	2.40	1.48	1.43
2	2	644	OMG	C5-C6	2.39	1.53	1.44
2	2	576	A2M	C4-N9	-2.38	1.32	1.37
2	2	116	OMU	C6-N1	2.38	1.43	1.38
2	2	512	A2M	O5'-C5'	-2.37	1.38	1.44
2	2	1850	MA6	C5-N7	-2.37	1.34	1.39
2	2	1490	OMG	C5-N7	-2.36	1.34	1.39
2	2	1678	A2M	C5-N7	-2.35	1.34	1.39
2	2	1031	A2M	O3'-C3'	2.34	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	436	OMG	C5-C6	2.34	1.53	1.44
2	2	683	OMG	C2-N1	2.34	1.43	1.37
2	2	509	OMG	C5-C6	2.33	1.53	1.44
2	2	590	A2M	O3'-C3'	2.33	1.48	1.43
2	2	36	PSU	C2-N3	-2.32	1.33	1.37
2	2	601	OMG	C5-C6	2.31	1.53	1.44
2	2	1272	OMC	C5-C4	2.30	1.48	1.42
2	2	1447	OMG	C5-C6	2.30	1.52	1.44
2	2	1850	MA6	C5-C6	2.30	1.47	1.41
2	2	601	OMG	C2-N1	2.27	1.43	1.37
2	2	1031	A2M	O5'-C5'	-2.26	1.39	1.44
2	2	99	A2M	O3'-C3'	2.26	1.48	1.43
2	2	462	OMC	C5-C4	2.24	1.48	1.42
2	2	1703	OMC	C5-C4	2.24	1.48	1.42
2	2	1832	6MZ	C4-N9	-2.24	1.32	1.37
2	2	1328	OMG	C5-C6	2.24	1.52	1.44
2	2	822	PSU	O4'-C1'	-2.23	1.40	1.43
2	2	1347	PSU	C2-N3	-2.23	1.33	1.37
2	2	1328	OMG	C6-N1	2.22	1.43	1.38
2	2	166	A2M	O5'-C5'	-2.21	1.39	1.44
2	2	1851	MA6	C4-N9	-2.20	1.32	1.37
2	2	436	OMG	C2-N1	2.20	1.43	1.37
2	2	509	OMG	C2-N1	2.19	1.43	1.37
2	2	468	A2M	C4-N9	-2.18	1.32	1.37
2	2	651	PSU	O4'-C1'	-2.18	1.40	1.43
2	2	484	A2M	C4-N9	-2.17	1.32	1.37
18	X	62	HY3	C4-C3	2.16	1.56	1.52
2	2	1643	PSU	C2-N3	-2.16	1.33	1.37
2	2	172	OMU	C6-N1	2.16	1.43	1.38
35	A	2	SAC	OAC-C1A	-2.16	1.18	1.23
2	2	1447	OMG	C6-N1	2.16	1.42	1.38
2	2	683	OMG	C5-C6	2.15	1.52	1.44
2	2	1136	PSU	C4-N3	2.15	1.42	1.38
2	2	1442	OMU	C5-C4	2.14	1.48	1.43
2	2	1174	PSU	C2-N3	-2.13	1.33	1.37
2	2	1248	B8N	O4'-C1'	-2.12	1.40	1.43
2	2	1643	PSU	C2'-C1'	-2.12	1.51	1.53
2	2	36	PSU	C2-N1	-2.12	1.33	1.36
2	2	1031	A2M	C4-N9	-2.11	1.33	1.37
2	2	576	A2M	O5'-C5'	-2.10	1.39	1.44
2	2	174	OMC	C5-C4	2.09	1.47	1.42
2	2	27	A2M	C8-N7	2.08	1.35	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1383	A2M	O5'-C5'	-2.07	1.39	1.44
2	2	1326	OMU	C5-C4	2.06	1.48	1.43
2	2	1177	PSU	C2-N3	-2.06	1.34	1.37
2	2	468	A2M	O5'-C5'	-2.05	1.39	1.44
2	2	1391	OMC	C5-C4	2.04	1.47	1.42
2	2	644	OMG	C2-N1	2.03	1.42	1.37
2	2	644	OMG	C6-N1	2.02	1.42	1.38
2	2	1678	A2M	C8-N7	2.02	1.35	1.31
2	2	681	PSU	O4'-C1'	-2.02	1.41	1.43
2	2	668	A2M	C8-N7	2.02	1.35	1.31
2	2	1177	PSU	C2-N1	-2.01	1.34	1.36
2	2	121	OMU	C5-C4	2.01	1.48	1.43
2	2	1136	PSU	O4'-C1'	-2.01	1.41	1.43
2	2	1851	MA6	C5-N7	-2.01	1.35	1.39

All (497) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1639	7MG	N9-C4-N3	8.72	138.51	125.47
2	2	468	A2M	N6-C6-N1	-6.94	103.14	118.35
2	2	590	A2M	N6-C6-N1	-6.78	103.51	118.35
2	2	1328	OMG	C1'-N9-C8	-6.77	107.43	126.70
2	2	590	A2M	C5-C4-N3	-6.64	118.09	126.75
2	2	159	A2M	N6-C6-N1	-6.62	103.85	118.35
2	2	1326	OMU	C4-N3-C2	-6.52	117.98	126.58
2	2	1031	A2M	N3-C2-N1	-6.32	118.72	128.60
2	2	1447	OMG	C1'-N9-C8	-6.29	108.81	126.70
2	2	468	A2M	C5-C6-N6	6.21	136.94	123.43
2	2	1678	A2M	C5-C4-N3	-6.19	118.68	126.75
2	2	27	A2M	C5-C4-N3	-6.19	118.68	126.75
2	2	512	A2M	N9-C8-N7	-6.18	105.46	113.91
2	2	166	A2M	N6-C6-N1	-6.17	104.83	118.35
2	2	1832	6MZ	N1-C2-N3	-6.16	118.96	128.60
2	2	1031	A2M	N6-C6-N1	-6.15	104.88	118.35
2	2	99	A2M	N3-C2-N1	-6.13	119.01	128.60
2	2	468	A2M	N9-C8-N7	-6.12	105.54	113.91
2	2	576	A2M	N6-C6-N1	-6.11	104.98	118.35
2	2	159	A2M	C5-C6-N6	6.10	136.71	123.43
2	2	1347	PSU	N1-C2-N3	6.04	121.97	115.13
2	2	512	A2M	N3-C2-N1	-5.99	119.23	128.60
2	2	1031	A2M	N9-C8-N7	-5.96	105.76	113.91
2	2	159	A2M	N9-C8-N7	-5.93	105.81	113.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1850	MA6	C5-C4-N3	-5.92	119.02	126.75
2	2	1490	OMG	C5-C4-N3	-5.90	118.88	128.46
2	2	590	A2M	N3-C2-N1	-5.86	119.44	128.60
2	2	484	A2M	C5-C4-N3	-5.84	119.13	126.75
2	2	512	A2M	C4-N9-C8	5.82	112.03	105.73
2	2	590	A2M	N3-C4-N9	5.80	136.64	127.08
2	2	1643	PSU	N1-C2-N3	5.80	121.70	115.13
2	2	1442	OMU	C4-N3-C2	-5.80	118.93	126.58
2	2	166	A2M	N9-C8-N7	-5.80	105.98	113.91
2	2	166	A2M	N3-C2-N1	-5.79	119.54	128.60
2	2	1031	A2M	C5-C6-N6	5.73	135.89	123.43
2	2	1383	A2M	N6-C6-N1	-5.71	105.84	118.35
2	2	512	A2M	N6-C6-N1	-5.71	105.84	118.35
2	2	1850	MA6	N1-C6-N6	5.70	123.32	117.08
2	2	1383	A2M	N9-C8-N7	-5.70	106.12	113.91
2	2	576	A2M	C5-C6-N6	5.69	135.80	123.43
2	2	99	A2M	N6-C6-N1	-5.68	105.92	118.35
2	2	1174	PSU	N1-C2-N3	5.66	121.54	115.13
2	2	354	OMU	C4-N3-C2	-5.65	119.13	126.58
2	2	1031	A2M	C4-N9-C1'	-5.63	113.18	126.59
2	2	36	PSU	N1-C2-N3	5.62	121.50	115.13
2	2	590	A2M	C5-C6-N6	5.62	135.67	123.43
2	2	99	A2M	N9-C8-N7	-5.60	106.25	113.91
2	2	99	A2M	N3-C4-N9	5.60	136.31	127.08
2	2	1851	MA6	C5-C4-N3	-5.59	119.46	126.75
2	2	1177	PSU	N1-C2-N3	5.54	121.41	115.13
2	2	1328	OMG	C1'-N9-C4	5.53	142.93	126.50
2	2	651	PSU	N1-C2-N3	5.53	121.39	115.13
2	2	166	A2M	C5-C6-N6	5.52	135.43	123.43
2	2	436	OMG	C1'-N9-C8	-5.49	111.06	126.70
2	2	468	A2M	N3-C2-N1	-5.49	120.02	128.60
2	2	1244	PSU	C4-N3-C2	-5.48	118.44	126.34
2	2	1383	A2M	N3-C2-N1	-5.46	120.06	128.60
2	2	576	A2M	N9-C8-N7	-5.45	106.46	113.91
2	2	159	A2M	C5-C4-N3	-5.44	119.65	126.75
2	2	576	A2M	N3-C2-N1	-5.42	120.13	128.60
2	2	590	A2M	N9-C8-N7	-5.41	106.52	113.91
2	2	1383	A2M	C4-N9-C8	5.40	111.58	105.73
2	2	1288	OMU	C4-N3-C2	-5.40	119.46	126.58
2	2	99	A2M	C5-C4-N3	-5.39	119.72	126.75
2	2	99	A2M	C4-N9-C8	5.38	111.56	105.73
2	2	172	OMU	C4-N3-C2	-5.38	119.48	126.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	512	A2M	N3-C4-N9	5.36	135.92	127.08
2	2	1639	7MG	N9-C8-N7	-5.33	95.75	103.38
2	2	1447	OMG	C1'-N9-C4	5.32	142.31	126.50
2	2	468	A2M	C4-N9-C8	5.32	111.49	105.73
2	2	1639	7MG	C5-C4-N3	-5.32	118.00	128.13
2	2	468	A2M	C4-N9-C1'	-5.30	113.95	126.59
2	2	512	A2M	C5-C4-N3	-5.29	119.84	126.75
2	2	863	PSU	C4-N3-C2	-5.28	118.73	126.34
2	2	1383	A2M	C5-C6-N6	5.26	134.88	123.43
2	2	99	A2M	C5-C6-N6	5.26	134.87	123.43
2	2	105	PSU	C4-N3-C2	-5.25	118.77	126.34
2	2	166	A2M	C4-N9-C1'	-5.25	114.09	126.59
2	2	668	A2M	C5-C4-N3	-5.23	119.93	126.75
2	2	121	OMU	C4-N3-C2	-5.23	119.69	126.58
2	2	105	PSU	N1-C2-N3	5.22	121.05	115.13
2	2	601	OMG	C1'-N9-C8	-5.20	111.89	126.70
2	2	159	A2M	C4-N9-C1'	-5.19	114.22	126.59
2	2	109	PSU	C4-N3-C2	-5.19	118.86	126.34
2	2	1337	4AC	CM7-C7-N4	5.19	124.26	115.29
2	2	1056	PSU	C4-N3-C2	-5.16	118.90	126.34
2	2	644	OMG	C1'-N9-C8	-5.14	112.06	126.70
2	2	576	A2M	C4-N9-C1'	-5.14	114.35	126.59
2	2	1383	A2M	C4-N9-C1'	-5.13	114.37	126.59
2	2	159	A2M	N3-C2-N1	-5.12	120.59	128.60
2	2	681	PSU	C4-N3-C2	-5.12	118.97	126.34
2	2	1031	A2M	C5-C4-N3	-5.09	120.11	126.75
2	2	651	PSU	C4-N3-C2	-5.07	119.04	126.34
2	2	1248	B8N	C5-C4-N3	5.07	125.55	116.17
2	2	649	PSU	C4-N3-C2	-5.05	119.06	126.34
2	2	1031	A2M	C4-N9-C8	5.05	111.20	105.73
2	2	1678	A2M	N3-C4-N9	5.04	135.38	127.08
2	2	166	A2M	C5-C4-N3	-5.03	120.19	126.75
2	2	1244	PSU	N1-C2-N3	5.01	120.81	115.13
2	2	576	A2M	C5-C4-N3	-4.99	120.24	126.75
2	2	1056	PSU	N1-C2-N3	4.98	120.77	115.13
2	2	686	PSU	C4-N3-C2	-4.98	119.17	126.34
2	2	512	A2M	C5-C6-N6	4.92	134.13	123.43
2	2	815	PSU	C4-N3-C2	-4.89	119.29	126.34
2	2	576	A2M	C4-N9-C8	4.89	111.03	105.73
2	2	1490	OMG	C2-N3-C4	4.88	121.00	112.30
2	2	683	OMG	C1'-N9-C8	-4.88	112.80	126.70
2	2	1850	MA6	N3-C4-N9	4.86	135.09	127.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	468	A2M	C5-C4-N3	-4.84	120.43	126.75
2	2	1238	PSU	C4-N3-C2	-4.84	119.37	126.34
2	2	686	PSU	N1-C2-N3	4.83	120.61	115.13
2	2	428	OMU	C4-N3-C2	-4.82	120.22	126.58
2	2	27	A2M	C2'-C1'-N9	-4.82	105.42	113.53
2	2	1383	A2M	C5-C4-N3	-4.81	120.47	126.75
2	2	814	PSU	C4-N3-C2	-4.81	119.41	126.34
2	2	509	OMG	C1'-N9-C8	-4.81	113.01	126.70
2	2	27	A2M	N3-C4-N9	4.80	134.99	127.08
2	2	119	PSU	C4-N3-C2	-4.79	119.44	126.34
2	2	1851	MA6	C10-N6-C6	-4.77	108.04	120.40
2	2	1625	PSU	C4-N3-C2	-4.74	119.51	126.34
2	2	1136	PSU	N1-C2-N3	4.72	120.48	115.13
2	2	1081	PSU	C4-N3-C2	-4.72	119.54	126.34
2	2	601	OMG	C2-N3-C4	4.70	120.67	112.30
2	2	863	PSU	N1-C2-N3	4.68	120.44	115.13
2	2	1383	A2M	N3-C4-N9	4.67	134.78	127.08
2	2	1046	PSU	C4-N3-C2	-4.66	119.62	126.34
2	2	572	PSU	N1-C2-N3	4.66	120.41	115.13
2	2	296	PSU	C4-N3-C2	-4.66	119.63	126.34
2	2	1045	PSU	C4-N3-C2	-4.65	119.63	126.34
2	2	1248	B8N	C4-N3-C2	-4.64	119.59	125.46
2	2	649	PSU	N1-C2-N3	4.64	120.39	115.13
2	2	166	A2M	C4-N9-C8	4.62	110.74	105.73
2	2	572	PSU	C4-N3-C2	-4.59	119.73	126.34
2	2	1832	6MZ	C5-C4-N3	-4.58	120.78	126.75
2	2	1031	A2M	N3-C4-N9	4.56	134.59	127.08
2	2	601	OMG	C1'-N9-C4	4.56	140.04	126.50
2	2	1625	PSU	N1-C2-N3	4.54	120.27	115.13
2	2	159	A2M	C4-N9-C8	4.52	110.62	105.73
2	2	93	PSU	C4-N3-C2	-4.51	119.83	126.34
2	2	822	PSU	C4-N3-C2	-4.50	119.85	126.34
2	2	815	PSU	N1-C2-N3	4.48	120.21	115.13
2	2	1692	PSU	C4-N3-C2	-4.48	119.89	126.34
2	2	1832	6MZ	N9-C8-N7	-4.48	107.79	113.91
2	2	512	A2M	C4-N9-C1'	-4.48	115.93	126.59
2	2	1851	MA6	C2-N1-C6	4.45	122.27	111.75
2	2	576	A2M	N3-C4-N9	4.43	134.38	127.08
2	2	1045	PSU	N1-C2-N3	4.43	120.15	115.13
2	2	1326	OMU	C5-C4-N3	4.41	121.44	114.84
2	2	590	A2M	C4-N9-C8	4.39	110.49	105.73
2	2	1445	PSU	C4-N3-C2	-4.39	120.02	126.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	468	A2M	N3-C4-N9	4.38	134.29	127.08
2	2	484	A2M	N3-C4-N9	4.37	134.28	127.08
2	2	1850	MA6	C2-N1-C6	4.37	122.07	111.75
2	2	681	PSU	N1-C2-N3	4.37	120.08	115.13
2	2	1232	PSU	N1-C2-N3	4.37	120.08	115.13
2	2	651	PSU	C6-C5-C4	4.36	121.25	118.20
2	2	1842	4AC	CM7-C7-N4	4.34	122.79	115.29
2	2	354	OMU	N3-C2-N1	4.33	120.64	114.89
2	2	1177	PSU	C4-N3-C2	-4.32	120.11	126.34
2	2	1136	PSU	C4-N3-C2	-4.32	120.11	126.34
2	2	406	PSU	N1-C2-N3	4.31	120.02	115.13
2	2	1692	PSU	N1-C2-N3	4.31	120.01	115.13
2	2	683	OMG	N9-C8-N7	-4.30	105.29	113.39
2	2	1490	OMG	N9-C4-N3	4.29	134.56	125.94
2	2	116	OMU	C4-N3-C2	-4.29	120.92	126.58
2	2	1238	PSU	N1-C2-N3	4.29	119.99	115.13
2	2	296	PSU	N1-C2-N3	4.29	119.99	115.13
2	2	436	OMG	C1'-N9-C4	4.27	139.20	126.50
2	2	1046	PSU	N1-C2-N3	4.27	119.97	115.13
2	2	1851	MA6	C9-N6-C6	-4.23	109.42	120.40
2	2	159	A2M	N3-C4-N9	4.23	134.06	127.08
2	2	822	PSU	N1-C2-N3	4.22	119.91	115.13
2	2	1328	OMG	C2-N3-C4	4.21	119.81	112.30
2	2	109	PSU	N1-C2-N3	4.20	119.89	115.13
2	2	651	PSU	O2-C2-N1	-4.20	118.17	122.79
2	2	166	A2M	N3-C4-N9	4.19	133.99	127.08
2	2	644	OMG	N9-C8-N7	-4.19	105.50	113.39
2	2	119	PSU	N1-C2-N3	4.18	119.86	115.13
2	2	1639	7MG	C2-N3-C4	4.18	119.74	112.30
2	2	1445	PSU	N1-C2-N3	4.17	119.86	115.13
2	2	159	A2M	C5-N7-C8	4.16	109.42	103.51
2	2	1248	B8N	C32-C31-N3	-4.15	104.22	112.00
2	2	590	A2M	C2-N3-C4	4.14	121.54	111.75
2	2	1232	PSU	C4-N3-C2	-4.13	120.39	126.34
2	2	668	A2M	N3-C4-N9	4.10	133.84	127.08
2	2	1328	OMG	C5-C4-N3	-4.05	121.89	128.46
2	2	93	PSU	N1-C2-N3	4.03	119.70	115.13
2	2	644	OMG	C1'-N9-C4	4.03	138.47	126.50
2	2	99	A2M	C4-N9-C1'	-4.03	117.00	126.59
2	2	121	OMU	N3-C2-N1	4.01	120.22	114.89
2	2	1678	A2M	C2-N3-C4	4.00	121.21	111.75
2	2	509	OMG	C1'-N9-C4	4.00	138.39	126.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1447	OMG	C2-N3-C4	3.98	119.39	112.30
2	2	1136	PSU	C6-C5-C4	3.98	120.98	118.20
2	2	509	OMG	C2-N3-C4	3.97	119.38	112.30
2	2	863	PSU	O2-C2-N1	-3.97	118.42	122.79
2	2	406	PSU	C4-N3-C2	-3.97	120.62	126.34
2	2	27	A2M	C2-N3-C4	3.97	121.12	111.75
2	2	354	OMU	C5-C4-N3	3.96	120.76	114.84
2	2	683	OMG	C2-N3-C4	3.93	119.31	112.30
2	2	1832	6MZ	C5-N7-C8	3.93	109.10	103.51
2	2	436	OMG	N9-C8-N7	-3.91	106.02	113.39
2	2	1442	OMU	N3-C2-N1	3.91	120.08	114.89
2	2	644	OMG	C2-N3-C4	3.89	119.23	112.30
2	2	1081	PSU	N1-C2-N3	3.88	119.53	115.13
2	2	1288	OMU	C5-C4-N3	3.88	120.64	114.84
2	2	1842	4AC	C5-C4-N4	3.87	129.63	122.92
2	2	1326	OMU	N3-C2-N1	3.85	120.00	114.89
2	2	1851	MA6	C4-C5-N7	-3.84	105.94	110.62
2	2	166	A2M	C5-N7-C8	3.81	108.93	103.51
2	2	1031	A2M	C5-N7-C8	3.81	108.92	103.51
2	2	484	A2M	C2-N3-C4	3.81	120.75	111.75
2	2	105	PSU	O2-C2-N1	-3.81	118.60	122.79
2	2	601	OMG	C5-C4-N3	-3.79	122.31	128.46
2	2	406	PSU	C6-N1-C2	-3.78	118.82	122.68
2	2	1442	OMU	C5-C4-N3	3.77	120.48	114.84
2	2	1850	MA6	C10-N6-C6	-3.76	110.65	120.40
2	2	1851	MA6	C2-N3-C4	3.76	120.63	111.75
2	2	1031	A2M	C1'-N9-C8	3.76	135.62	127.14
2	2	1174	PSU	C4-N3-C2	-3.75	120.94	126.34
2	2	590	A2M	C5-N7-C8	3.73	108.81	103.51
2	2	1851	MA6	N3-C4-N9	3.72	133.21	127.08
2	2	1347	PSU	C4-N3-C2	-3.72	120.98	126.34
2	2	1643	PSU	C4-N3-C2	-3.72	120.98	126.34
2	2	1328	OMG	N9-C8-N7	-3.71	106.41	113.39
2	2	1850	MA6	C9-N6-C6	-3.70	110.80	120.40
2	2	428	OMU	C5-C4-N3	3.70	120.37	114.84
2	2	814	PSU	N1-C2-N3	3.69	119.32	115.13
2	2	1031	A2M	C2-N3-C4	3.67	120.42	111.75
2	2	512	A2M	C5-N7-C8	3.65	108.69	103.51
2	2	99	A2M	C2-N3-C4	3.65	120.37	111.75
2	2	1056	PSU	C6-C5-C4	3.64	120.75	118.20
2	2	436	OMG	C2-N3-C4	3.64	118.78	112.30
2	2	468	A2M	C5-N7-C8	3.64	108.67	103.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	512	A2M	C2-N3-C4	3.60	120.25	111.75
2	2	1832	6MZ	C2-N3-C4	3.59	120.24	111.75
2	2	1850	MA6	C2-N3-C4	3.59	120.22	111.75
2	2	166	A2M	C2-N3-C4	3.57	120.19	111.75
2	2	172	OMU	N3-C2-N1	3.56	119.62	114.89
2	2	166	A2M	C1'-N9-C8	3.56	135.17	127.14
2	2	159	A2M	C1'-N9-C8	3.55	135.15	127.14
2	2	36	PSU	C4-N3-C2	-3.55	121.23	126.34
2	2	1328	OMG	C2-N1-C6	-3.54	118.65	125.10
17	V	1	AME	CT2-CT1-N	3.53	122.08	116.10
2	2	509	OMG	N9-C8-N7	-3.52	106.76	113.39
2	2	121	OMU	C5-C4-N3	3.52	120.10	114.84
2	2	601	OMG	N9-C8-N7	-3.51	106.77	113.39
2	2	1447	OMG	N9-C8-N7	-3.51	106.78	113.39
2	2	116	OMU	C5-C4-N3	3.50	120.08	114.84
2	2	159	A2M	C2-N3-C4	3.49	120.00	111.75
2	2	1447	OMG	C5-C4-N3	-3.49	122.81	128.46
2	2	1244	PSU	O2-C2-N1	-3.48	118.96	122.79
2	2	668	A2M	C4-C5-N7	-3.48	106.39	110.62
2	2	172	OMU	C5-C4-N3	3.47	120.04	114.84
2	2	27	A2M	N3-C2-N1	-3.47	123.17	128.60
2	2	509	OMG	C5-C4-N3	-3.47	122.83	128.46
2	2	668	A2M	C2-N3-C4	3.46	119.91	111.75
2	2	683	OMG	C1'-N9-C4	3.45	136.75	126.50
2	2	644	OMG	C6-C5-N7	3.44	136.65	130.25
2	2	1347	PSU	O2-C2-N1	-3.44	119.01	122.79
2	2	484	A2M	N3-C2-N1	-3.43	123.24	128.60
2	2	1832	6MZ	C9-N6-C6	3.42	125.82	122.87
2	2	1232	PSU	C6-N1-C2	-3.41	119.20	122.68
2	2	1337	4AC	C5-C4-N4	3.40	128.81	122.92
2	2	1288	OMU	O4-C4-C5	-3.38	119.22	125.16
2	2	27	A2M	C4-C5-N7	-3.38	106.50	110.62
2	2	1625	PSU	O2-C2-N1	-3.38	119.07	122.79
2	2	576	A2M	C5-N7-C8	3.37	108.30	103.51
2	2	1288	OMU	N3-C2-N1	3.36	119.35	114.89
2	2	1678	A2M	N3-C2-N1	-3.35	123.37	128.60
2	2	484	A2M	C4-C5-N7	-3.34	106.56	110.62
2	2	468	A2M	C2-N3-C4	3.33	119.61	111.75
2	2	99	A2M	C5-N7-C8	3.32	108.23	103.51
2	2	1850	MA6	C5-C6-N6	-3.32	119.52	125.30
2	2	1490	OMG	C6-C5-N7	3.32	136.41	130.25
2	2	576	A2M	C2-N3-C4	3.31	119.58	111.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1692	PSU	O2-C2-N1	-3.31	119.14	122.79
2	2	576	A2M	C1'-N9-C8	3.31	134.61	127.14
2	2	651	PSU	C6-N1-C2	-3.31	119.30	122.68
2	2	590	A2M	C4'-O4'-C1'	-3.30	102.19	109.47
2	2	468	A2M	C1'-N9-C8	3.28	134.55	127.14
2	2	1326	OMU	O4-C4-C5	-3.28	119.39	125.16
2	2	172	OMU	O4-C4-C5	-3.28	119.39	125.16
2	2	572	PSU	C6-N1-C2	-3.28	119.33	122.68
2	2	1045	PSU	C6-N1-C2	-3.28	119.33	122.68
2	2	1625	PSU	C6-N1-C2	-3.24	119.36	122.68
2	2	1445	PSU	C6-N1-C2	-3.24	119.37	122.68
2	2	1174	PSU	O2-C2-N1	-3.24	119.23	122.79
2	2	105	PSU	C6-N1-C2	-3.23	119.38	122.68
17	V	1	AME	CE-SD-CG	3.22	111.46	100.40
2	2	668	A2M	C4-N9-C8	3.21	109.21	105.73
2	2	1136	PSU	C6-N1-C2	-3.20	119.41	122.68
2	2	1248	B8N	N3-C2-N1	3.19	121.26	116.76
2	2	1046	PSU	C6-N1-C2	-3.18	119.43	122.68
2	2	686	PSU	C6-N1-C2	-3.18	119.44	122.68
2	2	822	PSU	C6-N1-C2	-3.18	119.44	122.68
2	2	121	OMU	O2-C2-N1	-3.16	118.58	122.79
2	2	1678	A2M	C4-C5-N7	-3.16	106.77	110.62
2	2	590	A2M	C4-N9-C1'	-3.16	119.07	126.59
2	2	1643	PSU	O2-C2-N1	-3.15	119.32	122.79
2	2	1056	PSU	C6-N1-C2	-3.15	119.46	122.68
2	2	1851	MA6	N1-C2-N3	-3.13	123.71	128.60
2	2	428	OMU	N3-C2-N1	3.11	119.02	114.89
2	2	668	A2M	N3-C2-N1	-3.11	123.74	128.60
2	2	1244	PSU	C6-N1-C2	-3.10	119.52	122.68
2	2	1850	MA6	N1-C2-N3	-3.08	123.78	128.60
2	2	1383	A2M	O4'-C1'-C2'	-3.08	101.17	106.57
2	2	1383	A2M	C1'-N9-C8	3.06	134.05	127.14
2	2	1383	A2M	C5-N7-C8	3.04	107.83	103.51
2	2	1678	A2M	C4-N9-C8	3.03	109.02	105.73
2	2	1832	6MZ	C4-C5-N7	-3.03	106.93	110.62
2	2	1383	A2M	C2-N3-C4	3.03	118.90	111.75
2	2	601	OMG	C5-C6-N1	3.02	120.87	113.19
2	2	116	OMU	N3-C2-N1	3.02	118.90	114.89
2	2	1328	OMG	C5-C6-N1	3.02	120.85	113.19
27	O	138	IAS	OXT-C-O	-3.00	117.27	124.09
2	2	683	OMG	C6-C5-N7	2.98	135.79	130.25
2	2	1045	PSU	C6-C5-C4	2.98	120.28	118.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	27	A2M	C5-N7-C8	2.98	107.74	103.51
2	2	509	OMG	C2-N1-C6	-2.97	119.68	125.10
2	2	601	OMG	C6-C5-N7	2.97	135.77	130.25
2	2	644	OMG	C5-C4-N3	-2.96	123.65	128.46
2	2	1177	PSU	O2-C2-N1	-2.96	119.54	122.79
2	2	436	OMG	C5-C4-N3	-2.93	123.71	128.46
2	2	428	OMU	O4-C4-C5	-2.93	120.01	125.16
2	2	644	OMG	C4-C5-N7	-2.92	106.10	110.72
2	2	1832	6MZ	C4-C5-C6	2.92	119.07	116.81
2	2	1678	A2M	C5-N7-C8	2.90	107.63	103.51
2	2	601	OMG	C2-N1-C6	-2.90	119.81	125.10
2	2	1328	OMG	O6-C6-C5	-2.89	118.93	126.60
2	2	1328	OMG	N2-C2-N1	2.89	122.86	116.71
2	2	296	PSU	O2-C2-N1	-2.88	119.62	122.79
2	2	1337	4AC	O7-C7-N4	-2.87	117.17	121.82
2	2	668	A2M	C5-N7-C8	2.87	107.59	103.51
2	2	512	A2M	C2'-C1'-N9	-2.86	108.71	113.53
2	2	1442	OMU	O4-C4-C5	-2.86	120.13	125.16
2	2	1244	PSU	C6-C5-C4	2.85	120.19	118.20
2	2	683	OMG	C5-C6-N1	2.85	120.42	113.19
2	2	509	OMG	C2'-C1'-N9	-2.84	108.71	114.22
2	2	1850	MA6	C4-C5-N7	-2.83	107.17	110.62
2	2	1851	MA6	C5-N7-C8	2.82	107.52	103.51
2	2	436	OMG	C2'-C1'-N9	-2.82	108.75	114.22
2	2	683	OMG	C5-C4-N3	-2.82	123.89	128.46
2	2	105	PSU	C6-C5-C4	2.81	120.16	118.20
2	2	436	OMG	C6-C5-N7	2.80	135.45	130.25
2	2	572	PSU	C6-C5-C4	2.77	120.14	118.20
2	2	509	OMG	C5-C6-N1	2.76	120.21	113.19
2	2	296	PSU	C6-N1-C2	-2.76	119.86	122.68
2	2	172	OMU	O2-C2-N1	-2.75	119.13	122.79
2	2	36	PSU	O2-C2-N1	-2.73	119.78	122.79
2	2	686	PSU	O2-C2-N1	-2.72	119.79	122.79
2	2	668	A2M	O4'-C1'-N9	-2.72	102.70	108.06
2	2	1850	MA6	C2'-C1'-N9	-2.70	106.45	113.30
2	2	644	OMG	C8-N7-C5	2.70	109.13	104.24
2	2	644	OMG	C5-C6-N1	2.67	119.98	113.19
2	2	509	OMG	C6-C5-N7	2.67	135.22	130.25
2	2	649	PSU	C6-N1-C2	-2.67	119.95	122.68
2	2	1851	MA6	C10-N6-C9	-2.64	107.61	116.12
2	2	863	PSU	C6-N1-C2	-2.64	119.98	122.68
2	2	668	A2M	C6-C5-N7	2.64	136.93	132.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	484	A2M	C5-N7-C8	2.64	107.25	103.51
2	2	1490	OMG	C4-C5-N7	-2.62	106.57	110.72
2	2	1447	OMG	N2-C2-N1	2.62	122.29	116.71
2	2	1447	OMG	C2-N1-C6	-2.62	120.33	125.10
2	2	1851	MA6	C2'-C1'-N9	-2.61	106.69	113.30
2	2	1238	PSU	C6-N1-C2	-2.60	120.02	122.68
2	2	1851	MA6	C6-C5-N7	2.60	137.64	133.28
2	2	1639	7MG	C5-C6-N1	2.59	115.56	110.99
2	2	644	OMG	C2-N1-C6	-2.59	120.38	125.10
2	2	1248	B8N	C31-N3-C4	2.57	121.10	117.31
2	2	1445	PSU	O2-C2-N1	-2.56	119.97	122.79
2	2	1447	OMG	C5-C6-N1	2.56	119.68	113.19
2	2	436	OMG	C5-C6-N1	2.55	119.67	113.19
2	2	1326	OMU	O2-C2-N1	-2.55	119.40	122.79
2	2	1447	OMG	C6-C5-N7	2.54	134.98	130.25
2	2	116	OMU	O4-C4-C5	-2.54	120.69	125.16
2	2	1045	PSU	O2-C2-N1	-2.54	119.99	122.79
2	2	683	OMG	C8-N7-C5	2.53	108.81	104.24
2	2	683	OMG	O6-C6-C5	-2.53	119.90	126.60
2	2	863	PSU	C6-C5-C4	2.52	119.96	118.20
2	2	1081	PSU	O4'-C1'-C2'	2.52	108.70	105.14
2	2	1832	6MZ	N3-C4-N9	2.51	131.22	127.08
2	2	27	A2M	C4-N9-C8	2.51	108.45	105.73
2	2	683	OMG	C2-N1-C6	-2.50	120.53	125.10
2	2	681	PSU	C6-N1-C2	-2.50	120.12	122.68
2	2	686	PSU	C6-C5-C4	2.50	119.94	118.20
2	2	1639	7MG	O4'-C1'-N9	2.49	112.69	109.30
2	2	119	PSU	C6-N1-C2	-2.48	120.15	122.68
2	2	1692	PSU	C6-N1-C2	-2.48	120.15	122.68
2	2	119	PSU	C6-C5-C4	2.47	119.93	118.20
2	2	1383	A2M	C6-C5-C4	2.47	120.50	117.18
27	O	138	IAS	OXT-C-CA	2.46	121.77	113.38
2	2	683	OMG	N2-C2-N1	2.46	121.95	116.71
2	2	601	OMG	N2-C2-N1	2.46	121.95	116.71
2	2	1643	PSU	C3'-C2'-C1'	2.46	104.50	101.64
2	2	590	A2M	C6-C5-C4	2.46	120.49	117.18
2	2	1850	MA6	C4-N9-C8	2.45	108.38	105.73
2	2	576	A2M	C6-C5-C4	2.44	120.47	117.18
2	2	436	OMG	N2-C2-N1	2.44	121.91	116.71
2	2	815	PSU	C6-N1-C2	-2.44	120.19	122.68
2	2	668	A2M	N9-C8-N7	-2.43	110.59	113.91
2	2	1842	4AC	O2-C2-N3	-2.43	118.38	122.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	406	PSU	C6-C5-C4	2.43	119.90	118.20
2	2	159	A2M	C6-C5-C4	2.42	120.44	117.18
2	2	159	A2M	C2'-C1'-N9	-2.40	109.50	113.53
2	2	590	A2M	O4'-C4'-C3'	-2.39	100.38	105.11
2	2	1678	A2M	N9-C8-N7	-2.39	110.64	113.91
2	2	601	OMG	C4-C5-N7	-2.39	106.94	110.72
2	2	484	A2M	C6-C5-N7	2.38	136.46	132.02
2	2	1447	OMG	C4-C5-N7	-2.38	106.95	110.72
2	2	436	OMG	C8-N7-C5	2.37	108.53	104.24
2	2	121	OMU	O4-C4-C5	-2.36	121.00	125.16
2	2	683	OMG	N1-C2-N3	-2.36	118.91	123.32
2	2	99	A2M	C6-C5-C4	2.35	120.34	117.18
2	2	1850	MA6	C5-N7-C8	2.34	106.84	103.51
2	2	649	PSU	O2-C2-N1	-2.34	120.22	122.79
2	2	116	OMU	O2-C2-N1	-2.34	119.68	122.79
2	2	1447	OMG	C8-N7-C5	2.33	108.47	104.24
2	2	93	PSU	C6-N1-C2	-2.33	120.30	122.68
2	2	509	OMG	C4-C5-N7	-2.32	107.05	110.72
2	2	815	PSU	C6-C5-C4	2.32	119.82	118.20
2	2	1490	OMG	C2'-C1'-N9	-2.32	109.73	114.22
2	2	509	OMG	C5-C4-N9	2.31	109.83	105.63
2	2	1081	PSU	C6-N1-C2	-2.31	120.32	122.68
2	2	814	PSU	O2-C2-N1	-2.31	120.25	122.79
2	2	644	OMG	C5-C4-N9	2.31	109.82	105.63
2	2	601	OMG	C8-N7-C5	2.31	108.42	104.24
2	2	601	OMG	C5-C4-N9	2.30	109.80	105.63
2	2	668	A2M	C2-N1-C6	2.30	122.71	118.77
2	2	683	OMG	C8-N9-C4	2.29	110.41	106.05
2	2	27	A2M	C6-C5-N7	2.29	136.29	132.02
2	2	1851	MA6	C4-N9-C8	2.29	108.21	105.73
2	2	601	OMG	N1-C2-N3	-2.29	119.05	123.32
2	2	354	OMU	O2-C2-N1	-2.28	119.75	122.79
2	2	512	A2M	C6-C5-C4	2.28	120.25	117.18
2	2	1337	4AC	C5-C4-N3	-2.28	118.93	122.59
2	2	93	PSU	O2-C2-N1	-2.27	120.29	122.79
2	2	1832	6MZ	C4-N9-C8	2.27	108.19	105.73
2	2	354	OMU	C2'-C1'-N1	-2.27	109.82	114.22
2	2	159	A2M	C4-C5-N7	-2.26	107.86	110.62
2	2	601	OMG	O6-C6-C5	-2.26	120.60	126.60
2	2	1678	A2M	C6-C5-N7	2.25	136.20	132.02
2	2	509	OMG	N2-C2-N1	2.24	121.49	116.71
2	2	512	A2M	O4'-C1'-C2'	-2.24	102.64	106.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1447	OMG	O6-C6-C5	-2.24	120.66	126.60
2	2	1490	OMG	O6-C6-C5	-2.24	120.67	126.60
35	A	2	SAC	C2A-C1A-N	2.23	119.87	116.10
35	A	2	SAC	O-C-CA	-2.22	118.96	124.78
2	2	354	OMU	O4-C4-C5	-2.22	121.27	125.16
2	2	1177	PSU	C5-C6-N1	-2.21	118.79	122.11
2	2	484	A2M	C2-N1-C6	2.21	122.56	118.77
2	2	1328	OMG	C8-N7-C5	2.21	108.24	104.24
2	2	27	A2M	O4'-C1'-N9	2.21	112.41	108.06
2	2	590	A2M	O4'-C1'-N9	2.20	112.40	108.06
2	2	1639	7MG	C5-C4-N9	-2.20	103.50	106.35
2	2	119	PSU	O2-C2-N1	-2.19	120.38	122.79
2	2	683	OMG	C4-C5-N7	-2.18	107.27	110.72
2	2	1347	PSU	C3'-C2'-C1'	2.18	104.18	101.64
2	2	436	OMG	C2-N1-C6	-2.18	121.12	125.10
2	2	428	OMU	O2-C2-N1	-2.18	119.89	122.79
2	2	512	A2M	C1'-N9-C8	2.17	132.03	127.14
2	2	1056	PSU	O2-C2-N1	-2.16	120.41	122.79
2	2	1442	OMU	O2-C2-N1	-2.16	119.91	122.79
2	2	822	PSU	O4'-C1'-C2'	2.16	108.19	105.14
2	2	436	OMG	C4-C5-N7	-2.16	107.31	110.72
2	2	649	PSU	C6-C5-C4	2.16	119.70	118.20
2	2	1842	4AC	O7-C7-CM7	-2.15	118.06	122.06
2	2	27	A2M	N9-C8-N7	-2.15	110.97	113.91
2	2	1238	PSU	O2-C2-N1	-2.14	120.43	122.79
27	O	138	IAS	CA-CB-CG	-2.13	105.28	114.50
2	2	484	A2M	C4-N9-C8	2.13	108.04	105.73
2	2	1851	MA6	N9-C8-N7	-2.12	111.01	113.91
2	2	436	OMG	O6-C6-C5	-2.12	120.97	126.60
2	2	1328	OMG	N9-C4-N3	2.12	130.19	125.94
2	2	296	PSU	C6-C5-C4	2.11	119.68	118.20
2	2	1337	4AC	O2-C2-N3	-2.11	118.89	122.33
2	2	109	PSU	C5-C4-N3	2.11	121.35	116.58
2	2	1625	PSU	C6-C5-C4	2.10	119.66	118.20
2	2	36	PSU	C3'-C2'-C1'	2.09	104.07	101.64
2	2	436	OMG	N1-C2-N3	-2.06	119.47	123.32
2	2	27	A2M	C2-N1-C6	2.06	122.31	118.77
2	2	509	OMG	O6-C6-C5	-2.06	121.14	126.60
2	2	166	A2M	O4'-C1'-C2'	-2.05	102.97	106.57
2	2	644	OMG	N1-C2-N3	-2.05	119.50	123.32
2	2	1232	PSU	O2-C2-N1	-2.05	120.54	122.79
2	2	1081	PSU	O4-C4-N3	-2.04	116.20	120.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1081	PSU	C5-C4-N3	2.03	121.17	116.58
2	2	576	A2M	O4'-C1'-C2'	-2.03	103.01	106.57
2	2	1248	B8N	O36-C34-O35	-2.03	119.49	124.09
2	2	1031	A2M	C6-C5-C4	2.03	119.91	117.18
2	2	1337	4AC	C6-C5-C4	2.02	119.44	116.96
2	2	681	PSU	C6-C5-C4	2.02	119.61	118.20
2	2	1383	A2M	C2'-C3'-C4'	-2.02	97.61	101.99
2	2	172	OMU	O2'-C2'-C1'	2.01	113.01	109.08
2	2	1248	B8N	O4'-C1'-C2'	2.01	107.98	105.14
2	2	109	PSU	C6-C5-C4	2.00	119.60	118.20
2	2	509	OMG	C8-N7-C5	2.00	107.86	104.24

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	X	62	HY3	O-C-CA-C3
2	2	27	A2M	C1'-C2'-O2'-CM'
2	2	116	OMU	C1'-C2'-O2'-CM2
2	2	174	OMC	C1'-C2'-O2'-CM2
2	2	468	A2M	C1'-C2'-O2'-CM'
2	2	484	A2M	C1'-C2'-O2'-CM'
2	2	1248	B8N	O4'-C4'-C5'-O5'
2	2	1248	B8N	C3'-C4'-C5'-O5'
2	2	1678	A2M	C1'-C2'-O2'-CM'
2	2	1850	MA6	C5-C6-N6-C9
2	2	1851	MA6	O4'-C4'-C5'-O5'
2	2	1851	MA6	C5-C6-N6-C9
2	2	1851	MA6	N1-C6-N6-C9
27	O	138	IAS	CA-CB-CG-OD1
2	2	668	A2M	O4'-C4'-C5'-O5'
2	2	668	A2M	C3'-C4'-C5'-O5'
2	2	1447	OMG	C3'-C4'-C5'-O5'
2	2	1851	MA6	C3'-C4'-C5'-O5'
17	V	1	AME	CT2-CT1-N-CA
17	V	1	AME	OT-CT1-N-CA
2	2	1850	MA6	N1-C6-N6-C9
2	2	172	OMU	C3'-C2'-O2'-CM2
17	V	1	AME	N-CA-CB-CG
2	2	1447	OMG	O4'-C4'-C5'-O5'
2	2	576	A2M	C3'-C4'-C5'-O5'
2	2	1851	MA6	C5-C6-N6-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	2	428	OMU	C2'-C1'-N1-C6
2	2	99	A2M	O4'-C4'-C5'-O5'
2	2	1337	4AC	O7-C7-N4-C4
2	2	1337	4AC	CM7-C7-N4-C4
2	2	1842	4AC	O7-C7-N4-C4
2	2	1842	4AC	CM7-C7-N4-C4
2	2	644	OMG	C4'-C5'-O5'-P
2	2	668	A2M	C2'-C1'-N9-C8
2	2	428	OMU	O4'-C1'-N1-C6
2	2	1851	MA6	C4'-C5'-O5'-P
2	2	1490	OMG	C4'-C5'-O5'-P
2	2	428	OMU	O4'-C1'-N1-C2
2	2	1347	PSU	O4'-C4'-C5'-O5'
2	2	99	A2M	C3'-C4'-C5'-O5'
2	2	576	A2M	O4'-C4'-C5'-O5'
2	2	428	OMU	C2'-C1'-N1-C2
27	O	138	IAS	OXT-C-CA-N
2	2	1081	PSU	C4'-C5'-O5'-P

There are no ring outliers.

24 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	468	A2M	1	0
2	2	1842	4AC	4	0
2	2	462	OMC	2	0
2	2	296	PSU	1	0
2	2	484	A2M	1	0
2	2	509	OMG	1	0
2	2	576	A2M	2	0
2	2	1383	A2M	1	0
2	2	668	A2M	1	0
2	2	1046	PSU	1	0
2	2	174	OMC	1	0
2	2	1288	OMU	1	0
2	2	1639	7MG	1	0
2	2	683	OMG	1	0
2	2	1643	PSU	1	0
2	2	1174	PSU	2	0
2	2	1232	PSU	2	0
2	2	1850	MA6	2	0
2	2	27	A2M	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	1442	OMU	1	0
2	2	116	OMU	3	0
2	2	1031	A2M	1	0
2	2	436	OMG	1	0
2	2	159	A2M	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 173 ligands modelled in this entry, 173 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

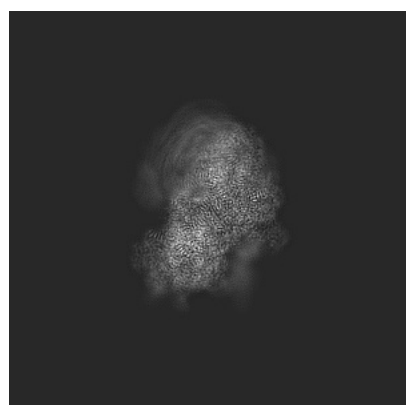
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14317. These allow visual inspection of the internal detail of the map and identification of artifacts.

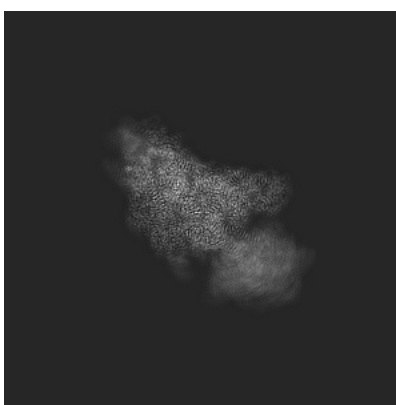
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

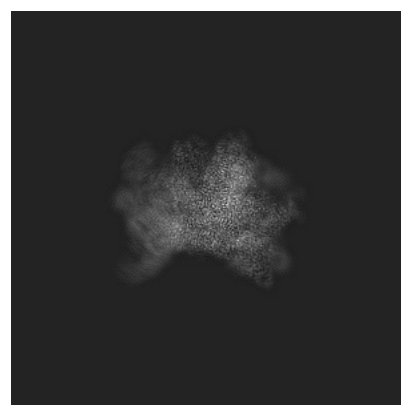
6.1.1 Primary map



X



Y

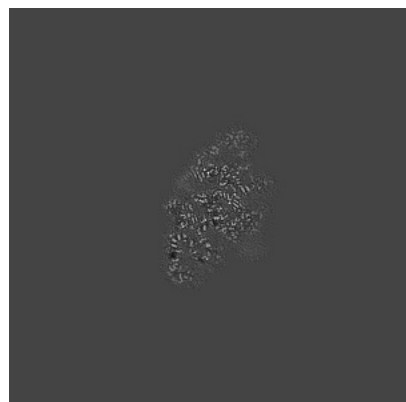


Z

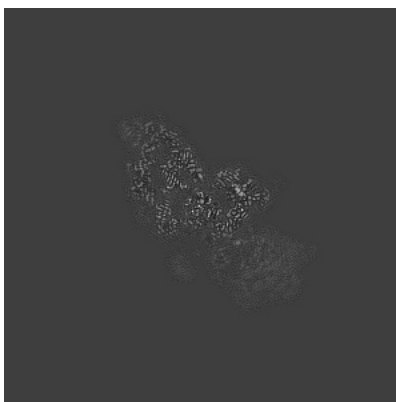
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

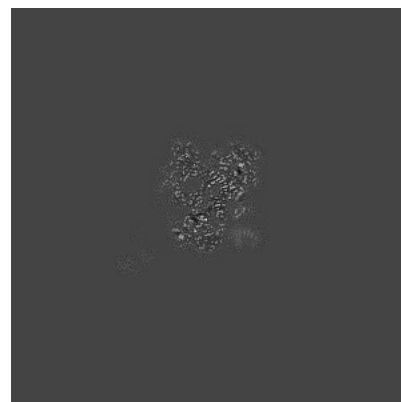
6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

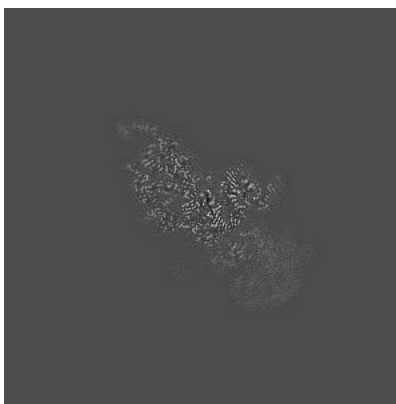
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

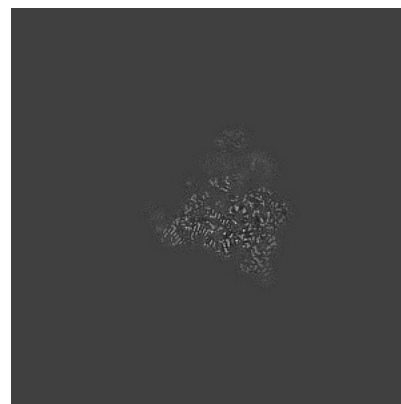
6.3.1 Primary map



X Index: 279



Y Index: 264

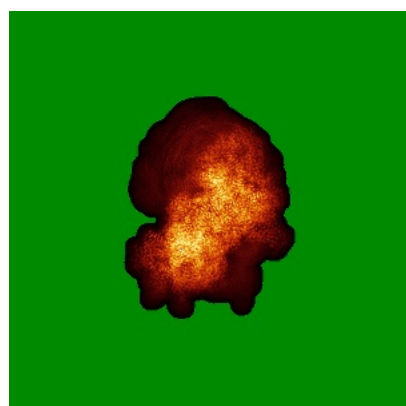


Z Index: 213

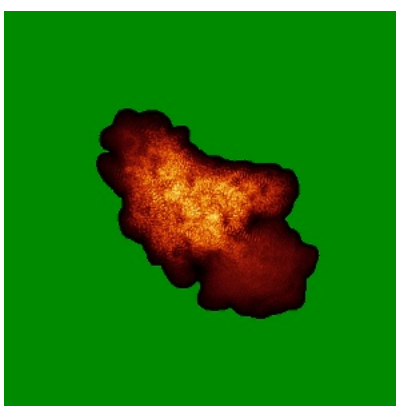
The images above show the largest variance slices of the map in three orthogonal directions.

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

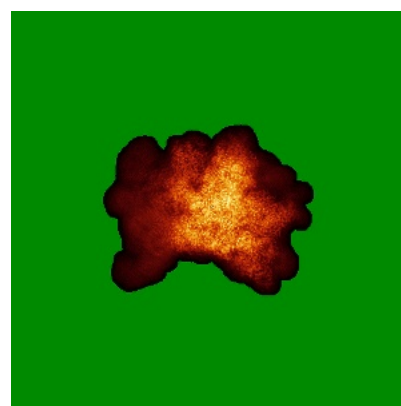
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

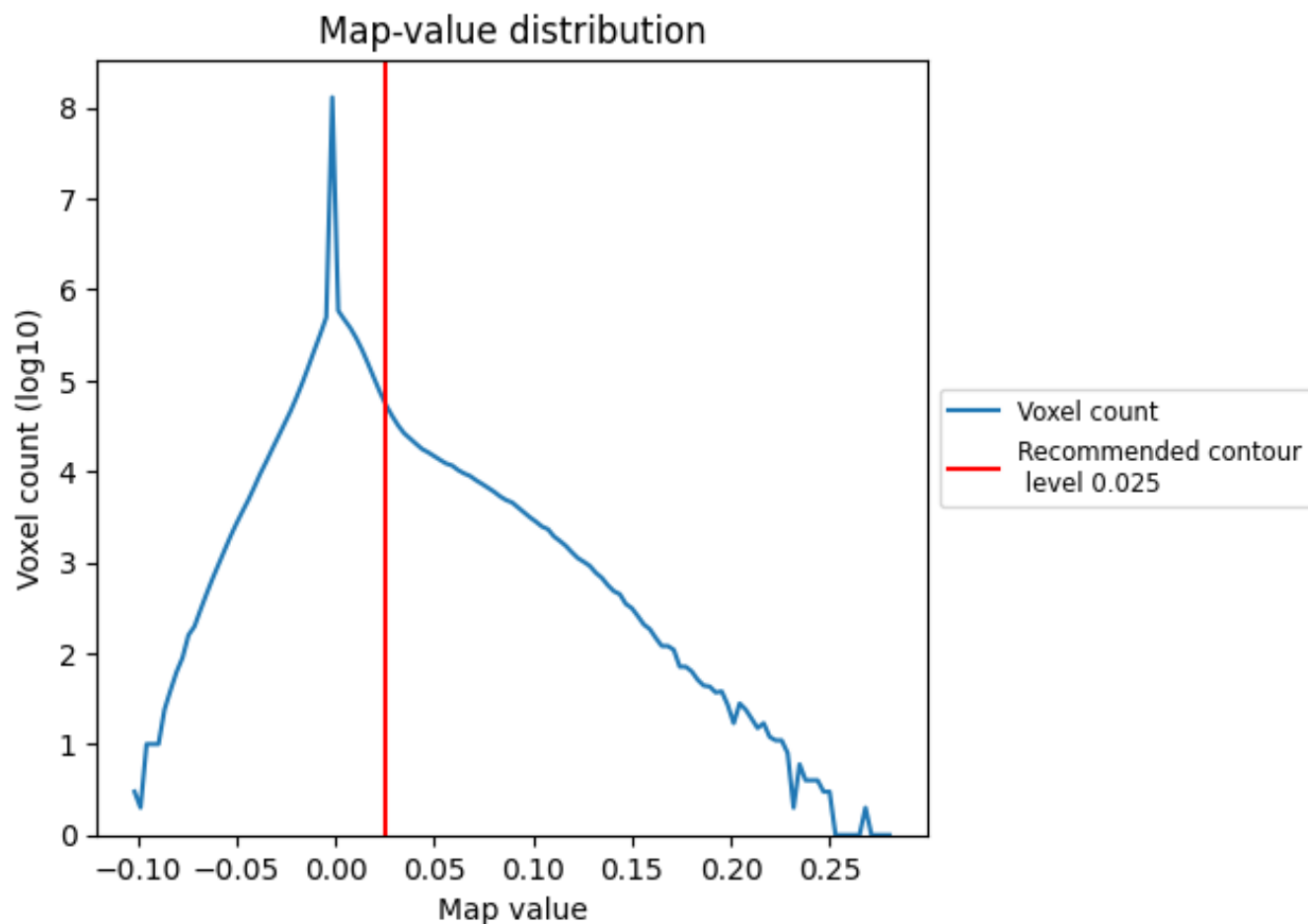
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

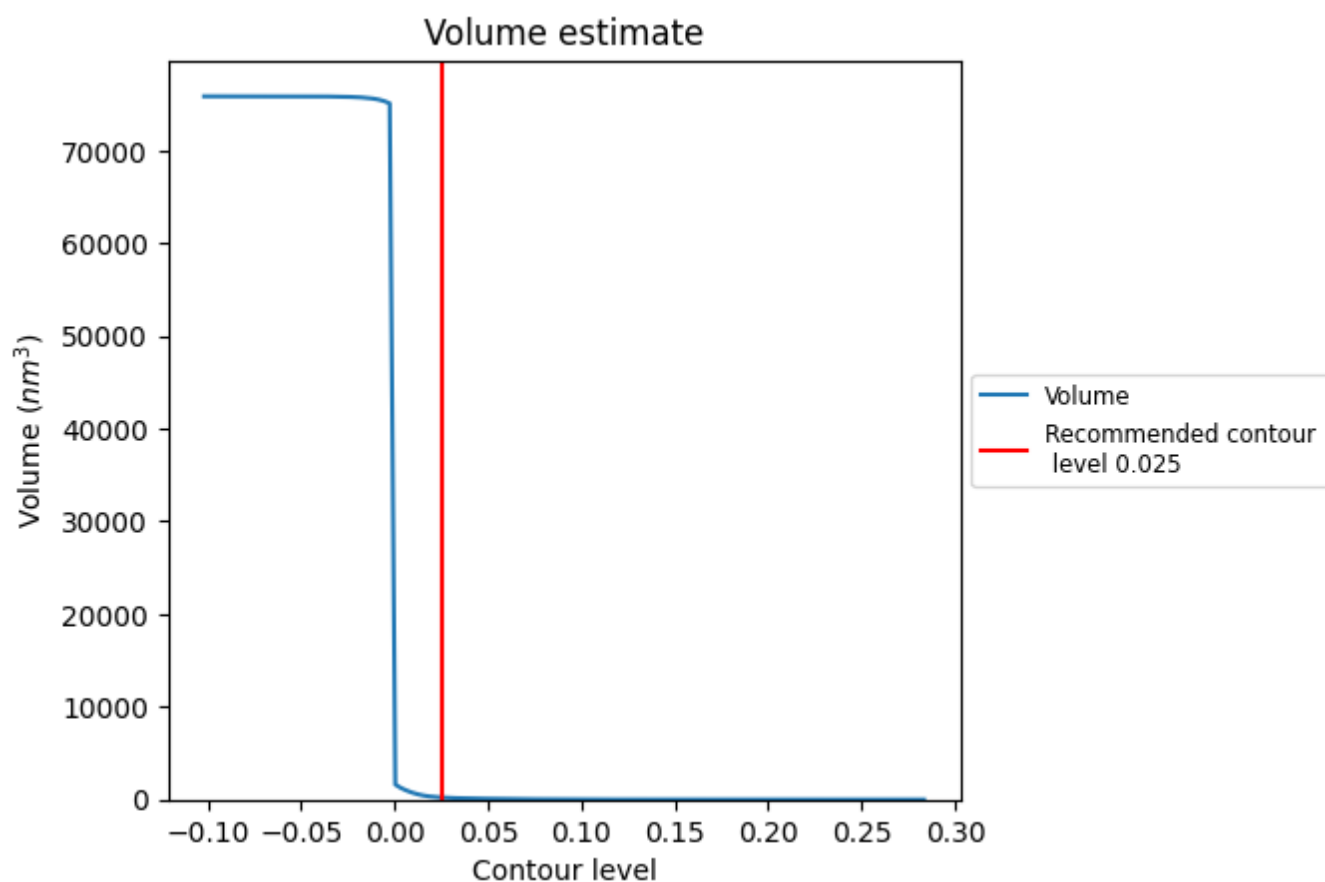
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

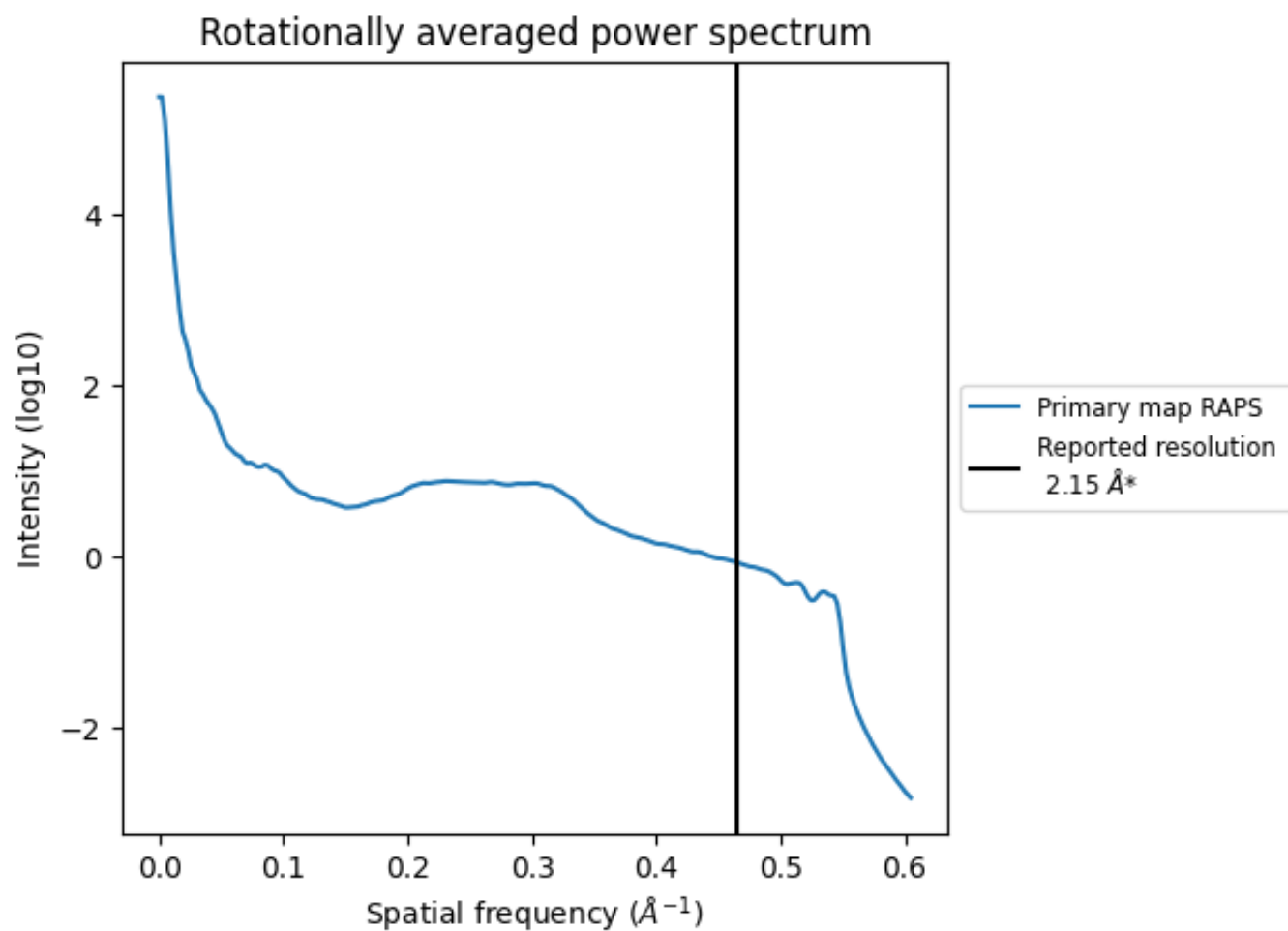
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 225 nm^3 ; this corresponds to an approximate mass of 203 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 ⓘ

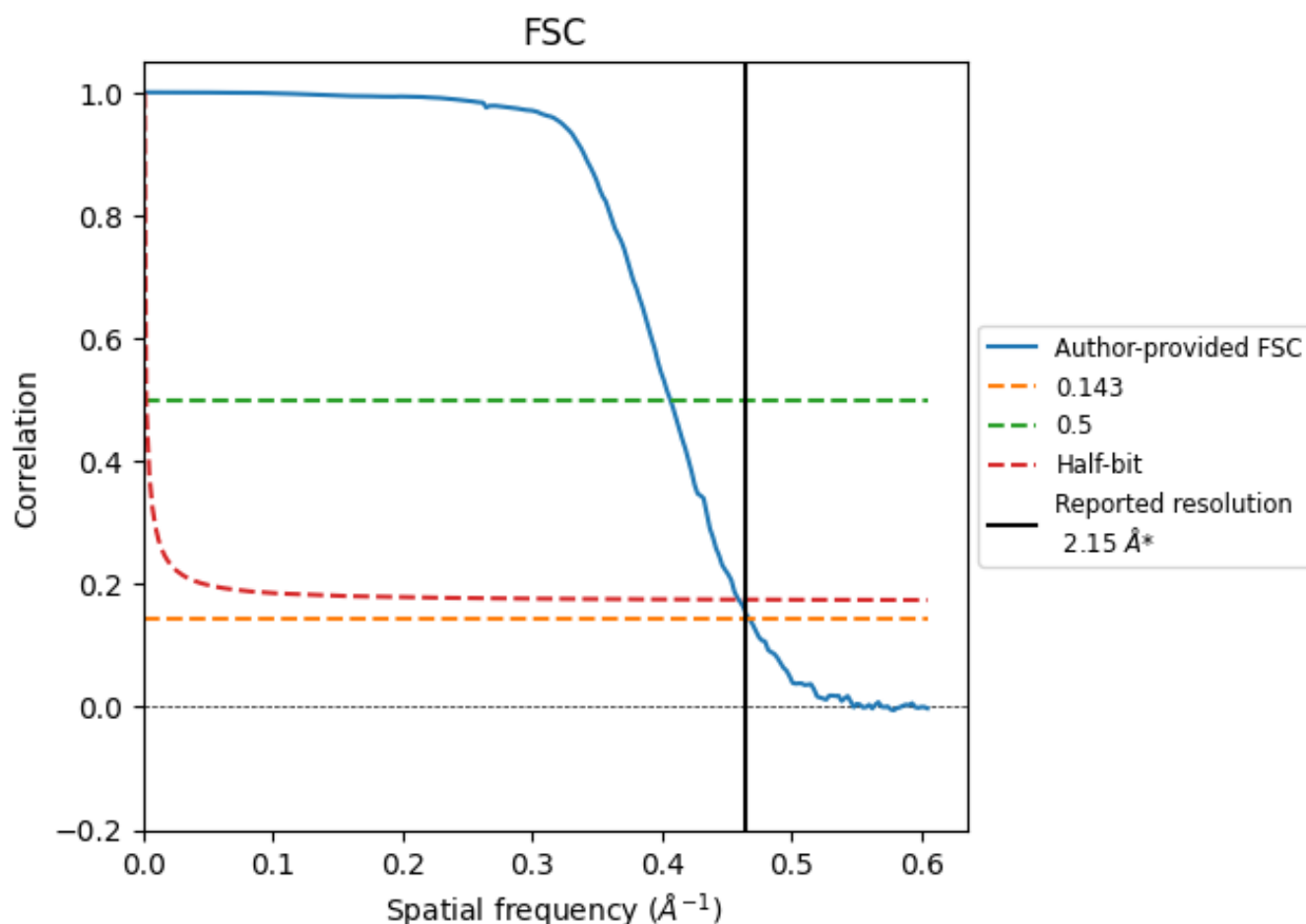


*Reported resolution corresponds to spatial frequency of 0.465 Å⁻¹

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 0.465 Å⁻¹

8.2 Resolution estimates [i](#)

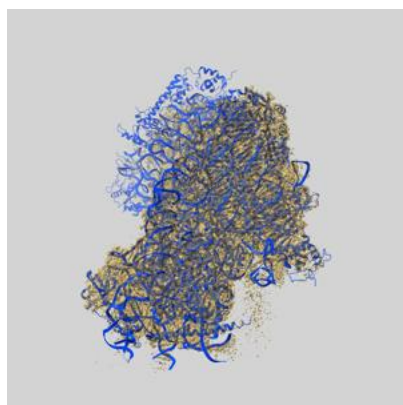
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.15	-	-
Author-provided FSC curve	2.14	2.46	2.18
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

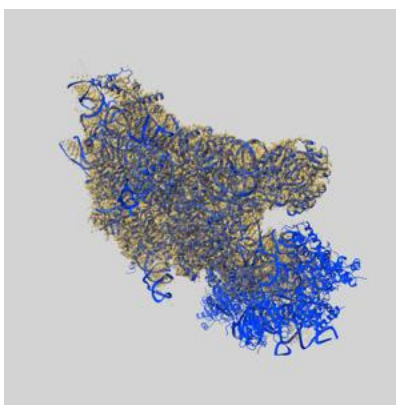
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14317 and PDB model 7R4X. Per-residue inclusion information can be found in section [3](#) on page [13](#).

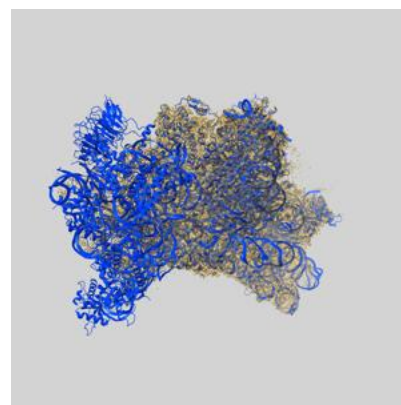
9.1 Map-model overlay [i](#)



X



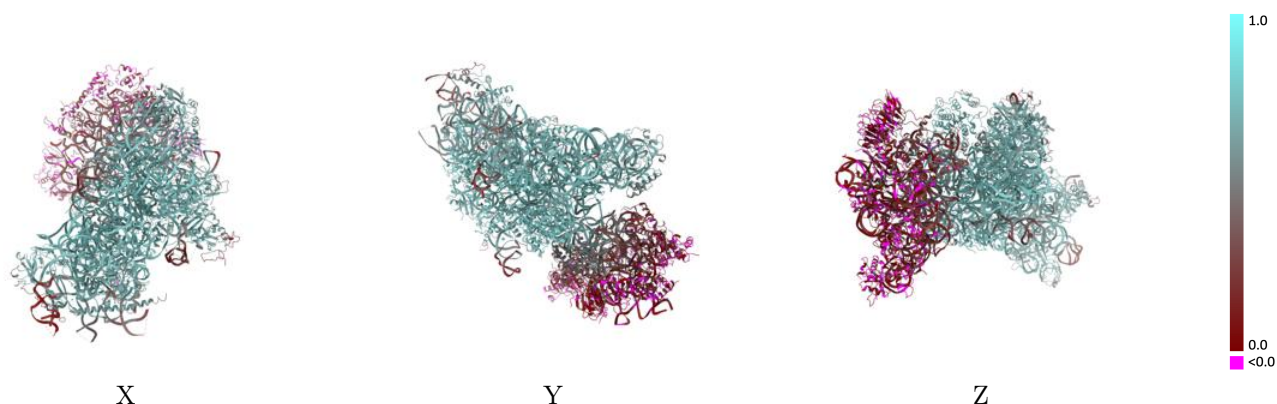
Y



Z

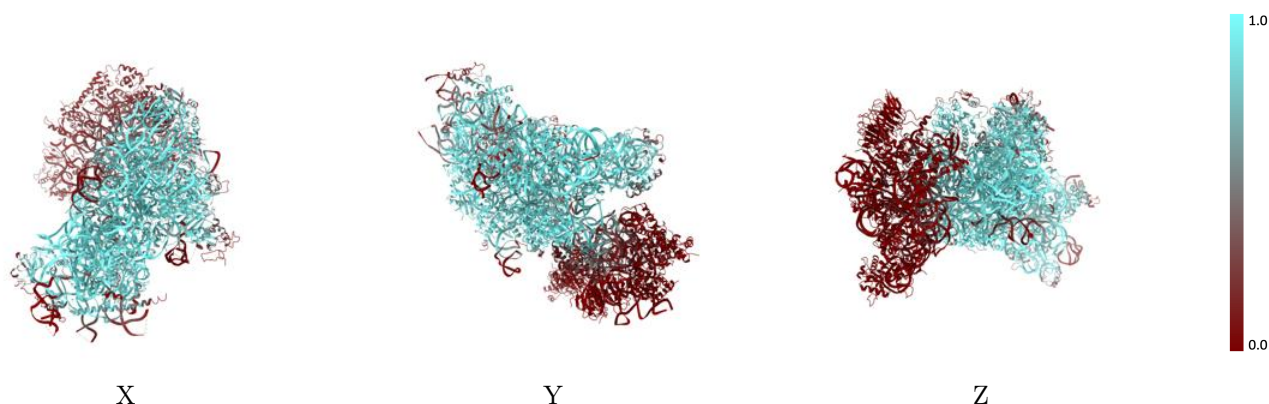
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



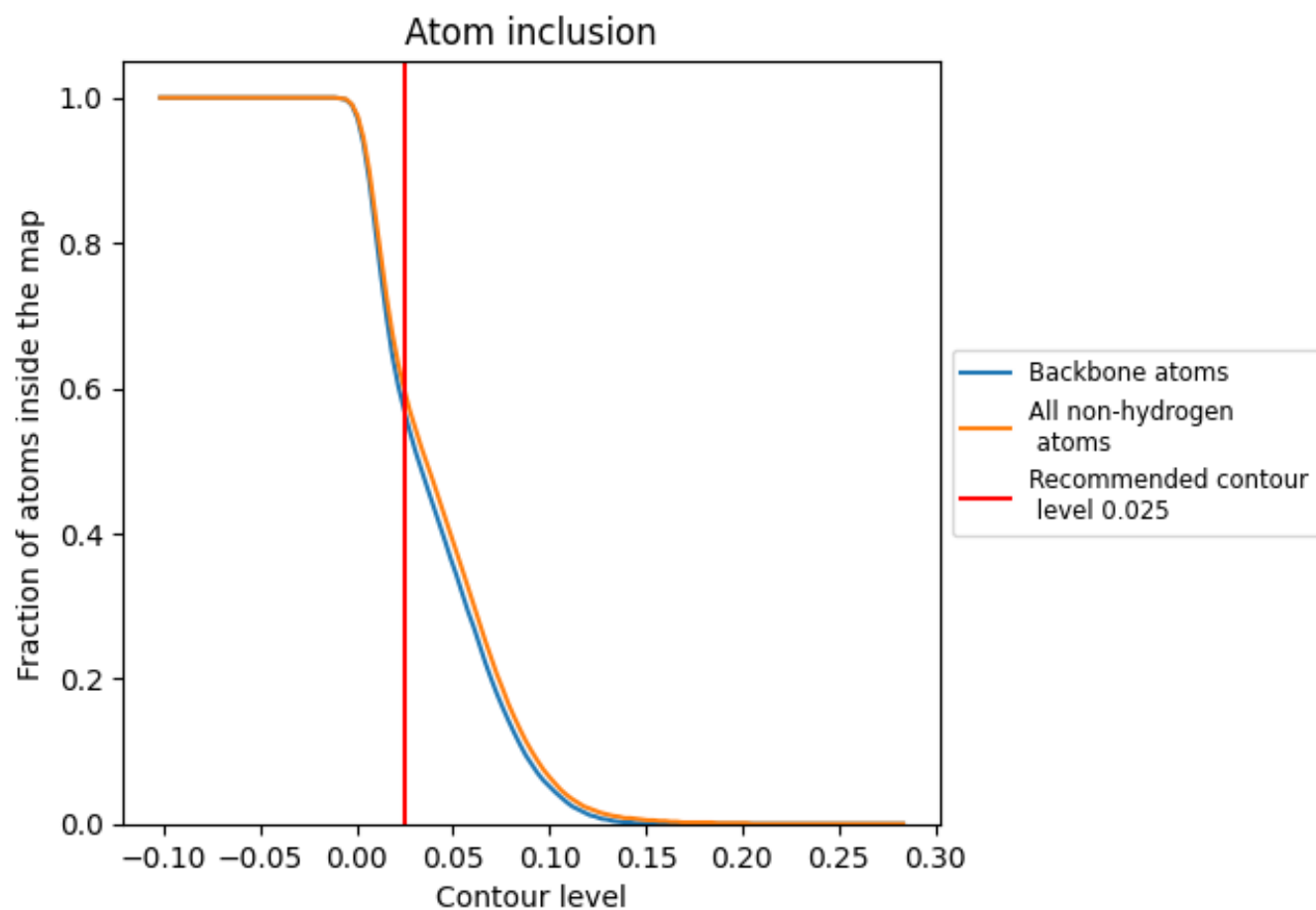
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion ⓘ



At the recommended contour level, 57% of all backbone atoms, 60% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5950	 0.5210
2	 0.6770	 0.5580
A	 0.9030	 0.7170
B	 0.7650	 0.6480
C	 0.9130	 0.7440
D	 0.1730	 0.3590
E	 0.9420	 0.7390
F	 0.0210	 0.1930
G	 0.6250	 0.6060
H	 0.5390	 0.5700
I	 0.7720	 0.6420
J	 0.8950	 0.7330
K	 0.0290	 0.1770
L	 0.8970	 0.7170
M	 0.0010	 0.0580
N	 0.8610	 0.6950
O	 0.8390	 0.6690
P	 0.0060	 0.1180
Q	 0.0500	 0.1560
R	 0.2950	 0.4730
S	 0.0050	 0.0860
T	 0.0050	 0.1020
U	 0.1150	 0.2440
V	 0.8940	 0.7250
W	 0.9680	 0.7720
X	 0.9490	 0.7620
Y	 0.8870	 0.7050
Z	 0.0000	 0.0570
a	 0.8450	 0.6970
b	 0.7610	 0.6650
c	 0.0490	 0.2810
d	 0.2170	 0.3440
e	 0.7350	 0.6540
f	 0.0000	 0.0280
g	 0.0070	 0.1120
n	 0.8010	 0.6940

