



Full wwPDB EM Validation Report ⓘ

Mar 18, 2024 – 03:56 PM JST

PDB ID : 8JIW
EMDB ID : EMD-36332
Title : Atomic structure of wheat ribosome reveals unique features of the plant ribosomes
Authors : Mishra, R.K.; Sharma, P.; Hussain, T.
Deposited on : 2023-05-28
Resolution : 2.88 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.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

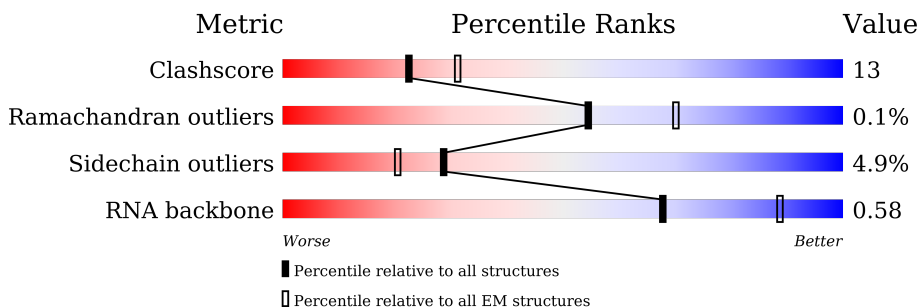
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.88 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.








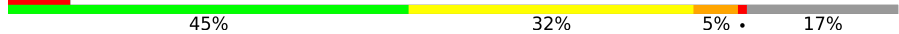





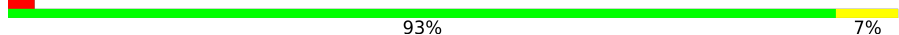

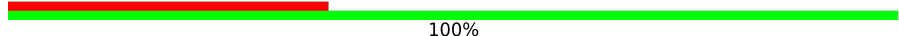





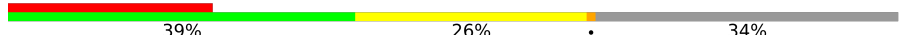





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	Ad	1811	 69% 17% 13%
2	BA	304	 35% 27% 36%
3	BB	263	 54% 25% 19%
4	BC	279	 54% 24% 21%
5	BE	265	 71% 29%
6	BG	250	 63% 27% 8%
7	BH	192	 64% 28% 5%

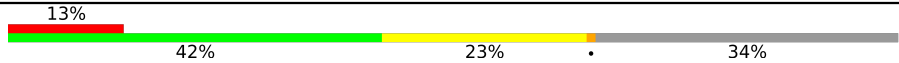
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Mol	Chain	Length	Quality of chain
8	BI	224	
9	BJ	195	
10	BL	161	
11	BN	151	
12	BO	151	
13	BR	143	
14	BV	82	
15	BW	130	
16	BX	142	
17	BY	137	
18	Ba	139	
19	Bb	86	
20	Be	62	
21	Cn	25	
22	BD	227	
23	BF	200	
24	BK	188	
25	BP	153	
26	BQ	149	
27	BS	152	
28	BT	155	
29	BU	117	
30	Bc	65	
31	Bd	56	
32	Bg	335	

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Mol	Chain	Length	Quality of chain										
33	BZ	98	 <p>A horizontal bar chart showing the quality distribution of chain BZ. The bar is divided into four segments: red (13%), green (42%), yellow (23%), and grey (34%).</p> <table border="1"><thead><tr><th>Quality Category</th><th>Percentage</th></tr></thead><tbody><tr><td>Red</td><td>13%</td></tr><tr><td>Green</td><td>42%</td></tr><tr><td>Yellow</td><td>23%</td></tr><tr><td>Grey</td><td>34%</td></tr></tbody></table>	Quality Category	Percentage	Red	13%	Green	42%	Yellow	23%	Grey	34%
Quality Category	Percentage												
Red	13%												
Green	42%												
Yellow	23%												
Grey	34%												

2 Entry composition [i](#)

There are 36 unique types of molecules in this entry. The entry contains 68755 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	Ad	1571	33567	15010	6022	10964	1571	0	0

- Molecule 2 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	BA	195	1554	987	276	279	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	BB	213	1740	1109	313	309	9	0	0

- Molecule 4 is a protein called S5 DRBM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	BC	220	1703	1096	303	295	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	BE	263	2088	1334	391	356	7	0	0

- Molecule 6 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	BG	229	1847	1152	365	322	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	BH	182	1368	879	240	248	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	BI	186	1504	932	301	267	4	0	0

- Molecule 9 is a protein called 30S ribosomal protein S4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	BJ	183	1504	952	300	248	4	0	0

- Molecule 10 is a protein called 40S ribosomal protein S11 N-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	BL	152	1207	766	230	205	6	0	0

- Molecule 11 is a protein called Ribosomal protein S13/S15 N-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	BN	149	1191	763	223	203	2	0	0

- Molecule 12 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	BO	130	983	603	195	181	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	BR	119	969	604	182	177	6	0	0

- Molecule 14 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	BV	81	636	393	118	122	3	0	0

- Molecule 15 is a protein called 30S ribosomal protein S8, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	BW	129	1032	659	188	180	5	0	0

- Molecule 16 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	BX	139	1077	684	208	182	3	0	0

- Molecule 17 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	BY	124	1011	645	196	168	2	0	0

- Molecule 18 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	Ba	98	791	487	172	125	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	Bb	86	663	416	120	119	8	0	0

- Molecule 20 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
20	Be	47	376	230	86	60	0	0

- Molecule 21 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Cn	25	Total	C	N	O	S	0	0
			237	145	62	27	3		

- Molecule 22 is a protein called KH type-2 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BD	208	Total	C	N	O	S	0	0
			1623	1030	295	289	9		

- Molecule 23 is a protein called Ribosomal protein S7 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BF	178	Total	C	N	O	S	0	0
			1416	888	263	258	7		

- Molecule 24 is a protein called Plectin/S10 N-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BK	82	Total	C	N	O	S	0	0
			711	467	118	123	3		

- Molecule 25 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BP	70	Total	C	N	O	S	0	0
			567	363	110	89	5		

- Molecule 26 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BQ	139	Total	C	N	O	S	0	0
			1108	704	213	186	5		

- Molecule 27 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BS	100	Total	C	N	O	S	0	0
			822	510	173	134	5		

- Molecule 28 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BT	137	Total	C	N	O	S	0	0
			1081	680	205	192	4		

- Molecule 29 is a protein called Ribosomal protein S10 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BU	101	Total	C	N	O	S	0	0
			793	495	148	146	4		

- Molecule 30 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Bc	61	Total	C	N	O	S	0	0
			489	301	100	86	2		

- Molecule 31 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Bd	50	Total	C	N	O	S	0	0
			403	250	82	65	6		

- Molecule 32 is a protein called Mitogen-activated protein kinase.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Bg	271	Total	C	N	O	S	0	0
			2086	1325	363	389	9		

- Molecule 33 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BZ	65	Total	C	N	O	S	0	0
			521	330	94	96	1		

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
34	Ad	14	Total	K	0
			14	14	
34	BT	1	Total	K	0
			1	1	
34	Bd	1	Total	K	0
			1	1	

- Molecule 35 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
35	Ad	69	Total 69	Mg 69	0
35	BS	1	Total 1	Mg 1	0

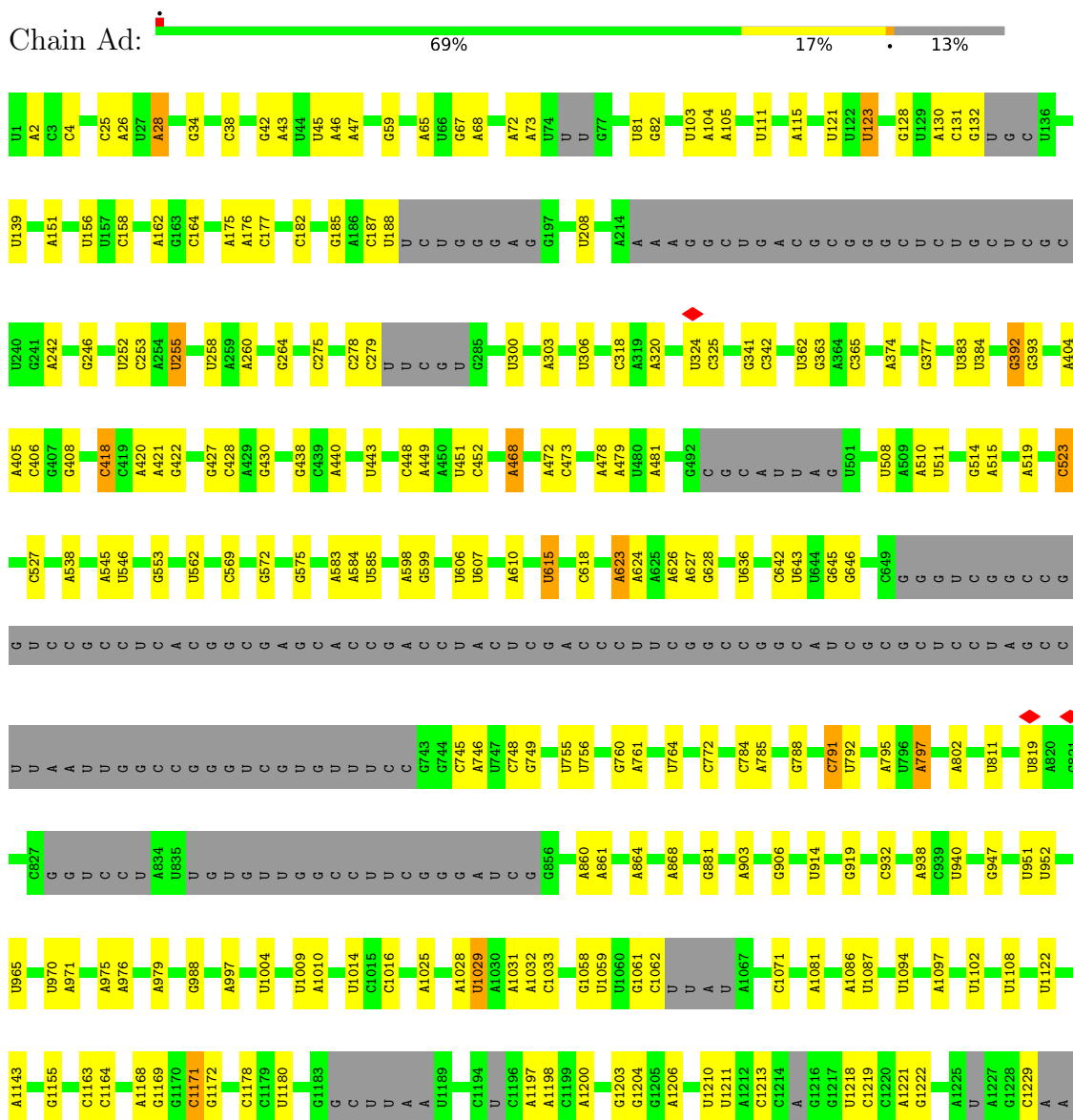
- Molecule 36 is ZINC ION (three-letter code: ZN) (formula: Zn).

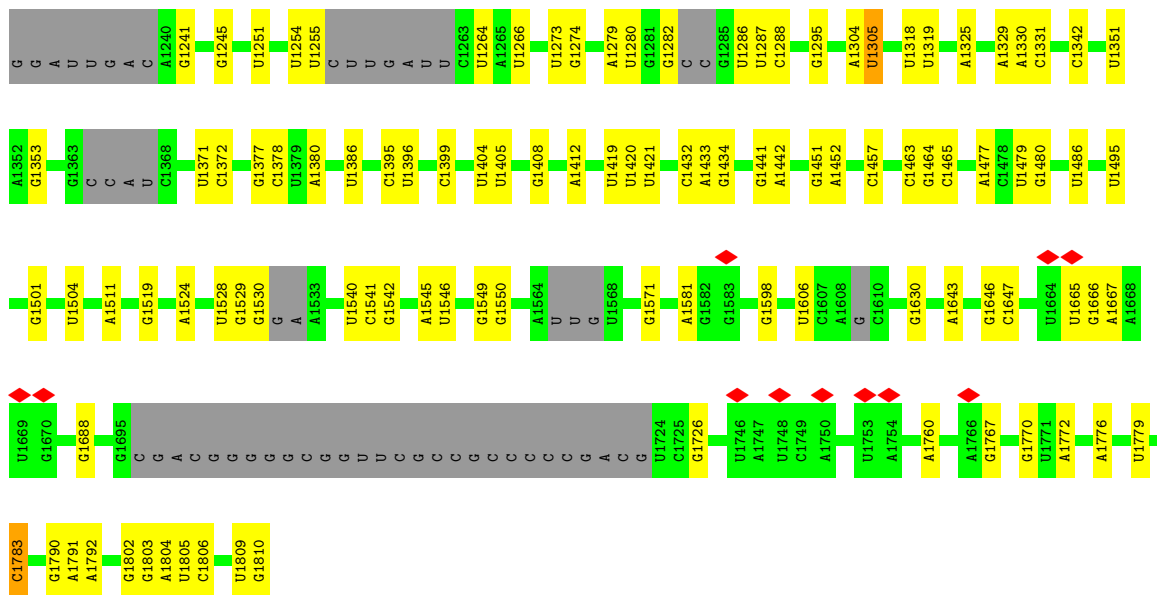
Mol	Chain	Residues	Atoms		AltConf
36	Bd	1	Total 1	Zn 1	0

3 Residue-property plots [i](#)

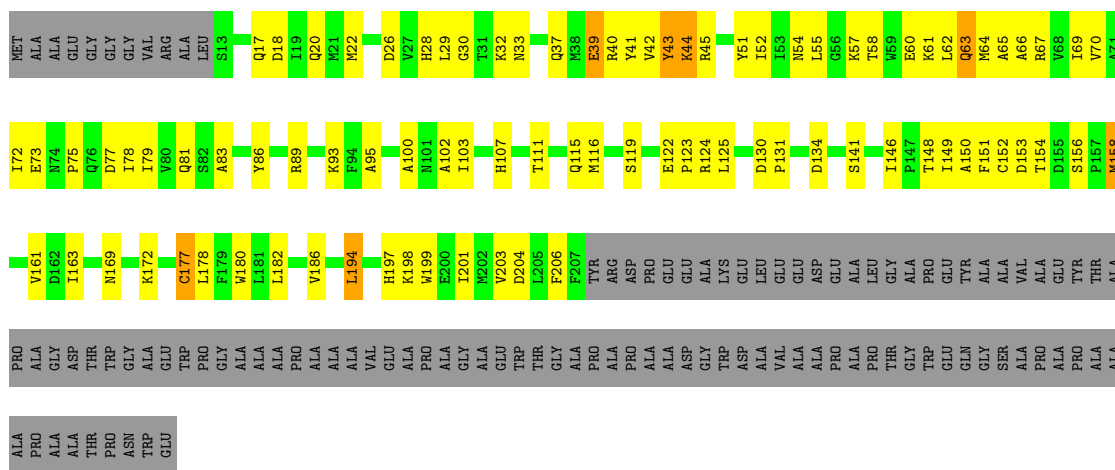
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 18S rRNA

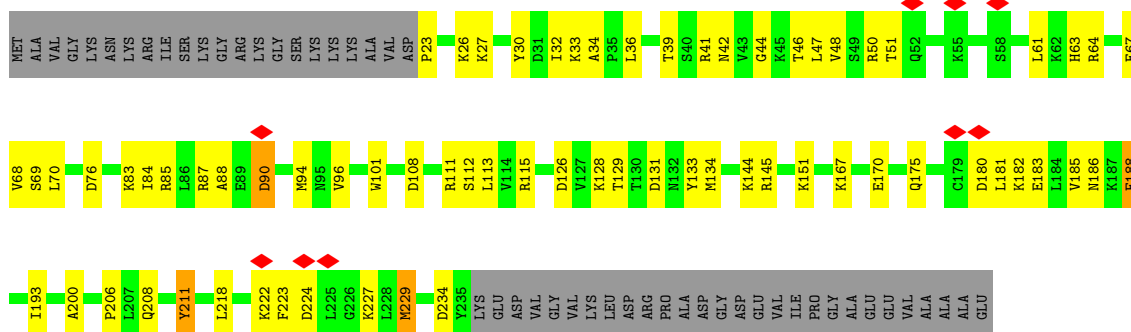




• Molecule 2: 40S ribosomal protein SA

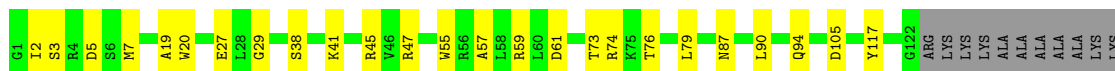


• Molecule 3: 40S ribosomal protein S3a

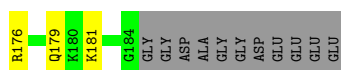
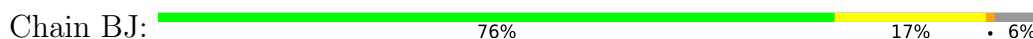




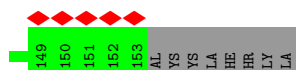
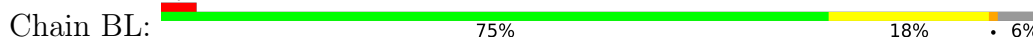
• Molecule 8: 40S ribosomal protein S8



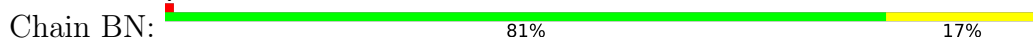
• Molecule 9: 30S ribosomal protein S4, chloroplastic



• Molecule 10: 40S ribosomal protein S11 N-terminal domain-containing protein



• Molecule 11: Ribosomal protein S13/S15 N-terminal domain-containing protein



• Molecule 12: 40S ribosomal protein S14





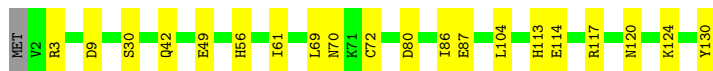
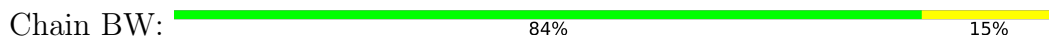
• Molecule 13: 40S ribosomal protein S17



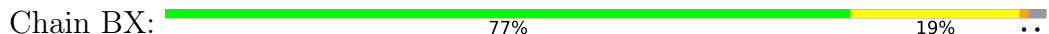
• Molecule 14: 40S ribosomal protein S21



• Molecule 15: 30S ribosomal protein S8, chloroplastic



• Molecule 16: 40S ribosomal protein S23

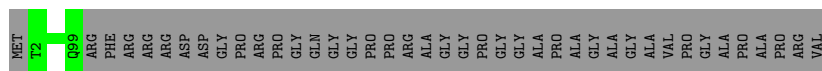


• Molecule 17: 40S ribosomal protein S24

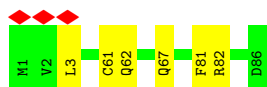


• Molecule 18: 40S ribosomal protein S26

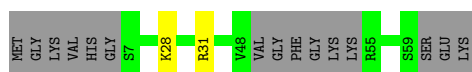




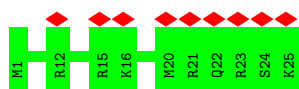
• Molecule 19: 40S ribosomal protein S27



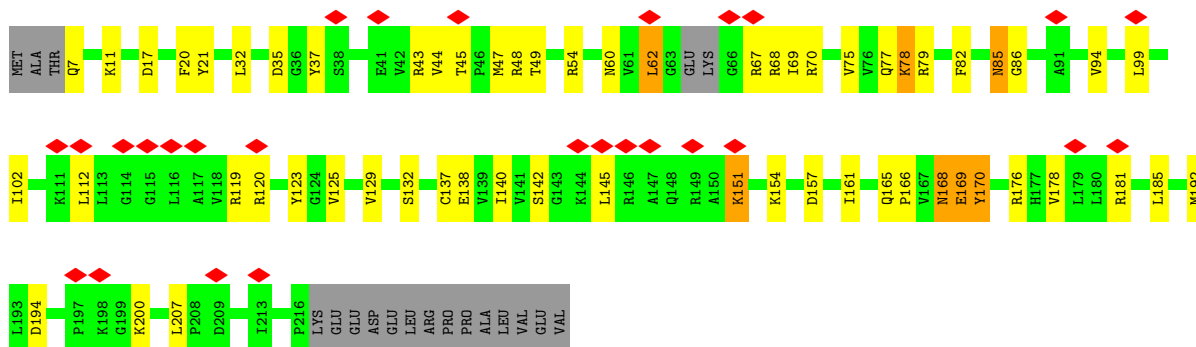
• Molecule 20: 40S ribosomal protein S30



• Molecule 21: 60S ribosomal protein L41

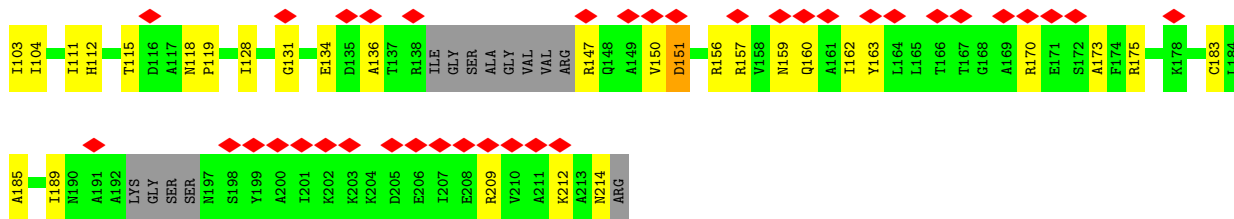


• Molecule 22: KH type-2 domain-containing protein

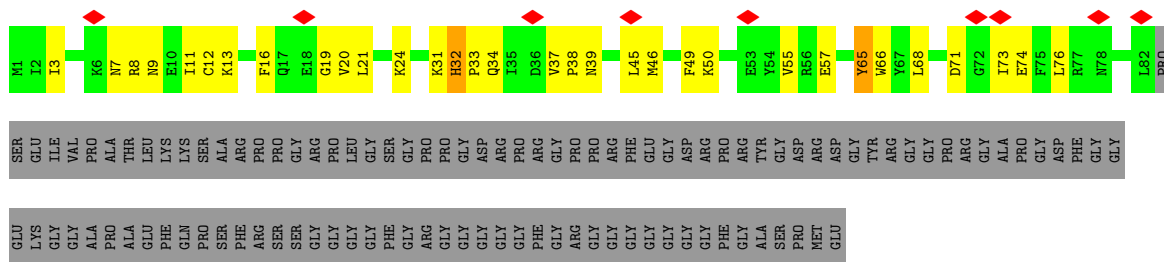
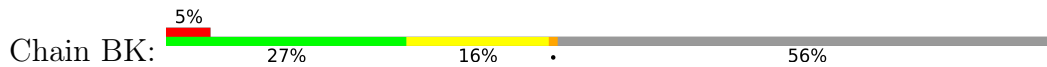


• Molecule 23: Ribosomal protein S7 domain-containing protein

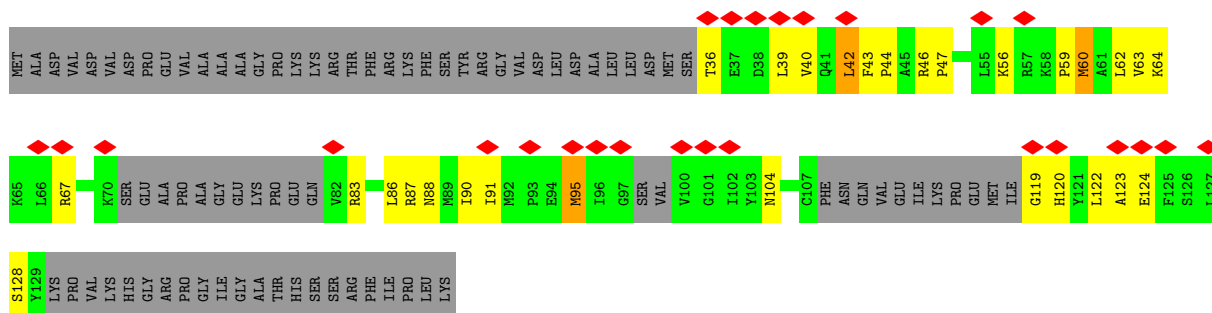
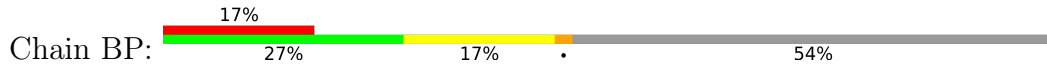




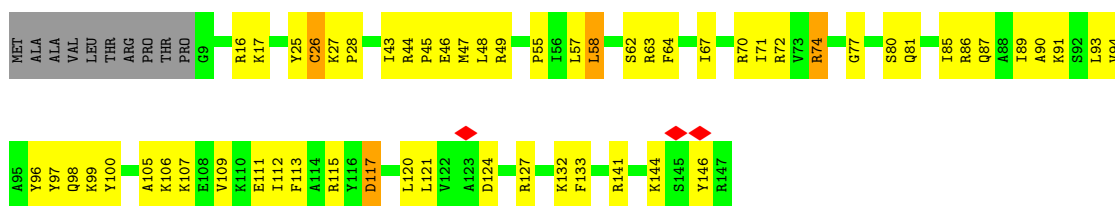
• Molecule 24: Plectin/S10 N-terminal domain-containing protein



• Molecule 25: 40S ribosomal protein S15

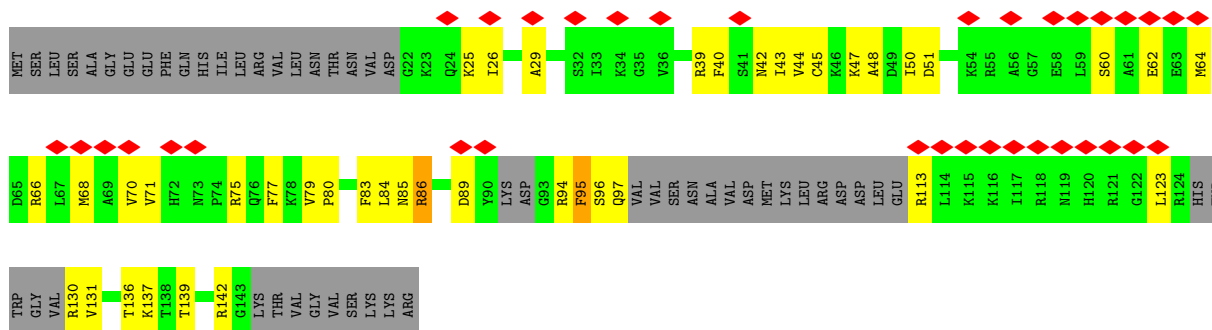


• Molecule 26: 40S ribosomal protein S16

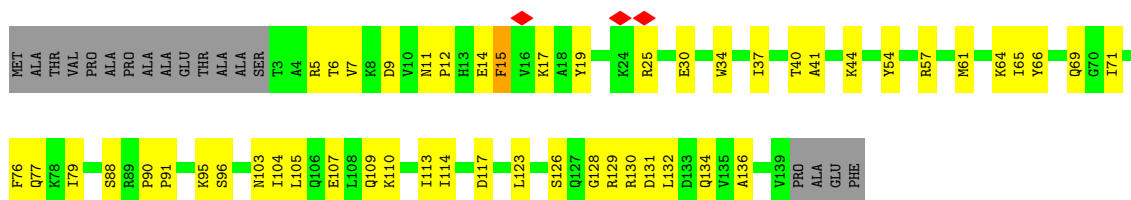


• Molecule 27: 40S ribosomal protein S18

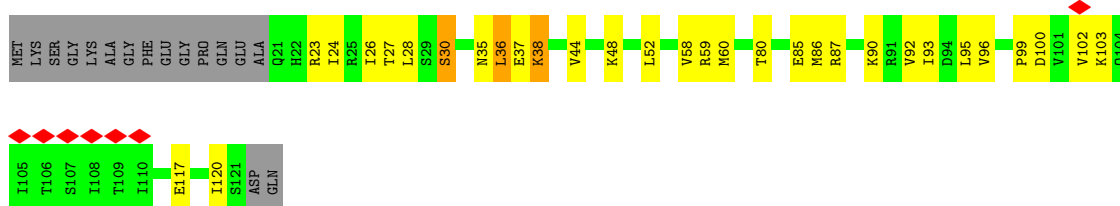




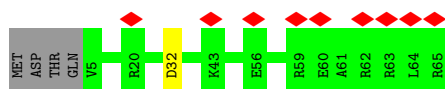
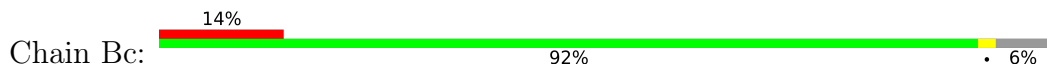
• Molecule 28: 40S ribosomal protein S19



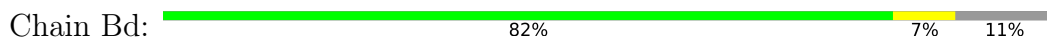
• Molecule 29: Ribosomal protein S10 domain-containing protein



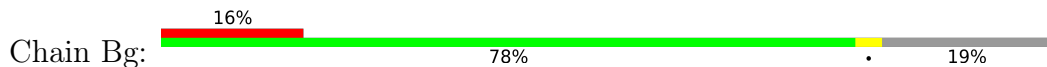
• Molecule 30: 40S ribosomal protein S28

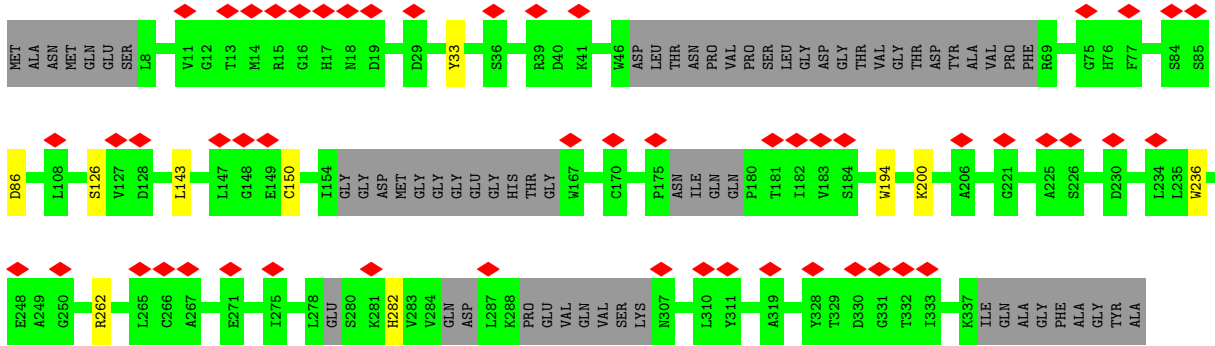


• Molecule 31: 40S ribosomal protein S29

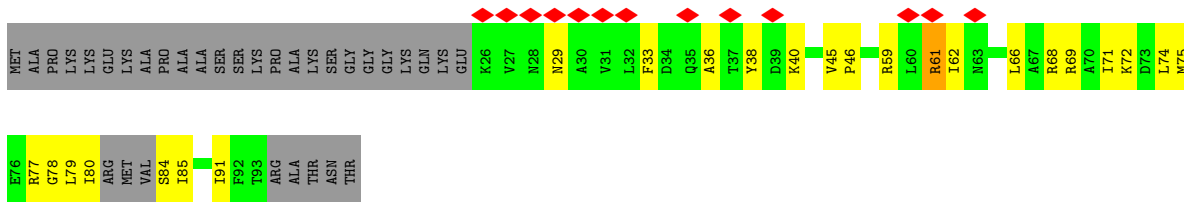


• Molecule 32: Mitogen-activated protein kinase





• Molecule 33: 40S ribosomal protein S25



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	105563	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 ($e^-/\text{\AA}^2$)	44.60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	4.553	Depositor
Minimum map value	-1.846	Depositor
Average map value	-0.004	Depositor
Map value standard deviation	0.119	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	449.40002, 449.40002, 449.40002	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, OMU, K, MG, A2M, MA6, OMG, ZN, OMC

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	Ad	0.30	0/36448	0.80	35/56766 (0.1%)
2	BA	0.29	0/1587	0.60	1/2147 (0.0%)
3	BB	0.26	0/1770	0.56	0/2378
4	BC	0.29	0/1740	0.52	0/2351
5	BE	0.28	0/2129	0.55	0/2855
6	BG	0.28	0/1867	0.62	1/2480 (0.0%)
7	BH	0.27	0/1394	0.56	0/1894
8	BI	0.27	0/1526	0.56	0/2038
9	BJ	0.28	0/1532	0.56	0/2050
10	BL	0.29	0/1233	0.52	0/1652
11	BN	0.25	0/1215	0.49	0/1634
12	BO	0.27	0/996	0.61	0/1336
13	BR	0.26	0/979	0.64	0/1306
14	BV	0.27	0/645	0.54	0/867
15	BW	0.29	0/1050	0.53	0/1405
16	BX	0.28	0/1096	0.52	0/1460
17	BY	0.28	0/1025	0.57	1/1359 (0.1%)
18	Ba	0.28	0/806	0.59	0/1077
19	Bb	0.26	0/674	0.54	0/905
20	Be	0.24	0/380	0.56	0/502
21	Cn	0.24	0/238	0.66	0/300
22	BD	0.26	0/1647	0.56	0/2215
23	BF	0.24	0/1435	0.51	0/1932
24	BK	0.25	0/730	0.49	0/983
25	BP	0.26	0/575	0.59	0/762
26	BQ	0.53	2/1126 (0.2%)	0.80	4/1502 (0.3%)
27	BS	0.24	0/831	0.57	0/1095
28	BT	0.26	0/1103	0.56	0/1482
29	BU	0.24	0/802	0.54	0/1081
30	Bc	0.24	0/490	0.65	0/652
31	Bd	0.26	0/413	0.56	0/549
32	Bg	0.24	0/2129	0.50	0/2889

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BZ	0.24	0/526	0.56	0/706
All	All	0.29	2/72137 (0.0%)	0.70	42/104610 (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
2	BA	0	1
7	BH	0	1
13	BR	0	2
19	Bb	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BQ	45	PRO	CG-CD	-12.96	1.07	1.50
26	BQ	45	PRO	N-CD	7.33	1.58	1.47

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BQ	45	PRO	N-CD-CG	-14.74	81.09	103.20
26	BQ	45	PRO	CA-N-CD	-11.06	96.01	111.50
1	Ad	1395	C	C2-N1-C1'	7.71	127.28	118.80
1	Ad	1218	U	C2-N1-C1'	7.37	126.54	117.70
1	Ad	1071	C	N3-C2-O2	-7.12	116.91	121.90
26	BQ	45	PRO	CA-CB-CG	-6.80	91.08	104.00
1	Ad	791	C	C2-N1-C1'	6.43	125.87	118.80
1	Ad	1251	U	N1-C2-O2	6.35	127.24	122.80
1	Ad	1251	U	N3-C2-O2	-6.32	117.78	122.20
6	BG	27	LEU	CA-CB-CG	6.30	129.80	115.30
1	Ad	932	C	N3-C2-O2	-6.30	117.49	121.90
1	Ad	932	C	N1-C2-O2	6.14	122.58	118.90
1	Ad	1218	U	N1-C2-O2	6.10	127.07	122.80
1	Ad	1395	C	N1-C2-O2	6.08	122.55	118.90
1	Ad	1251	U	C2-N1-C1'	6.08	124.99	117.70
1	Ad	791	C	N1-C2-O2	5.99	122.49	118.90
1	Ad	1457	C	N3-C2-O2	-5.91	117.76	121.90
1	Ad	1219	C	C2-N1-C1'	5.86	125.24	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ad	1171	C	C2-N1-C1'	5.82	125.20	118.80
1	Ad	1071	C	N1-C2-O2	5.78	122.37	118.90
1	Ad	1395	C	C6-N1-C2	-5.62	118.05	120.30
1	Ad	523	C	C2-N1-C1'	5.60	124.96	118.80
17	BY	45	LEU	CA-CB-CG	5.51	127.97	115.30
1	Ad	1218	U	N3-C2-O2	-5.47	118.37	122.20
1	Ad	970	U	C2-N1-C1'	5.43	124.22	117.70
26	BQ	45	PRO	N-CA-CB	-5.36	96.70	102.60
1	Ad	523	C	N1-C2-O2	5.34	122.11	118.90
1	Ad	1783	C	N3-C2-O2	-5.34	118.16	121.90
1	Ad	1395	C	N3-C2-O2	-5.33	118.17	121.90
1	Ad	1178	C	N1-C2-O2	5.32	122.09	118.90
2	BA	158	MET	CB-CG-SD	5.31	128.32	112.40
1	Ad	1219	C	N1-C2-O2	5.27	122.06	118.90
1	Ad	1264	U	C2-N1-C1'	5.26	124.02	117.70
1	Ad	1305	U	C2-N1-C1'	5.25	124.01	117.70
1	Ad	527	C	C2-N1-C1'	5.24	124.57	118.80
1	Ad	1783	C	N1-C2-O2	5.23	122.04	118.90
1	Ad	791	C	N3-C2-O2	-5.18	118.27	121.90
1	Ad	1372	C	C2-N1-C1'	5.16	124.47	118.80
1	Ad	1395	C	C6-N1-C1'	-5.12	114.65	120.80
1	Ad	1783	C	C2-N1-C1'	5.09	124.40	118.80
1	Ad	1171	C	N1-C2-O2	5.04	121.92	118.90
1	Ad	1372	C	N1-C2-O2	5.01	121.91	118.90

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	BA	43	TYR	Peptide
7	BH	103	ARG	Peptide
13	BR	73	LEU	Peptide
13	BR	74	GLN	Peptide
19	Bb	62	GLN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Ad	33567	0	16962	0	0
2	BA	1554	0	1565	64	0
3	BB	1740	0	1806	48	0
4	BC	1703	0	1790	49	0
5	BE	2088	0	2189	52	0
6	BG	1847	0	1989	47	0
7	BH	1368	0	1304	47	0
8	BI	1504	0	1548	25	0
9	BJ	1504	0	1571	22	0
10	BL	1207	0	1262	18	0
11	BN	1191	0	1284	13	0
12	BO	983	0	1012	20	0
13	BR	969	0	1013	41	0
14	BV	636	0	626	21	0
15	BW	1032	0	1068	12	0
16	BX	1077	0	1140	15	0
17	BY	1011	0	1095	15	0
18	Ba	791	0	815	0	0
19	Bb	663	0	683	0	0
20	Be	376	0	406	0	0
21	Cn	237	0	289	0	0
22	BD	1623	0	1696	32	0
23	BF	1416	0	1454	41	0
24	BK	711	0	712	28	0
25	BP	567	0	597	19	0
26	BQ	1108	0	1171	44	0
27	BS	822	0	862	30	0
28	BT	1081	0	1101	41	0
29	BU	793	0	851	25	0
30	Bc	489	0	532	0	0
31	Bd	403	0	394	0	0
32	Bg	2086	0	2057	0	0
33	BZ	521	0	548	18	0
34	Ad	14	0	0	0	0
34	BT	1	0	0	0	0
34	Bd	1	0	0	0	0
35	Ad	69	0	0	0	0
35	BS	1	0	0	0	0
36	Bd	1	0	0	0	0
All	All	68755	0	53392	747	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 13.

All (747) 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)
13:BR:10:LYS:HG2	13:BR:53:PHE:HE1	1.36	0.89
5:BE:87:MET:HE1	5:BE:123:LEU:HB2	1.62	0.81
12:BO:95:ILE:HD13	12:BO:126:ILE:HG23	1.66	0.77
7:BH:99:ARG:HD2	7:BH:122:VAL:HG13	1.69	0.74
27:BS:80:PRO:HG3	28:BT:37:ILE:HG12	1.70	0.74
2:BA:72:ILE:HD11	2:BA:78:ILE:HD11	1.71	0.73
5:BE:199:GLU:OE2	5:BE:201:HIS:NE2	2.21	0.72
25:BP:60:MET:HA	25:BP:63:VAL:HG22	1.71	0.71
13:BR:20:TYR:HE1	13:BR:23:ARG:HB3	1.56	0.71
24:BK:46:MET:HG2	24:BK:66:TRP:CE2	2.25	0.71
10:BL:114:SER:HG	10:BL:116:CYS:HG	1.39	0.71
26:BQ:63:ARG:HH22	26:BQ:105:ALA:HB1	1.54	0.71
3:BB:182:LYS:O	3:BB:186:ASN:ND2	2.24	0.71
33:BZ:69:ARG:HA	33:BZ:72:LYS:HD3	1.72	0.71
10:BL:35:ARG:NH2	10:BL:55:TYR:O	2.17	0.70
2:BA:54:ASN:HA	13:BR:105:MET:HE3	1.72	0.70
3:BB:36:LEU:HA	3:BB:41:ARG:HE	1.56	0.70
13:BR:40:ILE:HG22	13:BR:42:GLN:HE22	1.56	0.70
29:BU:58:VAL:HB	29:BU:92:VAL:HG23	1.72	0.70
16:BX:100:LEU:HB3	16:BX:123:LYS:HB2	1.73	0.70
27:BS:84:LEU:HD23	27:BS:97:GLN:HG2	1.72	0.70
4:BC:163:GLY:HA2	14:BV:3:ASN:HD21	1.56	0.70
6:BG:135:ARG:HG2	6:BG:178:PRO:HG3	1.73	0.70
23:BF:25:GLY:N	23:BF:36:GLU:OE2	2.24	0.70
28:BT:41:ALA:HB3	28:BT:44:LYS:HG3	1.73	0.70
7:BH:105:PRO:HG2	7:BH:113:ARG:HG2	1.74	0.69
5:BE:48:LEU:HD12	5:BE:61:VAL:HG13	1.74	0.69
28:BT:131:ASP:HA	28:BT:134:GLN:HE21	1.56	0.69
2:BA:39:GLU:HA	2:BA:42:VAL:HG22	1.75	0.69
6:BG:67:VAL:HB	6:BG:101:GLY:HA2	1.74	0.69
26:BQ:97:TYR:HB2	26:BQ:106:LYS:HB2	1.74	0.69
33:BZ:45:VAL:HG13	33:BZ:46:PRO:HD3	1.73	0.69
4:BC:183:MET:HG2	4:BC:212:THR:HG22	1.75	0.69
13:BR:66:VAL:HG23	13:BR:68:GLY:H	1.57	0.69
2:BA:130:ASP:OD1	2:BA:169:ASN:ND2	2.26	0.68
14:BV:21:ASN:O	14:BV:21:ASN:ND2	2.26	0.68
22:BD:119:ARG:H	22:BD:119:ARG:HD2	1.58	0.68
23:BF:37:ASP:OD1	23:BF:118:ASN:ND2	2.27	0.68
24:BK:8:ARG:NH2	24:BK:9:ASN:OD1	2.26	0.68
2:BA:122:GLU:OE2	2:BA:122:GLU:N	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:BK:24:LYS:O	24:BK:39:ASN:ND2	2.28	0.67
23:BF:91:GLY:HA2	23:BF:94:ASN:HD21	1.57	0.67
15:BW:87:GLU:OE2	15:BW:117:ARG:NH2	2.26	0.67
2:BA:149:ILE:HG12	2:BA:163:ILE:HB	1.76	0.67
3:BB:47:LEU:HB2	12:BO:51:GLU:HG3	1.77	0.67
5:BE:48:LEU:HD13	5:BE:64:ILE:HD11	1.76	0.67
9:BJ:135:HIS:ND1	9:BJ:164:SER:OG	2.25	0.67
7:BH:105:PRO:HG3	7:BH:111:VAL:HG13	1.77	0.67
4:BC:134:GLU:N	4:BC:134:GLU:OE1	2.28	0.67
28:BT:113:ILE:HG23	28:BT:114:ILE:HG23	1.77	0.67
33:BZ:84:SER:N	33:BZ:91:ILE:O	2.28	0.66
5:BE:130:GLN:OE1	5:BE:130:GLN:N	2.28	0.66
24:BK:8:ARG:NH1	24:BK:12:CYS:SG	2.68	0.66
28:BT:7:VAL:HA	28:BT:15:PHE:HE2	1.58	0.66
3:BB:144:LYS:HB2	3:BB:208:GLN:HB3	1.77	0.66
13:BR:6:THR:HG22	13:BR:8:THR:H	1.59	0.66
8:BI:76:THR:OG1	8:BI:105:ASP:OD1	2.12	0.66
26:BQ:90:ALA:O	26:BQ:94:VAL:HG23	1.96	0.66
10:BL:57:ASP:OD1	10:BL:84:ARG:NH1	2.30	0.65
9:BJ:140:ARG:O	9:BJ:140:ARG:NH1	2.29	0.65
13:BR:11:LYS:O	13:BR:15:GLN:HG2	1.96	0.65
28:BT:65:ILE:HD13	28:BT:114:ILE:HG21	1.79	0.65
6:BG:173:LYS:HE2	6:BG:173:LYS:HA	1.78	0.65
2:BA:69:ILE:HD11	2:BA:186:VAL:HG21	1.78	0.64
3:BB:32:ILE:HD13	3:BB:96:VAL:HG21	1.79	0.64
10:BL:125:VAL:HG12	10:BL:144:VAL:HG22	1.79	0.64
23:BF:50:ALA:HB3	23:BF:78:PRO:HA	1.77	0.64
9:BJ:153:GLU:O	9:BJ:156:LYS:NZ	2.30	0.64
13:BR:10:LYS:HG2	13:BR:53:PHE:CE1	2.27	0.64
14:BV:65:ASP:OD1	14:BV:66:GLY:N	2.30	0.64
4:BC:167:THR:HG21	4:BC:186:ALA:H	1.63	0.64
8:BI:147:SER:O	8:BI:151:GLN:NE2	2.31	0.64
9:BJ:159:ASP:OD1	9:BJ:160:PHE:N	2.30	0.64
22:BD:112:LEU:HD11	22:BD:178:VAL:HG21	1.79	0.64
5:BE:45:ILE:HD12	5:BE:61:VAL:HG21	1.79	0.63
3:BB:229:MET:HE2	3:BB:229:MET:H	1.63	0.63
6:BG:32:ILE:HG23	6:BG:53:MET:HA	1.80	0.63
3:BB:145:ARG:NH2	3:BB:151:LYS:O	2.32	0.63
28:BT:105:LEU:O	28:BT:109:GLN:HG3	1.99	0.63
16:BX:97:ASP:OD2	16:BX:98:GLU:N	2.31	0.63
8:BI:7:MET:HE3	8:BI:20:TRP:H	1.62	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BD:44:VAL:HG12	22:BD:49:THR:HG22	1.81	0.62
2:BA:153:ASP:OD1	2:BA:154:THR:N	2.32	0.62
7:BH:103:ARG:O	7:BH:103:ARG:NE	2.32	0.62
10:BL:114:SER:OG	10:BL:116:CYS:SG	2.51	0.62
29:BU:37:GLU:OE2	29:BU:59:ARG:NH1	2.29	0.62
5:BE:233:LYS:NZ	5:BE:234:PRO:O	2.33	0.62
2:BA:32:LYS:O	2:BA:45:ARG:NH2	2.32	0.61
5:BE:60:GLU:HA	5:BE:63:SER:HB3	1.80	0.61
27:BS:48:ALA:HB2	27:BS:70:VAL:HG21	1.82	0.61
4:BC:72:LEU:O	14:BV:15:ARG:NH1	2.33	0.61
17:BY:96:ARG:O	17:BY:100:ASN:ND2	2.33	0.61
22:BD:129:VAL:O	22:BD:132:SER:OG	2.17	0.61
6:BG:45:PHE:HE1	6:BG:123:LEU:HD21	1.64	0.61
3:BB:44:GLY:HA3	12:BO:47:LEU:HD11	1.83	0.61
33:BZ:36:ALA:O	33:BZ:40:LYS:HG2	2.00	0.61
3:BB:144:LYS:HB3	3:BB:206:PRO:HB2	1.82	0.61
16:BX:65:ILE:O	16:BX:67:LYS:NZ	2.33	0.61
29:BU:95:LEU:HD23	29:BU:102:VAL:HG22	1.82	0.61
3:BB:167:LYS:NZ	3:BB:200:ALA:O	2.33	0.61
6:BG:219:GLN:OE1	6:BG:220:ARG:NH1	2.34	0.61
8:BI:87:ASN:HB3	8:BI:90:LEU:HG	1.81	0.61
6:BG:105:SER:OG	6:BG:107:ASP:OD1	2.19	0.60
16:BX:52:GLU:HG2	16:BX:70:ARG:HB3	1.81	0.60
13:BR:80:ARG:O	13:BR:80:ARG:NH1	2.34	0.60
4:BC:87:CYS:HB3	4:BC:90:LEU:HD21	1.81	0.60
26:BQ:133:PHE:HE2	29:BU:80:THR:HA	1.66	0.60
5:BE:41:CYS:HA	5:BE:85:GLY:HA2	1.82	0.60
22:BD:181:ARG:O	22:BD:181:ARG:NH1	2.30	0.60
25:BP:43:PHE:HD1	25:BP:44:PRO:HD2	1.66	0.60
10:BL:89:ARG:NH1	10:BL:91:ASN:OD1	2.34	0.60
14:BV:78:GLU:O	14:BV:80:LYS:NZ	2.30	0.60
28:BT:107:GLU:HA	28:BT:110:LYS:HD2	1.82	0.60
24:BK:16:PHE:HE2	24:BK:73:ILE:HG13	1.66	0.60
2:BA:204:ASP:N	2:BA:204:ASP:OD1	2.28	0.60
3:BB:33:LYS:NZ	3:BB:42:ASN:OD1	2.35	0.60
4:BC:156:GLY:N	4:BC:167:THR:O	2.32	0.59
7:BH:94:VAL:HG21	7:BH:130:VAL:HG13	1.82	0.59
4:BC:175:LYS:NZ	4:BC:177:GLY:O	2.31	0.59
2:BA:28:HIS:HB3	2:BA:55:LEU:HD11	1.84	0.59
7:BH:136:ILE:HG23	7:BH:153:ILE:HG23	1.85	0.59
7:BH:113:ARG:HH12	7:BH:119:LEU:H	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BD:102:ILE:HG13	22:BD:176:ARG:HH22	1.67	0.59
27:BS:51:ASP:OD1	27:BS:51:ASP:N	2.35	0.59
12:BO:67:ASP:O	12:BO:70:SER:OG	2.19	0.59
2:BA:64:MET:HA	2:BA:67:ARG:HD2	1.83	0.59
3:BB:26:LYS:HE3	3:BB:26:LYS:HA	1.85	0.58
3:BB:46:THR:OG1	12:BO:46:ASP:OD2	2.16	0.58
4:BC:154:ARG:HB2	4:BC:236:TYR:CD2	2.38	0.58
14:BV:69:ASP:O	14:BV:73:GLN:HG2	2.03	0.58
22:BD:67:ARG:HH21	22:BD:68:ARG:HH11	1.50	0.58
16:BX:67:LYS:HB3	16:BX:90:LEU:HD22	1.84	0.58
4:BC:68:GLU:N	4:BC:68:GLU:OE1	2.37	0.58
6:BG:43:GLU:OE2	6:BG:44:GLU:N	2.36	0.58
11:BN:5:HIS:HB3	11:BN:117:LEU:HD13	1.85	0.58
13:BR:98:VAL:HG23	13:BR:102:THR:HB	1.84	0.58
24:BK:46:MET:HE1	24:BK:55:VAL:HG11	1.86	0.58
4:BC:242:ASP:HB2	14:BV:1:MET:HG2	1.83	0.58
23:BF:83:LEU:HD23	23:BF:162:ILE:HG23	1.84	0.58
2:BA:18:ASP:O	2:BA:22:MET:HG3	2.04	0.58
2:BA:60:GLU:HA	2:BA:63:GLN:HB3	1.86	0.58
6:BG:164:ARG:NE	6:BG:175:SER:OG	2.32	0.58
13:BR:12:THR:O	13:BR:16:VAL:HG12	2.04	0.58
3:BB:64:ARG:HA	3:BB:88:ALA:H	1.68	0.58
8:BI:2:ILE:HD12	8:BI:2:ILE:H	1.69	0.57
6:BG:135:ARG:NE	6:BG:161:THR:OG1	2.37	0.57
14:BV:21:ASN:C	14:BV:21:ASN:HD22	2.06	0.57
16:BX:138:GLU:N	16:BX:138:GLU:OE1	2.38	0.57
26:BQ:77:GLY:N	26:BQ:80:SER:OG	2.37	0.57
26:BQ:17:LYS:HD2	26:BQ:80:SER:HA	1.86	0.57
29:BU:28:LEU:HB3	29:BU:36:LEU:HD21	1.86	0.57
3:BB:27:LYS:HA	3:BB:48:VAL:O	2.05	0.57
3:BB:50:ARG:HG2	3:BB:51:THR:HG22	1.86	0.57
4:BC:191:GLY:N	4:BC:209:ASP:OD2	2.30	0.57
8:BI:5:ASP:HB3	8:BI:27:GLU:OE1	2.04	0.57
26:BQ:98:GLN:O	26:BQ:98:GLN:NE2	2.37	0.57
3:BB:68:VAL:HG23	3:BB:84:ILE:HB	1.85	0.57
28:BT:130:ARG:O	28:BT:130:ARG:NH1	2.38	0.57
28:BT:131:ASP:OD2	28:BT:134:GLN:NE2	2.37	0.57
2:BA:124:ARG:NH1	4:BC:254:TYR:O	2.38	0.57
10:BL:23:THR:HG22	10:BL:24:LYS:H	1.70	0.57
24:BK:3:ILE:HG21	24:BK:45:LEU:HD11	1.87	0.56
5:BE:54:TYR:O	17:BY:20:ASN:ND2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:BN:84:ILE:HD12	11:BN:149:LEU:HD21	1.88	0.56
23:BF:61:PRO:HB3	23:BF:80:ILE:HG13	1.87	0.56
9:BJ:90:GLU:OE1	9:BJ:90:GLU:N	2.37	0.56
26:BQ:71:ILE:HG21	26:BQ:85:ILE:HD13	1.88	0.56
26:BQ:85:ILE:O	26:BQ:89:ILE:HG22	2.04	0.56
7:BH:145:LEU:HA	15:BW:42:GLN:HE21	1.70	0.56
8:BI:2:ILE:O	8:BI:29:GLY:N	2.34	0.56
8:BI:199:GLU:OE1	10:BL:11:LYS:NZ	2.29	0.56
13:BR:57:LEU:O	13:BR:61:ILE:HG13	2.05	0.56
22:BD:62:LEU:HA	22:BD:69:ILE:HD11	1.87	0.56
23:BF:42:ASP:OD1	23:BF:44:SER:OG	2.20	0.56
3:BB:180:ASP:N	3:BB:180:ASP:OD1	2.38	0.56
12:BO:74:ALA:HB1	12:BO:115:ALA:HB2	1.87	0.56
23:BF:111:ILE:HD12	23:BF:189:ILE:HG23	1.87	0.56
24:BK:55:VAL:HG11	24:BK:66:TRP:HB3	1.88	0.56
4:BC:90:LEU:HD12	4:BC:118:VAL:HG22	1.87	0.56
17:BY:54:GLU:N	17:BY:54:GLU:OE1	2.39	0.55
28:BT:54:TYR:OH	28:BT:107:GLU:OE1	2.24	0.55
5:BE:249:ILE:O	5:BE:253:ARG:HG2	2.06	0.55
25:BP:62:LEU:HD22	25:BP:86:LEU:HD11	1.89	0.55
6:BG:221:LEU:O	6:BG:225:ARG:NH1	2.38	0.55
23:BF:112:HIS:HB2	23:BF:119:PRO:HD3	1.88	0.55
13:BR:108:PHE:HD2	13:BR:109:LEU:HG	1.71	0.55
2:BA:37:GLN:HG3	2:BA:158:MET:HG2	1.88	0.55
13:BR:87:GLU:OE1	13:BR:87:GLU:N	2.40	0.55
28:BT:76:PHE:HA	28:BT:79:ILE:HG22	1.89	0.55
22:BD:77:GLN:HA	22:BD:82:PHE:HB2	1.88	0.55
2:BA:69:ILE:HG22	2:BA:125:LEU:HD21	1.89	0.55
26:BQ:43:ILE:HB	26:BQ:49:ARG:HG3	1.89	0.55
13:BR:70:SER:OG	13:BR:71:LEU:N	2.40	0.54
23:BF:136:ALA:HB3	23:BF:147:ARG:HH21	1.71	0.54
23:BF:185:ALA:O	23:BF:189:ILE:HG12	2.06	0.54
9:BJ:171:ALA:O	9:BJ:176:ARG:NH1	2.40	0.54
4:BC:70:ILE:HG23	4:BC:75:LEU:HB2	1.88	0.54
6:BG:25:ARG:O	6:BG:28:TYR:HB2	2.08	0.54
14:BV:81:GLN:N	14:BV:81:GLN:OE1	2.41	0.54
4:BC:59:VAL:HG21	4:BC:82:ILE:HG23	1.90	0.54
6:BG:51:LYS:HB3	6:BG:114:VAL:HG12	1.90	0.54
14:BV:7:ASP:OD1	14:BV:7:ASP:N	2.40	0.54
13:BR:45:ARG:HA	13:BR:48:ASN:HD22	1.73	0.54
2:BA:151:PHE:CD1	2:BA:178:LEU:HD21	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BC:236:TYR:OH	14:BV:12:TYR:O	2.23	0.54
10:BL:32:GLU:OE2	10:BL:32:GLU:N	2.41	0.54
2:BA:131:PRO:HG2	2:BA:156:SER:HB2	1.90	0.54
4:BC:237:GLY:HA2	14:BV:23:ILE:HD11	1.89	0.54
25:BP:47:PRO:HA	25:BP:90:ILE:HD13	1.90	0.54
29:BU:100:ASP:HA	29:BU:103:LYS:HD2	1.90	0.54
8:BI:117:TYR:CD2	8:BI:161:ARG:HG3	2.43	0.53
12:BO:84:ARG:O	12:BO:84:ARG:HD3	2.08	0.53
2:BA:33:ASN:OD1	2:BA:33:ASN:N	2.41	0.53
8:BI:5:ASP:HB2	8:BI:7:MET:H	1.73	0.53
11:BN:6:SER:OG	11:BN:7:ARG:N	2.40	0.53
5:BE:212:ASP:OD1	5:BE:213:ALA:N	2.42	0.53
9:BJ:84:ARG:HG2	9:BJ:151:ARG:HD3	1.90	0.53
27:BS:40:PHE:O	27:BS:44:VAL:HG13	2.08	0.53
28:BT:69:GLN:N	28:BT:69:GLN:OE1	2.41	0.53
2:BA:43:TYR:HB3	2:BA:52:ILE:HG23	1.90	0.53
4:BC:197:VAL:HB	4:BC:198:PRO:HD3	1.90	0.53
5:BE:21:ASP:OD1	5:BE:21:ASP:N	2.42	0.53
5:BE:115:ARG:HE	5:BE:116:ASP:H	1.55	0.53
10:BL:38:LYS:NZ	10:BL:61:PRO:O	2.38	0.53
23:BF:80:ILE:HD11	23:BF:104:ILE:HG12	1.91	0.53
6:BG:9:THR:OG1	6:BG:10:THR:N	2.43	0.52
12:BO:97:LEU:HD12	12:BO:98:ARG:N	2.24	0.52
14:BV:16:LYS:HA	14:BV:23:ILE:HA	1.90	0.52
23:BF:91:GLY:HA2	23:BF:94:ASN:ND2	2.22	0.52
2:BA:148:THR:OG1	2:BA:161:VAL:HA	2.08	0.52
2:BA:198:LYS:HZ3	2:BA:201:ILE:HA	1.74	0.52
6:BG:61:PHE:CE2	6:BG:98:SER:HB2	2.44	0.52
22:BD:165:GLN:OE1	22:BD:168:ASN:ND2	2.35	0.52
2:BA:141:SER:HB2	2:BA:146:ILE:HB	1.91	0.52
5:BE:186:GLY:O	5:BE:189:THR:OG1	2.28	0.52
26:BQ:98:GLN:HG3	26:BQ:99:LYS:HD3	1.92	0.52
4:BC:167:THR:HG23	4:BC:209:ASP:O	2.10	0.52
7:BH:105:PRO:HD2	7:BH:113:ARG:HD3	1.92	0.52
29:BU:60:MET:HG2	29:BU:90:LYS:HD2	1.90	0.52
5:BE:199:GLU:HG2	5:BE:207:THR:HB	1.91	0.52
13:BR:53:PHE:O	13:BR:57:LEU:HG	2.10	0.52
3:BB:39:THR:O	3:BB:41:ARG:NH1	2.43	0.52
25:BP:43:PHE:CD1	25:BP:44:PRO:HD2	2.44	0.52
26:BQ:44:ARG:HH12	28:BT:12:PRO:HD2	1.75	0.52
27:BS:84:LEU:HA	27:BS:97:GLN:NE2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:BJ:171:ALA:HB1	9:BJ:175:LYS:HB3	1.92	0.52
13:BR:20:TYR:CE1	13:BR:23:ARG:HB3	2.43	0.52
13:BR:99:ASP:OD1	13:BR:102:THR:OG1	2.24	0.52
17:BY:86:GLU:OE1	17:BY:86:GLU:N	2.25	0.52
2:BA:111:THR:OG1	2:BA:119:SER:O	2.27	0.51
5:BE:151:ASP:OD1	6:BG:220:ARG:NH2	2.43	0.51
16:BX:72:GLN:HG3	16:BX:79:LYS:HG3	1.91	0.51
22:BD:78:LYS:HE2	24:BK:20:VAL:HB	1.92	0.51
16:BX:43:SER:OG	16:BX:45:HIS:O	2.26	0.51
3:BB:229:MET:HE2	3:BB:229:MET:N	2.25	0.51
12:BO:99:ALA:H	12:BO:133:THR:HG23	1.75	0.51
23:BF:29:LEU:HB3	23:BF:33:TRP:HB2	1.91	0.51
26:BQ:55:PRO:HG2	26:BQ:89:ILE:HG23	1.92	0.51
33:BZ:45:VAL:CG1	33:BZ:46:PRO:HD3	2.40	0.51
3:BB:181:LEU:O	3:BB:185:VAL:HG22	2.09	0.51
12:BO:77:ALA:O	12:BO:81:VAL:HG13	2.10	0.51
26:BQ:16:ARG:O	26:BQ:87:GLN:NE2	2.44	0.51
28:BT:11:ASN:ND2	28:BT:14:GLU:OE1	2.30	0.51
29:BU:60:MET:HB3	29:BU:90:LYS:HB3	1.92	0.51
2:BA:194:LEU:HD12	2:BA:194:LEU:H	1.75	0.51
8:BI:148:ASN:HA	8:BI:151:GLN:HE21	1.75	0.51
22:BD:48:ARG:NH1	22:BD:85:ASN:O	2.43	0.51
27:BS:48:ALA:HB3	27:BS:50:ILE:HG12	1.91	0.51
23:BF:87:LEU:O	23:BF:170:ARG:NH2	2.44	0.51
13:BR:9:VAL:HA	13:BR:12:THR:HG22	1.93	0.51
33:BZ:45:VAL:HG21	33:BZ:74:LEU:HD13	1.93	0.51
23:BF:134:GLU:HG3	23:BF:151:ASP:HA	1.93	0.51
4:BC:236:TYR:HE1	14:BV:14:PRO:HG3	1.74	0.51
13:BR:31:ASN:OD1	13:BR:55:THR:OG1	2.24	0.51
16:BX:24:ASP:HB3	16:BX:27:TYR:HB3	1.92	0.50
5:BE:18:TRP:HH2	5:BE:31:PRO:HG3	1.75	0.50
6:BG:135:ARG:HD2	6:BG:136:GLY:H	1.76	0.50
13:BR:30:THR:HA	13:BR:33:LYS:HG2	1.94	0.50
6:BG:123:LEU:O	6:BG:127:THR:OG1	2.29	0.50
12:BO:31:ALA:HB2	12:BO:93:LEU:HD12	1.93	0.50
13:BR:72:LYS:HE2	13:BR:76:GLU:HA	1.93	0.50
23:BF:67:TYR:HA	23:BF:73:ARG:HG2	1.93	0.50
7:BH:16:PRO:HB2	7:BH:20:GLU:OE1	2.12	0.50
7:BH:80:LEU:O	7:BH:84:LEU:N	2.38	0.50
15:BW:3:ARG:NH1	15:BW:9:ASP:OD2	2.44	0.50
5:BE:171:ASP:OD1	5:BE:171:ASP:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BH:20:GLU:N	7:BH:20:GLU:OE2	2.44	0.50
7:BH:99:ARG:NH1	7:BH:126:ILE:HG22	2.27	0.50
7:BH:168:GLU:OE2	7:BH:168:GLU:N	2.40	0.50
11:BN:130:LYS:NZ	11:BN:139:TRP:O	2.28	0.50
22:BD:75:VAL:O	22:BD:79:ARG:HB3	2.12	0.50
23:BF:61:PRO:HB3	23:BF:80:ILE:HG23	1.93	0.50
24:BK:9:ASN:O	24:BK:13:LYS:HG2	2.11	0.50
26:BQ:28:PRO:HA	26:BQ:67:ILE:HG23	1.94	0.50
4:BC:93:GLU:HG2	4:BC:204:PHE:CZ	2.47	0.50
10:BL:127:ILE:HG22	10:BL:141:VAL:HA	1.93	0.50
27:BS:47:LYS:HZ1	27:BS:79:VAL:HG23	1.76	0.50
2:BA:17:GLN:O	2:BA:20:GLN:HG2	2.12	0.49
17:BY:48:ARG:O	17:BY:52:ILE:HG23	2.11	0.49
28:BT:19:TYR:OH	28:BT:131:ASP:OD1	2.18	0.49
15:BW:69:LEU:HD11	15:BW:72:CYS:HB3	1.93	0.49
29:BU:23:ARG:HD2	29:BU:96:VAL:HG12	1.93	0.49
2:BA:89:ARG:HG3	2:BA:204:ASP:HA	1.93	0.49
6:BG:32:ILE:HD11	6:BG:63:MET:HE3	1.94	0.49
8:BI:164:ASP:OD1	8:BI:166:HIS:N	2.42	0.49
22:BD:170:TYR:CZ	22:BD:207:LEU:HG	2.47	0.49
33:BZ:29:ASN:ND2	33:BZ:62:ILE:O	2.44	0.49
5:BE:165:GLU:H	5:BE:165:GLU:CD	2.14	0.49
8:BI:5:ASP:OD1	8:BI:5:ASP:N	2.34	0.49
13:BR:53:PHE:CE2	13:BR:57:LEU:HD21	2.47	0.49
22:BD:49:THR:N	22:BD:86:GLY:O	2.44	0.49
22:BD:140:ILE:HG12	22:BD:154:LYS:HG2	1.93	0.49
2:BA:124:ARG:HH12	4:BC:258:THR:HG22	1.78	0.49
7:BH:123:HIS:O	7:BH:174:TYR:OH	2.20	0.49
26:BQ:105:ALA:O	26:BQ:109:VAL:HG12	2.12	0.49
3:BB:133:TYR:CD2	3:BB:181:LEU:HD11	2.48	0.49
5:BE:12:LEU:HD21	5:BE:22:LYS:HG3	1.95	0.49
29:BU:30:SER:HB3	29:BU:36:LEU:HG	1.94	0.49
2:BA:83:ALA:HB2	2:BA:134:ASP:HB3	1.94	0.49
28:BT:130:ARG:HH22	28:BT:134:GLN:HB3	1.77	0.49
4:BC:229:PHE:O	4:BC:233:MET:HG3	2.13	0.49
8:BI:164:ASP:OD1	8:BI:165:SER:N	2.46	0.49
2:BA:93:LYS:HE2	2:BA:204:ASP:HB3	1.95	0.49
3:BB:129:THR:HG23	3:BB:131:ASP:H	1.77	0.49
24:BK:32:HIS:N	24:BK:37:VAL:O	2.42	0.49
25:BP:40:VAL:HA	25:BP:43:PHE:HB2	1.95	0.49
27:BS:48:ALA:HB1	27:BS:66:ARG:HG2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BZ:61:ARG:O	33:BZ:61:ARG:NE	2.46	0.49
13:BR:106:LEU:HD12	13:BR:111:MET:O	2.13	0.48
23:BF:87:LEU:HD12	23:BF:170:ARG:HH21	1.78	0.48
24:BK:21:LEU:HB2	24:BK:66:TRP:HB2	1.95	0.48
28:BT:71:ILE:HB	28:BT:76:PHE:HE1	1.78	0.48
15:BW:70:ASN:ND2	15:BW:130:TYR:OXT	2.43	0.48
16:BX:86:ASN:HB3	16:BX:133:PHE:CD1	2.47	0.48
2:BA:72:ILE:O	2:BA:73:GLU:HG3	2.13	0.48
6:BG:33:SER:HA	6:BG:51:LYS:HE2	1.94	0.48
7:BH:70:ARG:NH2	7:BH:129:ASP:OD2	2.47	0.48
2:BA:30:GLY:N	2:BA:51:TYR:O	2.46	0.48
26:BQ:113:PHE:CD2	26:BQ:120:LEU:HD23	2.48	0.48
2:BA:79:ILE:HD12	2:BA:79:ILE:H	1.78	0.48
4:BC:57:ARG:NH2	4:BC:260:ILE:O	2.47	0.48
5:BE:204:THR:OG1	5:BE:205:PHE:N	2.46	0.48
17:BY:13:ARG:HD3	17:BY:15:ARG:HH21	1.79	0.48
7:BH:120:THR:HA	7:BH:123:HIS:CD2	2.49	0.48
12:BO:79:GLN:O	12:BO:83:THR:HG23	2.13	0.48
28:BT:30:GLU:HG2	28:BT:107:GLU:OE2	2.14	0.48
7:BH:45:TYR:CD2	7:BH:46:ILE:HG13	2.48	0.48
7:BH:145:LEU:HA	15:BW:42:GLN:NE2	2.28	0.48
23:BF:27:VAL:HG22	23:BF:59:PHE:HE1	1.78	0.48
23:BF:66:ARG:HE	23:BF:66:ARG:HA	1.78	0.48
26:BQ:133:PHE:O	26:BQ:141:ARG:NH1	2.47	0.48
2:BA:177:CYS:SG	2:BA:178:LEU:N	2.86	0.48
23:BF:111:ILE:O	23:BF:115:THR:OG1	2.28	0.48
5:BE:58:TYR:HD1	5:BE:58:TYR:O	1.96	0.48
5:BE:255:ARG:HD2	5:BE:255:ARG:O	2.13	0.48
10:BL:121:GLU:OE1	10:BL:121:GLU:N	2.46	0.48
13:BR:108:PHE:CD2	13:BR:109:LEU:HG	2.48	0.48
24:BK:71:ASP:HA	24:BK:74:GLU:HG2	1.94	0.48
2:BA:182:LEU:O	2:BA:186:VAL:HG23	2.14	0.47
4:BC:92:ASP:OD1	4:BC:118:VAL:HG23	2.13	0.47
13:BR:27:ASP:HB3	13:BR:30:THR:HG23	1.96	0.47
23:BF:209:ARG:HA	23:BF:212:LYS:HE3	1.96	0.47
25:BP:87:ARG:HD3	25:BP:123:ALA:HA	1.96	0.47
2:BA:201:ILE:O	2:BA:203:VAL:HG13	2.13	0.47
4:BC:93:GLU:HG2	4:BC:204:PHE:HZ	1.79	0.47
5:BE:163:ASP:OD1	5:BE:164:LEU:N	2.46	0.47
6:BG:38:GLY:HA3	6:BG:45:PHE:HB3	1.96	0.47
6:BG:50:PHE:HB3	6:BG:113:LEU:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:BF:98:ILE:HD12	26:BQ:48:LEU:HD11	1.95	0.47
25:BP:39:LEU:HD12	25:BP:40:VAL:HG13	1.96	0.47
4:BC:94:VAL:HG12	4:BC:116:VAL:HG22	1.97	0.47
5:BE:97:GLU:HB3	5:BE:99:TYR:CZ	2.50	0.47
23:BF:45:LEU:HD21	23:BF:157:ARG:HE	1.79	0.47
25:BP:64:LYS:HE2	25:BP:67:ARG:HH21	1.78	0.47
26:BQ:25:TYR:HB2	26:BQ:72:ARG:HH22	1.80	0.47
27:BS:94:ARG:NH1	27:BS:95:PHE:HB2	2.29	0.47
27:BS:130:ARG:HD3	27:BS:131:VAL:N	2.29	0.47
3:BB:23:PRO:HA	12:BO:88:LEU:HD21	1.96	0.47
3:BB:183:GLU:HA	3:BB:186:ASN:HB2	1.97	0.47
4:BC:89:GLY:O	4:BC:120:ASP:HB3	2.14	0.47
26:BQ:70:ARG:HH21	26:BQ:72:ARG:CZ	2.27	0.47
5:BE:174:LYS:HE3	5:BE:174:LYS:HB3	1.69	0.47
15:BW:80:ASP:OD1	15:BW:124:LYS:NZ	2.42	0.47
22:BD:161:ILE:HG22	22:BD:192:MET:HE1	1.96	0.47
23:BF:88:MET:HB3	23:BF:94:ASN:HA	1.97	0.47
28:BT:126:SER:O	28:BT:129:ARG:NH1	2.48	0.47
29:BU:99:PRO:HB2	29:BU:103:LYS:HE3	1.96	0.47
6:BG:89:ARG:HB3	6:BG:93:GLU:OE2	2.15	0.47
5:BE:44:LEU:HD23	5:BE:82:TYR:HB3	1.96	0.47
6:BG:5:ILE:HD12	6:BG:126:LEU:HD21	1.97	0.47
7:BH:146:ASP:OD1	7:BH:146:ASP:N	2.39	0.47
25:BP:120:HIS:CD2	25:BP:124:GLU:HB2	2.50	0.47
27:BS:136:THR:HA	27:BS:139:THR:HG22	1.97	0.47
3:BB:128:LYS:HB2	3:BB:134:MET:SD	2.55	0.46
4:BC:180:THR:OG1	4:BC:215:ARG:HB3	2.15	0.46
5:BE:248:ILE:O	5:BE:252:GLN:HG2	2.15	0.46
17:BY:94:LYS:O	17:BY:98:ILE:HG12	2.14	0.46
26:BQ:58:LEU:HD21	26:BQ:112:ILE:HG22	1.96	0.46
4:BC:157:TYR:OH	14:BV:3:ASN:ND2	2.48	0.46
6:BG:208:SER:O	6:BG:212:GLU:HG2	2.16	0.46
13:BR:55:THR:HG23	13:BR:59:ARG:NH1	2.30	0.46
28:BT:113:ILE:HG13	28:BT:128:GLY:HA3	1.96	0.46
2:BA:26:ASP:HB3	2:BA:29:LEU:HD11	1.97	0.46
8:BI:38:SER:HB3	8:BI:59:ARG:HG2	1.97	0.46
8:BI:155:GLU:OE1	8:BI:155:GLU:N	2.48	0.46
23:BF:156:ARG:NH1	23:BF:160:GLN:OE1	2.48	0.46
26:BQ:44:ARG:HH12	28:BT:12:PRO:CD	2.28	0.46
2:BA:115:GLN:HG2	2:BA:116:MET:SD	2.55	0.46
7:BH:144:ARG:NH2	7:BH:146:ASP:OD2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:BJ:102:THR:HG23	9:BJ:104:GLU:HG2	1.98	0.46
26:BQ:86:ARG:NH2	26:BQ:117:ASP:OD2	2.49	0.46
26:BQ:133:PHE:CE2	29:BU:80:THR:HA	2.50	0.46
7:BH:21:ASP:OD1	7:BH:22:THR:N	2.49	0.46
17:BY:98:ILE:HG21	17:BY:105:LYS:HE3	1.97	0.46
22:BD:32:LEU:HB2	22:BD:37:TYR:HB2	1.98	0.46
24:BK:46:MET:HA	24:BK:49:PHE:CD1	2.51	0.46
6:BG:157:SER:O	6:BG:157:SER:OG	2.27	0.46
7:BH:151:ILE:HB	7:BH:182:VAL:HG22	1.97	0.46
8:BI:57:ALA:HB2	8:BI:188:GLY:HA2	1.98	0.46
24:BK:46:MET:HA	24:BK:49:PHE:HD1	1.80	0.46
3:BB:34:ALA:HB3	3:BB:41:ARG:HA	1.96	0.46
7:BH:73:PHE:O	7:BH:77:HIS:N	2.47	0.46
27:BS:26:ILE:HD12	27:BS:26:ILE:H	1.80	0.46
2:BA:180:TRP:CZ2	2:BA:198:LYS:HE3	2.51	0.46
4:BC:246:GLU:OE1	4:BC:246:GLU:HA	2.16	0.46
13:BR:29:HIS:HA	13:BR:32:LYS:HG2	1.97	0.46
23:BF:175:ARG:HD2	23:BF:175:ARG:HA	1.75	0.46
26:BQ:107:LYS:O	26:BQ:111:GLU:HG2	2.15	0.46
26:BQ:124:ASP:O	26:BQ:127:ARG:NH2	2.36	0.46
28:BT:54:TYR:HE2	28:BT:104:ILE:HD13	1.80	0.46
28:BT:64:LYS:HE3	28:BT:79:ILE:HD11	1.98	0.46
2:BA:86:TYR:HE2	2:BA:172:LYS:HA	1.81	0.46
2:BA:150:ALA:HB3	2:BA:161:VAL:HG21	1.98	0.46
7:BH:126:ILE:O	7:BH:130:VAL:HG23	2.16	0.46
22:BD:157:ASP:OD1	22:BD:157:ASP:N	2.49	0.46
26:BQ:94:VAL:HG21	26:BQ:121:LEU:HD11	1.98	0.46
2:BA:79:ILE:HD12	2:BA:123:PRO:HB3	1.98	0.46
3:BB:33:LYS:HA	3:BB:33:LYS:HD3	1.55	0.46
4:BC:200:LYS:HA	4:BC:200:LYS:HD3	1.78	0.46
5:BE:68:ARG:HB3	5:BE:76:VAL:HG11	1.98	0.46
5:BE:206:GLU:HG2	5:BE:222:LEU:HD22	1.98	0.46
10:BL:35:ARG:NE	10:BL:53:GLY:O	2.41	0.46
11:BN:49:GLN:HA	11:BN:52:VAL:HG12	1.98	0.46
12:BO:97:LEU:HD12	12:BO:98:ARG:H	1.80	0.46
23:BF:131:GLY:O	23:BF:157:ARG:NH1	2.49	0.46
27:BS:40:PHE:O	27:BS:43:ILE:HG22	2.16	0.46
28:BT:117:ASP:HB3	28:BT:123:LEU:HG	1.97	0.46
33:BZ:45:VAL:HG11	33:BZ:79:LEU:HD13	1.97	0.46
3:BB:87:ARG:HB2	3:BB:101:TRP:HB2	1.98	0.45
5:BE:141:THR:OG1	5:BE:143:ASP:OD1	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BB:133:TYR:CG	3:BB:181:LEU:HD11	2.51	0.45
7:BH:127:LEU:HD21	7:BH:153:ILE:HD11	1.99	0.45
28:BT:7:VAL:HA	28:BT:15:PHE:CE2	2.45	0.45
2:BA:65:ALA:O	2:BA:69:ILE:HG23	2.15	0.45
5:BE:36:HIS:CG	5:BE:85:GLY:HA3	2.52	0.45
6:BG:167:LEU:HD23	6:BG:173:LYS:HE2	1.99	0.45
25:BP:87:ARG:HA	25:BP:122:LEU:HB2	1.99	0.45
7:BH:144:ARG:HA	15:BW:49:GLU:OE1	2.17	0.45
24:BK:7:ASN:O	24:BK:11:ILE:HG12	2.15	0.45
28:BT:54:TYR:CE2	28:BT:104:ILE:HD13	2.52	0.45
3:BB:108:ASP:O	3:BB:112:SER:OG	2.30	0.45
6:BG:172:LYS:HD2	6:BG:172:LYS:HA	1.72	0.45
22:BD:54:ARG:HH21	22:BD:94:VAL:HA	1.81	0.45
27:BS:60:SER:OG	27:BS:62:GLU:OE1	2.33	0.45
4:BC:259:ASP:OD1	4:BC:259:ASP:N	2.48	0.45
6:BG:30:LYS:NZ	6:BG:35:GLU:O	2.50	0.45
7:BH:70:ARG:O	7:BH:74:ARG:HG2	2.17	0.45
17:BY:85:LEU:O	17:BY:89:LYS:HG2	2.16	0.45
22:BD:137:CYS:SG	22:BD:138:GLU:N	2.90	0.45
23:BF:45:LEU:HD13	23:BF:128:ILE:HD11	1.98	0.45
25:BP:56:LYS:C	25:BP:59:PRO:HD2	2.36	0.45
26:BQ:93:LEU:O	26:BQ:96:TYR:HB2	2.17	0.45
2:BA:79:ILE:CD1	2:BA:123:PRO:HB3	2.47	0.45
3:BB:224:ASP:OD2	3:BB:227:LYS:NZ	2.42	0.45
5:BE:165:GLU:OE2	5:BE:165:GLU:N	2.35	0.45
6:BG:10:THR:O	6:BG:131:LYS:NZ	2.49	0.45
24:BK:50:LYS:HE3	24:BK:57:GLU:HG3	1.99	0.45
28:BT:15:PHE:CZ	28:BT:136:ALA:HB2	2.52	0.45
2:BA:66:ALA:O	2:BA:70:VAL:HG12	2.16	0.45
5:BE:95:THR:HG22	17:BY:21:ARG:HD3	1.98	0.45
5:BE:196:LYS:HD2	5:BE:196:LYS:HA	1.64	0.45
6:BG:106:GLN:OE1	6:BG:106:GLN:N	2.30	0.45
7:BH:158:LYS:O	7:BH:158:LYS:HG2	2.16	0.45
8:BI:73:THR:O	8:BI:74:ARG:NH1	2.49	0.45
12:BO:98:ARG:HB3	12:BO:132:VAL:HG23	1.98	0.45
6:BG:57:ASP:O	6:BG:109:SER:OG	2.28	0.45
26:BQ:25:TYR:CE2	26:BQ:27:LYS:HE3	2.52	0.45
29:BU:36:LEU:HA	29:BU:36:LEU:HD23	1.71	0.45
8:BI:155:GLU:HA	8:BI:158:GLN:HB2	1.99	0.44
13:BR:73:LEU:HD12	13:BR:78:ARG:HD3	1.98	0.44
23:BF:97:LYS:O	23:BF:101:VAL:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:BL:23:THR:HG21	10:BL:33:GLY:O	2.17	0.44
11:BN:107:LYS:HA	11:BN:107:LYS:HD2	1.69	0.44
2:BA:58:THR:O	2:BA:62:LEU:HG	2.18	0.44
27:BS:83:PHE:CD1	28:BT:37:ILE:HD11	2.53	0.44
3:BB:30:TYR:CD2	3:BB:61:LEU:HD11	2.53	0.44
11:BN:62:LEU:O	11:BN:65:SER:OG	2.31	0.44
16:BX:92:PHE:O	16:BX:139:LYS:NZ	2.40	0.44
17:BY:86:GLU:H	17:BY:86:GLU:CD	2.15	0.44
2:BA:77:ASP:HB2	2:BA:123:PRO:HA	2.00	0.44
16:BX:17:ARG:O	16:BX:21:ARG:HG2	2.18	0.44
28:BT:77:GLN:HG2	28:BT:95:LYS:HE2	2.00	0.44
3:BB:113:LEU:HD11	3:BB:211:TYR:OH	2.18	0.44
10:BL:22:THR:OG1	10:BL:23:THR:N	2.50	0.44
22:BD:78:LYS:HZ3	24:BK:20:VAL:C	2.21	0.44
5:BE:143:ASP:OD1	5:BE:143:ASP:N	2.49	0.44
14:BV:76:LYS:HE2	14:BV:81:GLN:HG3	2.00	0.44
2:BA:60:GLU:OE2	2:BA:60:GLU:N	2.47	0.44
2:BA:122:GLU:OE1	4:BC:54:LYS:HB2	2.18	0.44
3:BB:222:LYS:HD2	3:BB:222:LYS:HA	1.71	0.44
6:BG:57:ASP:CG	6:BG:100:ARG:HE	2.17	0.44
14:BV:78:GLU:OE1	14:BV:78:GLU:N	2.44	0.44
16:BX:28:LYS:O	16:BX:32:LEU:HB2	2.18	0.44
25:BP:104:ASN:ND2	25:BP:128:SER:HA	2.32	0.44
27:BS:25:LYS:O	27:BS:29:ALA:N	2.51	0.44
28:BT:71:ILE:HB	28:BT:76:PHE:CE1	2.53	0.44
29:BU:28:LEU:HB3	29:BU:36:LEU:CD2	2.48	0.44
3:BB:185:VAL:HA	3:BB:188:PHE:HB2	2.00	0.44
7:BH:113:ARG:HG3	7:BH:113:ARG:O	2.17	0.44
7:BH:162:ASN:HB2	7:BH:165:TYR:HE1	1.83	0.44
12:BO:46:ASP:OD1	12:BO:47:LEU:N	2.50	0.44
13:BR:98:VAL:HG11	13:BR:118:GLU:H	1.83	0.44
33:BZ:74:LEU:O	33:BZ:78:GLY:N	2.33	0.44
7:BH:158:LYS:HE2	7:BH:158:LYS:HB3	1.82	0.43
8:BI:45:ARG:HB2	8:BI:55:TRP:CZ3	2.53	0.43
22:BD:145:LEU:HG	22:BD:151:LYS:HE3	1.99	0.43
27:BS:80:PRO:HG2	27:BS:83:PHE:HB2	2.00	0.43
3:BB:90:ASP:HB2	3:BB:223:PHE:CZ	2.53	0.43
9:BJ:147:SER:O	9:BJ:147:SER:OG	2.36	0.43
11:BN:87:ASP:OD1	11:BN:87:ASP:N	2.51	0.43
17:BY:60:CYS:HB3	17:BY:82:TYR:HB2	1.99	0.43
22:BD:125:VAL:O	22:BD:129:VAL:HG22	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BI:171:PHE:HE1	8:BI:176:LEU:HD11	1.82	0.43
23:BF:101:VAL:HG13	26:BQ:47:MET:HE1	2.00	0.43
5:BE:163:ASP:OD2	5:BE:166:THR:OG1	2.35	0.43
14:BV:59:ARG:HA	14:BV:64:ALA:HB2	2.00	0.43
23:BF:173:ALA:HB2	23:BF:183:CYS:SG	2.59	0.43
29:BU:85:GLU:OE2	29:BU:87:ARG:HG2	2.18	0.43
2:BA:124:ARG:HH22	4:BC:258:THR:HG21	1.83	0.43
6:BG:111:ILE:HG22	6:BG:113:LEU:HD22	1.99	0.43
8:BI:79:LEU:HD12	8:BI:175:ARG:HB3	2.00	0.43
22:BD:166:PRO:HA	22:BD:169:GLU:OE2	2.19	0.43
24:BK:32:HIS:HB3	24:BK:37:VAL:HG13	2.01	0.43
28:BT:130:ARG:NH2	28:BT:134:GLN:HB3	2.33	0.43
33:BZ:74:LEU:HD11	33:BZ:80:ILE:HG23	1.99	0.43
4:BC:91:LYS:HA	4:BC:91:LYS:HD2	1.88	0.43
4:BC:118:VAL:HG21	4:BC:147:LYS:HG3	2.01	0.43
6:BG:189:LEU:O	6:BG:193:ARG:HG3	2.17	0.43
10:BL:59:LYS:NZ	10:BL:133:LEU:O	2.51	0.43
13:BR:29:HIS:O	13:BR:33:LYS:HG2	2.18	0.43
13:BR:71:LEU:HG	13:BR:72:LYS:HG3	2.01	0.43
13:BR:73:LEU:HD12	13:BR:73:LEU:H	1.84	0.43
24:BK:19:GLY:O	24:BK:68:LEU:HD13	2.19	0.43
27:BS:47:LYS:NZ	27:BS:77:PHE:O	2.33	0.43
27:BS:85:ASN:OD1	27:BS:85:ASN:N	2.51	0.43
2:BA:79:ILE:CG2	2:BA:103:ILE:HG12	2.48	0.43
5:BE:173:ILE:HG23	5:BE:230:LYS:HD2	1.99	0.43
6:BG:143:ILE:HG21	6:BG:155:VAL:HB	2.00	0.43
13:BR:109:LEU:HD12	13:BR:110:GLY:N	2.34	0.43
15:BW:30:SER:HB2	15:BW:61:ILE:HG13	2.01	0.43
4:BC:127:LEU:HD11	4:BC:225:VAL:HG13	2.00	0.43
4:BC:151:VAL:HG12	14:BV:27:LYS:HE2	2.01	0.43
6:BG:68:LEU:O	6:BG:101:GLY:HA3	2.19	0.43
9:BJ:70:ARG:HG2	9:BJ:74:GLU:OE2	2.19	0.43
11:BN:23:PRO:HG2	11:BN:26:VAL:HG23	2.01	0.43
15:BW:120:ASN:ND2	15:BW:120:ASN:O	2.52	0.43
22:BD:35:ASP:OD1	22:BD:60:ASN:HB3	2.19	0.43
24:BK:32:HIS:CE1	24:BK:34:GLN:H	2.37	0.43
26:BQ:112:ILE:HA	26:BQ:115:ARG:HG2	2.00	0.43
29:BU:27:THR:OG1	29:BU:117:GLU:HB2	2.19	0.43
6:BG:200:LYS:HA	6:BG:200:LYS:HD2	1.80	0.43
22:BD:120:ARG:HA	22:BD:123:TYR:CD2	2.54	0.43
24:BK:31:LYS:HE2	24:BK:31:LYS:HB2	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:BK:55:VAL:CG1	24:BK:66:TRP:HB3	2.48	0.43
28:BT:14:GLU:HA	28:BT:17:LYS:HG2	1.99	0.43
33:BZ:38:TYR:OH	33:BZ:77:ARG:NH2	2.52	0.43
2:BA:93:LYS:C	2:BA:95:ALA:H	2.21	0.43
5:BE:19:MET:H	5:BE:19:MET:HG2	1.59	0.43
7:BH:164:GLU:OE1	7:BH:164:GLU:N	2.52	0.43
7:BH:176:ARG:HE	7:BH:176:ARG:HB3	1.55	0.43
16:BX:52:GLU:HG3	16:BX:54:ILE:HG23	2.01	0.43
33:BZ:84:SER:OG	33:BZ:85:ILE:N	2.52	0.43
2:BA:41:TYR:OH	2:BA:61:LYS:NZ	2.51	0.42
3:BB:32:ILE:HD11	3:BB:46:THR:HB	2.01	0.42
7:BH:88:PHE:O	7:BH:91:LYS:HE3	2.19	0.42
17:BY:65:LYS:HD2	17:BY:78:PHE:HE2	1.83	0.42
29:BU:52:LEU:HB3	29:BU:95:LEU:HD11	2.00	0.42
3:BB:67:GLU:OE2	3:BB:85:ARG:NH1	2.51	0.42
4:BC:144:ILE:HD13	4:BC:144:ILE:HA	1.87	0.42
9:BJ:23:LYS:HD3	9:BJ:23:LYS:HA	1.89	0.42
13:BR:74:GLN:HG3	13:BR:80:ARG:HB2	2.00	0.42
25:BP:39:LEU:O	25:BP:42:LEU:HD23	2.18	0.42
25:BP:43:PHE:HE1	25:BP:119:GLY:HA2	1.83	0.42
9:BJ:109:ARG:NH2	9:BJ:155:GLU:OE1	2.52	0.42
26:BQ:46:GLU:O	26:BQ:49:ARG:HB2	2.19	0.42
33:BZ:68:ARG:O	33:BZ:71:ILE:HG22	2.20	0.42
4:BC:232:LEU:HD23	4:BC:232:LEU:HA	1.86	0.42
5:BE:92:ILE:HB	5:BE:97:GLU:HB2	2.01	0.42
7:BH:62:VAL:HG13	7:BH:94:VAL:HG13	2.02	0.42
25:BP:36:THR:HG22	25:BP:39:LEU:HD21	2.00	0.42
26:BQ:81:GLN:O	26:BQ:85:ILE:HG22	2.18	0.42
2:BA:17:GLN:N	2:BA:17:GLN:OE1	2.52	0.42
3:BB:134:MET:O	3:BB:218:LEU:N	2.51	0.42
4:BC:263:LYS:N	4:BC:264:PRO:HD3	2.35	0.42
6:BG:18:ILE:HG13	6:BG:24:LEU:HD21	2.01	0.42
17:BY:56:LYS:HA	17:BY:56:LYS:HE2	2.00	0.42
26:BQ:26:CYS:SG	26:BQ:27:LYS:N	2.92	0.42
26:BQ:64:PHE:CZ	26:BQ:93:LEU:HD22	2.54	0.42
26:BQ:144:LYS:HE2	26:BQ:146:TYR:HE1	1.84	0.42
29:BU:24:ILE:HG21	29:BU:102:VAL:HG11	2.01	0.42
29:BU:24:ILE:HD13	29:BU:24:ILE:HA	1.88	0.42
33:BZ:29:ASN:HA	33:BZ:61:ARG:HD2	2.00	0.42
2:BA:75:PRO:O	2:BA:100:ALA:HA	2.19	0.42
3:BB:167:LYS:HA	3:BB:170:GLU:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BD:142:SER:O	22:BD:185:LEU:HD12	2.19	0.42
3:BB:63:HIS:ND1	12:BO:50:ARG:HD3	2.34	0.42
7:BH:97:ALA:O	7:BH:99:ARG:NH1	2.52	0.42
25:BP:104:ASN:O	25:BP:128:SER:HB2	2.19	0.42
26:BQ:132:LYS:HB2	26:BQ:141:ARG:HH12	1.85	0.42
27:BS:86:ARG:CZ	27:BS:89:ASP:HB2	2.49	0.42
3:BB:64:ARG:HA	3:BB:88:ALA:N	2.33	0.42
5:BE:206:GLU:HB3	5:BE:222:LEU:HB2	2.02	0.42
7:BH:45:TYR:HD1	7:BH:45:TYR:H	1.68	0.42
9:BJ:84:ARG:O	9:BJ:152:VAL:HG22	2.20	0.42
22:BD:99:LEU:HD23	22:BD:99:LEU:HA	1.88	0.42
23:BF:61:PRO:HA	23:BF:81:GLU:HG2	2.02	0.42
24:BK:16:PHE:CD2	24:BK:76:LEU:HD13	2.54	0.42
2:BA:81:GLN:HE22	2:BA:107:HIS:CD2	2.37	0.42
4:BC:57:ARG:HH21	4:BC:261:LEU:HA	1.84	0.42
5:BE:22:LYS:HB3	5:BE:22:LYS:HE2	1.74	0.42
7:BH:45:TYR:CE2	7:BH:46:ILE:HG13	2.55	0.42
7:BH:88:PHE:O	7:BH:88:PHE:HD1	2.03	0.42
10:BL:37:TRP:NE1	10:BL:51:ILE:HG23	2.35	0.42
11:BN:125:LEU:HD12	11:BN:125:LEU:HA	1.83	0.42
22:BD:75:VAL:HG13	24:BK:65:TYR:CZ	2.55	0.42
23:BF:103:ILE:HD13	23:BF:103:ILE:HA	1.87	0.42
28:BT:66:TYR:CD1	28:BT:132:LEU:HD23	2.55	0.42
28:BT:104:ILE:HA	28:BT:107:GLU:HG3	2.01	0.42
29:BU:35:ASN:O	29:BU:38:LYS:HG3	2.20	0.42
29:BU:86:MET:SD	29:BU:86:MET:N	2.93	0.42
4:BC:195:ALA:O	4:BC:199:LYS:HB2	2.20	0.42
7:BH:77:HIS:HB3	7:BH:132:TYR:CE2	2.54	0.42
16:BX:52:GLU:HA	16:BX:95:GLU:OE2	2.19	0.42
3:BB:83:LYS:HE2	3:BB:83:LYS:HB2	1.88	0.41
8:BI:7:MET:HE3	8:BI:19:ALA:HA	2.01	0.41
8:BI:201:GLU:HA	8:BI:204:MET:HB2	2.02	0.41
24:BK:37:VAL:HG22	24:BK:38:PRO:O	2.20	0.41
26:BQ:46:GLU:O	26:BQ:49:ARG:CB	2.67	0.41
27:BS:130:ARG:HD3	27:BS:131:VAL:H	1.85	0.41
28:BT:6:THR:O	28:BT:9:ASP:N	2.49	0.41
5:BE:260:GLN:O	5:BE:262:ALA:N	2.53	0.41
12:BO:131:ASP:OD1	12:BO:133:THR:OG1	2.30	0.41
15:BW:86:ILE:HD12	15:BW:104:LEU:HD11	2.02	0.41
23:BF:59:PHE:CE2	26:BQ:57:LEU:HD23	2.55	0.41
27:BS:64:MET:O	27:BS:68:MET:HG3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BG:23:LYS:HB3	6:BG:23:LYS:HE3	1.90	0.41
6:BG:120:GLU:OE2	6:BG:120:GLU:N	2.53	0.41
28:BT:57:ARG:HA	28:BT:57:ARG:HD3	1.88	0.41
29:BU:26:ILE:HG22	29:BU:93:ILE:HB	2.02	0.41
2:BA:54:ASN:O	2:BA:58:THR:HG23	2.20	0.41
2:BA:79:ILE:HG21	2:BA:103:ILE:HG12	2.01	0.41
4:BC:80:HIS:CG	4:BC:144:ILE:HD12	2.55	0.41
5:BE:58:TYR:O	5:BE:58:TYR:CD1	2.72	0.41
5:BE:60:GLU:O	5:BE:64:ILE:HG23	2.21	0.41
5:BE:246:LEU:O	5:BE:250:GLU:HG3	2.20	0.41
6:BG:166:PHE:HZ	6:BG:174:VAL:HG12	1.85	0.41
23:BF:50:ALA:HB1	23:BF:56:HIS:HB3	2.02	0.41
26:BQ:74:ARG:HE	26:BQ:74:ARG:HB3	1.63	0.41
28:BT:40:THR:O	28:BT:96:SER:OG	2.32	0.41
28:BT:90:PRO:HA	28:BT:91:PRO:HD3	1.98	0.41
7:BH:84:LEU:HD12	7:BH:84:LEU:HA	1.90	0.41
9:BJ:120:MET:HB3	9:BJ:160:PHE:CZ	2.54	0.41
11:BN:19:LYS:NZ	11:BN:21:THR:HB	2.35	0.41
15:BW:113:HIS:NE2	15:BW:114:GLU:OE2	2.54	0.41
25:BP:91:ILE:HG12	25:BP:95:MET:HE2	2.03	0.41
27:BS:136:THR:O	27:BS:136:THR:OG1	2.32	0.41
2:BA:39:GLU:HA	2:BA:42:VAL:CG2	2.46	0.41
3:BB:69:SER:O	3:BB:70:LEU:HB3	2.21	0.41
4:BC:55:LEU:HD12	4:BC:55:LEU:HA	1.87	0.41
6:BG:57:ASP:OD2	6:BG:100:ARG:NE	2.33	0.41
7:BH:119:LEU:O	7:BH:120:THR:OG1	2.31	0.41
7:BH:131:VAL:HG12	7:BH:170:PHE:CE2	2.55	0.41
9:BJ:61:LEU:HD11	9:BJ:74:GLU:HB2	2.02	0.41
9:BJ:175:LYS:O	9:BJ:179:GLN:HG2	2.21	0.41
12:BO:78:SER:O	12:BO:81:VAL:HG22	2.19	0.41
13:BR:15:GLN:HB3	13:BR:19:LYS:NZ	2.35	0.41
25:BP:46:ARG:HB3	25:BP:47:PRO:HD3	2.01	0.41
28:BT:17:LYS:HE2	28:BT:17:LYS:HB3	1.86	0.41
2:BA:44:LYS:H	2:BA:52:ILE:HG22	1.85	0.41
13:BR:30:THR:HA	13:BR:33:LYS:HD3	2.02	0.41
17:BY:12:LEU:HD22	17:BY:32:VAL:HG22	2.03	0.41
27:BS:39:ARG:HA	27:BS:39:ARG:HD2	1.93	0.41
27:BS:42:ASN:HA	27:BS:45:CYS:SG	2.60	0.41
27:BS:123:LEU:HD23	27:BS:123:LEU:HA	1.93	0.41
29:BU:24:ILE:HD13	29:BU:120:ILE:HA	2.02	0.41
3:BB:175:GLN:HB2	3:BB:193:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BC:73:HIS:HA	14:BV:15:ARG:NH1	2.36	0.41
5:BE:104:ASP:OD1	5:BE:105:THR:N	2.53	0.41
6:BG:61:PHE:HE2	6:BG:98:SER:HB2	1.84	0.41
6:BG:135:ARG:HG3	6:BG:136:GLY:O	2.21	0.41
7:BH:159:GLU:H	7:BH:159:GLU:HG2	1.62	0.41
9:BJ:27:ASP:OD1	9:BJ:27:ASP:N	2.53	0.41
11:BN:115:LEU:O	11:BN:119:GLU:HG2	2.20	0.41
12:BO:38:ASN:O	12:BO:68:GLU:HB2	2.21	0.41
13:BR:94:ASP:O	13:BR:95:GLU:HG3	2.20	0.41
23:BF:87:LEU:HD12	23:BF:170:ARG:NH2	2.36	0.41
23:BF:101:VAL:O	23:BF:104:ILE:HG22	2.21	0.41
24:BK:46:MET:HG2	24:BK:66:TRP:CD2	2.56	0.41
26:BQ:91:LYS:HB3	26:BQ:91:LYS:HE3	1.94	0.41
29:BU:44:VAL:O	29:BU:48:LYS:HG2	2.21	0.41
5:BE:116:ASP:OD1	5:BE:117:GLU:N	2.54	0.41
5:BE:253:ARG:HA	5:BE:256:ASP:OD2	2.21	0.41
14:BV:16:LYS:HB3	14:BV:16:LYS:HE3	1.89	0.41
23:BF:83:LEU:HD23	23:BF:83:LEU:HA	1.81	0.41
28:BT:131:ASP:CA	28:BT:134:GLN:HE21	2.30	0.41
29:BU:48:LYS:HA	29:BU:48:LYS:HD2	1.81	0.41
2:BA:57:LYS:HE2	2:BA:57:LYS:HB3	1.67	0.40
6:BG:63:MET:SD	6:BG:108:LEU:HD21	2.61	0.40
2:BA:102:ALA:C	2:BA:103:ILE:HD13	2.42	0.40
3:BB:64:ARG:HB3	3:BB:87:ARG:HD2	2.03	0.40
5:BE:151:ASP:HA	6:BG:216:LEU:HD21	2.03	0.40
7:BH:69:LEU:C	7:BH:72:PRO:HD2	2.42	0.40
11:BN:60:ILE:HG23	11:BN:66:VAL:HG21	2.02	0.40
22:BD:45:THR:OG1	22:BD:48:ARG:HB2	2.21	0.40
22:BD:67:ARG:O	22:BD:70:ARG:HG2	2.20	0.40
27:BS:44:VAL:HG11	27:BS:71:VAL:HG22	2.03	0.40
3:BB:129:THR:HG22	3:BB:133:TYR:H	1.85	0.40
9:BJ:181:LYS:HB2	9:BJ:181:LYS:HE2	1.77	0.40
27:BS:84:LEU:HB3	27:BS:96:SER:O	2.21	0.40
4:BC:175:LYS:HB2	4:BC:180:THR:HG22	2.04	0.40
5:BE:93:PRO:O	5:BE:95:THR:N	2.54	0.40
7:BH:101:ILE:HG12	7:BH:119:LEU:HG	2.03	0.40
9:BJ:51:LEU:HD13	9:BJ:106:PHE:CE1	2.56	0.40
9:BJ:104:GLU:OE1	9:BJ:104:GLU:N	2.46	0.40
13:BR:44:LYS:HE2	13:BR:47:ARG:HH12	1.86	0.40
23:BF:101:VAL:HG13	26:BQ:47:MET:CE	2.52	0.40
24:BK:11:ILE:HD11	24:BK:37:VAL:HG11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BS:75:ARG:NH1	27:BS:95:PHE:O	2.55	0.40
33:BZ:71:ILE:O	33:BZ:75:MET:HG3	2.22	0.40
2:BA:55:LEU:HD12	2:BA:55:LEU:H	1.87	0.40
8:BI:61:ASP:OD1	8:BI:61:ASP:N	2.50	0.40
9:BJ:15:LYS:O	9:BJ:16:LYS:HB2	2.22	0.40
10:BL:17:LEU:HD23	10:BL:17:LEU:HA	1.94	0.40
13:BR:70:SER:O	13:BR:71:LEU:HB3	2.22	0.40
26:BQ:25:TYR:HE2	26:BQ:27:LYS:HE3	1.85	0.40
33:BZ:62:ILE:HD12	33:BZ:62:ILE:HA	1.88	0.40
33:BZ:66:LEU:HD22	33:BZ:69:ARG:HD3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	BA	193/304 (64%)	173 (90%)	20 (10%)	0	100	100
3	BB	211/263 (80%)	185 (88%)	26 (12%)	0	100	100
4	BC	218/279 (78%)	198 (91%)	20 (9%)	0	100	100
5	BE	261/265 (98%)	225 (86%)	35 (13%)	1 (0%)	34	64
6	BG	227/250 (91%)	195 (86%)	32 (14%)	0	100	100
7	BH	180/192 (94%)	145 (81%)	34 (19%)	1 (1%)	25	55
8	BI	182/224 (81%)	175 (96%)	7 (4%)	0	100	100
9	BJ	181/195 (93%)	177 (98%)	4 (2%)	0	100	100
10	BL	150/161 (93%)	138 (92%)	12 (8%)	0	100	100
11	BN	147/151 (97%)	145 (99%)	2 (1%)	0	100	100
12	BO	128/151 (85%)	120 (94%)	8 (6%)	0	100	100
13	BR	117/143 (82%)	102 (87%)	14 (12%)	1 (1%)	17	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	BV	79/82 (96%)	76 (96%)	3 (4%)	0	100	100
15	BW	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
16	BX	137/142 (96%)	130 (95%)	7 (5%)	0	100	100
17	BY	122/137 (89%)	120 (98%)	2 (2%)	0	100	100
18	Ba	96/139 (69%)	96 (100%)	0	0	100	100
19	Bb	84/86 (98%)	74 (88%)	10 (12%)	0	100	100
20	Be	43/62 (69%)	43 (100%)	0	0	100	100
21	Cn	23/25 (92%)	23 (100%)	0	0	100	100
22	BD	204/227 (90%)	198 (97%)	6 (3%)	0	100	100
23	BF	172/200 (86%)	160 (93%)	12 (7%)	0	100	100
24	BK	80/188 (43%)	80 (100%)	0	0	100	100
25	BP	62/153 (40%)	56 (90%)	6 (10%)	0	100	100
26	BQ	137/149 (92%)	132 (96%)	5 (4%)	0	100	100
27	BS	92/152 (60%)	85 (92%)	7 (8%)	0	100	100
28	BT	135/155 (87%)	131 (97%)	4 (3%)	0	100	100
29	BU	99/117 (85%)	96 (97%)	3 (3%)	0	100	100
30	Bc	59/65 (91%)	58 (98%)	1 (2%)	0	100	100
31	Bd	48/56 (86%)	45 (94%)	3 (6%)	0	100	100
32	Bg	257/335 (77%)	247 (96%)	10 (4%)	0	100	100
33	BZ	61/98 (62%)	58 (95%)	3 (5%)	0	100	100
All	All	4312/5276 (82%)	4007 (93%)	302 (7%)	3 (0%)	54	80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	BE	261	ALA
7	BH	66	PRO
13	BR	71	LEU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	BA	167/228 (73%)	157 (94%)	10 (6%)	19	46
3	BB	191/228 (84%)	181 (95%)	10 (5%)	23	53
4	BC	185/221 (84%)	172 (93%)	13 (7%)	15	39
5	BE	223/224 (100%)	217 (97%)	6 (3%)	44	75
6	BG	201/215 (94%)	194 (96%)	7 (4%)	36	68
7	BH	134/171 (78%)	123 (92%)	11 (8%)	11	31
8	BI	159/180 (88%)	154 (97%)	5 (3%)	40	72
9	BJ	155/162 (96%)	150 (97%)	5 (3%)	39	71
10	BL	131/137 (96%)	125 (95%)	6 (5%)	27	58
11	BN	130/131 (99%)	127 (98%)	3 (2%)	50	79
12	BO	102/121 (84%)	95 (93%)	7 (7%)	15	39
13	BR	107/124 (86%)	98 (92%)	9 (8%)	11	30
14	BV	67/68 (98%)	63 (94%)	4 (6%)	19	46
15	BW	111/112 (99%)	110 (99%)	1 (1%)	78	92
16	BX	110/113 (97%)	105 (96%)	5 (4%)	27	59
17	BY	107/116 (92%)	103 (96%)	4 (4%)	34	66
18	Ba	85/108 (79%)	85 (100%)	0	100	100
19	Bb	78/78 (100%)	73 (94%)	5 (6%)	17	43
20	Be	38/49 (78%)	36 (95%)	2 (5%)	22	52
21	Cn	24/24 (100%)	24 (100%)	0	100	100
22	BD	174/192 (91%)	158 (91%)	16 (9%)	9	25
23	BF	153/169 (90%)	143 (94%)	10 (6%)	17	42
24	BK	78/143 (54%)	75 (96%)	3 (4%)	33	65
25	BP	59/130 (45%)	54 (92%)	5 (8%)	10	29
26	BQ	111/120 (92%)	105 (95%)	6 (5%)	22	51
27	BS	86/133 (65%)	81 (94%)	5 (6%)	20	48
28	BT	113/124 (91%)	106 (94%)	7 (6%)	18	45
29	BU	95/106 (90%)	92 (97%)	3 (3%)	39	71
30	Bc	54/58 (93%)	53 (98%)	1 (2%)	57	82
31	Bd	43/48 (90%)	39 (91%)	4 (9%)	9	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	Bg	229/278 (82%)	219 (96%)	10 (4%)	28	59
33	BZ	59/83 (71%)	56 (95%)	3 (5%)	24	53
All	All	3759/4394 (86%)	3573 (95%)	186 (5%)	29	55

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	BA	39	GLU
2	BA	40	ARG
2	BA	44	LYS
2	BA	63	GLN
2	BA	152	CYS
2	BA	177	CYS
2	BA	194	LEU
2	BA	197	HIS
2	BA	199	TRP
2	BA	206	PHE
3	BB	76	ASP
3	BB	90	ASP
3	BB	94	MET
3	BB	111	ARG
3	BB	115	ARG
3	BB	126	ASP
3	BB	188	PHE
3	BB	211	TYR
3	BB	229	MET
3	BB	234	ASP
4	BC	48	LYS
4	BC	57	ARG
4	BC	66	LYS
4	BC	87	CYS
4	BC	109	ARG
4	BC	133	LYS
4	BC	200	LYS
4	BC	217	SER
4	BC	224	PHE
4	BC	231	CYS
4	BC	236	TYR
4	BC	243	PHE
4	BC	244	TRP
5	BE	7	LYS

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Mol	Chain	Res	Type
5	BE	75	LYS
5	BE	103	TYR
5	BE	187	ARG
5	BE	197	ASN
5	BE	242	LYS
6	BG	21	ASP
6	BG	28	TYR
6	BG	43	GLU
6	BG	96	ARG
6	BG	107	ASP
6	BG	158	TYR
6	BG	228	ARG
7	BH	12	LYS
7	BH	27	PHE
7	BH	28	PHE
7	BH	51	GLN
7	BH	88	PHE
7	BH	89	SER
7	BH	92	ASP
7	BH	124	ASP
7	BH	165	TYR
7	BH	174	TYR
7	BH	176	ARG
8	BI	3	SER
8	BI	41	LYS
8	BI	47	ARG
8	BI	94	GLN
8	BI	175	ARG
9	BJ	10	TYR
9	BJ	24	GLU
9	BJ	27	ASP
9	BJ	59	ARG
9	BJ	96	ASP
10	BL	7	LYS
10	BL	17	LEU
10	BL	60	CYS
10	BL	69	ARG
10	BL	114	SER
10	BL	131	ARG
11	BN	4	MET
11	BN	12	SER
11	BN	69	SER

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Mol	Chain	Res	Type
12	BO	39	ASP
12	BO	63	LYS
12	BO	66	ARG
12	BO	103	ASN
12	BO	128	ARG
12	BO	142	ARG
12	BO	143	LYS
13	BR	20	TYR
13	BR	23	ARG
13	BR	45	ARG
13	BR	53	PHE
13	BR	73	LEU
13	BR	83	ASP
13	BR	88	LYS
13	BR	89	SER
13	BR	95	GLU
14	BV	4	GLU
14	BV	21	ASN
14	BV	48	ARG
14	BV	74	LYS
15	BW	56	HIS
16	BX	32	LEU
16	BX	79	LYS
16	BX	104	PHE
16	BX	107	LYS
16	BX	118	ARG
17	BY	23	LEU
17	BY	89	LYS
17	BY	105	LYS
17	BY	127	LYS
19	Bb	3	LEU
19	Bb	61	CYS
19	Bb	67	GLN
19	Bb	81	PHE
19	Bb	82	ARG
20	Be	28	LYS
20	Be	31	ARG
22	BD	7	GLN
22	BD	11	LYS
22	BD	17	ASP
22	BD	20	PHE
22	BD	21	TYR

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Mol	Chain	Res	Type
22	BD	43	ARG
22	BD	47	MET
22	BD	62	LEU
22	BD	78	LYS
22	BD	85	ASN
22	BD	151	LYS
22	BD	168	ASN
22	BD	169	GLU
22	BD	170	TYR
22	BD	194	ASP
22	BD	200	LYS
23	BF	30	PHE
23	BF	60	LEU
23	BF	66	ARG
23	BF	83	LEU
23	BF	94	ASN
23	BF	150	VAL
23	BF	151	ASP
23	BF	159	ASN
23	BF	163	TYR
23	BF	214	ASN
24	BK	32	HIS
24	BK	33	PRO
24	BK	65	TYR
25	BP	42	LEU
25	BP	60	MET
25	BP	83	ARG
25	BP	88	ASN
25	BP	95	MET
26	BQ	26	CYS
26	BQ	58	LEU
26	BQ	62	SER
26	BQ	74	ARG
26	BQ	100	TYR
26	BQ	117	ASP
27	BS	86	ARG
27	BS	95	PHE
27	BS	113	ARG
27	BS	137	LYS
27	BS	142	ARG
28	BT	5	ARG
28	BT	15	PHE

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Mol	Chain	Res	Type
28	BT	25	ARG
28	BT	34	TRP
28	BT	61	MET
28	BT	88	SER
28	BT	103	ASN
29	BU	30	SER
29	BU	36	LEU
29	BU	38	LYS
30	Bc	32	ASP
31	Bd	19	ARG
31	Bd	24	CYS
31	Bd	43	PHE
31	Bd	45	SER
32	Bg	33	TYR
32	Bg	86	ASP
32	Bg	126	SER
32	Bg	143	LEU
32	Bg	150	CYS
32	Bg	194	TRP
32	Bg	200	LYS
32	Bg	236	TRP
32	Bg	262	ARG
32	Bg	282	HIS
33	BZ	33	PHE
33	BZ	59	ARG
33	BZ	61	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	BA	107	HIS
8	BI	148	ASN
8	BI	151	GLN
13	BR	42	GLN
14	BV	3	ASN
23	BF	94	ASN
28	BT	134	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	Ad	1546/1811 (85%)	281 (18%)	0

All (281) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	Ad	2	A
1	Ad	4	C
1	Ad	25	C
1	Ad	26	A
1	Ad	28	A2M
1	Ad	34	G
1	Ad	42	G
1	Ad	43	A
1	Ad	45	U
1	Ad	46	A
1	Ad	47	A
1	Ad	59	G
1	Ad	65	A
1	Ad	67	G
1	Ad	68	A
1	Ad	72	A
1	Ad	73	A
1	Ad	81	U
1	Ad	82	G
1	Ad	104	A
1	Ad	105	A
1	Ad	115	A
1	Ad	123	OMU
1	Ad	128	G
1	Ad	130	A
1	Ad	131	C
1	Ad	132	G
1	Ad	139	U
1	Ad	151	A
1	Ad	156	U
1	Ad	158	C
1	Ad	164	C
1	Ad	175	A
1	Ad	176	A
1	Ad	177	C
1	Ad	182	C
1	Ad	185	G
1	Ad	187	C

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Mol	Chain	Res	Type
1	Ad	188	U
1	Ad	242	A
1	Ad	252	U
1	Ad	253	C
1	Ad	255	PSU
1	Ad	260	A
1	Ad	264	G
1	Ad	275	C
1	Ad	278	C
1	Ad	279	C
1	Ad	303	A
1	Ad	318	C
1	Ad	320	A
1	Ad	324	U
1	Ad	325	C
1	Ad	341	G
1	Ad	342	C
1	Ad	363	G
1	Ad	365	C
1	Ad	374	A
1	Ad	377	G
1	Ad	384	U
1	Ad	392	OMG
1	Ad	393	G
1	Ad	404	A
1	Ad	405	A
1	Ad	406	C
1	Ad	408	G
1	Ad	418	OMC
1	Ad	420	A
1	Ad	421	A
1	Ad	422	G
1	Ad	427	G
1	Ad	428	C
1	Ad	430	G
1	Ad	438	G
1	Ad	443	U
1	Ad	448	C
1	Ad	449	A
1	Ad	452	C
1	Ad	468	A2M
1	Ad	472	A

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Mol	Chain	Res	Type
1	Ad	478	A
1	Ad	479	A
1	Ad	481	A
1	Ad	508	U
1	Ad	510	A
1	Ad	511	U
1	Ad	514	G
1	Ad	515	A
1	Ad	519	A
1	Ad	523	C
1	Ad	538	A
1	Ad	546	U
1	Ad	553	G
1	Ad	562	U
1	Ad	569	C
1	Ad	572	G
1	Ad	575	G
1	Ad	583	A
1	Ad	584	A
1	Ad	598	A
1	Ad	607	U
1	Ad	610	A
1	Ad	615	OMU
1	Ad	618	C
1	Ad	623	A2M
1	Ad	624	A
1	Ad	626	A
1	Ad	627	A
1	Ad	628	G
1	Ad	642	C
1	Ad	643	U
1	Ad	645	G
1	Ad	646	G
1	Ad	745	C
1	Ad	746	A
1	Ad	748	C
1	Ad	749	G
1	Ad	756	U
1	Ad	760	G
1	Ad	761	A
1	Ad	772	C
1	Ad	784	C

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Mol	Chain	Res	Type
1	Ad	785	A
1	Ad	788	G
1	Ad	791	C
1	Ad	792	U
1	Ad	795	A
1	Ad	797	A2M
1	Ad	819	U
1	Ad	860	A
1	Ad	861	A
1	Ad	864	A
1	Ad	868	A
1	Ad	881	G
1	Ad	903	A
1	Ad	906	G
1	Ad	919	G
1	Ad	938	A
1	Ad	940	U
1	Ad	947	G
1	Ad	965	U
1	Ad	971	A
1	Ad	975	A
1	Ad	976	A
1	Ad	988	G
1	Ad	997	A
1	Ad	1009	U
1	Ad	1010	A
1	Ad	1016	C
1	Ad	1025	A
1	Ad	1028	A
1	Ad	1029	PSU
1	Ad	1031	A
1	Ad	1032	A
1	Ad	1033	C
1	Ad	1058	G
1	Ad	1059	U
1	Ad	1061	G
1	Ad	1062	C
1	Ad	1081	A
1	Ad	1086	A
1	Ad	1087	U
1	Ad	1094	U
1	Ad	1097	A

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Mol	Chain	Res	Type
1	Ad	1102	U
1	Ad	1143	A
1	Ad	1155	G
1	Ad	1163	C
1	Ad	1164	C
1	Ad	1168	A
1	Ad	1169	G
1	Ad	1171	C
1	Ad	1172	G
1	Ad	1180	U
1	Ad	1197	A
1	Ad	1198	A
1	Ad	1200	A
1	Ad	1203	G
1	Ad	1204	G
1	Ad	1206	A
1	Ad	1210	U
1	Ad	1211	U
1	Ad	1213	C
1	Ad	1221	A
1	Ad	1222	G
1	Ad	1229	C
1	Ad	1241	G
1	Ad	1245	G
1	Ad	1254	U
1	Ad	1255	U
1	Ad	1266	U
1	Ad	1273	U
1	Ad	1274	G
1	Ad	1279	A
1	Ad	1280	U
1	Ad	1282	G
1	Ad	1286	U
1	Ad	1287	U
1	Ad	1288	C
1	Ad	1295	G
1	Ad	1304	A
1	Ad	1305	U
1	Ad	1318	U
1	Ad	1319	U
1	Ad	1325	A
1	Ad	1329	A

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Mol	Chain	Res	Type
1	Ad	1330	A
1	Ad	1331	C
1	Ad	1342	C
1	Ad	1351	U
1	Ad	1353	G
1	Ad	1371	U
1	Ad	1377	G
1	Ad	1378	C
1	Ad	1380	A
1	Ad	1386	U
1	Ad	1396	U
1	Ad	1399	C
1	Ad	1404	U
1	Ad	1405	U
1	Ad	1408	G
1	Ad	1412	A
1	Ad	1419	U
1	Ad	1420	U
1	Ad	1421	U
1	Ad	1432	C
1	Ad	1433	A
1	Ad	1434	G
1	Ad	1441	G
1	Ad	1442	A
1	Ad	1451	G
1	Ad	1452	A
1	Ad	1463	C
1	Ad	1464	G
1	Ad	1465	C
1	Ad	1477	A
1	Ad	1479	U
1	Ad	1480	G
1	Ad	1486	U
1	Ad	1495	U
1	Ad	1501	G
1	Ad	1504	U
1	Ad	1511	A
1	Ad	1519	G
1	Ad	1524	A
1	Ad	1528	U
1	Ad	1529	G
1	Ad	1530	G

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Mol	Chain	Res	Type
1	Ad	1540	U
1	Ad	1541	C
1	Ad	1542	G
1	Ad	1545	A
1	Ad	1546	U
1	Ad	1549	G
1	Ad	1550	G
1	Ad	1571	G
1	Ad	1581	A
1	Ad	1598	G
1	Ad	1606	U
1	Ad	1630	G
1	Ad	1643	A
1	Ad	1646	G
1	Ad	1665	U
1	Ad	1666	G
1	Ad	1667	A
1	Ad	1688	G
1	Ad	1726	G
1	Ad	1767	G
1	Ad	1770	G
1	Ad	1772	A
1	Ad	1776	A
1	Ad	1779	U
1	Ad	1783	C
1	Ad	1790	G
1	Ad	1802	G
1	Ad	1803	G
1	Ad	1804	A
1	Ad	1805	U
1	Ad	1806	C
1	Ad	1809	U
1	Ad	1810	G

There are no RNA pucker outliers to report.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	Ad	451	1	18,21,22	4.38	7 (38%)	22,30,33	1.70	4 (18%)
1	MA6	Ad	1791	1	19,26,27	1.00	1 (5%)	18,38,41	4.73	3 (16%)
1	PSU	Ad	258	1	18,21,22	4.38	7 (38%)	22,30,33	1.75	5 (22%)
1	PSU	Ad	1004	1	18,21,22	4.45	7 (38%)	22,30,33	1.72	4 (18%)
1	PSU	Ad	585	1	18,21,22	4.44	7 (38%)	22,30,33	1.75	5 (22%)
1	PSU	Ad	1108	1	18,21,22	4.40	7 (38%)	22,30,33	1.79	4 (18%)
1	A2M	Ad	545	1	18,25,26	4.22	7 (38%)	18,36,39	2.32	4 (22%)
1	OMG	Ad	246	1	18,26,27	2.59	8 (44%)	19,38,41	1.51	4 (21%)
1	OMC	Ad	38	1	19,22,23	3.13	8 (42%)	26,31,34	1.07	2 (7%)
1	PSU	Ad	111	34,1	18,21,22	4.38	7 (38%)	22,30,33	1.76	5 (22%)
1	PSU	Ad	255	35,1	18,21,22	4.42	7 (38%)	22,30,33	1.69	4 (18%)
1	PSU	Ad	755	1	18,21,22	4.42	7 (38%)	22,30,33	1.87	4 (18%)
1	PSU	Ad	764	1	18,21,22	4.39	7 (38%)	22,30,33	1.88	5 (22%)
1	PSU	Ad	952	1	18,21,22	4.44	7 (38%)	22,30,33	1.71	4 (18%)
1	A2M	Ad	28	35,1	18,25,26	4.21	7 (38%)	18,36,39	2.42	5 (27%)
1	A2M	Ad	802	1	18,25,26	4.21	7 (38%)	18,36,39	2.24	4 (22%)
1	A2M	Ad	979	1	18,25,26	4.27	8 (44%)	18,36,39	2.61	5 (27%)
1	PSU	Ad	914	1	18,21,22	4.46	7 (38%)	22,30,33	1.69	3 (13%)
1	PSU	Ad	103	1	18,21,22	4.37	7 (38%)	22,30,33	1.87	5 (22%)
1	OMC	Ad	1647	1	19,22,23	3.14	8 (42%)	26,31,34	1.09	2 (7%)
1	A2M	Ad	623	35,1	18,25,26	4.14	7 (38%)	18,36,39	2.24	4 (22%)
1	OMU	Ad	1014	1	19,22,23	3.27	7 (36%)	26,31,34	1.68	5 (19%)
1	OMG	Ad	392	1	18,26,27	2.54	8 (44%)	19,38,41	1.56	4 (21%)
1	OMG	Ad	599	1	18,26,27	2.55	8 (44%)	19,38,41	1.50	4 (21%)
1	PSU	Ad	811	1	18,21,22	4.42	7 (38%)	22,30,33	1.76	5 (22%)
1	OMU	Ad	615	1	19,22,23	3.27	8 (42%)	26,31,34	1.87	6 (23%)
1	A2M	Ad	440	1	18,25,26	4.16	7 (38%)	18,36,39	2.30	4 (22%)
1	PSU	Ad	1122	1	18,21,22	4.45	7 (38%)	22,30,33	1.72	4 (18%)
1	PSU	Ad	300	1	18,21,22	4.42	7 (38%)	22,30,33	1.76	5 (22%)
1	PSU	Ad	362	1	18,21,22	4.37	7 (38%)	22,30,33	1.75	4 (18%)
1	PSU	Ad	951	1	18,21,22	4.43	7 (38%)	22,30,33	1.72	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	Ad	1029	1	18,21,22	4.42	7 (38%)	22,30,33	1.76	3 (13%)
1	PSU	Ad	383	35,1	18,21,22	4.39	7 (38%)	22,30,33	1.78	5 (22%)
1	A2M	Ad	1760	1	18,25,26	4.28	7 (38%)	18,36,39	2.34	4 (22%)
1	OMC	Ad	473	1	19,22,23	3.09	8 (42%)	26,31,34	0.74	0
1	MA6	Ad	1792	1	19,26,27	1.03	1 (5%)	18,38,41	5.00	3 (16%)
1	A2M	Ad	797	1	18,25,26	4.28	7 (38%)	18,36,39	2.41	4 (22%)
1	OMC	Ad	418	1	19,22,23	3.13	8 (42%)	26,31,34	1.32	4 (15%)
1	OMU	Ad	123	1	19,22,23	3.29	7 (36%)	26,31,34	1.72	5 (19%)
1	A2M	Ad	468	1	18,25,26	4.23	7 (38%)	18,36,39	2.27	4 (22%)
1	PSU	Ad	306	1	18,21,22	4.34	7 (38%)	22,30,33	1.71	4 (18%)
1	PSU	Ad	606	1	18,21,22	4.37	7 (38%)	22,30,33	1.70	5 (22%)
1	PSU	Ad	636	1	18,21,22	4.42	7 (38%)	22,30,33	1.72	3 (13%)
1	PSU	Ad	121	1	18,21,22	4.38	7 (38%)	22,30,33	1.73	4 (18%)
1	A2M	Ad	162	1	18,25,26	4.23	8 (44%)	18,36,39	2.26	4 (22%)
1	PSU	Ad	208	1	18,21,22	4.41	7 (38%)	22,30,33	1.76	5 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	Ad	451	1	-	2/7/25/26	0/2/2/2
1	MA6	Ad	1791	1	-	2/7/29/30	0/3/3/3
1	PSU	Ad	258	1	-	2/7/25/26	0/2/2/2
1	PSU	Ad	1004	1	-	3/7/25/26	0/2/2/2
1	PSU	Ad	585	1	-	0/7/25/26	0/2/2/2
1	PSU	Ad	1108	1	-	2/7/25/26	0/2/2/2
1	A2M	Ad	545	1	-	1/5/27/28	0/3/3/3
1	OMG	Ad	246	1	-	3/5/27/28	0/3/3/3
1	OMC	Ad	38	1	-	3/9/27/28	0/2/2/2
1	PSU	Ad	111	34,1	-	2/7/25/26	0/2/2/2
1	PSU	Ad	255	35,1	-	3/7/25/26	0/2/2/2
1	PSU	Ad	755	1	-	4/7/25/26	0/2/2/2
1	PSU	Ad	764	1	-	0/7/25/26	0/2/2/2
1	PSU	Ad	952	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	Ad	28	35,1	-	2/5/27/28	0/3/3/3
1	A2M	Ad	802	1	-	0/5/27/28	0/3/3/3
1	A2M	Ad	979	1	-	0/5/27/28	0/3/3/3
1	PSU	Ad	914	1	-	2/7/25/26	0/2/2/2
1	PSU	Ad	103	1	-	0/7/25/26	0/2/2/2
1	OMC	Ad	1647	1	-	4/9/27/28	0/2/2/2
1	A2M	Ad	623	35,1	-	3/5/27/28	0/3/3/3
1	OMU	Ad	1014	1	-	0/9/27/28	0/2/2/2
1	OMG	Ad	392	1	-	0/5/27/28	0/3/3/3
1	OMG	Ad	599	1	-	4/5/27/28	0/3/3/3
1	PSU	Ad	811	1	-	2/7/25/26	0/2/2/2
1	OMU	Ad	615	1	-	4/9/27/28	0/2/2/2
1	A2M	Ad	440	1	-	1/5/27/28	0/3/3/3
1	PSU	Ad	1122	1	-	2/7/25/26	0/2/2/2
1	PSU	Ad	300	1	-	2/7/25/26	0/2/2/2
1	PSU	Ad	362	1	-	2/7/25/26	0/2/2/2
1	PSU	Ad	951	1	-	2/7/25/26	0/2/2/2
1	PSU	Ad	1029	1	-	7/7/25/26	0/2/2/2
1	PSU	Ad	383	35,1	-	2/7/25/26	0/2/2/2
1	A2M	Ad	1760	1	-	1/5/27/28	0/3/3/3
1	OMC	Ad	473	1	-	0/9/27/28	0/2/2/2
1	MA6	Ad	1792	1	-	6/7/29/30	0/3/3/3
1	A2M	Ad	797	1	-	2/5/27/28	0/3/3/3
1	OMC	Ad	418	1	-	6/9/27/28	0/2/2/2
1	OMU	Ad	123	1	-	3/9/27/28	0/2/2/2
1	A2M	Ad	468	1	-	2/5/27/28	0/3/3/3
1	PSU	Ad	306	1	-	2/7/25/26	0/2/2/2
1	PSU	Ad	606	1	-	1/7/25/26	0/2/2/2
1	PSU	Ad	636	1	-	3/7/25/26	0/2/2/2
1	PSU	Ad	121	1	-	5/7/25/26	0/2/2/2
1	A2M	Ad	162	1	-	1/5/27/28	0/3/3/3
1	PSU	Ad	208	1	-	3/7/25/26	0/2/2/2

All (320) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Ad	797	A2M	O4'-C1'	15.40	1.62	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Ad	979	A2M	O4'-C1'	15.38	1.62	1.41
1	Ad	1760	A2M	O4'-C1'	15.37	1.62	1.41
1	Ad	162	A2M	O4'-C1'	15.19	1.62	1.41
1	Ad	468	A2M	O4'-C1'	15.17	1.62	1.41
1	Ad	802	A2M	O4'-C1'	15.13	1.62	1.41
1	Ad	545	A2M	O4'-C1'	15.11	1.62	1.41
1	Ad	28	A2M	O4'-C1'	15.09	1.62	1.41
1	Ad	440	A2M	O4'-C1'	14.78	1.61	1.41
1	Ad	623	A2M	O4'-C1'	14.46	1.61	1.41
1	Ad	914	PSU	C6-C5	11.00	1.48	1.35
1	Ad	1004	PSU	C6-C5	10.95	1.48	1.35
1	Ad	585	PSU	C6-C5	10.94	1.48	1.35
1	Ad	1122	PSU	C6-C5	10.89	1.48	1.35
1	Ad	755	PSU	C6-C5	10.88	1.48	1.35
1	Ad	952	PSU	C6-C5	10.86	1.48	1.35
1	Ad	951	PSU	C6-C5	10.83	1.47	1.35
1	Ad	811	PSU	C6-C5	10.83	1.47	1.35
1	Ad	1029	PSU	C6-C5	10.78	1.47	1.35
1	Ad	300	PSU	C6-C5	10.77	1.47	1.35
1	Ad	208	PSU	C6-C5	10.77	1.47	1.35
1	Ad	255	PSU	C6-C5	10.75	1.47	1.35
1	Ad	383	PSU	C6-C5	10.75	1.47	1.35
1	Ad	1108	PSU	C6-C5	10.75	1.47	1.35
1	Ad	111	PSU	C6-C5	10.71	1.47	1.35
1	Ad	258	PSU	C6-C5	10.71	1.47	1.35
1	Ad	636	PSU	C6-C5	10.71	1.47	1.35
1	Ad	362	PSU	C6-C5	10.67	1.47	1.35
1	Ad	451	PSU	C6-C5	10.67	1.47	1.35
1	Ad	103	PSU	C6-C5	10.66	1.47	1.35
1	Ad	764	PSU	C6-C5	10.65	1.47	1.35
1	Ad	606	PSU	C6-C5	10.61	1.47	1.35
1	Ad	121	PSU	C6-C5	10.56	1.47	1.35
1	Ad	306	PSU	C6-C5	10.52	1.47	1.35
1	Ad	636	PSU	C2-N1	9.72	1.49	1.36
1	Ad	952	PSU	C2-N1	9.68	1.49	1.36
1	Ad	121	PSU	C2-N1	9.67	1.49	1.36
1	Ad	300	PSU	C2-N1	9.67	1.49	1.36
1	Ad	914	PSU	C2-N1	9.66	1.49	1.36
1	Ad	951	PSU	C2-N1	9.65	1.49	1.36
1	Ad	1122	PSU	C2-N1	9.64	1.49	1.36
1	Ad	1004	PSU	C2-N1	9.64	1.49	1.36
1	Ad	255	PSU	C2-N1	9.63	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Ad	208	PSU	C2-N1	9.61	1.49	1.36
1	Ad	755	PSU	C2-N1	9.61	1.49	1.36
1	Ad	764	PSU	C2-N1	9.60	1.49	1.36
1	Ad	1029	PSU	C2-N1	9.59	1.49	1.36
1	Ad	585	PSU	C2-N1	9.58	1.49	1.36
1	Ad	1108	PSU	C2-N1	9.57	1.49	1.36
1	Ad	111	PSU	C2-N1	9.56	1.49	1.36
1	Ad	451	PSU	C2-N1	9.55	1.49	1.36
1	Ad	811	PSU	C2-N1	9.55	1.49	1.36
1	Ad	606	PSU	C2-N1	9.53	1.49	1.36
1	Ad	103	PSU	C2-N1	9.52	1.49	1.36
1	Ad	362	PSU	C2-N1	9.50	1.49	1.36
1	Ad	258	PSU	C2-N1	9.49	1.49	1.36
1	Ad	383	PSU	C2-N1	9.47	1.49	1.36
1	Ad	306	PSU	C2-N1	9.36	1.49	1.36
1	Ad	615	OMU	C2-N1	8.08	1.51	1.38
1	Ad	1014	OMU	C2-N3	7.81	1.51	1.38
1	Ad	123	OMU	C2-N1	7.76	1.50	1.38
1	Ad	123	OMU	C2-N3	7.73	1.51	1.38
1	Ad	615	OMU	C2-N3	7.71	1.51	1.38
1	Ad	1014	OMU	C2-N1	7.64	1.50	1.38
1	Ad	418	OMC	C2-N3	7.51	1.51	1.36
1	Ad	1647	OMC	C2-N3	7.34	1.51	1.36
1	Ad	473	OMC	C2-N3	7.32	1.51	1.36
1	Ad	38	OMC	C2-N3	7.29	1.51	1.36
1	Ad	764	PSU	C2-N3	6.99	1.49	1.37
1	Ad	585	PSU	C2-N3	6.91	1.49	1.37
1	Ad	1122	PSU	C2-N3	6.91	1.49	1.37
1	Ad	811	PSU	C2-N3	6.91	1.49	1.37
1	Ad	258	PSU	C2-N3	6.90	1.49	1.37
1	Ad	952	PSU	C2-N3	6.90	1.49	1.37
1	Ad	914	PSU	C2-N3	6.90	1.49	1.37
1	Ad	606	PSU	C2-N3	6.89	1.49	1.37
1	Ad	383	PSU	C2-N3	6.88	1.49	1.37
1	Ad	208	PSU	C2-N3	6.88	1.49	1.37
1	Ad	103	PSU	C2-N3	6.87	1.49	1.37
1	Ad	1004	PSU	C2-N3	6.86	1.49	1.37
1	Ad	951	PSU	C2-N3	6.86	1.49	1.37
1	Ad	300	PSU	C2-N3	6.83	1.49	1.37
1	Ad	255	PSU	C2-N3	6.79	1.49	1.37
1	Ad	1108	PSU	C2-N3	6.77	1.49	1.37
1	Ad	121	PSU	C2-N3	6.76	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Ad	623	A2M	O4'-C4'	-6.76	1.29	1.45
1	Ad	111	PSU	C2-N3	6.73	1.49	1.37
1	Ad	362	PSU	C2-N3	6.72	1.49	1.37
1	Ad	306	PSU	C2-N3	6.71	1.49	1.37
1	Ad	1029	PSU	C2-N3	6.67	1.48	1.37
1	Ad	636	PSU	C2-N3	6.60	1.48	1.37
1	Ad	451	PSU	C2-N3	6.59	1.48	1.37
1	Ad	38	OMC	C6-C5	6.56	1.50	1.35
1	Ad	440	A2M	O4'-C4'	-6.51	1.30	1.45
1	Ad	473	OMC	C6-C5	6.49	1.50	1.35
1	Ad	755	PSU	C2-N3	6.48	1.48	1.37
1	Ad	1647	OMC	C6-C5	6.48	1.50	1.35
1	Ad	1760	A2M	O4'-C4'	-6.43	1.30	1.45
1	Ad	545	A2M	O4'-C4'	-6.39	1.30	1.45
1	Ad	162	A2M	O4'-C4'	-6.38	1.30	1.45
1	Ad	797	A2M	O4'-C4'	-6.35	1.30	1.45
1	Ad	979	A2M	O4'-C4'	-6.35	1.30	1.45
1	Ad	468	A2M	O4'-C4'	-6.32	1.30	1.45
1	Ad	123	OMU	C6-C5	6.30	1.49	1.35
1	Ad	802	A2M	O4'-C4'	-6.29	1.30	1.45
1	Ad	28	A2M	O4'-C4'	-6.29	1.30	1.45
1	Ad	1014	OMU	C6-C5	6.23	1.49	1.35
1	Ad	418	OMC	C6-C5	6.16	1.49	1.35
1	Ad	615	OMU	C6-C5	6.06	1.49	1.35
1	Ad	636	PSU	O4-C4	-5.99	1.12	1.23
1	Ad	755	PSU	O4-C4	-5.95	1.12	1.23
1	Ad	1108	PSU	O4-C4	-5.78	1.12	1.23
1	Ad	306	PSU	O4-C4	-5.77	1.12	1.23
1	Ad	1029	PSU	O4-C4	-5.76	1.12	1.23
1	Ad	362	PSU	O4-C4	-5.74	1.12	1.23
1	Ad	1004	PSU	O4-C4	-5.70	1.12	1.23
1	Ad	1122	PSU	O4-C4	-5.67	1.12	1.23
1	Ad	451	PSU	O4-C4	-5.67	1.12	1.23
1	Ad	111	PSU	O4-C4	-5.65	1.12	1.23
1	Ad	208	PSU	O4-C4	-5.63	1.12	1.23
1	Ad	121	PSU	O4-C4	-5.62	1.12	1.23
1	Ad	952	PSU	O4-C4	-5.62	1.12	1.23
1	Ad	811	PSU	O4-C4	-5.60	1.12	1.23
1	Ad	383	PSU	O4-C4	-5.59	1.12	1.23
1	Ad	300	PSU	O4-C4	-5.59	1.13	1.23
1	Ad	951	PSU	O4-C4	-5.56	1.13	1.23
1	Ad	255	PSU	O4-C4	-5.52	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Ad	764	PSU	O4-C4	-5.50	1.13	1.23
1	Ad	258	PSU	O4-C4	-5.50	1.13	1.23
1	Ad	103	PSU	O4-C4	-5.48	1.13	1.23
1	Ad	246	OMG	C2-N3	5.48	1.46	1.33
1	Ad	914	PSU	O4-C4	-5.47	1.13	1.23
1	Ad	585	PSU	O4-C4	-5.47	1.13	1.23
1	Ad	606	PSU	O4-C4	-5.42	1.13	1.23
1	Ad	418	OMC	C4-N3	5.41	1.45	1.34
1	Ad	914	PSU	C6-N1	5.38	1.45	1.36
1	Ad	1122	PSU	C6-N1	5.33	1.45	1.36
1	Ad	599	OMG	C2-N3	5.33	1.46	1.33
1	Ad	1029	PSU	C6-N1	5.30	1.45	1.36
1	Ad	952	PSU	C6-N1	5.30	1.45	1.36
1	Ad	755	PSU	C6-N1	5.29	1.45	1.36
1	Ad	255	PSU	C6-N1	5.29	1.45	1.36
1	Ad	1004	PSU	C6-N1	5.28	1.45	1.36
1	Ad	636	PSU	C6-N1	5.28	1.45	1.36
1	Ad	951	PSU	C6-N1	5.27	1.45	1.36
1	Ad	300	PSU	C6-N1	5.26	1.45	1.36
1	Ad	451	PSU	C6-N1	5.24	1.44	1.36
1	Ad	121	PSU	C6-N1	5.23	1.44	1.36
1	Ad	585	PSU	C6-N1	5.21	1.44	1.36
1	Ad	811	PSU	C6-N1	5.20	1.44	1.36
1	Ad	208	PSU	C6-N1	5.19	1.44	1.36
1	Ad	473	OMC	C4-N3	5.18	1.44	1.34
1	Ad	258	PSU	C6-N1	5.15	1.44	1.36
1	Ad	111	PSU	C6-N1	5.15	1.44	1.36
1	Ad	103	PSU	C6-N1	5.15	1.44	1.36
1	Ad	362	PSU	C6-N1	5.15	1.44	1.36
1	Ad	1647	OMC	C4-N3	5.14	1.44	1.34
1	Ad	383	PSU	C6-N1	5.14	1.44	1.36
1	Ad	392	OMG	C2-N3	5.14	1.45	1.33
1	Ad	764	PSU	C6-N1	5.14	1.44	1.36
1	Ad	306	PSU	C6-N1	5.13	1.44	1.36
1	Ad	1108	PSU	C6-N1	5.13	1.44	1.36
1	Ad	606	PSU	C6-N1	5.12	1.44	1.36
1	Ad	38	OMC	C4-N3	5.00	1.44	1.34
1	Ad	246	OMG	C4-N3	4.98	1.49	1.37
1	Ad	599	OMG	C4-N3	4.92	1.49	1.37
1	Ad	392	OMG	C4-N3	4.79	1.49	1.37
1	Ad	246	OMG	C2-N2	4.79	1.45	1.34
1	Ad	1647	OMC	C2-N1	4.74	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Ad	392	OMG	C2-N2	4.72	1.45	1.34
1	Ad	418	OMC	C2-N1	4.70	1.50	1.40
1	Ad	599	OMG	C2-N2	4.69	1.45	1.34
1	Ad	38	OMC	C2-N1	4.67	1.50	1.40
1	Ad	473	OMC	C2-N1	4.29	1.49	1.40
1	Ad	585	PSU	C4-N3	4.19	1.46	1.38
1	Ad	914	PSU	C4-N3	4.18	1.46	1.38
1	Ad	255	PSU	C4-N3	4.17	1.46	1.38
1	Ad	258	PSU	C4-N3	4.17	1.46	1.38
1	Ad	952	PSU	C4-N3	4.16	1.46	1.38
1	Ad	811	PSU	C4-N3	4.12	1.46	1.38
1	Ad	1122	PSU	C4-N3	4.12	1.46	1.38
1	Ad	951	PSU	C4-N3	4.12	1.46	1.38
1	Ad	300	PSU	C4-N3	4.10	1.46	1.38
1	Ad	1014	OMU	C4-N3	4.10	1.45	1.38
1	Ad	1004	PSU	C4-N3	4.10	1.46	1.38
1	Ad	208	PSU	C4-N3	4.08	1.46	1.38
1	Ad	383	PSU	C4-N3	4.08	1.46	1.38
1	Ad	103	PSU	C4-N3	4.07	1.46	1.38
1	Ad	764	PSU	C4-N3	4.06	1.46	1.38
1	Ad	1029	PSU	C4-N3	4.06	1.46	1.38
1	Ad	306	PSU	C4-N3	4.06	1.46	1.38
1	Ad	121	PSU	C4-N3	4.05	1.46	1.38
1	Ad	606	PSU	C4-N3	4.04	1.46	1.38
1	Ad	418	OMC	C4-N4	4.03	1.43	1.33
1	Ad	111	PSU	C4-N3	3.98	1.46	1.38
1	Ad	1108	PSU	C4-N3	3.97	1.46	1.38
1	Ad	451	PSU	C4-N3	3.97	1.46	1.38
1	Ad	362	PSU	C4-N3	3.94	1.46	1.38
1	Ad	123	OMU	C4-N3	3.93	1.45	1.38
1	Ad	755	PSU	C4-N3	3.93	1.46	1.38
1	Ad	636	PSU	C4-N3	3.92	1.46	1.38
1	Ad	1647	OMC	C4-N4	3.88	1.43	1.33
1	Ad	38	OMC	C4-N4	3.85	1.43	1.33
1	Ad	392	OMG	C6-N1	3.76	1.43	1.37
1	Ad	473	OMC	C4-N4	3.74	1.42	1.33
1	Ad	615	OMU	C4-N3	3.71	1.45	1.38
1	Ad	246	OMG	C6-N1	3.64	1.43	1.37
1	Ad	755	PSU	O2-C2	-3.61	1.15	1.23
1	Ad	599	OMG	C6-N1	3.60	1.43	1.37
1	Ad	103	PSU	O2-C2	-3.54	1.16	1.23
1	Ad	1029	PSU	O2-C2	-3.53	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Ad	636	PSU	O2-C2	-3.49	1.16	1.23
1	Ad	362	PSU	O2-C2	-3.49	1.16	1.23
1	Ad	306	PSU	O2-C2	-3.48	1.16	1.23
1	Ad	1108	PSU	O2-C2	-3.48	1.16	1.23
1	Ad	451	PSU	O2-C2	-3.47	1.16	1.23
1	Ad	811	PSU	O2-C2	-3.47	1.16	1.23
1	Ad	111	PSU	O2-C2	-3.47	1.16	1.23
1	Ad	1647	OMC	C6-N1	3.47	1.46	1.38
1	Ad	585	PSU	O2-C2	-3.46	1.16	1.23
1	Ad	383	PSU	O2-C2	-3.46	1.16	1.23
1	Ad	914	PSU	O2-C2	-3.46	1.16	1.23
1	Ad	1122	PSU	O2-C2	-3.45	1.16	1.23
1	Ad	255	PSU	O2-C2	-3.44	1.16	1.23
1	Ad	300	PSU	O2-C2	-3.44	1.16	1.23
1	Ad	1004	PSU	O2-C2	-3.44	1.16	1.23
1	Ad	258	PSU	O2-C2	-3.44	1.16	1.23
1	Ad	208	PSU	O2-C2	-3.44	1.16	1.23
1	Ad	121	PSU	O2-C2	-3.44	1.16	1.23
1	Ad	951	PSU	O2-C2	-3.41	1.16	1.23
1	Ad	764	PSU	O2-C2	-3.41	1.16	1.23
1	Ad	952	PSU	O2-C2	-3.41	1.16	1.23
1	Ad	606	PSU	O2-C2	-3.40	1.16	1.23
1	Ad	38	OMC	C6-N1	3.40	1.46	1.38
1	Ad	473	OMC	C6-N1	3.39	1.46	1.38
1	Ad	28	A2M	O3'-C3'	-3.21	1.35	1.43
1	Ad	418	OMC	C6-N1	3.19	1.45	1.38
1	Ad	162	A2M	C6-N6	3.14	1.45	1.34
1	Ad	1760	A2M	C6-N6	3.14	1.45	1.34
1	Ad	797	A2M	C6-N6	3.14	1.45	1.34
1	Ad	545	A2M	C6-N6	3.13	1.45	1.34
1	Ad	802	A2M	C6-N6	3.13	1.45	1.34
1	Ad	1760	A2M	O3'-C3'	-3.11	1.35	1.43
1	Ad	468	A2M	C6-N6	3.11	1.45	1.34
1	Ad	440	A2M	C6-N6	3.10	1.45	1.34
1	Ad	623	A2M	C6-N6	3.08	1.45	1.34
1	Ad	28	A2M	C6-N6	3.06	1.45	1.34
1	Ad	162	A2M	O3'-C3'	-3.06	1.35	1.43
1	Ad	468	A2M	O3'-C3'	-3.05	1.35	1.43
1	Ad	623	A2M	O3'-C3'	-3.04	1.35	1.43
1	Ad	979	A2M	O3'-C3'	-3.03	1.35	1.43
1	Ad	979	A2M	C6-N6	3.02	1.45	1.34
1	Ad	545	A2M	O3'-C3'	-2.99	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Ad	797	A2M	O3'-C3'	-2.98	1.35	1.43
1	Ad	623	A2M	O2'-C2'	2.94	1.50	1.42
1	Ad	599	OMG	C5-C6	2.93	1.53	1.47
1	Ad	802	A2M	O3'-C3'	-2.93	1.36	1.43
1	Ad	615	OMU	O4-C4	-2.92	1.18	1.24
1	Ad	440	A2M	O3'-C3'	-2.92	1.36	1.43
1	Ad	246	OMG	C5-C6	2.88	1.53	1.47
1	Ad	1014	OMU	C6-N1	2.87	1.44	1.38
1	Ad	392	OMG	C5-C4	-2.86	1.35	1.43
1	Ad	123	OMU	C6-N1	2.86	1.44	1.38
1	Ad	392	OMG	C5-C6	2.86	1.53	1.47
1	Ad	38	OMC	O2-C2	-2.85	1.18	1.23
1	Ad	123	OMU	O4-C4	-2.85	1.19	1.24
1	Ad	1760	A2M	O2'-C2'	2.84	1.49	1.42
1	Ad	802	A2M	C5-C4	-2.84	1.33	1.40
1	Ad	1014	OMU	O4-C4	-2.81	1.19	1.24
1	Ad	623	A2M	C5-C4	-2.80	1.33	1.40
1	Ad	468	A2M	C5-C4	-2.80	1.33	1.40
1	Ad	545	A2M	O2'-C2'	2.77	1.49	1.42
1	Ad	162	A2M	C5-C4	-2.77	1.33	1.40
1	Ad	440	A2M	C5-C4	-2.77	1.33	1.40
1	Ad	797	A2M	O2'-C2'	2.76	1.49	1.42
1	Ad	1647	OMC	O2-C2	-2.76	1.18	1.23
1	Ad	440	A2M	O2'-C2'	2.75	1.49	1.42
1	Ad	123	OMU	C5-C4	2.73	1.49	1.43
1	Ad	468	A2M	O2'-C2'	2.73	1.49	1.42
1	Ad	418	OMC	O2-C2	-2.73	1.18	1.23
1	Ad	545	A2M	C5-C4	-2.73	1.33	1.40
1	Ad	1791	MA6	C5-C4	-2.72	1.33	1.40
1	Ad	979	A2M	O2'-C2'	2.72	1.49	1.42
1	Ad	162	A2M	O2'-C2'	2.71	1.49	1.42
1	Ad	28	A2M	C5-C4	-2.70	1.33	1.40
1	Ad	1760	A2M	C5-C4	-2.70	1.33	1.40
1	Ad	246	OMG	C2-N1	2.69	1.44	1.37
1	Ad	1014	OMU	C5-C4	2.69	1.49	1.43
1	Ad	615	OMU	C6-N1	2.67	1.44	1.38
1	Ad	797	A2M	C5-C4	-2.67	1.33	1.40
1	Ad	473	OMC	O2-C2	-2.67	1.18	1.23
1	Ad	392	OMG	C2-N1	2.66	1.44	1.37
1	Ad	599	OMG	C5-C4	-2.65	1.36	1.43
1	Ad	28	A2M	O2'-C2'	2.65	1.49	1.42
1	Ad	979	A2M	C5-C4	-2.65	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Ad	599	OMG	C2-N1	2.64	1.44	1.37
1	Ad	615	OMU	C5-C4	2.60	1.49	1.43
1	Ad	1792	MA6	C5-C4	-2.60	1.34	1.40
1	Ad	802	A2M	O2'-C2'	2.60	1.49	1.42
1	Ad	246	OMG	C5-C4	-2.56	1.36	1.43
1	Ad	38	OMC	C5-C4	2.47	1.48	1.42
1	Ad	1647	OMC	C5-C4	2.42	1.48	1.42
1	Ad	246	OMG	O6-C6	-2.41	1.18	1.23
1	Ad	473	OMC	C5-C4	2.40	1.48	1.42
1	Ad	623	A2M	O5'-C5'	-2.32	1.39	1.44
1	Ad	599	OMG	O6-C6	-2.30	1.18	1.23
1	Ad	418	OMC	C5-C4	2.29	1.48	1.42
1	Ad	392	OMG	O6-C6	-2.26	1.18	1.23
1	Ad	545	A2M	C2-N3	2.12	1.35	1.32
1	Ad	979	A2M	C2-N3	2.12	1.35	1.32
1	Ad	797	A2M	C2-N3	2.11	1.35	1.32
1	Ad	1760	A2M	C2-N3	2.08	1.35	1.32
1	Ad	28	A2M	O5'-C5'	-2.07	1.39	1.44
1	Ad	802	A2M	C2-N3	2.06	1.35	1.32
1	Ad	162	A2M	O5'-C5'	-2.04	1.39	1.44
1	Ad	162	A2M	C2-N3	2.04	1.35	1.32
1	Ad	440	A2M	C2-N3	2.04	1.35	1.32
1	Ad	979	A2M	O5'-C5'	-2.02	1.39	1.44
1	Ad	615	OMU	O2-C2	-2.02	1.19	1.23
1	Ad	468	A2M	C2-N3	2.01	1.35	1.32

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ad	1792	MA6	C1'-N9-C4	14.83	152.70	126.64
1	Ad	1791	MA6	N1-C6-N6	-14.23	102.08	117.06
1	Ad	1792	MA6	N1-C6-N6	-13.93	102.39	117.06
1	Ad	1791	MA6	C1'-N9-C4	12.67	148.90	126.64
1	Ad	979	A2M	C1'-N9-C4	6.50	138.06	126.64
1	Ad	797	A2M	C1'-N9-C4	5.97	137.13	126.64
1	Ad	1791	MA6	N3-C2-N1	-5.68	119.81	128.68
1	Ad	545	A2M	C1'-N9-C4	5.64	136.56	126.64
1	Ad	468	A2M	N3-C2-N1	-5.62	119.89	128.68
1	Ad	1760	A2M	N3-C2-N1	-5.61	119.92	128.68
1	Ad	545	A2M	N3-C2-N1	-5.60	119.92	128.68
1	Ad	162	A2M	N3-C2-N1	-5.59	119.93	128.68
1	Ad	1760	A2M	C1'-N9-C4	5.55	136.39	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ad	28	A2M	C1'-N9-C4	5.50	136.31	126.64
1	Ad	802	A2M	N3-C2-N1	-5.50	120.08	128.68
1	Ad	1792	MA6	N3-C2-N1	-5.45	120.16	128.68
1	Ad	28	A2M	N3-C2-N1	-5.45	120.16	128.68
1	Ad	440	A2M	C1'-N9-C4	5.45	136.21	126.64
1	Ad	623	A2M	N3-C2-N1	-5.44	120.17	128.68
1	Ad	797	A2M	N3-C2-N1	-5.43	120.19	128.68
1	Ad	440	A2M	N3-C2-N1	-5.37	120.28	128.68
1	Ad	979	A2M	N3-C2-N1	-5.36	120.30	128.68
1	Ad	468	A2M	C1'-N9-C4	5.36	136.06	126.64
1	Ad	162	A2M	C1'-N9-C4	5.23	135.82	126.64
1	Ad	615	OMU	C4-N3-C2	-5.21	119.71	126.58
1	Ad	123	OMU	C4-N3-C2	-5.20	119.72	126.58
1	Ad	802	A2M	C1'-N9-C4	5.15	135.69	126.64
1	Ad	1014	OMU	C4-N3-C2	-5.11	119.83	126.58
1	Ad	623	A2M	C1'-N9-C4	5.05	135.51	126.64
1	Ad	755	PSU	C4-N3-C2	-4.90	119.28	126.34
1	Ad	636	PSU	C4-N3-C2	-4.76	119.47	126.34
1	Ad	1029	PSU	C4-N3-C2	-4.75	119.49	126.34
1	Ad	103	PSU	C4-N3-C2	-4.70	119.56	126.34
1	Ad	1108	PSU	C4-N3-C2	-4.70	119.57	126.34
1	Ad	362	PSU	C4-N3-C2	-4.67	119.61	126.34
1	Ad	306	PSU	C4-N3-C2	-4.66	119.62	126.34
1	Ad	451	PSU	C4-N3-C2	-4.66	119.63	126.34
1	Ad	111	PSU	C4-N3-C2	-4.63	119.67	126.34
1	Ad	764	PSU	C4-N3-C2	-4.62	119.68	126.34
1	Ad	300	PSU	C4-N3-C2	-4.60	119.71	126.34
1	Ad	811	PSU	C4-N3-C2	-4.58	119.74	126.34
1	Ad	121	PSU	C4-N3-C2	-4.57	119.75	126.34
1	Ad	255	PSU	C4-N3-C2	-4.54	119.80	126.34
1	Ad	383	PSU	C4-N3-C2	-4.52	119.82	126.34
1	Ad	1004	PSU	C4-N3-C2	-4.52	119.82	126.34
1	Ad	952	PSU	C4-N3-C2	-4.52	119.82	126.34
1	Ad	208	PSU	C4-N3-C2	-4.52	119.83	126.34
1	Ad	1122	PSU	C4-N3-C2	-4.51	119.83	126.34
1	Ad	951	PSU	C4-N3-C2	-4.50	119.86	126.34
1	Ad	979	A2M	C5-C6-N6	-4.49	113.53	120.35
1	Ad	258	PSU	C4-N3-C2	-4.47	119.91	126.34
1	Ad	585	PSU	C4-N3-C2	-4.43	119.96	126.34
1	Ad	606	PSU	C4-N3-C2	-4.42	119.97	126.34
1	Ad	914	PSU	C4-N3-C2	-4.30	120.14	126.34
1	Ad	103	PSU	N1-C2-N3	4.27	119.97	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ad	764	PSU	N1-C2-N3	4.22	119.92	115.13
1	Ad	383	PSU	N1-C2-N3	4.14	119.82	115.13
1	Ad	755	PSU	N1-C2-N3	4.14	119.82	115.13
1	Ad	1108	PSU	N1-C2-N3	4.12	119.80	115.13
1	Ad	797	A2M	C5-C6-N6	-4.11	114.10	120.35
1	Ad	28	A2M	C5-C6-N6	-4.11	114.11	120.35
1	Ad	585	PSU	N1-C2-N3	4.09	119.76	115.13
1	Ad	811	PSU	N1-C2-N3	4.08	119.76	115.13
1	Ad	545	A2M	C5-C6-N6	-4.06	114.18	120.35
1	Ad	300	PSU	N1-C2-N3	4.06	119.73	115.13
1	Ad	606	PSU	N1-C2-N3	4.06	119.73	115.13
1	Ad	615	OMU	N3-C2-N1	4.06	120.28	114.89
1	Ad	111	PSU	N1-C2-N3	4.06	119.72	115.13
1	Ad	362	PSU	N1-C2-N3	4.04	119.71	115.13
1	Ad	208	PSU	N1-C2-N3	4.01	119.67	115.13
1	Ad	1004	PSU	N1-C2-N3	3.99	119.66	115.13
1	Ad	1029	PSU	N1-C2-N3	3.99	119.65	115.13
1	Ad	162	A2M	C5-C6-N6	-3.99	114.30	120.35
1	Ad	468	A2M	C5-C6-N6	-3.98	114.30	120.35
1	Ad	914	PSU	N1-C2-N3	3.97	119.63	115.13
1	Ad	1122	PSU	N1-C2-N3	3.96	119.62	115.13
1	Ad	123	OMU	N3-C2-N1	3.95	120.13	114.89
1	Ad	258	PSU	N1-C2-N3	3.95	119.60	115.13
1	Ad	121	PSU	N1-C2-N3	3.94	119.60	115.13
1	Ad	440	A2M	C5-C6-N6	-3.93	114.38	120.35
1	Ad	951	PSU	N1-C2-N3	3.93	119.59	115.13
1	Ad	802	A2M	C5-C6-N6	-3.89	114.45	120.35
1	Ad	636	PSU	N1-C2-N3	3.89	119.53	115.13
1	Ad	255	PSU	N1-C2-N3	3.88	119.53	115.13
1	Ad	952	PSU	N1-C2-N3	3.85	119.50	115.13
1	Ad	451	PSU	N1-C2-N3	3.84	119.48	115.13
1	Ad	1760	A2M	C5-C6-N6	-3.84	114.52	120.35
1	Ad	979	A2M	N6-C6-N1	3.79	126.43	118.57
1	Ad	306	PSU	N1-C2-N3	3.79	119.42	115.13
1	Ad	623	A2M	C5-C6-N6	-3.71	114.71	120.35
1	Ad	1014	OMU	N3-C2-N1	3.71	119.82	114.89
1	Ad	615	OMU	C1'-N1-C2	3.69	124.25	117.57
1	Ad	797	A2M	N6-C6-N1	3.58	126.00	118.57
1	Ad	28	A2M	N6-C6-N1	3.54	125.92	118.57
1	Ad	246	OMG	C5-C6-N1	3.50	120.14	113.95
1	Ad	392	OMG	C5-C6-N1	3.45	120.04	113.95
1	Ad	599	OMG	C5-C6-N1	3.44	120.02	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ad	468	A2M	N6-C6-N1	3.42	125.67	118.57
1	Ad	545	A2M	N6-C6-N1	3.41	125.65	118.57
1	Ad	162	A2M	N6-C6-N1	3.40	125.62	118.57
1	Ad	1760	A2M	N6-C6-N1	3.35	125.53	118.57
1	Ad	418	OMC	C1'-N1-C2	3.35	125.89	118.42
1	Ad	440	A2M	N6-C6-N1	3.33	125.48	118.57
1	Ad	764	PSU	C6-C5-C4	3.33	120.52	118.20
1	Ad	802	A2M	N6-C6-N1	3.29	125.41	118.57
1	Ad	623	A2M	N6-C6-N1	3.27	125.36	118.57
1	Ad	1014	OMU	C5-C4-N3	3.27	119.73	114.84
1	Ad	123	OMU	C5-C4-N3	3.25	119.70	114.84
1	Ad	979	A2M	O4'-C4'-C3'	-3.05	99.08	105.11
1	Ad	103	PSU	C6-C5-C4	3.05	120.33	118.20
1	Ad	914	PSU	C6-N1-C2	-3.01	119.61	122.68
1	Ad	764	PSU	C6-N1-C2	-2.99	119.62	122.68
1	Ad	606	PSU	C6-N1-C2	-2.95	119.66	122.68
1	Ad	615	OMU	C5-C4-N3	2.94	119.24	114.84
1	Ad	585	PSU	C6-N1-C2	-2.94	119.68	122.68
1	Ad	383	PSU	C6-N1-C2	-2.93	119.68	122.68
1	Ad	599	OMG	C2-N1-C6	-2.93	119.70	125.10
1	Ad	103	PSU	C6-N1-C2	-2.92	119.70	122.68
1	Ad	246	OMG	C2-N1-C6	-2.92	119.72	125.10
1	Ad	1014	OMU	O4-C4-C5	-2.88	120.09	125.16
1	Ad	1122	PSU	C6-N1-C2	-2.88	119.74	122.68
1	Ad	811	PSU	C6-N1-C2	-2.86	119.76	122.68
1	Ad	1004	PSU	C6-N1-C2	-2.85	119.77	122.68
1	Ad	1108	PSU	C6-N1-C2	-2.82	119.80	122.68
1	Ad	418	OMC	C1'-N1-C6	-2.82	114.69	120.84
1	Ad	300	PSU	C6-N1-C2	-2.82	119.80	122.68
1	Ad	208	PSU	C6-N1-C2	-2.82	119.80	122.68
1	Ad	392	OMG	C2-N1-C6	-2.81	119.92	125.10
1	Ad	121	PSU	C6-N1-C2	-2.78	119.84	122.68
1	Ad	111	PSU	C6-N1-C2	-2.77	119.85	122.68
1	Ad	258	PSU	C6-N1-C2	-2.76	119.86	122.68
1	Ad	951	PSU	C6-N1-C2	-2.74	119.88	122.68
1	Ad	123	OMU	O4-C4-C5	-2.72	120.38	125.16
1	Ad	392	OMG	C8-N7-C5	2.72	108.16	102.99
1	Ad	362	PSU	C6-N1-C2	-2.71	119.91	122.68
1	Ad	38	OMC	O2-C2-N3	-2.68	117.98	122.33
1	Ad	599	OMG	C8-N7-C5	2.67	108.07	102.99
1	Ad	952	PSU	C6-N1-C2	-2.64	119.98	122.68
1	Ad	755	PSU	C6-N1-C2	-2.64	119.98	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ad	1647	OMC	C1'-N1-C2	2.63	124.29	118.42
1	Ad	1029	PSU	C6-N1-C2	-2.60	120.02	122.68
1	Ad	255	PSU	C6-N1-C2	-2.60	120.03	122.68
1	Ad	1647	OMC	O2-C2-N3	-2.58	118.13	122.33
1	Ad	615	OMU	O4-C4-C5	-2.57	120.64	125.16
1	Ad	636	PSU	C6-N1-C2	-2.54	120.08	122.68
1	Ad	246	OMG	C8-N7-C5	2.53	107.80	102.99
1	Ad	103	PSU	O2-C2-N1	-2.43	120.12	122.79
1	Ad	383	PSU	O2-C2-N1	-2.42	120.13	122.79
1	Ad	258	PSU	O2-C2-N1	-2.40	120.15	122.79
1	Ad	606	PSU	O2-C2-N1	-2.40	120.15	122.79
1	Ad	764	PSU	O2-C2-N1	-2.39	120.16	122.79
1	Ad	28	A2M	C5'-C4'-C3'	-2.38	106.27	115.18
1	Ad	451	PSU	C6-N1-C2	-2.34	120.29	122.68
1	Ad	811	PSU	O2-C2-N1	-2.34	120.21	122.79
1	Ad	306	PSU	C6-N1-C2	-2.32	120.31	122.68
1	Ad	246	OMG	O6-C6-C5	-2.31	119.85	124.37
1	Ad	392	OMG	O6-C6-C5	-2.31	119.86	124.37
1	Ad	585	PSU	O2-C2-N1	-2.31	120.25	122.79
1	Ad	306	PSU	O2-C2-N1	-2.31	120.25	122.79
1	Ad	208	PSU	O2-C2-N1	-2.30	120.26	122.79
1	Ad	1108	PSU	O2-C2-N1	-2.28	120.28	122.79
1	Ad	606	PSU	C6-C5-C4	2.26	119.78	118.20
1	Ad	258	PSU	C6-C5-C4	2.23	119.76	118.20
1	Ad	208	PSU	C6-C5-C4	2.22	119.75	118.20
1	Ad	38	OMC	C1'-N1-C2	2.20	123.33	118.42
1	Ad	418	OMC	N4-C4-N3	2.19	121.81	117.97
1	Ad	952	PSU	O2-C2-N1	-2.19	120.38	122.79
1	Ad	451	PSU	O4'-C1'-C2'	2.19	108.23	105.14
1	Ad	599	OMG	O6-C6-C5	-2.19	120.10	124.37
1	Ad	1122	PSU	O2-C2-N1	-2.18	120.39	122.79
1	Ad	300	PSU	O2-C2-N1	-2.17	120.40	122.79
1	Ad	383	PSU	C6-C5-C4	2.16	119.71	118.20
1	Ad	615	OMU	O2-C2-N3	-2.14	117.51	121.50
1	Ad	111	PSU	O2-C2-N1	-2.12	120.46	122.79
1	Ad	951	PSU	O2-C2-N1	-2.12	120.46	122.79
1	Ad	123	OMU	C1'-N1-C2	2.11	121.39	117.57
1	Ad	111	PSU	C6-C5-C4	2.10	119.67	118.20
1	Ad	951	PSU	O4'-C1'-C2'	2.10	108.11	105.14
1	Ad	1014	OMU	C1'-N1-C2	2.07	121.32	117.57
1	Ad	418	OMC	O2-C2-N3	-2.06	118.98	122.33
1	Ad	255	PSU	O2-C2-N1	-2.06	120.52	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ad	362	PSU	O2-C2-N1	-2.04	120.55	122.79
1	Ad	585	PSU	C6-C5-C4	2.03	119.61	118.20
1	Ad	1004	PSU	O2-C2-N1	-2.02	120.56	122.79
1	Ad	755	PSU	O3'-C3'-C2'	2.02	118.36	111.82
1	Ad	811	PSU	C6-C5-C4	2.02	119.61	118.20
1	Ad	300	PSU	C6-C5-C4	2.02	119.61	118.20
1	Ad	121	PSU	C6-C5-C4	2.01	119.61	118.20

There are no chirality outliers.

All (103) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	Ad	28	A2M	C3'-C4'-C5'-O5'
1	Ad	38	OMC	O4'-C1'-N1-C2
1	Ad	38	OMC	O4'-C1'-N1-C6
1	Ad	38	OMC	C1'-C2'-O2'-CM2
1	Ad	111	PSU	O4'-C1'-C5-C4
1	Ad	111	PSU	O4'-C1'-C5-C6
1	Ad	121	PSU	C2'-C1'-C5-C4
1	Ad	121	PSU	O4'-C1'-C5-C4
1	Ad	121	PSU	O4'-C1'-C5-C6
1	Ad	123	OMU	C1'-C2'-O2'-CM2
1	Ad	123	OMU	C3'-C4'-C5'-O5'
1	Ad	123	OMU	O4'-C4'-C5'-O5'
1	Ad	162	A2M	C1'-C2'-O2'-CM'
1	Ad	208	PSU	C2'-C1'-C5-C4
1	Ad	208	PSU	O4'-C1'-C5-C4
1	Ad	208	PSU	O4'-C1'-C5-C6
1	Ad	246	OMG	C1'-C2'-O2'-CM2
1	Ad	255	PSU	O4'-C1'-C5-C4
1	Ad	255	PSU	C2'-C1'-C5-C6
1	Ad	255	PSU	O4'-C1'-C5-C6
1	Ad	258	PSU	O4'-C1'-C5-C4
1	Ad	258	PSU	O4'-C1'-C5-C6
1	Ad	300	PSU	O4'-C1'-C5-C4
1	Ad	300	PSU	O4'-C1'-C5-C6
1	Ad	306	PSU	O4'-C1'-C5-C4
1	Ad	306	PSU	O4'-C1'-C5-C6
1	Ad	362	PSU	O4'-C1'-C5-C4
1	Ad	362	PSU	O4'-C1'-C5-C6
1	Ad	383	PSU	O4'-C1'-C5-C4
1	Ad	383	PSU	O4'-C1'-C5-C6

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Mol	Chain	Res	Type	Atoms
1	Ad	418	OMC	O4'-C1'-N1-C2
1	Ad	418	OMC	O4'-C1'-N1-C6
1	Ad	418	OMC	C3'-C4'-C5'-O5'
1	Ad	418	OMC	O4'-C4'-C5'-O5'
1	Ad	440	A2M	C1'-C2'-O2'-CM'
1	Ad	451	PSU	O4'-C1'-C5-C4
1	Ad	451	PSU	O4'-C1'-C5-C6
1	Ad	468	A2M	O4'-C4'-C5'-O5'
1	Ad	599	OMG	C1'-C2'-O2'-CM2
1	Ad	615	OMU	O4'-C1'-N1-C2
1	Ad	615	OMU	O4'-C1'-N1-C6
1	Ad	615	OMU	O4'-C4'-C5'-O5'
1	Ad	623	A2M	C1'-C2'-O2'-CM'
1	Ad	636	PSU	C2'-C1'-C5-C4
1	Ad	636	PSU	O4'-C1'-C5-C4
1	Ad	636	PSU	O4'-C1'-C5-C6
1	Ad	755	PSU	O4'-C1'-C5-C4
1	Ad	755	PSU	O4'-C1'-C5-C6
1	Ad	797	A2M	O4'-C4'-C5'-O5'
1	Ad	811	PSU	O4'-C1'-C5-C4
1	Ad	811	PSU	O4'-C1'-C5-C6
1	Ad	914	PSU	O4'-C1'-C5-C4
1	Ad	914	PSU	O4'-C1'-C5-C6
1	Ad	951	PSU	O4'-C1'-C5-C4
1	Ad	951	PSU	O4'-C1'-C5-C6
1	Ad	952	PSU	O4'-C1'-C5-C4
1	Ad	952	PSU	O4'-C1'-C5-C6
1	Ad	1004	PSU	C2'-C1'-C5-C4
1	Ad	1004	PSU	O4'-C1'-C5-C4
1	Ad	1004	PSU	O4'-C1'-C5-C6
1	Ad	1029	PSU	C2'-C1'-C5-C4
1	Ad	1029	PSU	O4'-C1'-C5-C4
1	Ad	1029	PSU	C2'-C1'-C5-C6
1	Ad	1029	PSU	O4'-C1'-C5-C6
1	Ad	1108	PSU	O4'-C1'-C5-C4
1	Ad	1108	PSU	O4'-C1'-C5-C6
1	Ad	1122	PSU	O4'-C1'-C5-C4
1	Ad	1122	PSU	O4'-C1'-C5-C6
1	Ad	1647	OMC	O4'-C1'-N1-C2
1	Ad	1647	OMC	O4'-C1'-N1-C6
1	Ad	1760	A2M	C1'-C2'-O2'-CM'
1	Ad	1791	MA6	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	Ad	1791	MA6	C3'-C4'-C5'-O5'
1	Ad	1792	MA6	O4'-C4'-C5'-O5'
1	Ad	1792	MA6	C3'-C4'-C5'-O5'
1	Ad	1792	MA6	C5-C6-N6-C9
1	Ad	28	A2M	O4'-C4'-C5'-O5'
1	Ad	615	OMU	C3'-C4'-C5'-O5'
1	Ad	797	A2M	C3'-C4'-C5'-O5'
1	Ad	1029	PSU	O4'-C4'-C5'-O5'
1	Ad	468	A2M	C3'-C4'-C5'-O5'
1	Ad	1029	PSU	C3'-C4'-C5'-O5'
1	Ad	623	A2M	C3'-C4'-C5'-O5'
1	Ad	1647	OMC	C3'-C4'-C5'-O5'
1	Ad	623	A2M	O4'-C4'-C5'-O5'
1	Ad	755	PSU	O4'-C4'-C5'-O5'
1	Ad	1792	MA6	C5-C6-N6-C10
1	Ad	755	PSU	C3'-C4'-C5'-O5'
1	Ad	1792	MA6	N1-C6-N6-C9
1	Ad	1647	OMC	O4'-C4'-C5'-O5'
1	Ad	1792	MA6	C4'-C5'-O5'-P
1	Ad	246	OMG	O4'-C4'-C5'-O5'
1	Ad	599	OMG	C3'-C4'-C5'-O5'
1	Ad	599	OMG	C4'-C5'-O5'-P
1	Ad	1029	PSU	C4'-C5'-O5'-P
1	Ad	418	OMC	C4'-C5'-O5'-P
1	Ad	121	PSU	O4'-C4'-C5'-O5'
1	Ad	418	OMC	C2'-C1'-N1-C6
1	Ad	606	PSU	O4'-C1'-C5-C6
1	Ad	246	OMG	C3'-C4'-C5'-O5'
1	Ad	599	OMG	O4'-C4'-C5'-O5'
1	Ad	545	A2M	C3'-C2'-O2'-CM'
1	Ad	121	PSU	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 87 ligands modelled in this entry, 87 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

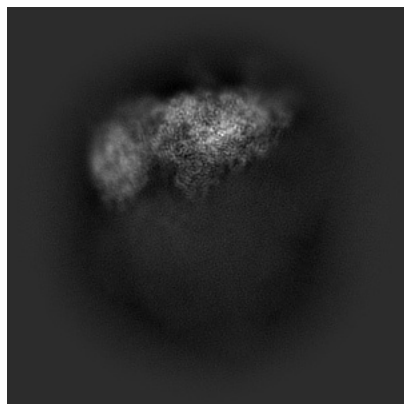
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36332. These allow visual inspection of the internal detail of the map and identification of artifacts.

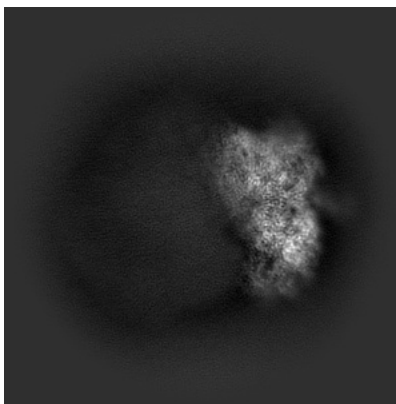
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

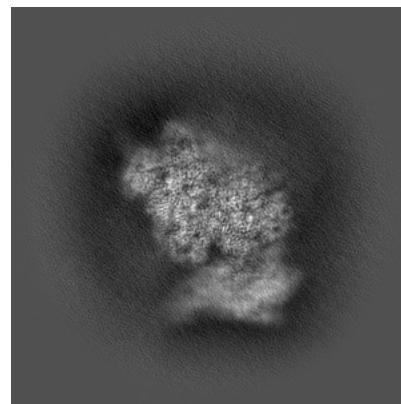
6.1.1 Primary map



X

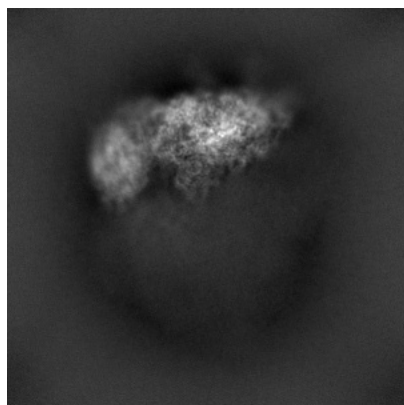


Y

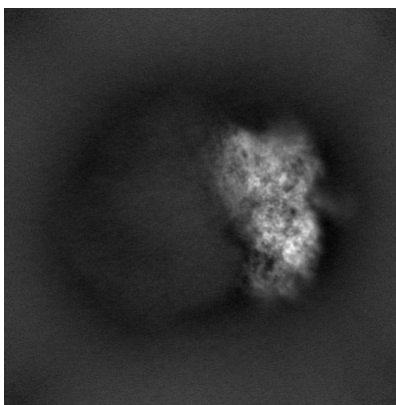


Z

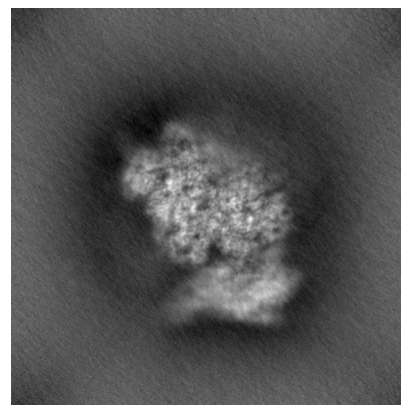
6.1.2 Raw map



X



Y

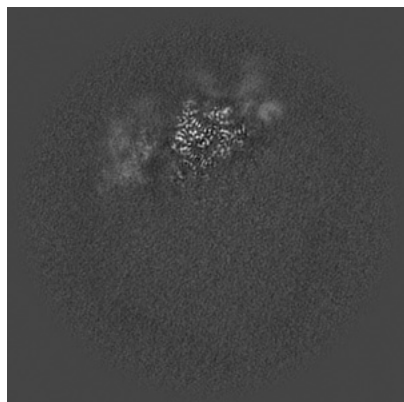


Z

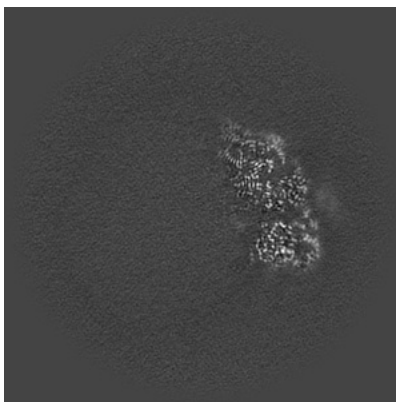
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

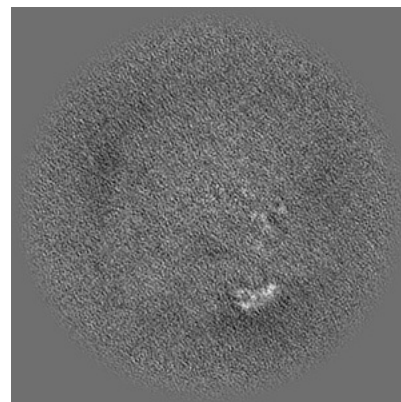
6.2.1 Primary map



X Index: 210

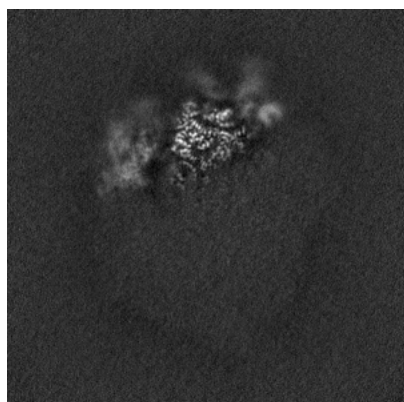


Y Index: 210

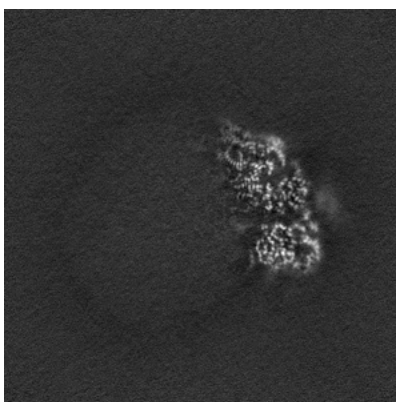


Z Index: 210

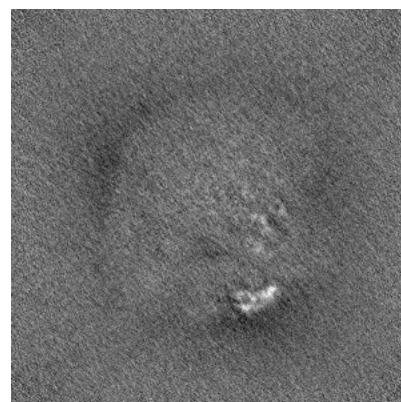
6.2.2 Raw map



X Index: 210



Y Index: 210

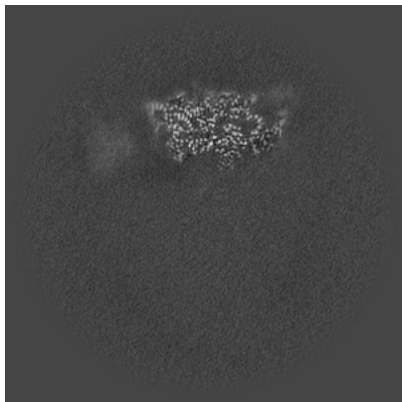


Z Index: 210

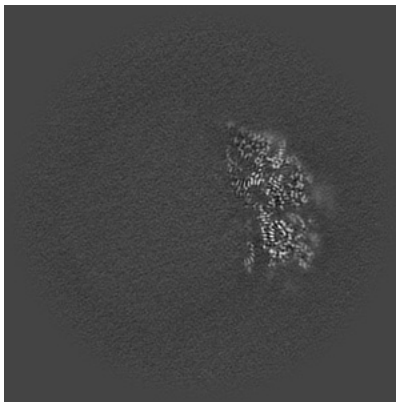
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

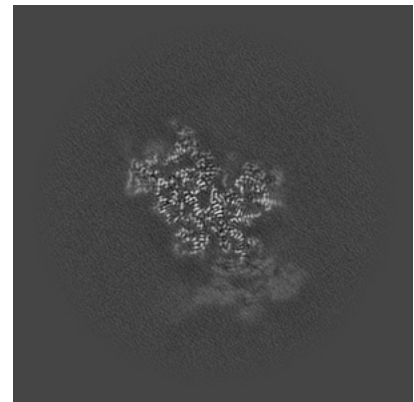
6.3.1 Primary map



X Index: 178

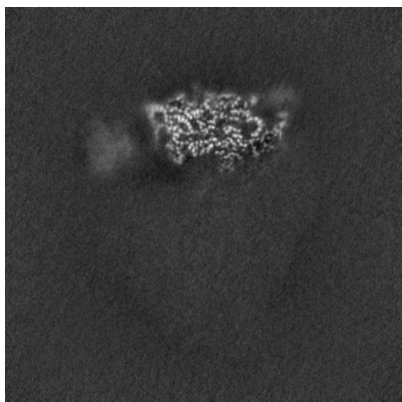


Y Index: 215

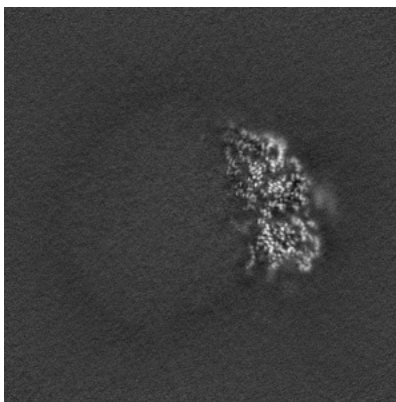


Z Index: 290

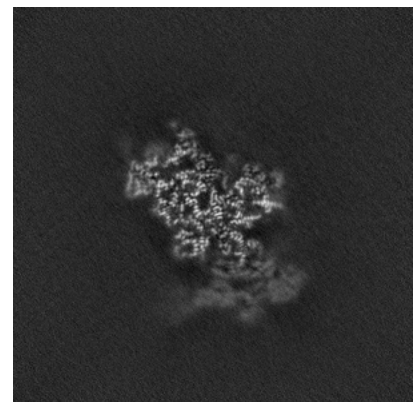
6.3.2 Raw map



X Index: 178



Y Index: 213

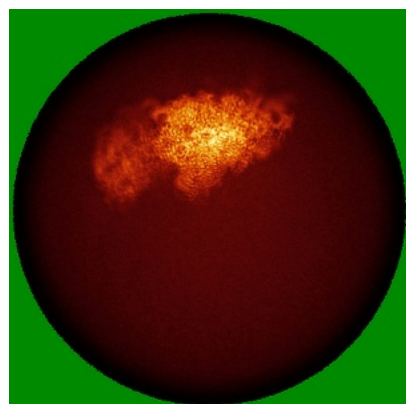


Z Index: 290

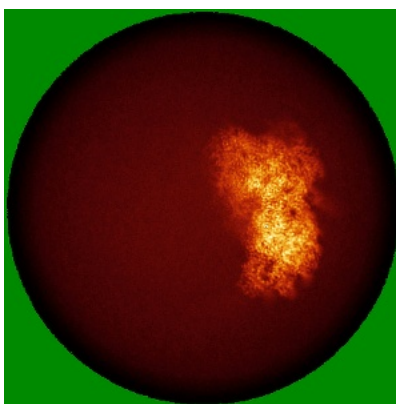
The images above show the largest variance slices of the map in three orthogonal directions.

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

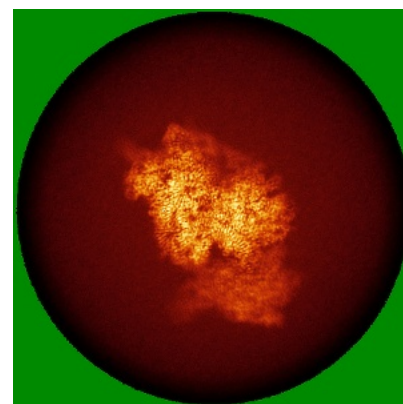
6.4.1 Primary map



X

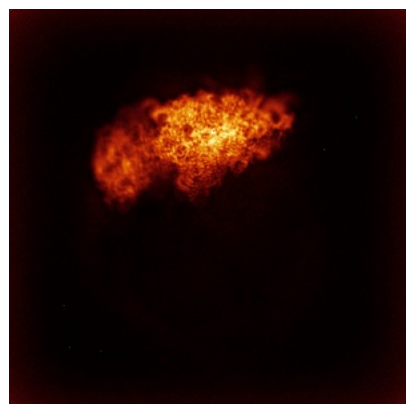


Y

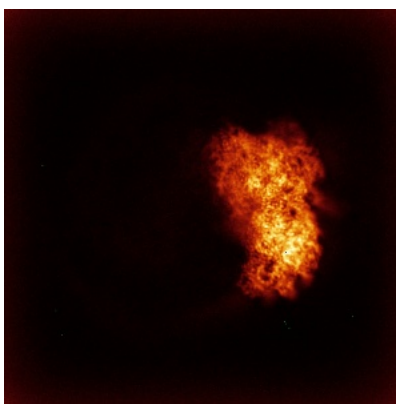


Z

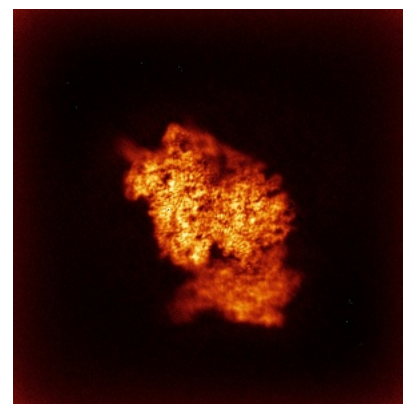
6.4.2 Raw map



X



Y

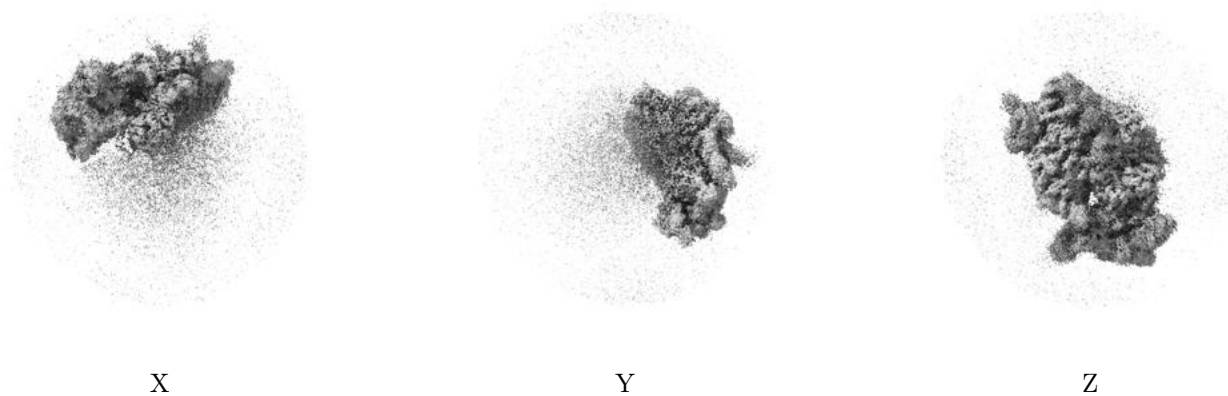


Z

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

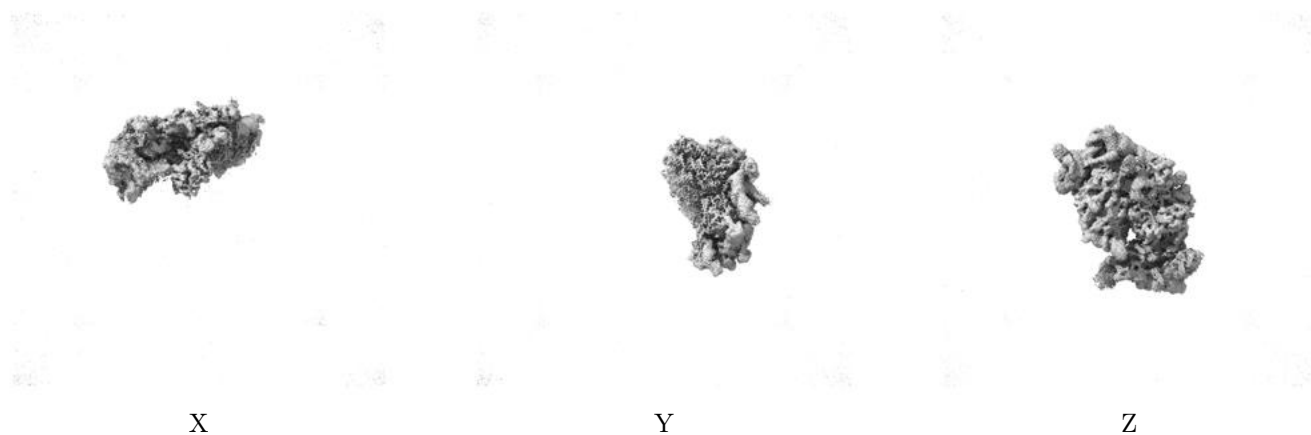
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

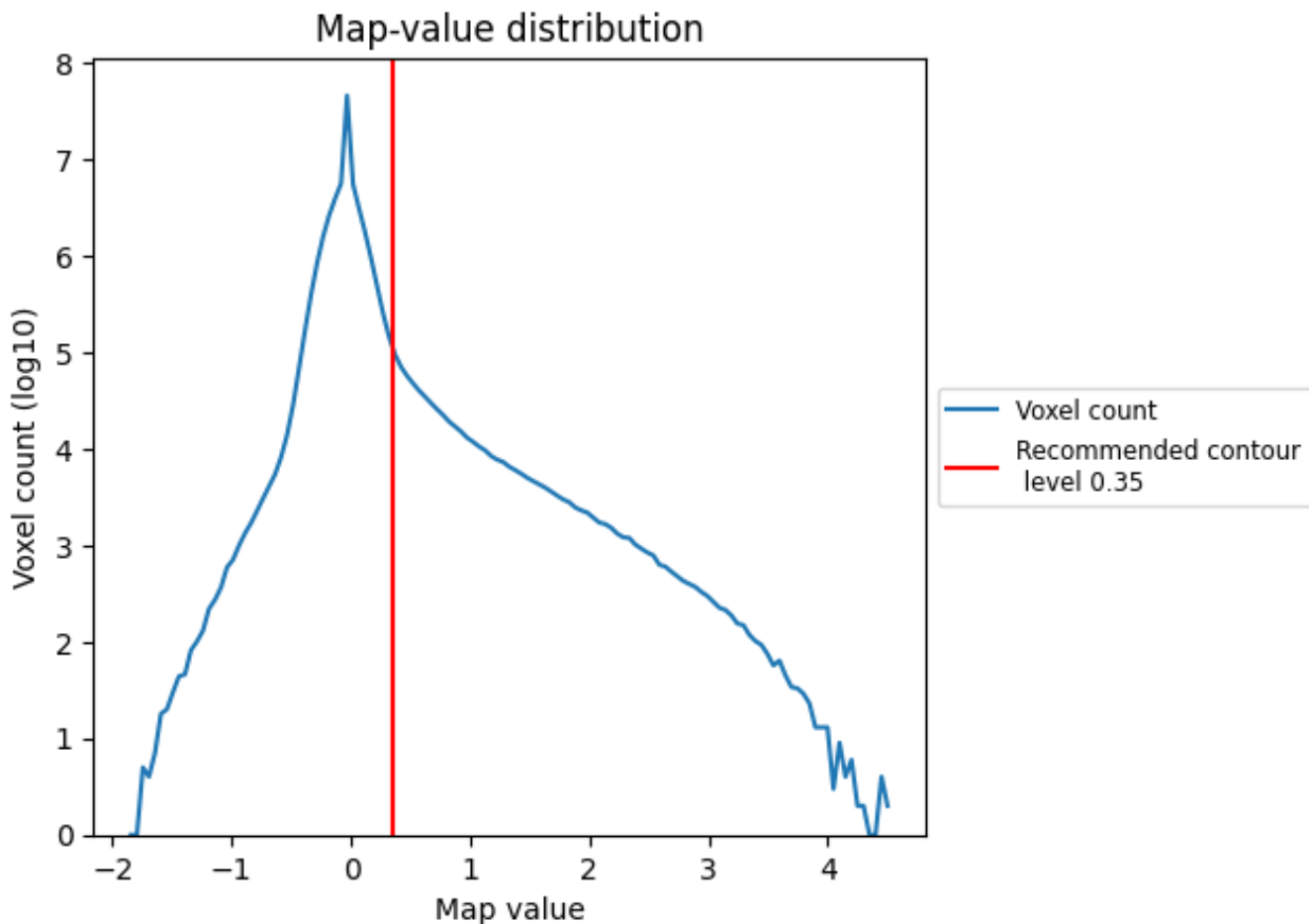
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

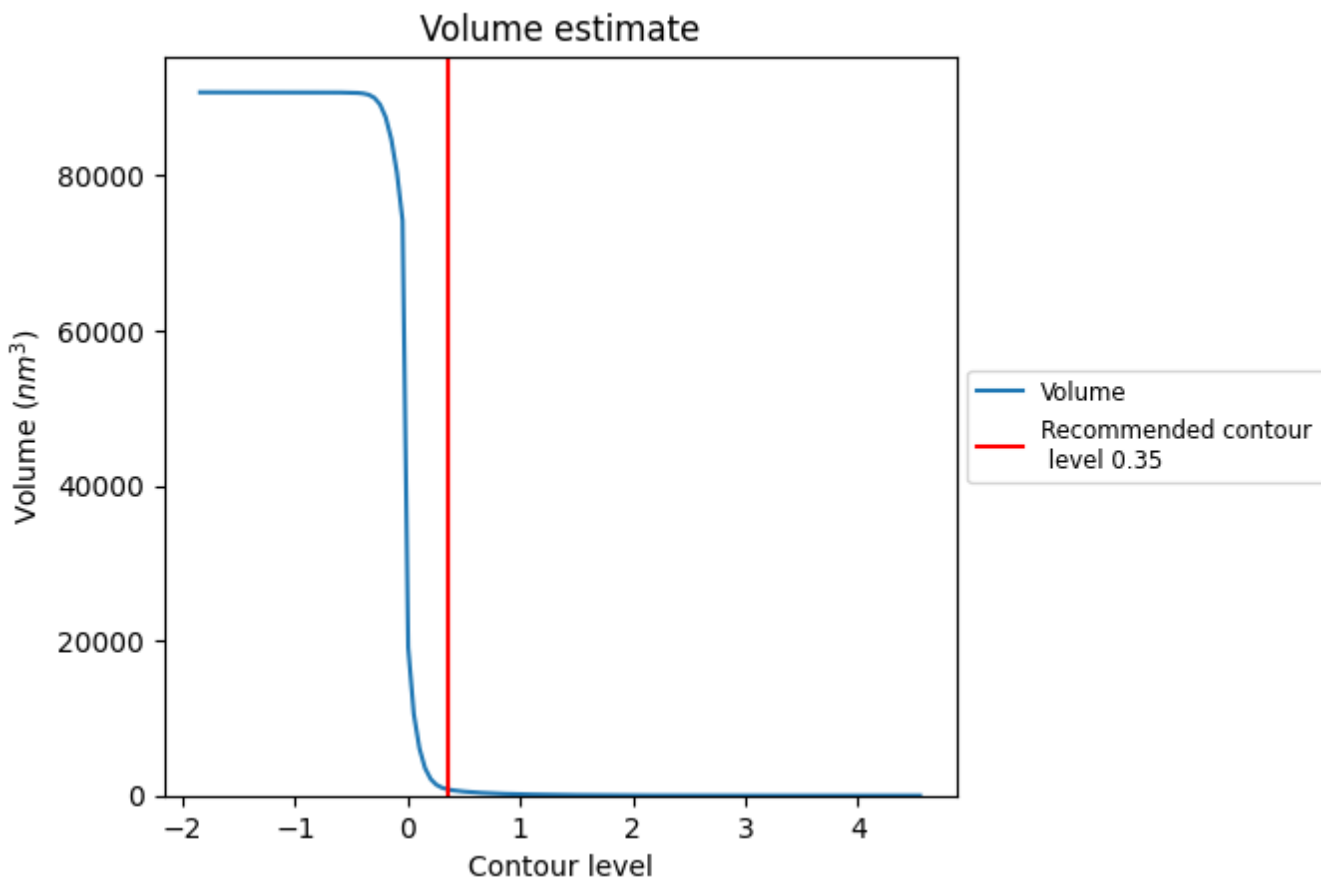
This section contains the results of statistical analysis of the map.

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.

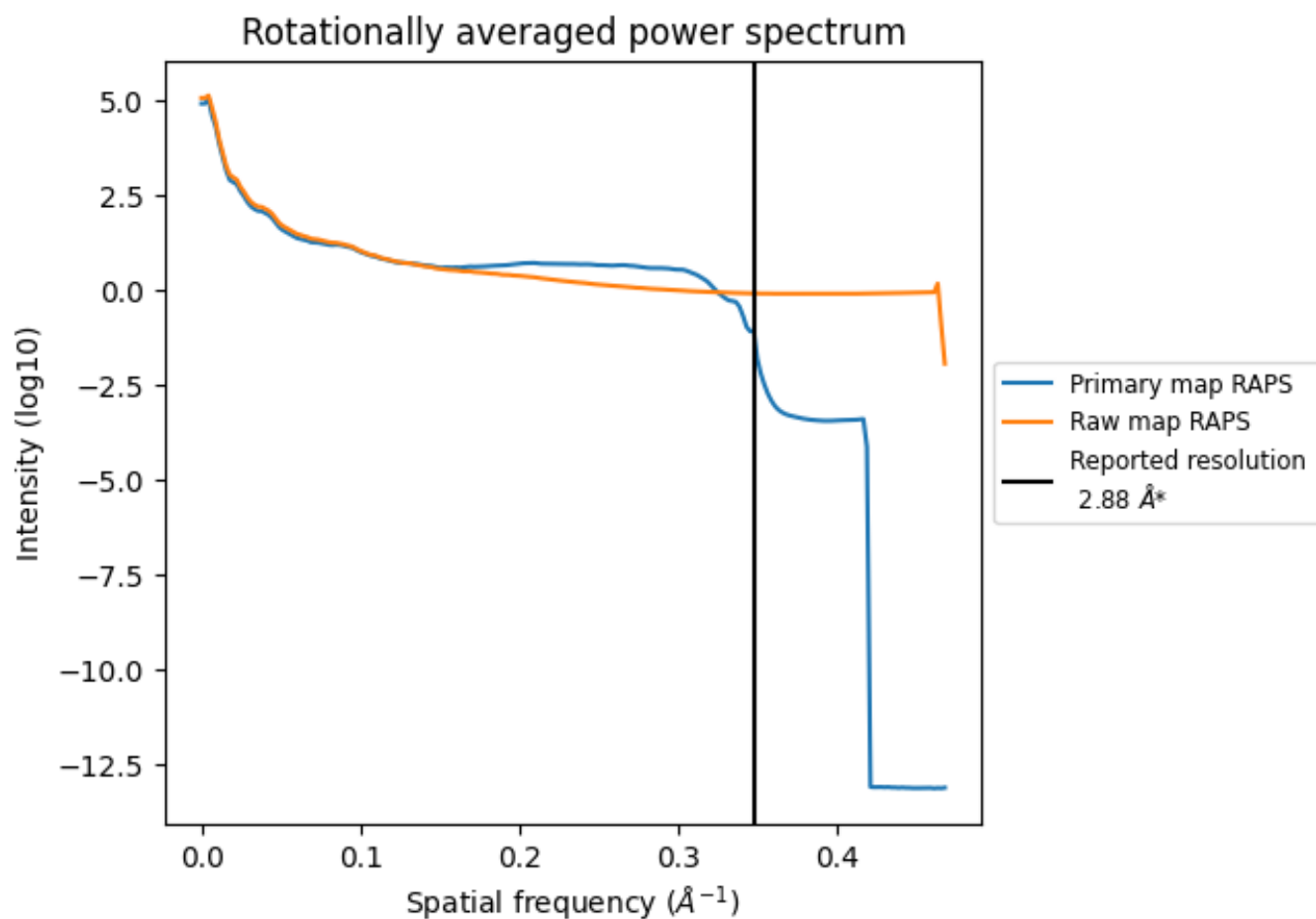
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 824 nm³; this corresponds to an approximate mass of 744 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 i

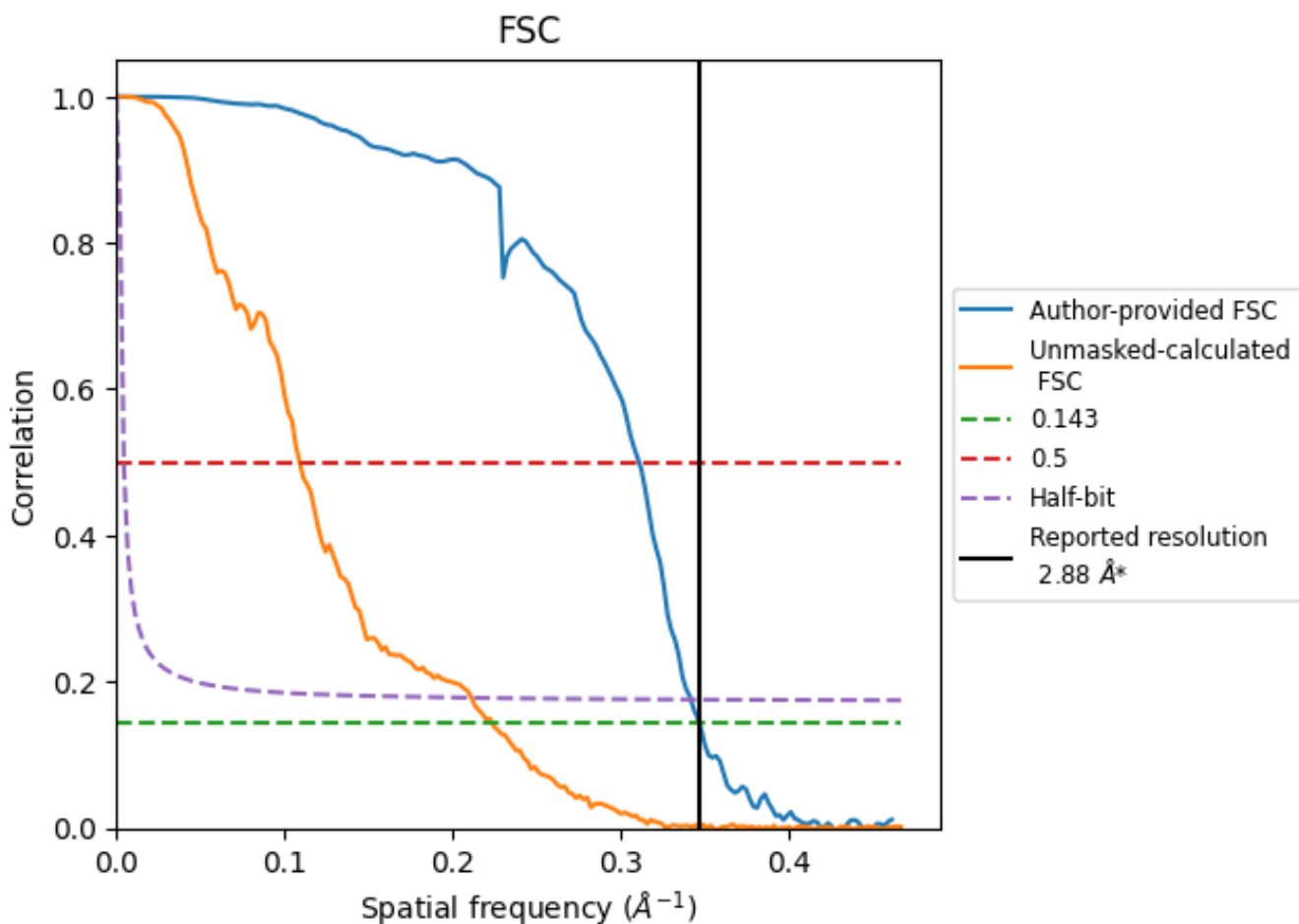


*Reported resolution corresponds to spatial frequency of 0.347 Å⁻¹

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 0.347 \AA^{-1}

8.2 Resolution estimates [i](#)

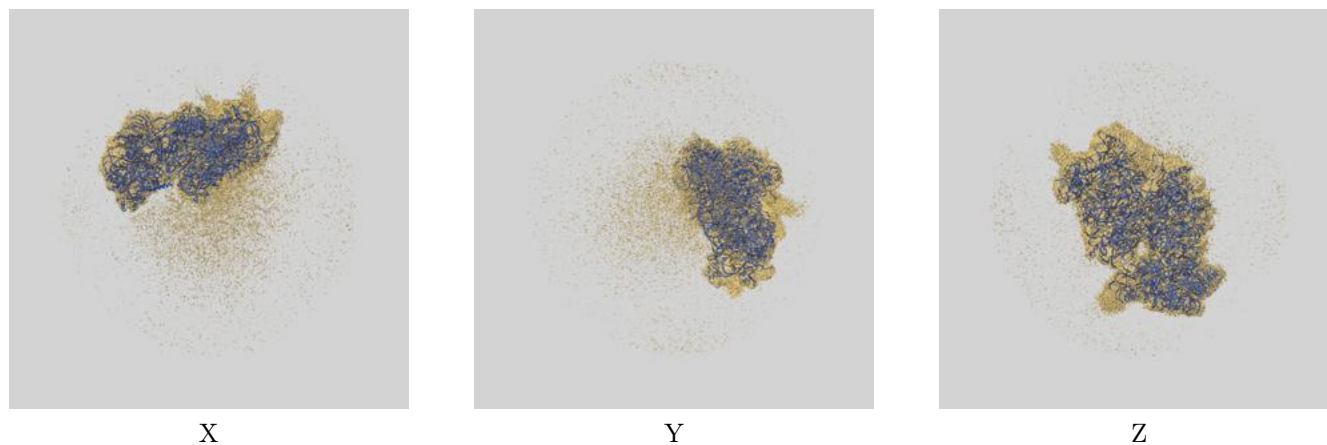
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.88	-	-
Author-provided FSC curve	2.88	3.21	2.92
Unmasked-calculated*	4.47	9.16	4.73

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.47 differs from the reported value 2.88 by more than 10 %

9 Map-model fit [i](#)

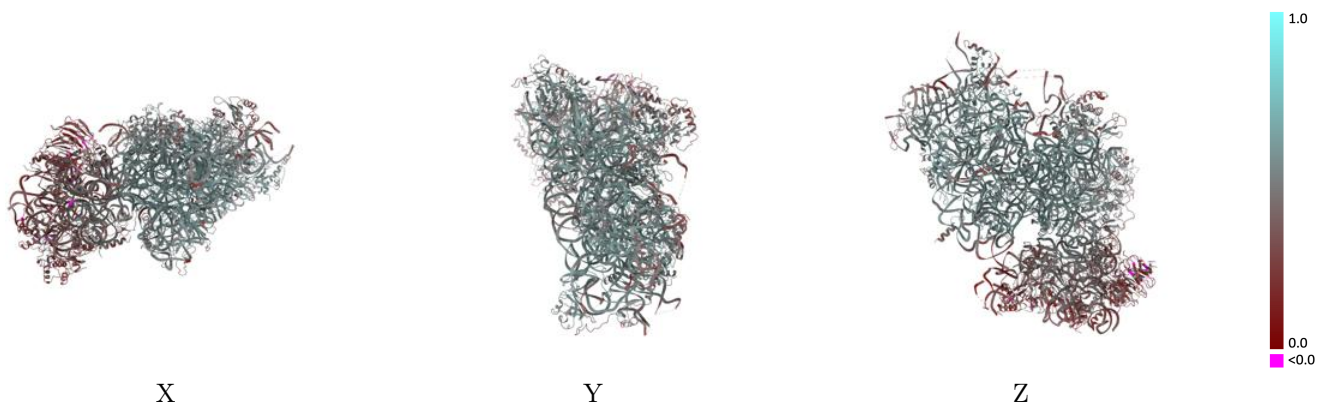
This section contains information regarding the fit between EMDB map EMD-36332 and PDB model 8JIW. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.35 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 [\(i\)](#)



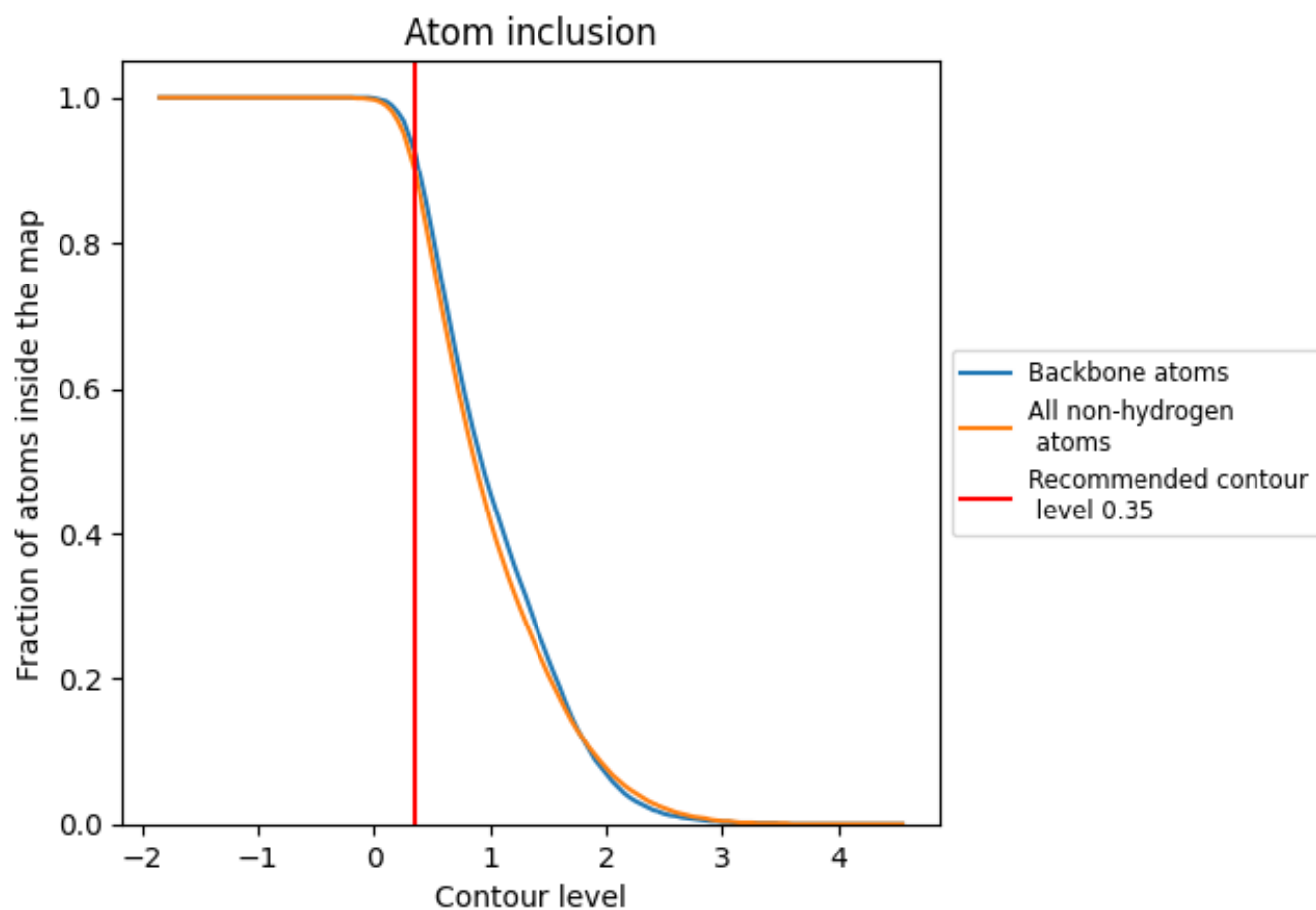
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).





































































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 90% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9000	 0.4810
Ad	 0.9460	 0.5000
BA	 0.9430	 0.4900
BB	 0.8350	 0.5090
BC	 0.9530	 0.5430
BD	 0.7110	 0.3660
BE	 0.9640	 0.5440
BF	 0.6800	 0.3890
BG	 0.9350	 0.4900
BH	 0.8950	 0.4310
BI	 0.8830	 0.5570
BJ	 0.9730	 0.5350
BK	 0.7860	 0.2760
BL	 0.8910	 0.5620
BN	 0.8530	 0.5470
BO	 0.9150	 0.5340
BP	 0.5790	 0.2930
BQ	 0.8710	 0.3750
BR	 0.8000	 0.3710
BS	 0.5590	 0.3180
BT	 0.9070	 0.3450
BU	 0.8100	 0.3630
BV	 0.9600	 0.5290
BW	 0.9740	 0.5760
BX	 0.9420	 0.5790
BY	 0.9640	 0.5400
BZ	 0.6780	 0.3030
Ba	 0.9650	 0.5610
Bb	 0.9210	 0.4830
Bc	 0.7630	 0.4290
Bd	 0.8480	 0.4010
Be	 0.9810	 0.5560
Bg	 0.6490	 0.2840
Cn	 0.5870	 0.5650

