



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:08 AM UTC

PDB ID : 6GAZ / pdb_00006gaz
EMDB ID : EMD-4369
Title : Unique features of mammalian mitochondrial translation initiation revealed by cryo-EM. This file contains the 28S ribosomal subunit.
Authors : Kummer, E.; Leibundgut, M.; Boehringer, D.; Ban, N.
Deposited on : 2018-04-13
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

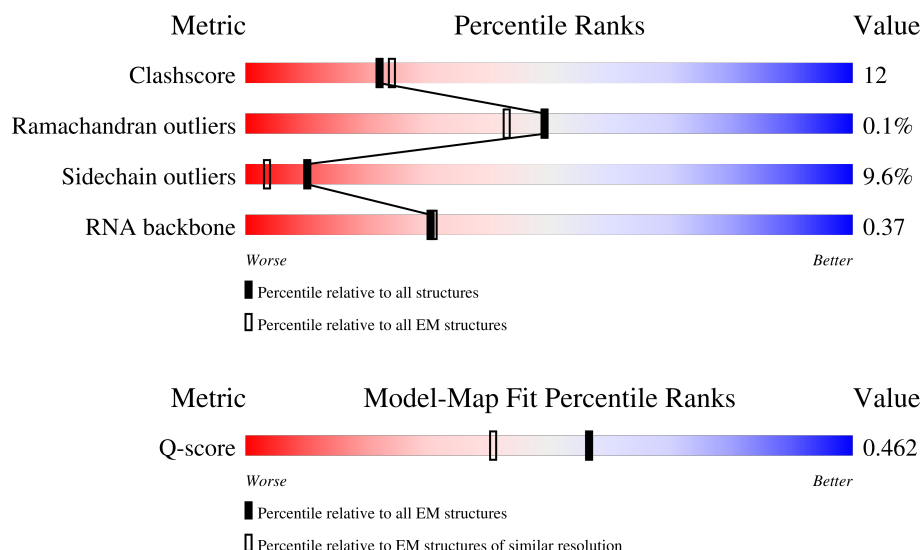
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



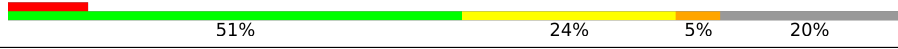
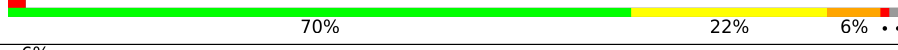
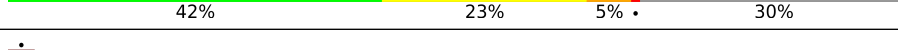
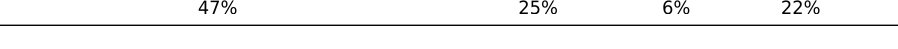
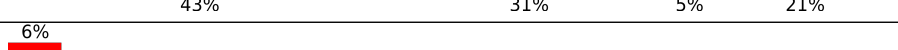
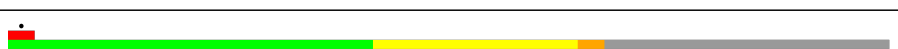
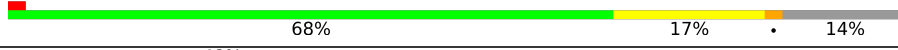
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	BC	657	
2	BT	292	
3	AA	962	

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Mol	Chain	Length	Quality of chain
4	AB	289	
5	AC	167	
6	AE	430	
7	AF	124	
8	AG	242	
9	AI	397	
10	AJ	201	
11	AK	196	
12	AL	139	
13	AN	128	
14	AO	239	
15	AP	135	
16	AQ	130	
17	AR	143	
18	AU	87	
19	AV	71	
20	AX	201	
21	AZ	18	
22	Aa	382	
23	Ab	190	
24	Ac	173	
25	Ad	205	
26	Ae	390	
27	Af	188	
28	Ag	397	

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Mol	Chain	Length	Quality of chain
29	Ah	387	
30	Ai	106	
31	Aj	218	
32	Ak	325	
33	Am	118	
34	An	199	
35	Ao	692	
36	Ap	258	

2 Entry composition

There are 44 unique types of molecules in this entry. The entry contains 73172 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Translation initiation factor IF-2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	BC	571	Total	C	N	O	S	0	0
			4364	2743	765	839	17		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	71	SER	-	expression tag	UNP P46199
BC	72	GLY	-	expression tag	UNP P46199
BC	73	GLY	-	expression tag	UNP P46199
BC	74	SER	-	expression tag	UNP P46199
BC	75	GLY	-	expression tag	UNP P46199
BC	76	SER	-	expression tag	UNP P46199
BC	77	GLY	-	expression tag	UNP P46199

- Molecule 2 is a protein called Mitochondrial ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	BT	17	Total	C	N	O	0	0
			109	72	19	18		

- Molecule 3 is a RNA chain called 12S ribosomal RNA, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AA	960	Total	C	N	O	P	0	0
			20411	9162	3708	6581	960		

- Molecule 4 is a protein called Mitochondrial ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AB	220	Total	C	N	O	S	0	0
			1762	1126	326	304	6		

- Molecule 5 is a protein called Mitochondrial ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AC	132	Total	C	N	O	S	0	0
			1075	695	195	181	4		

- Molecule 6 is a protein called Mitochondrial ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AE	343	Total	C	N	O	S	0	0
			2732	1707	527	487	11		

- Molecule 7 is a protein called Mitochondrial ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AF	122	Total	C	N	O	S	0	0
			981	620	178	177	6		

- Molecule 8 is a protein called Mitochondrial ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AG	208	Total	C	N	O	S	0	0
			1721	1097	314	299	11		

- Molecule 9 is a protein called Mitochondrial ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	328	Total	C	N	O	S	0	0
			2650	1678	478	481	13		

- Molecule 10 is a protein called Mitochondrial ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	140	Total	C	N	O	S	0	0
			1155	746	197	208	4		

- Molecule 11 is a protein called Mitochondrial ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	137	Total	C	N	O	S	0	0
			1007	631	193	180	3		

- Molecule 12 is a protein called Mitochondrial ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	109	Total	C	N	O	S	0	0
			840	524	172	138	6		

- Molecule 13 is a protein called Mitochondrial ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AN	101	Total	C	N	O	S	0	0
			858	534	174	144	6		

- Molecule 14 is a protein called Mitochondrial ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AO	175	Total	C	N	O	S	0	0
			1448	919	272	248	9		

- Molecule 15 is a protein called bS16m, MRPS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AP	117	Total	C	N	O	S	0	0
			932	588	184	155	5		

- Molecule 16 is a protein called Mitochondrial ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AQ	112	Total	C	N	O	S	0	0
			875	568	153	151	3		

- Molecule 17 is a protein called Mitochondrial ribosomal protein S18C.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AR	97	Total	C	N	O	S	0	0
			784	507	132	138	7		

- Molecule 18 is a protein called Mitochondrial ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AU	86	Total	C	N	O	S	0	0
			734	453	148	125	8		

- Molecule 19 is a RNA chain called P-site fMet-tRNA^{Met}, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AV	71	Total	C	N	O	P	0	0
			1498	673	264	491	70		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AV	69	C	-	insertion	GB 1208989970
AV	70	C	-	insertion	GB 1208989970
AV	71	A	-	insertion	GB 1208989970

- Molecule 20 is a RNA chain called MT-CO3 mRNA, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AX	17	Total	C	N	O	P	0	0
			354	161	65	112	16		

- Molecule 21 is a protein called unassigned secondary structure elements.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	AZ	18	Total	C	N	O	0	0
			90	54	18	18		

- Molecule 22 is a protein called Mitochondrial ribosomal protein S22.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Aa	292	Total	C	N	O	S	0	0
			2378	1518	409	442	9		

- Molecule 23 is a protein called Mitochondrial ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Ab	135	Total	C	N	O	S	0	0
			1101	709	199	192	1		

- Molecule 24 is a protein called Mitochondrial ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Ac	169	Total	C	N	O	S	0	0
			1367	876	236	245	10		

- Molecule 25 is a protein called Mitochondrial ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Ad	177	Total	C	N	O	S	0	0
			1467	904	288	273	2		

- Molecule 26 is a protein called Mitochondrial ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Ae	388	Total	C	N	O	S	0	0
			3109	1971	535	589	14		

- Molecule 27 is a protein called Mitoribosomal protein ms28, mrps28.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Af	99	Total	C	N	O	S	0	0
			778	494	134	146	4		

- Molecule 28 is a protein called Death associated protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Ag	353	Total	C	N	O	S	0	0
			2875	1837	515	513	10		

- Molecule 29 is a protein called mS31, MRPS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Ah	120	Total	C	N	O	S	0	0
			1015	659	168	185	3		

- Molecule 30 is a protein called Mitochondrial ribosomal protein S33.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Ai	99	Total	C	N	O	S	0	0
			824	522	156	143	3		

- Molecule 31 is a protein called Mitochondrial ribosomal protein S34.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Aj	213	Total	C	N	O	S	0	0
			1788	1131	338	311	8		

- Molecule 32 is a protein called Mitochondrial ribosomal protein S35.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Ak	275	Total	C	N	O	S	0	0
			2222	1414	380	419	9		

- Molecule 33 is a protein called Mitochondrial ribosomal protein S37.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Am	116	Total	C	N	O	S	0	0
			930	577	185	160	8		

- Molecule 34 is a protein called Aurora kinase A interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	An	72	Total	C	N	O	S	0	0
			639	407	139	92	1		

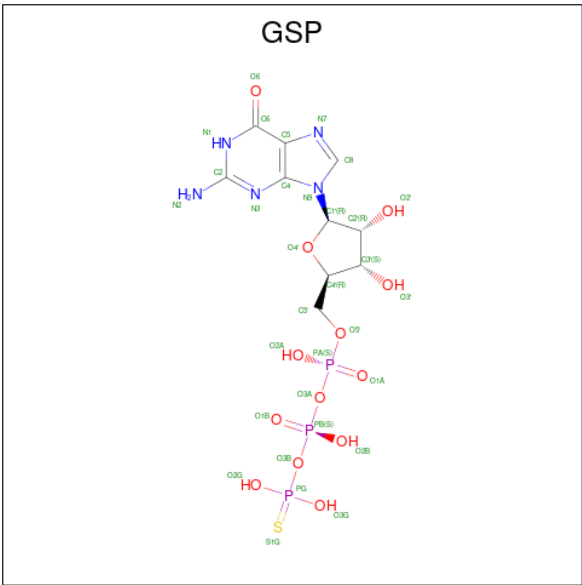
- Molecule 35 is a protein called Mitochondrial ribosomal protein S39.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Ao	572	Total	C	N	O	S	0	0
			4527	2899	770	834	24		

- Molecule 36 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Ap	190	Total	C	N	O	S	0	0
			1564	991	292	273	8		

- Molecule 37 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (CCD ID: GSP) (formula: C₁₀H₁₆N₅O₁₃P₃S).



Mol	Chain	Residues	Atoms						AltConf
37	BC	1	Total	C	N	O	P	S	0
			32	10	5	13	3	1	

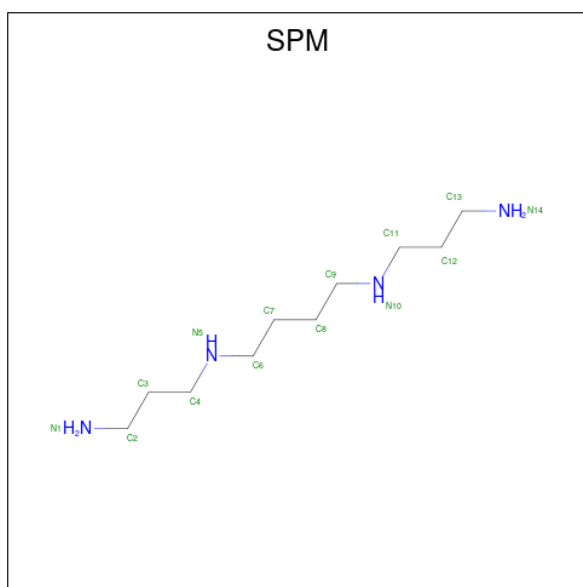
- Molecule 38 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
38	BC	2	Total	Mg	0
			2	2	
38	AA	105	Total	Mg	0
			105	105	
38	AB	1	Total	Mg	0
			1	1	
38	AX	1	Total	Mg	0
			1	1	
38	Ag	1	Total	Mg	0
			1	1	
38	An	1	Total	Mg	0
			1	1	

- Molecule 39 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
39	BC	1	Total	Na	0
			1	1	

- Molecule 40 is SPERMINE (CCD ID: SPM) (formula: C₁₀H₂₆N₄).

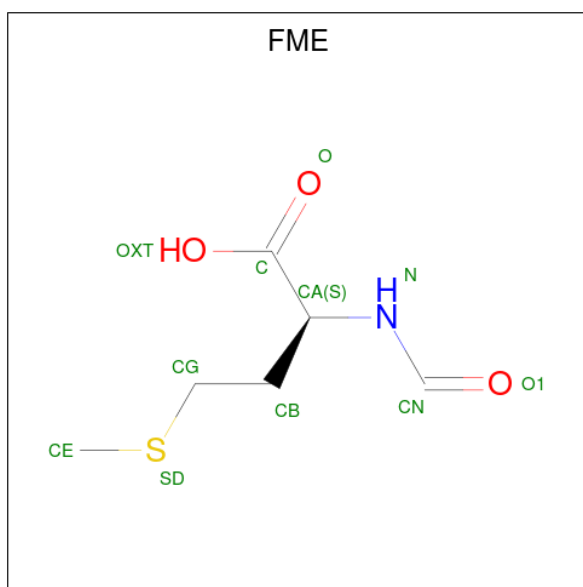


Mol	Chain	Residues	Atoms			AltConf
40	AA	1	Total	C	N	0
			14	10	4	

- Molecule 41 is ZINC ION (CCD ID: ZN) (formula: Zn).

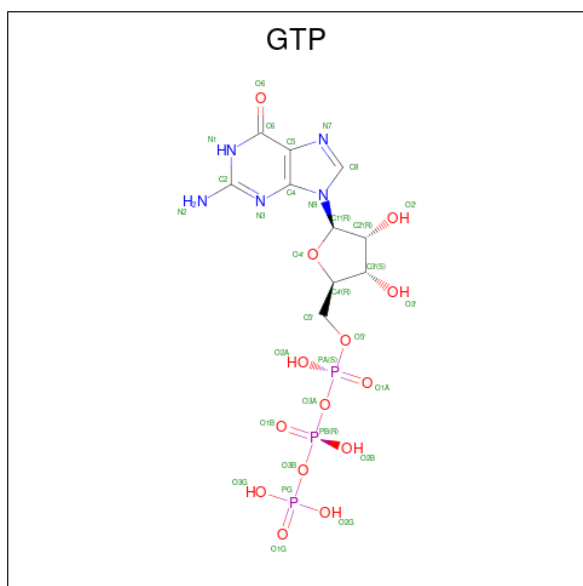
Mol	Chain	Residues	Atoms		AltConf
41	AR	1	Total	Zn	0
			1	1	
41	Ac	1	Total	Zn	0
			1	1	
41	Ap	1	Total	Zn	0
			1	1	

- Molecule 42 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: C₆H₁₁NO₃S).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
42	AV	1	10	6	1	2	1	0

- Molecule 43 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
43	Ag	1	32	10	5	14	3	0

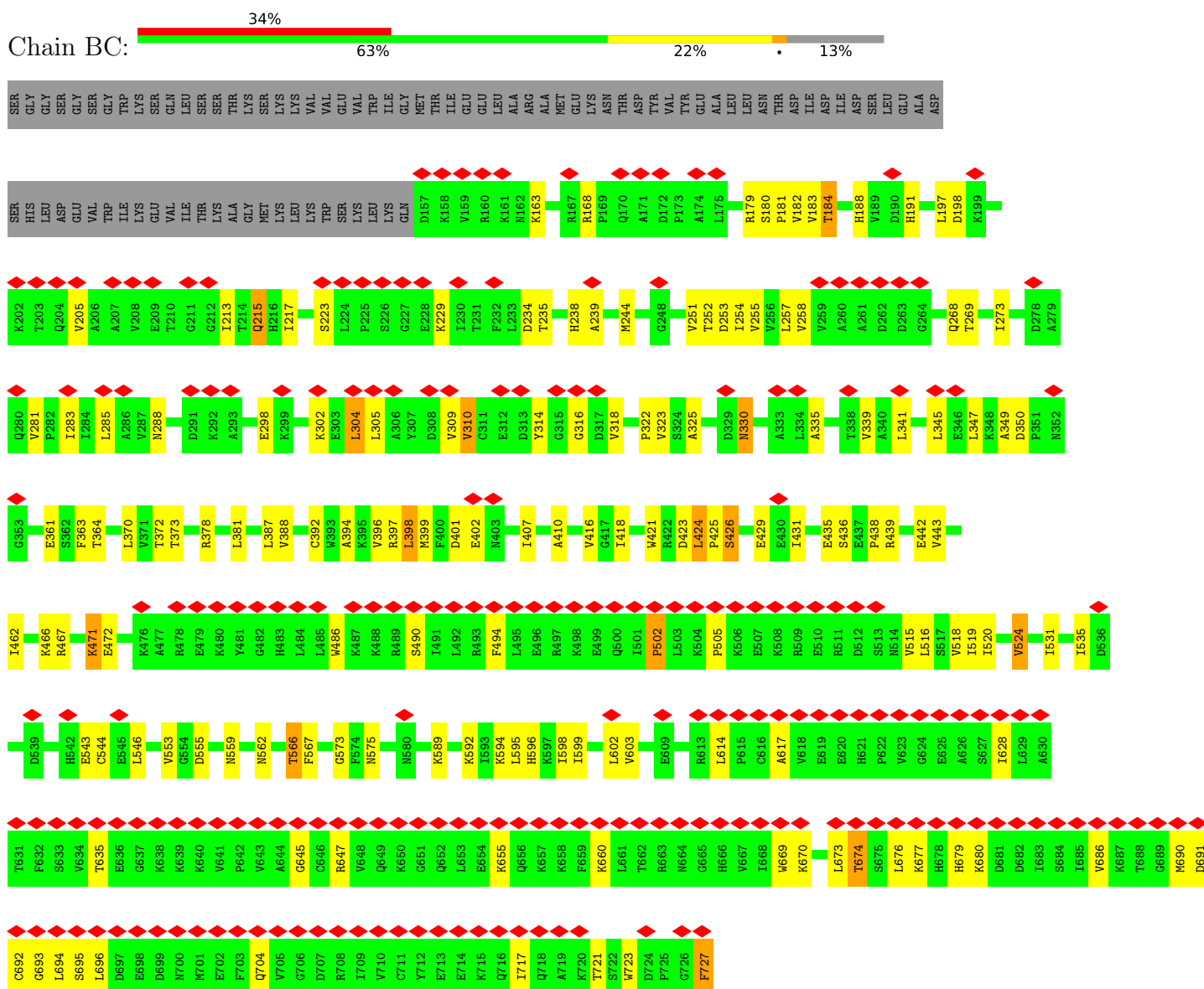
- Molecule 44 is water.

Mol	Chain	Residues	Atoms		AltConf
44	BC	2	Total 2	O 2	0
44	Ag	3	Total 3	O 3	0

3 Residue-property plots

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

- Molecule 1: Translation initiation factor IF-2, mitochondrial



- Molecule 2: Mitochondrial ribosomal protein L19

94%

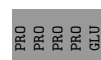
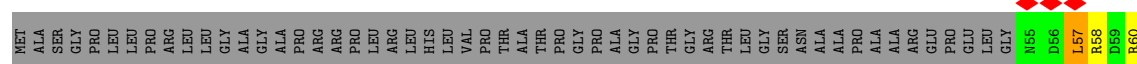
- Molecule 3: 12S ribosomal RNA, mitochondrial

57%

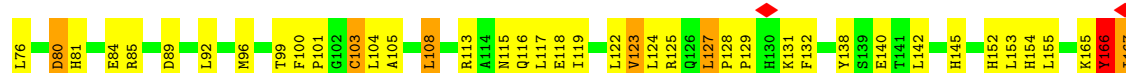
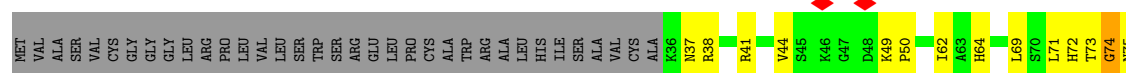




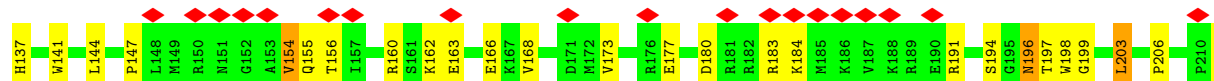
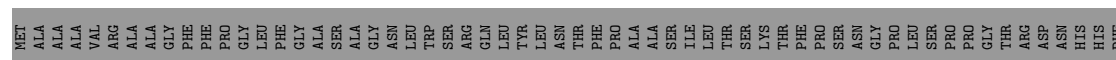
• Molecule 4: Mitochondrial ribosomal protein S2

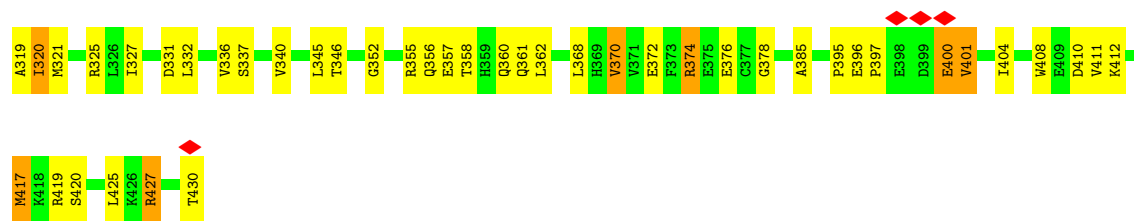


• Molecule 5: Mitochondrial ribosomal protein S24



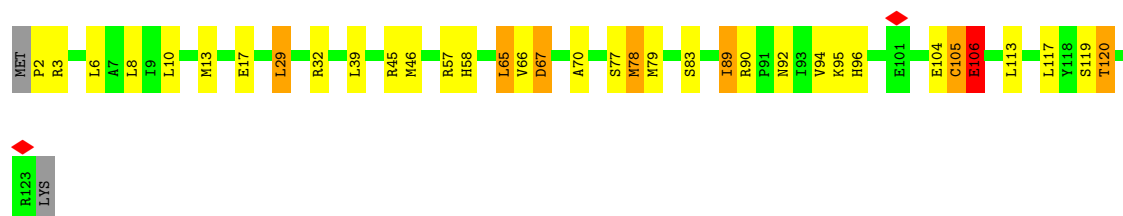
• Molecule 6: Mitochondrial ribosomal protein S5





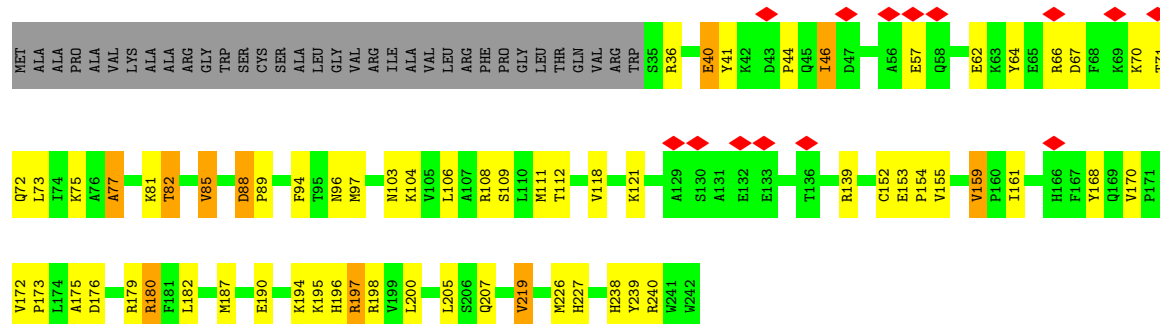
• Molecule 7: Mitochondrial ribosomal protein S6

Chain AF: 70% 22% 6% ••



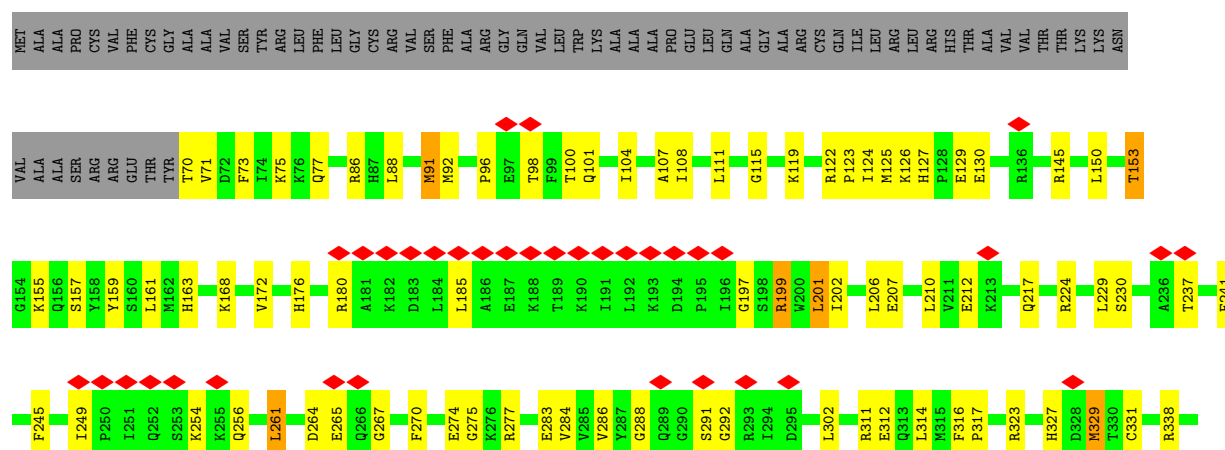
• Molecule 8: Mitochondrial ribosomal protein S7

Chain AG: 59% 23% 14% • 6%



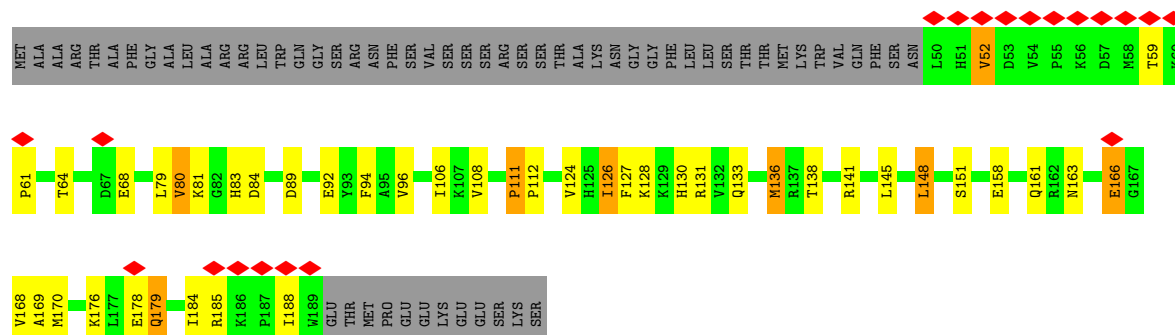
• Molecule 9: Mitochondrial ribosomal protein S9

Chain AI: 55% 25% 17% • 9%

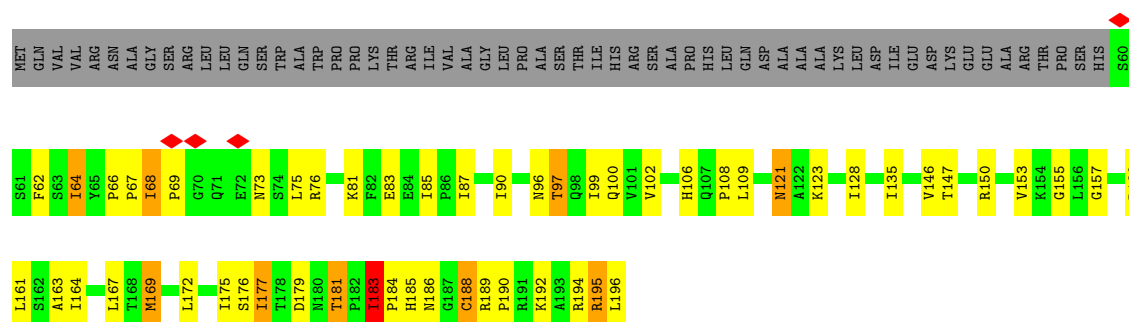




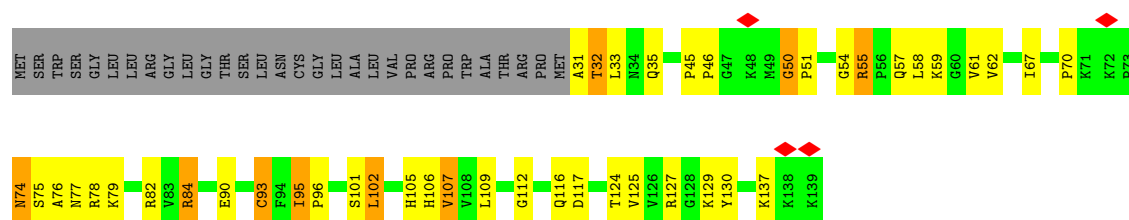
• Molecule 10: Mitochondrial ribosomal protein S10



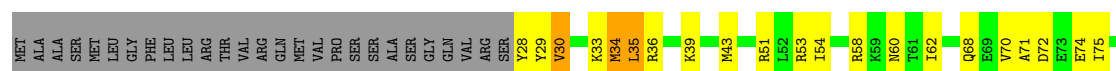
• Molecule 11: Mitochondrial ribosomal protein S11



• Molecule 12: Mitochondrial ribosomal protein S12

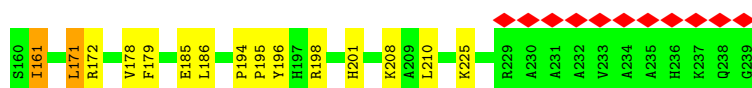
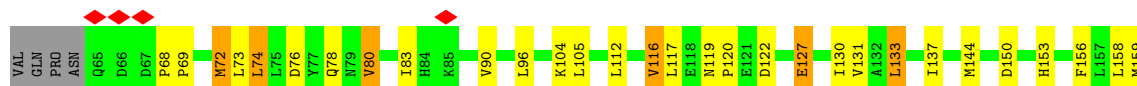
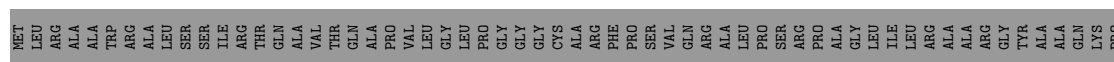


• Molecule 13: Mitochondrial ribosomal protein S14

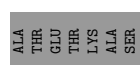




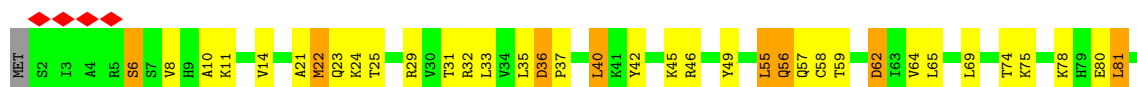
• Molecule 14: Mitochondrial ribosomal protein S15



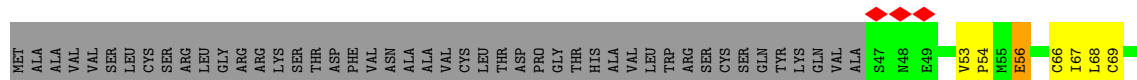
• Molecule 15: bS16m, MRPS16



• Molecule 16: Mitochondrial ribosomal protein S17



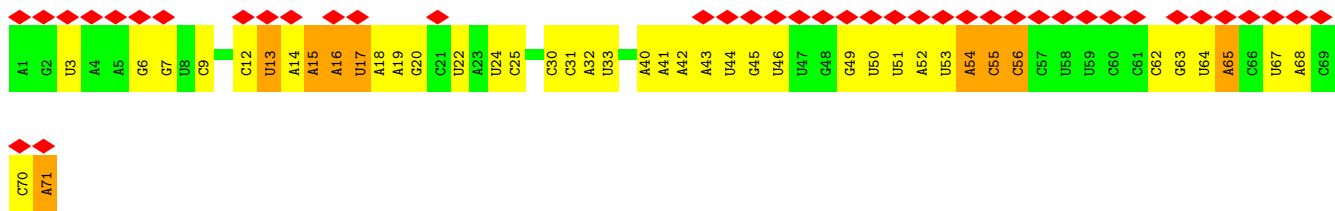
• Molecule 17: Mitochondrial ribosomal protein S18C



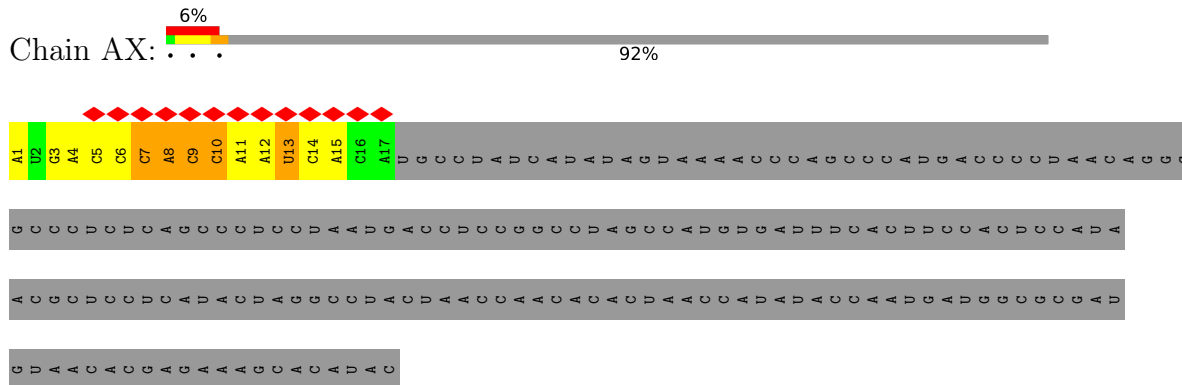
• Molecule 18: Mitochondrial ribosomal protein S21



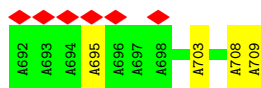
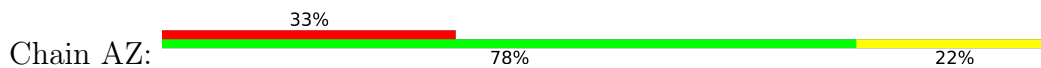
- Molecule 19: P-site fMet-tRNA^{Met}, mitochondrial



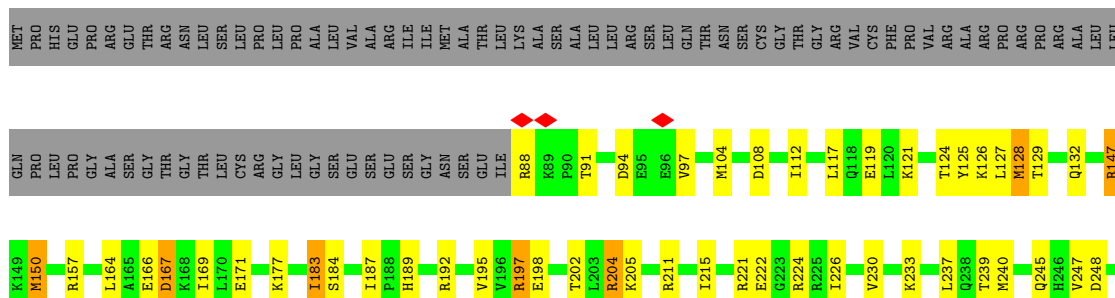
- Molecule 20: MT-CO3 mRNA, mitochondrial



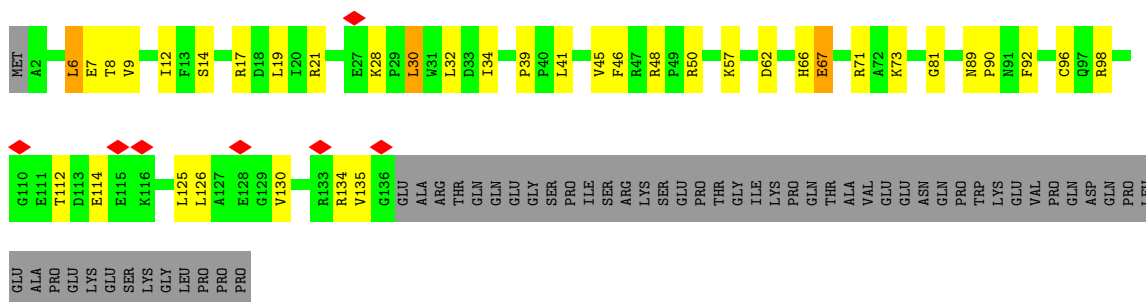
- Molecule 21: unassigned secondary structure elements



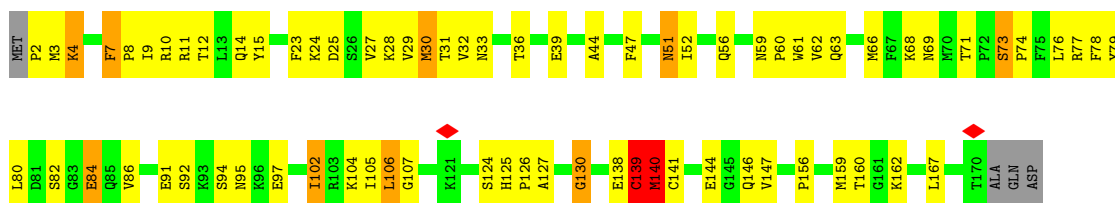
- Molecule 22: Mitochondrial ribosomal protein S22



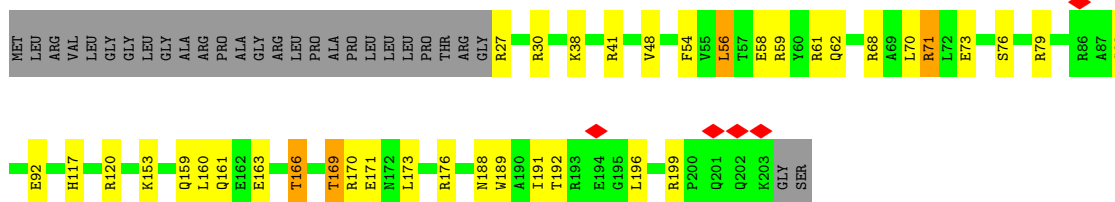
- Molecule 23: Mitochondrial ribosomal protein S23



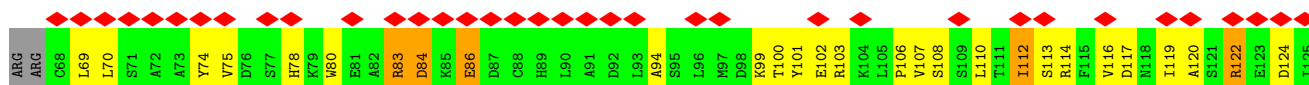
- Molecule 24: Mitochondrial ribosomal protein S25

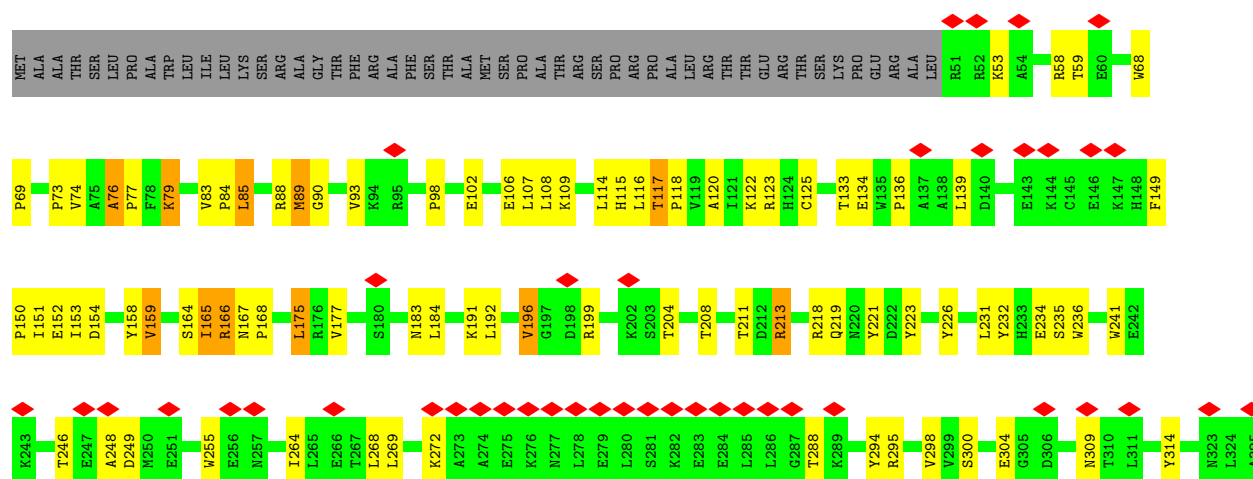


- Molecule 25: Mitochondrial ribosomal protein S26

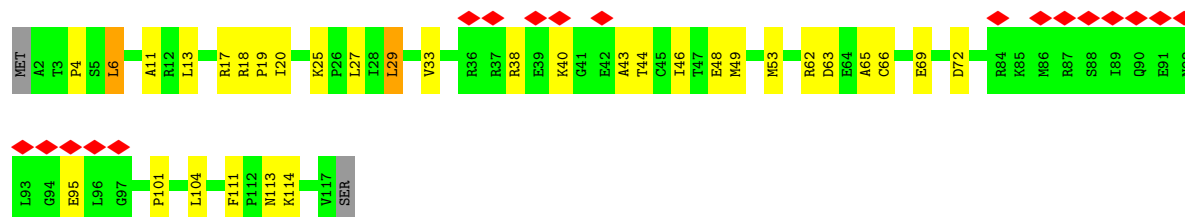
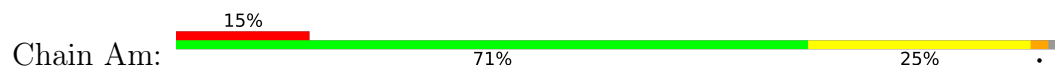


- Molecule 26: Mitochondrial ribosomal protein S27

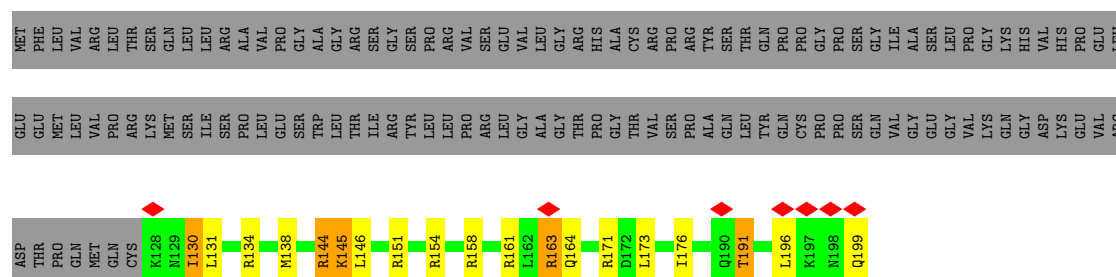




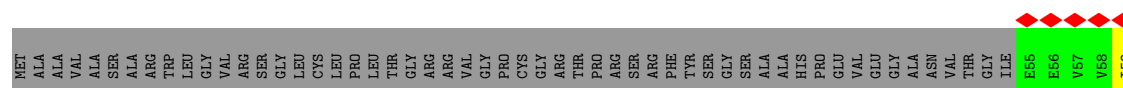
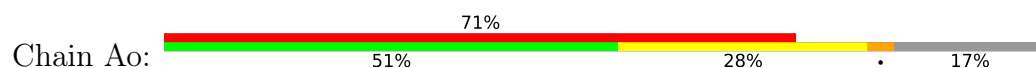
• Molecule 33: Mitochondrial ribosomal protein S37

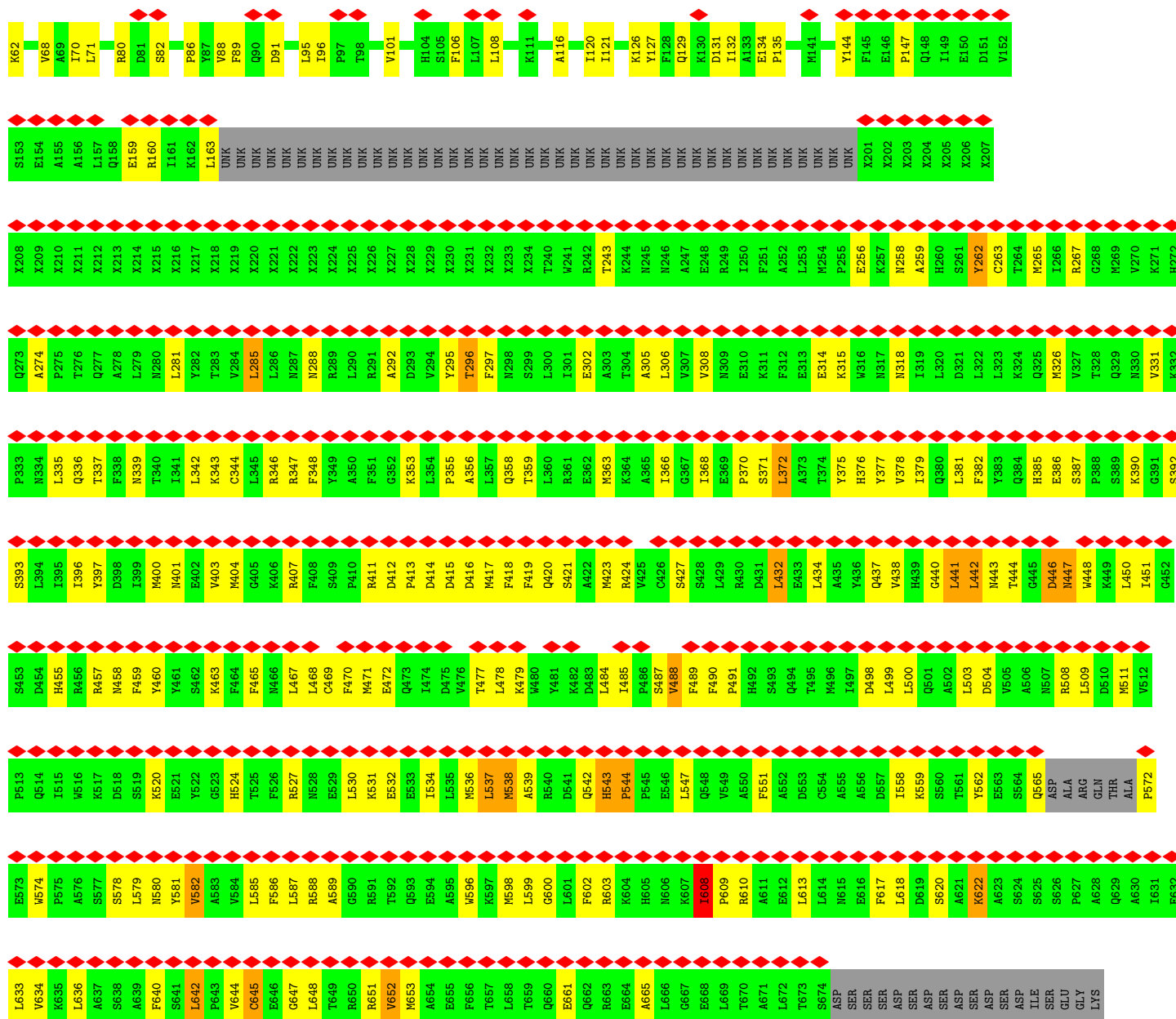


• Molecule 34: Aurora kinase A interacting protein 1

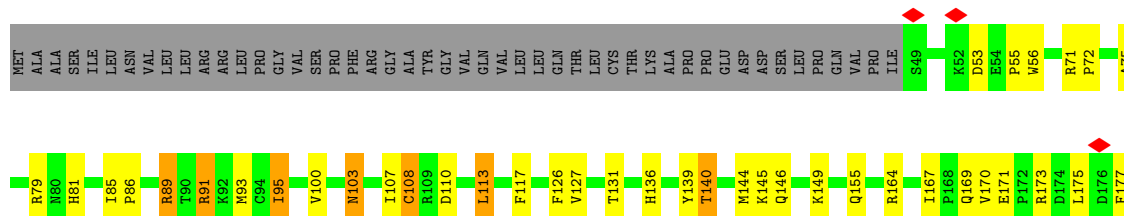


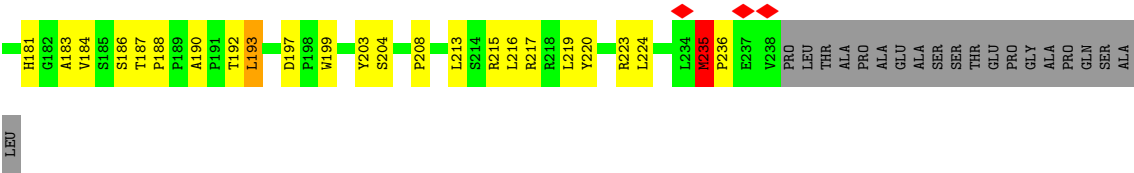
• Molecule 35: Mitochondrial ribosomal protein S39





• Molecule 36: 28S ribosomal protein S18b, mitochondrial





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	139206	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.610	Depositor
Minimum map value	-0.242	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.085	Depositor
Map size ($\text{\AA}$)	390.59, 390.59, 390.59	wwPDB
Map dimensions	281, 281, 281	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.39, 1.39, 1.39	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GSP, NA, GTP, MG, ZN, FME, SPM

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	BC	0.46	0/4432	0.85	4/5989 (0.1%)
2	BT	0.64	0/113	1.35	5/157 (3.2%)
3	AA	0.37	0/22852	0.48	0/35580
4	AB	0.72	0/1804	1.03	9/2445 (0.4%)
5	AC	0.50	0/1105	0.94	2/1496 (0.1%)
6	AE	0.59	0/2785	0.96	4/3735 (0.1%)
7	AF	0.58	0/999	1.00	4/1347 (0.3%)
8	AG	0.46	0/1763	0.87	4/2368 (0.2%)
9	AI	0.46	0/2707	0.83	3/3636 (0.1%)
10	AJ	0.58	1/1181 (0.1%)	0.96	2/1597 (0.1%)
11	AK	0.64	0/1027	1.26	12/1389 (0.9%)
12	AL	0.64	0/858	1.08	7/1152 (0.6%)
13	AN	0.55	0/874	0.94	2/1171 (0.2%)
14	AO	0.61	0/1473	1.00	7/1970 (0.4%)
15	AP	0.66	0/954	1.01	1/1284 (0.1%)
16	AQ	0.61	0/894	1.11	4/1213 (0.3%)
17	AR	0.72	0/802	1.09	4/1079 (0.4%)
18	AU	0.65	0/745	0.96	0/993
19	AV	0.23	0/1673	0.38	0/2602
20	AX	0.30	0/395	0.47	0/612
21	AZ	0.65	0/89	1.07	0/123
22	Aa	0.51	0/2428	0.91	3/3279 (0.1%)
23	Ab	0.54	0/1126	0.99	5/1514 (0.3%)
24	Ac	0.63	2/1399 (0.1%)	1.09	13/1881 (0.7%)
25	Ad	0.48	0/1490	0.86	2/2005 (0.1%)
26	Ae	0.45	0/3171	0.90	8/4292 (0.2%)
27	Af	0.56	0/790	0.90	1/1064 (0.1%)
28	Ag	0.37	0/2945	0.82	1/3984 (0.0%)
29	Ah	0.41	0/1045	0.81	0/1409
30	Ai	0.41	0/841	0.85	0/1121
31	Aj	0.43	0/1835	0.90	9/2484 (0.4%)
32	Ak	0.41	0/2268	0.89	9/3069 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Am	0.49	0/947	0.91	1/1268 (0.1%)
34	An	0.60	0/650	0.97	1/858 (0.1%)
35	Ao	0.53	0/4458	0.89	12/6036 (0.2%)
36	Ap	0.56	0/1616	1.02	14/2195 (0.6%)
All	All	0.48	3/76534 (0.0%)	0.80	153/108397 (0.1%)

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
26	Ae	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Ac	52	ILE	CA-CB	5.82	1.57	1.54
10	AJ	127	PHE	CA-C	-5.28	1.47	1.53
24	Ac	139	CYS	CB-SG	5.21	1.98	1.81

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	AK	66	PRO	CA-C-N	11.34	134.02	119.84
11	AK	66	PRO	C-N-CA	11.34	134.02	119.84
16	AQ	36	ASP	CA-C-N	9.65	129.37	118.85
16	AQ	36	ASP	C-N-CA	9.65	129.37	118.85
26	Ae	215	VAL	CA-C-N	-9.54	107.91	119.84
26	Ae	215	VAL	C-N-CA	-9.54	107.91	119.84
4	AB	227	ASN	CA-C-N	8.51	128.72	119.87
4	AB	227	ASN	C-N-CA	8.51	128.72	119.87
25	Ad	199	ARG	CA-C-N	8.28	127.92	119.56
25	Ad	199	ARG	C-N-CA	8.28	127.92	119.56
14	AO	68	PRO	CA-C-N	8.04	128.66	120.38
14	AO	68	PRO	C-N-CA	8.04	128.66	120.38
4	AB	183	GLY	CA-C-N	7.93	128.37	119.32
4	AB	183	GLY	C-N-CA	7.93	128.37	119.32
12	AL	50	GLY	CA-C-N	7.79	127.70	119.05
12	AL	50	GLY	C-N-CA	7.79	127.70	119.05
13	AN	96	ARG	CA-C-N	7.70	127.33	119.56
13	AN	96	ARG	C-N-CA	7.70	127.33	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AB	147	HIS	CA-C-N	-7.69	111.39	122.77
4	AB	147	HIS	C-N-CA	-7.69	111.39	122.77
11	AK	183	ILE	CA-C-N	-7.65	112.12	119.85
11	AK	183	ILE	C-N-CA	-7.65	112.12	119.85
7	AF	90	ARG	CA-C-N	7.65	130.15	120.51
7	AF	90	ARG	C-N-CA	7.65	130.15	120.51
35	Ao	642	LEU	CA-C-N	7.61	127.66	119.28
35	Ao	642	LEU	C-N-CA	7.61	127.66	119.28
32	AK	76	ALA	CA-C-N	7.59	127.26	119.82
32	AK	76	ALA	C-N-CA	7.59	127.26	119.82
24	Ac	7	PHE	CA-C-N	7.50	127.53	119.28
24	Ac	7	PHE	C-N-CA	7.50	127.53	119.28
36	Ap	71	ARG	CA-C-N	-7.25	113.34	120.52
36	Ap	71	ARG	C-N-CA	-7.25	113.34	120.52
1	BC	505	PRO	N-CA-CB	7.22	109.75	102.17
5	AC	166	TYR	CB-CA-C	-7.22	108.24	116.54
32	AK	149	PHE	CA-C-N	7.17	126.79	119.19
32	AK	149	PHE	C-N-CA	7.17	126.79	119.19
36	Ap	187	THR	CA-C-N	7.07	127.66	120.38
36	Ap	187	THR	C-N-CA	7.07	127.66	120.38
22	Aa	187	ILE	N-CA-C	7.06	115.87	108.95
7	AF	105	CYS	N-CA-C	-6.91	99.67	109.96
12	AL	112	GLY	N-CA-C	6.81	124.24	115.32
2	BT	68	PRO	N-CA-CB	6.76	110.35	103.25
6	AE	378	GLY	CA-C-N	6.69	126.82	119.87
6	AE	378	GLY	C-N-CA	6.69	126.82	119.87
35	Ao	274	ALA	CA-C-N	6.62	126.24	119.56
35	Ao	274	ALA	C-N-CA	6.62	126.24	119.56
6	AE	141	TRP	CA-C-N	6.56	126.80	119.32
6	AE	141	TRP	C-N-CA	6.56	126.80	119.32
35	Ao	415	ASP	N-CA-C	6.50	120.67	112.87
8	AG	36	ARG	N-CA-C	-6.45	105.04	113.17
35	Ao	490	PHE	CA-C-N	6.43	126.81	119.93
35	Ao	490	PHE	C-N-CA	6.43	126.81	119.93
12	AL	75	SER	N-CA-C	6.42	119.65	109.50
22	Aa	333	GLY	N-CA-C	-6.38	101.41	110.91
4	AB	149	GLN	N-CA-C	-6.34	97.30	110.80
1	BC	502	PRO	N-CA-CB	6.31	109.88	103.25
5	AC	74	GLY	N-CA-C	6.28	121.62	113.27
11	AK	157	GLY	CA-C-N	6.26	125.88	119.56
11	AK	157	GLY	C-N-CA	6.26	125.88	119.56
15	AP	26	CYS	N-CA-C	-6.25	99.80	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Ae	342	PRO	N-CA-CB	6.24	109.80	103.25
31	Aj	50	LEU	CA-C-N	6.11	126.13	119.90
31	Aj	50	LEU	C-N-CA	6.11	126.13	119.90
36	Ap	171	GLU	CA-C-N	-6.11	114.32	120.31
36	Ap	171	GLU	C-N-CA	-6.11	114.32	120.31
12	AL	95	ILE	CA-C-N	6.06	126.03	120.21
12	AL	95	ILE	C-N-CA	6.06	126.03	120.21
7	AF	106	GLU	N-CA-C	-6.04	105.40	112.89
34	An	151	ARG	N-CA-C	6.00	118.31	111.11
31	Aj	136	TYR	CA-C-N	-5.96	114.00	122.41
31	Aj	136	TYR	C-N-CA	-5.96	114.00	122.41
26	Ae	83	ARG	N-CA-C	5.94	119.71	112.23
17	AR	90	GLY	N-CA-C	-5.91	106.83	115.63
2	BT	59	LYS	CA-C-N	5.83	125.74	119.85
2	BT	59	LYS	C-N-CA	5.83	125.74	119.85
24	Ac	140	MET	N-CA-C	-5.83	105.82	113.17
31	Aj	7	ARG	CA-C-N	5.80	127.09	119.84
31	Aj	7	ARG	C-N-CA	5.80	127.09	119.84
9	AI	145	ARG	CA-C-N	5.76	125.53	119.76
9	AI	145	ARG	C-N-CA	5.76	125.53	119.76
11	AK	188	CYS	N-CA-C	5.72	118.65	110.24
23	Ab	81	GLY	CA-C-N	5.70	125.23	119.19
23	Ab	81	GLY	C-N-CA	5.70	125.23	119.19
28	Ag	82	LEU	N-CA-C	-5.68	102.28	110.40
23	Ab	9	VAL	N-CA-C	5.67	116.44	110.72
26	Ae	311	GLU	N-CA-C	5.66	118.70	109.24
8	AG	71	THR	N-CA-C	-5.64	104.12	111.74
32	Ak	79	LYS	CA-C-N	5.64	125.17	119.19
32	Ak	79	LYS	C-N-CA	5.64	125.17	119.19
24	Ac	139	CYS	N-CA-C	-5.63	103.21	110.19
16	AQ	58	CYS	N-CA-C	5.58	117.86	107.99
8	AG	77	ALA	CA-C-N	5.56	125.51	119.78
8	AG	77	ALA	C-N-CA	5.56	125.51	119.78
33	Am	20	ILE	N-CA-C	-5.55	106.26	111.48
11	AK	185	HIS	CA-C-N	5.52	132.08	121.54
11	AK	185	HIS	C-N-CA	5.52	132.08	121.54
17	AR	123	VAL	N-CA-C	5.51	117.42	111.58
14	AO	80	VAL	CA-C-N	5.50	125.77	119.83
14	AO	80	VAL	C-N-CA	5.50	125.77	119.83
36	Ap	117	PHE	N-CA-C	-5.50	106.53	113.18
32	Ak	83	VAL	CA-C-N	5.47	124.81	118.85
32	Ak	83	VAL	C-N-CA	5.47	124.81	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AB	241	SER	CA-C-N	5.46	126.01	120.38
4	AB	241	SER	C-N-CA	5.46	126.01	120.38
24	Ac	147	VAL	CA-C-N	5.44	125.34	119.85
24	Ac	147	VAL	C-N-CA	5.44	125.34	119.85
24	Ac	73	SER	CA-C-N	5.43	125.19	119.76
24	Ac	73	SER	C-N-CA	5.43	125.19	119.76
16	AQ	21	ALA	N-CA-C	5.42	118.69	111.75
12	AL	95	ILE	N-CA-C	5.41	113.39	107.60
35	Ao	543	HIS	CA-C-N	5.40	125.94	120.38
35	Ao	543	HIS	C-N-CA	5.40	125.94	120.38
36	Ap	81	HIS	N-CA-C	5.38	116.45	108.60
17	AR	76	LYS	CA-C-N	-5.33	115.91	122.84
17	AR	76	LYS	C-N-CA	-5.33	115.91	122.84
9	AI	387	GLY	N-CA-C	5.33	125.82	113.18
11	AK	90	ILE	CB-CA-C	-5.33	104.39	110.73
35	Ao	608	ILE	N-CA-C	5.33	113.75	107.84
36	Ap	188	PRO	CA-C-N	5.33	125.33	119.90
36	Ap	188	PRO	C-N-CA	5.33	125.33	119.90
24	Ac	130	GLY	CA-C-N	5.32	125.24	119.76
24	Ac	130	GLY	C-N-CA	5.32	125.24	119.76
26	Ae	86	GLU	N-CA-C	5.31	118.92	112.23
24	Ac	139	CYS	CA-CB-SG	5.29	126.56	114.40
14	AO	194	PRO	CA-C-N	-5.28	115.13	120.31
14	AO	194	PRO	C-N-CA	-5.28	115.13	120.31
24	Ac	144	GLU	N-CA-C	5.28	117.47	111.02
10	AJ	111	PRO	CA-C-N	5.27	125.28	119.90
10	AJ	111	PRO	C-N-CA	5.27	125.28	119.90
36	Ap	197	ASP	CA-C-N	5.27	125.27	119.90
36	Ap	197	ASP	C-N-CA	5.27	125.27	119.90
36	Ap	235	MET	CA-C-N	5.25	125.23	120.03
36	Ap	235	MET	C-N-CA	5.25	125.23	120.03
23	Ab	39	PRO	CA-C-N	5.20	125.48	119.92
23	Ab	39	PRO	C-N-CA	5.20	125.48	119.92
31	Aj	116	GLY	N-CA-C	5.17	117.82	110.74
31	Aj	167	PRO	CA-C-N	5.16	125.20	119.32
31	Aj	167	PRO	C-N-CA	5.16	125.20	119.32
35	Ao	544	PRO	CA-C-N	5.13	124.80	119.56
35	Ao	544	PRO	C-N-CA	5.13	124.80	119.56
32	Ak	184	LEU	N-CA-C	5.12	117.45	110.24
14	AO	74	LEU	N-CA-C	5.09	116.86	110.24
26	Ae	217	SER	N-CA-C	-5.08	105.87	111.71
1	BC	235	THR	CA-C-N	5.07	125.01	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BC	235	THR	C-N-CA	5.07	125.01	119.78
11	AK	189	ARG	CA-C-N	5.07	125.08	120.21
11	AK	189	ARG	C-N-CA	5.07	125.08	120.21
24	Ac	92	SER	N-CA-C	-5.06	106.88	113.16
26	Ae	317	GLY	N-CA-C	-5.03	106.67	112.50
22	Aa	171	GLU	N-CA-C	5.02	117.14	111.02
27	Af	109	VAL	N-CA-C	-5.02	101.83	108.96
2	BT	55	GLN	CA-C-N	5.01	123.32	119.66
2	BT	55	GLN	C-N-CA	5.01	123.32	119.66

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	Ae	313	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BC	4364	0	4371	108	0
2	BT	109	0	86	2	0
3	AA	20411	0	10345	220	0
4	AB	1762	0	1774	49	0
5	AC	1075	0	1087	32	0
6	AE	2732	0	2774	92	0
7	AF	981	0	1012	25	0
8	AG	1721	0	1747	53	0
9	AI	2650	0	2613	82	0
10	AJ	1155	0	1193	35	0
11	AK	1007	0	1042	42	0
12	AL	840	0	890	32	0
13	AN	858	0	883	39	0
14	AO	1448	0	1536	31	0
15	AP	932	0	951	22	0
16	AQ	875	0	931	31	0
17	AR	784	0	813	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	AU	734	0	745	35	0
19	AV	1498	0	765	23	0
20	AX	354	0	187	10	0
21	AZ	90	0	89	4	0
22	Aa	2378	0	2392	70	0
23	Ab	1101	0	1118	28	0
24	Ac	1367	0	1385	49	0
25	Ad	1467	0	1466	35	0
26	Ae	3109	0	3029	115	0
27	Af	778	0	791	21	0
28	Ag	2875	0	2886	78	0
29	Ah	1015	0	969	41	0
30	Ai	824	0	842	25	0
31	Aj	1788	0	1799	57	0
32	Ak	2222	0	2270	74	0
33	Am	930	0	959	22	0
34	An	639	0	709	14	0
35	Ao	4527	0	4391	185	0
36	Ap	1564	0	1531	32	0
37	BC	32	0	12	1	0
38	AA	105	0	0	0	0
38	AB	1	0	0	0	0
38	AX	1	0	0	0	0
38	Ag	1	0	0	0	0
38	An	1	0	0	0	0
38	BC	2	0	0	0	0
39	BC	1	0	0	0	0
40	AA	14	0	26	0	0
41	AR	1	0	0	0	0
41	Ac	1	0	0	0	0
41	Ap	1	0	0	0	0
42	AV	10	0	10	1	0
43	Ag	32	0	12	3	0
44	Ag	3	0	0	1	0
44	BC	2	0	0	0	0
All	All	73172	0	62431	1551	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 12.

All (1551) 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)
9:AI:254:LYS:HB3	9:AI:366:ARG:HH12	1.16	1.03
34:An:144:ARG:HG3	34:An:144:ARG:HH11	1.18	1.02
25:Ad:58:GLU:OE1	25:Ad:61:ARG:NH1	1.96	0.98
26:Ae:136:ARG:NH1	26:Ae:173:VAL:O	1.98	0.97
22:Aa:198:GLU:OE2	22:Aa:204:ARG:NH1	2.02	0.93
6:AE:427:ARG:HG2	6:AE:427:ARG:HH11	1.34	0.92
17:AR:141:TYR:O	18:AU:28:ARG:NH1	2.03	0.91
31:Aj:171:ARG:NH1	31:Aj:188:GLU:OE2	2.04	0.90
26:Ae:211:GLU:OE2	31:Aj:78:ARG:NH1	2.05	0.90
32:Ak:191:LYS:NZ	32:Ak:234:GLU:O	2.06	0.88
24:Ac:71:THR:HG22	24:Ac:73:SER:H	1.36	0.88
6:AE:283:GLU:OE2	23:Ab:21:ARG:NH1	2.07	0.88
21:AZ:703:ALA:HA	21:AZ:708:ALA:HB3	1.56	0.88
26:Ae:258:SER:HB3	26:Ae:311:GLU:HB3	1.53	0.88
9:AI:254:LYS:HB3	9:AI:366:ARG:NH1	1.89	0.87
22:Aa:335:SER:HB2	22:Aa:357:GLU:HG3	1.53	0.87
26:Ae:325:ARG:HH12	26:Ae:379:ARG:HH12	1.23	0.86
3:AA:255:G:OP1	6:AE:116:LYS:NZ	2.08	0.86
3:AA:882:A:H5'	26:Ae:108:SER:HB3	1.58	0.85
13:AN:125:ARG:HG2	13:AN:125:ARG:HH11	1.41	0.85
6:AE:197:THR:HG22	6:AE:199:GLY:H	1.41	0.85
22:Aa:184:SER:H	22:Aa:192:ARG:HH12	1.22	0.85
28:Ag:46:ALA:HB3	28:Ag:357:GLN:HG3	1.58	0.84
6:AE:411:VAL:HG21	24:Ac:2:PRO:HD3	1.59	0.84
35:Ao:346:ARG:NH1	35:Ao:377:TYR:O	2.10	0.84
25:Ad:166:THR:O	25:Ad:176:ARG:NH2	2.10	0.83
8:AG:73:LEU:HG	9:AI:254:LYS:NZ	1.93	0.83
3:AA:882:A:H2	3:AA:886:A:H61	1.23	0.83
35:Ao:346:ARG:NH1	35:Ao:381:LEU:HB2	1.94	0.83
9:AI:323:ARG:HH11	9:AI:327:HIS:HE1	1.22	0.83
15:AP:93:LEU:O	22:Aa:197:ARG:NH1	2.11	0.83
6:AE:317:HIS:HD2	6:AE:319:ALA:H	1.27	0.83
33:Am:11:ALA:HB2	33:Am:19:PRO:HG3	1.61	0.83
3:AA:601:A:OP1	35:Ao:126:LYS:NZ	2.12	0.83
22:Aa:298:VAL:HG21	22:Aa:325:LEU:HD13	1.61	0.83
31:Aj:52:MET:HG2	36:Ap:223:ARG:HH12	1.45	0.82
26:Ae:325:ARG:HH12	26:Ae:379:ARG:NH1	1.77	0.82
8:AG:73:LEU:HG	9:AI:254:LYS:HZ3	1.44	0.82
8:AG:180:ARG:HH11	8:AG:180:ARG:HB3	1.44	0.82
16:AQ:6:SER:O	16:AQ:11:LYS:NZ	2.13	0.82
31:Aj:132:GLU:HG2	31:Aj:133:GLN:HG3	1.63	0.81
18:AU:52:ARG:HG2	18:AU:52:ARG:HH11	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Ae:312:ASP:HB2	26:Ae:314:GLN:HE21	1.46	0.80
3:AA:956:G:O6	18:AU:50:ARG:NH2	2.14	0.80
3:AA:106:C:OP2	16:AQ:45:LYS:NZ	2.13	0.80
31:Aj:82:ARG:HG3	31:Aj:138:ASP:HB3	1.61	0.80
11:AK:76:ARG:NH1	11:AK:81:LYS:HG2	1.97	0.80
5:AC:96:MET:HG3	5:AC:108:LEU:HD21	1.65	0.79
26:Ae:181:ASN:OD1	26:Ae:419:ARG:NH1	2.16	0.79
16:AQ:95:VAL:CG1	25:Ad:120:ARG:HH12	1.95	0.79
7:AF:3:ARG:NH1	7:AF:70:ALA:O	2.15	0.79
12:AL:78:ARG:NH1	12:AL:117:ASP:OD2	2.16	0.78
29:Ah:323:HIS:HD2	29:Ah:361:LYS:HZ1	1.31	0.78
18:AU:50:ARG:HG3	18:AU:50:ARG:HH11	1.48	0.78
3:AA:213:G:OP1	24:Ac:162:LYS:NZ	2.16	0.78
8:AG:197:ARG:HG2	8:AG:197:ARG:HH11	1.49	0.77
9:AI:111:LEU:HD22	32:Ak:114:LEU:HD23	1.65	0.77
9:AI:150:LEU:O	9:AI:153:THR:OG1	2.02	0.77
3:AA:344:G:H1	11:AK:121:ASN:HB3	1.49	0.76
8:AG:94:PHE:HD1	8:AG:111:MET:HE1	1.49	0.76
15:AP:59:ASN:HD22	24:Ac:146:GLN:HE22	1.33	0.76
13:AN:53:ARG:HE	29:Ah:364:HIS:HD2	1.33	0.76
21:AZ:703:ALA:HB1	21:AZ:709:ALA:HB2	1.65	0.76
32:Ak:166:ARG:HB2	35:Ao:134:GLU:HG3	1.68	0.76
4:AB:81:ARG:HA	27:Af:84:MET:HE1	1.68	0.76
3:AA:826:C:H2'	3:AA:827:A:H8	1.50	0.75
32:Ak:196:VAL:HG12	32:Ak:199:ARG:HD3	1.68	0.75
3:AA:93:A:N3	25:Ad:79:ARG:NH2	2.34	0.75
24:Ac:23:PHE:H	24:Ac:59:ASN:HD21	1.33	0.75
6:AE:291:TYR:H	6:AE:356:GLN:HE21	1.33	0.75
26:Ae:157:LEU:HA	26:Ae:161:ALA:HB2	1.68	0.75
18:AU:50:ARG:HH11	18:AU:50:ARG:CG	2.00	0.75
7:AF:58:HIS:CD2	7:AF:89:ILE:HD11	2.23	0.74
24:Ac:36:THR:H	24:Ac:69:ASN:HD21	1.36	0.74
6:AE:292:HIS:HE1	6:AE:357:GLU:H	1.35	0.74
22:Aa:184:SER:H	22:Aa:192:ARG:NH1	1.86	0.74
28:Ag:264:VAL:HG21	28:Ag:307:LEU:HB3	1.70	0.74
31:Aj:99:ARG:HG3	31:Aj:115:TRP:HB2	1.70	0.74
35:Ao:574:TRP:HH2	35:Ao:579:LEU:HB2	1.52	0.74
13:AN:125:ARG:HH11	13:AN:125:ARG:CG	2.00	0.74
1:BC:660:LYS:HD3	1:BC:670:LYS:HZ3	1.53	0.74
35:Ao:617:PHE:HD2	35:Ao:633:LEU:HD11	1.51	0.74
6:AE:317:HIS:CD2	6:AE:319:ALA:H	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AA:103:G:OP1	16:AQ:78:LYS:NZ	2.20	0.73
11:AK:195:ARG:HG2	11:AK:195:ARG:HH11	1.52	0.73
9:AI:396:LYS:NZ	19:AV:31:C:OP2	2.15	0.73
3:AA:604:U:H1'	30:AI:95:ARG:HD3	1.70	0.73
35:Ao:544:PRO:HD2	35:Ao:547:LEU:HD12	1.69	0.73
35:Ao:551:PHE:HB3	35:Ao:585:LEU:HD13	1.69	0.73
3:AA:841:C:OP2	20:AX:8:A:N6	2.21	0.73
9:AI:119:LYS:HA	9:AI:122:ARG:HD2	1.70	0.73
4:AB:57:LEU:HB2	4:AB:270:TYR:HE2	1.52	0.73
35:Ao:579:LEU:HD21	35:Ao:599:LEU:HA	1.71	0.73
6:AE:160:ARG:NH1	6:AE:168:VAL:HG21	2.04	0.72
9:AI:329:MET:HE1	9:AI:349:MET:HG3	1.69	0.72
22:Aa:104:MET:HE3	22:Aa:310:GLN:HE22	1.54	0.72
13:AN:90:ARG:NH1	13:AN:95:SER:O	2.22	0.72
28:Ag:154:ILE:HD13	28:Ag:261:VAL:HG22	1.71	0.72
29:Ah:323:HIS:HD2	29:Ah:361:LYS:NZ	1.86	0.72
36:Ap:217:ARG:HG2	36:Ap:224:LEU:HD21	1.69	0.72
7:AF:65:LEU:HD21	17:AR:76:LYS:HD3	1.72	0.72
16:AQ:14:VAL:H	24:Ac:63:GLN:HE22	1.36	0.72
22:Aa:119:GLU:HA	36:Ap:131:THR:HG23	1.70	0.71
24:Ac:125:HIS:HD2	24:Ac:127:ALA:H	1.38	0.71
26:Ae:154:ARG:HD3	26:Ae:157:LEU:HD12	1.71	0.71
34:An:144:ARG:HG3	34:An:144:ARG:NH1	1.91	0.71
1:BC:660:LYS:HD3	1:BC:670:LYS:NZ	2.05	0.71
16:AQ:95:VAL:HG11	25:Ad:120:ARG:HH12	1.54	0.71
34:An:144:ARG:HH11	34:An:144:ARG:CG	2.00	0.71
12:AL:70:PRO:HB3	12:AL:117:ASP:HB3	1.70	0.70
17:AR:139:ILE:HD11	18:AU:32:MET:HG2	1.71	0.70
35:Ao:539:ALA:HB2	35:Ao:581:TYR:HE1	1.56	0.70
4:AB:57:LEU:HD23	4:AB:60:ARG:NH1	2.06	0.70
4:AB:141:ILE:HD13	4:AB:191:LEU:HD23	1.73	0.70
35:Ao:346:ARG:HD3	35:Ao:381:LEU:HG	1.73	0.70
4:AB:70:ASP:O	4:AB:73:ASN:N	2.18	0.70
35:Ao:335:LEU:HD11	35:Ao:370:PRO:HA	1.72	0.70
5:AC:132:PHE:HD2	35:Ao:95:LEU:HD21	1.56	0.70
35:Ao:82:SER:O	35:Ao:487:SER:OG	2.09	0.70
3:AA:562:A:O2'	3:AA:708:A:N6	2.23	0.70
26:Ae:300:LEU:HD13	26:Ae:374:ARG:HD2	1.74	0.70
3:AA:54:A:C8	25:Ad:27:ARG:NH1	2.59	0.69
18:AU:50:ARG:HG3	18:AU:50:ARG:NH1	2.03	0.69
35:Ao:558:ILE:HG23	35:Ao:562:TYR:CE2	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AI:397:ARG:NH1	19:AV:32:A:OP2	2.26	0.69
35:Ao:574:TRP:CH2	35:Ao:579:LEU:HB2	2.28	0.69
10:AJ:124:VAL:HG22	13:AN:109:ILE:HD13	1.75	0.69
23:Ab:30:LEU:HD12	23:Ab:30:LEU:H	1.55	0.69
3:AA:552:A:H2'	3:AA:553:G:C8	2.28	0.69
26:Ae:80:TRP:HB2	26:Ae:154:ARG:NH1	2.08	0.68
8:AG:64:TYR:HA	8:AG:67:ASP:HB2	1.75	0.68
19:AV:3:U:H3	19:AV:65:A:H61	1.41	0.68
28:Ag:173:ASN:O	28:Ag:176:ARG:NH1	2.26	0.68
1:BC:381:LEU:HB3	1:BC:410:ALA:HB3	1.76	0.68
22:Aa:347:LEU:HD11	22:Aa:368:LEU:HD11	1.76	0.68
29:Ah:323:HIS:CD2	29:Ah:361:LYS:NZ	2.62	0.68
35:Ao:446:ASP:O	35:Ao:450:LEU:HG	1.93	0.68
32:Ak:89:MET:HG2	32:Ak:90:GLY:H	1.58	0.68
17:AR:115:ALA:HB3	17:AR:121:MET:HE2	1.76	0.68
3:AA:471:U:OP2	23:Ab:50:ARG:NH2	2.24	0.68
26:Ae:286:ASN:HB3	31:Aj:70:ARG:HH12	1.58	0.68
17:AR:68:LEU:HD21	25:Ad:191:ILE:HD13	1.75	0.67
35:Ao:308:VAL:HG22	35:Ao:315:LYS:HG3	1.74	0.67
35:Ao:603:ARG:HD2	35:Ao:636:LEU:HD13	1.75	0.67
24:Ac:51:ASN:ND2	24:Ac:95:ASN:OD1	2.23	0.67
28:Ag:173:ASN:HB3	28:Ag:176:ARG:HD2	1.77	0.67
36:Ap:126:PHE:HE2	36:Ap:140:THR:HG21	1.60	0.67
6:AE:160:ARG:HH11	6:AE:168:VAL:HG21	1.60	0.67
10:AJ:52:VAL:HG21	35:Ao:479:LYS:HB3	1.75	0.67
17:AR:77:ASN:HB2	25:Ad:188:ASN:HA	1.74	0.67
23:Ab:73:LYS:NZ	23:Ab:114:GLU:HG3	2.10	0.67
11:AK:96:ASN:OD1	11:AK:97:THR:N	2.28	0.67
1:BC:543:GLU:HB3	1:BC:614:LEU:HD11	1.76	0.66
4:AB:57:LEU:HB2	4:AB:270:TYR:CE2	2.29	0.66
5:AC:75:ASN:HD21	13:AN:104:TRP:HE1	1.41	0.66
8:AG:94:PHE:CD1	8:AG:111:MET:HE1	2.30	0.66
35:Ao:558:ILE:HG23	35:Ao:562:TYR:HE2	1.59	0.66
9:AI:323:ARG:HH11	9:AI:327:HIS:CE1	2.10	0.66
1:BC:215:GLN:HE22	1:BC:598:ILE:HA	1.60	0.66
3:AA:90:U:H5'	25:Ad:68:ARG:HH21	1.61	0.66
36:Ap:181:HIS:HD2	36:Ap:183:ALA:H	1.44	0.66
10:AJ:161:GLN:HG2	10:AJ:170:MET:HE1	1.77	0.66
8:AG:152:CYS:SG	8:AG:219:VAL:HB	2.35	0.66
36:Ap:192:THR:HG21	36:Ap:199:TRP:HA	1.78	0.65
9:AI:199:ARG:HG2	9:AI:249:ILE:HG23	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AA:287:C:N3	24:Ac:11:ARG:NH2	2.44	0.65
11:AK:175:ILE:HG13	11:AK:176:SER:H	1.61	0.65
16:AQ:62:ASP:N	16:AQ:62:ASP:OD1	2.30	0.65
34:An:173:LEU:HD12	34:An:191:THR:HG23	1.77	0.65
17:AR:95:ARG:NH1	17:AR:102:GLY:HA2	2.12	0.65
22:Aa:221:ARG:NH1	22:Aa:224:ARG:HE	1.95	0.65
24:Ac:125:HIS:CD2	24:Ac:127:ALA:H	2.13	0.65
29:Ah:345:LEU:HD11	30:Ai:26:THR:HG21	1.78	0.65
35:Ao:485:ILE:HD12	35:Ao:491:PRO:HG3	1.77	0.65
7:AF:58:HIS:CG	7:AF:89:ILE:HD11	2.32	0.65
43:Ag:500:GTP:O2A	44:Ag:601:HOH:O	2.14	0.65
35:Ao:427:SER:HA	35:Ao:467:LEU:HD21	1.79	0.65
11:AK:177:ILE:HD11	18:AU:23:TYR:HD2	1.61	0.65
35:Ao:543:HIS:HD2	35:Ao:588:ARG:HG3	1.62	0.65
7:AF:104:GLU:N	7:AF:104:GLU:OE1	2.29	0.64
15:AP:42:PRO:HG2	15:AP:45:GLY:HA3	1.79	0.64
31:Aj:63:ARG:HH11	31:Aj:111:HIS:CE1	2.15	0.64
8:AG:159:VAL:HB	8:AG:172:VAL:HG21	1.79	0.64
28:Ag:252:LEU:HB2	28:Ag:254:ILE:HG22	1.78	0.64
32:Ak:151:ILE:HG12	32:Ak:177:VAL:HG22	1.79	0.64
8:AG:240:ARG:NH2	33:Am:44:THR:O	2.30	0.64
3:AA:201:A:H2'	3:AA:202:A:C8	2.33	0.64
28:Ag:205:GLU:OE2	28:Ag:248:ARG:NH1	2.31	0.64
35:Ao:539:ALA:HB2	35:Ao:581:TYR:CE1	2.32	0.64
36:Ap:108:CYS:SG	36:Ap:146:GLN:HG3	2.37	0.64
28:Ag:259:VAL:HB	28:Ag:305:ILE:HG22	1.78	0.64
28:Ag:312:THR:OG1	43:Ag:500:GTP:O1G	2.12	0.64
35:Ao:504:ASP:HB2	35:Ao:537:LEU:HD22	1.78	0.64
35:Ao:326:MET:HE1	35:Ao:337:THR:HG21	1.79	0.64
10:AJ:59:THR:HG22	10:AJ:61:PRO:HD3	1.80	0.64
9:AI:176:HIS:HE1	9:AI:185:LEU:HD22	1.62	0.64
35:Ao:343:LYS:HE2	35:Ao:347:ARG:HH21	1.62	0.64
1:BC:310:VAL:HB	1:BC:316:GLY:HA3	1.79	0.64
9:AI:91:MET:HB2	32:Ak:117:THR:HG21	1.80	0.64
17:AR:95:ARG:HH12	17:AR:102:GLY:HA2	1.62	0.64
35:Ao:608:ILE:HG13	35:Ao:642:LEU:HD21	1.79	0.64
4:AB:137:ARG:HD3	23:Ab:34:ILE:HD11	1.81	0.63
7:AF:67:ASP:OD1	7:AF:67:ASP:N	2.29	0.63
24:Ac:78:PHE:HB2	24:Ac:86:VAL:HB	1.78	0.63
4:AB:79:SER:H	4:AB:82:SER:HB3	1.64	0.63
6:AE:370:VAL:HG13	6:AE:385:ALA:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AK:100:GLN:HE21	11:AK:108:PRO:HB3	1.62	0.63
28:Ag:161:VAL:HG22	28:Ag:289:ILE:HD11	1.80	0.63
32:Ak:89:MET:HE2	32:Ak:107:LEU:HG	1.79	0.63
8:AG:238:HIS:HE1	11:AK:128:ILE:HG13	1.62	0.63
3:AA:876:A:H61	31:Aj:17:ARG:HH12	1.44	0.63
18:AU:66:MET:HE2	33:Am:4:PRO:HD3	1.81	0.63
22:Aa:192:ARG:O	22:Aa:211:ARG:NH2	2.27	0.63
24:Ac:76:LEU:HD13	24:Ac:102:ILE:HD11	1.79	0.63
26:Ae:270:LEU:HG	26:Ae:320:LEU:HD21	1.81	0.63
26:Ae:276:LEU:HD23	26:Ae:365:GLN:HG2	1.80	0.63
1:BC:617:ALA:HB3	1:BC:717:ILE:HB	1.81	0.63
13:AN:51:ARG:NH2	13:AN:83:CYS:HB3	2.14	0.63
22:Aa:279:GLY:HA2	22:Aa:281:TYR:HE1	1.64	0.63
3:AA:826:C:H2'	3:AA:827:A:C8	2.33	0.63
13:AN:60:ASN:O	13:AN:68:GLN:NE2	2.32	0.63
27:Af:153:ARG:NH1	27:Af:160:ASP:OD1	2.32	0.63
29:Ah:335:LYS:O	29:Ah:340:ARG:HG3	1.99	0.63
6:AE:316:CYS:HB2	6:AE:321:MET:HG3	1.80	0.63
18:AU:52:ARG:HH11	18:AU:52:ARG:CG	2.12	0.63
24:Ac:47:PHE:HA	24:Ac:51:ASN:HD22	1.64	0.63
12:AL:32:THR:H	12:AL:35:GLN:HE21	1.46	0.62
29:Ah:298:LYS:HE2	35:Ao:68:VAL:HG21	1.81	0.62
3:AA:901:A:O2'	34:An:171:ARG:NH1	2.32	0.62
9:AI:124:ILE:HG23	9:AI:126:LYS:HG3	1.81	0.62
9:AI:201:LEU:HD11	9:AI:245:PHE:HD1	1.64	0.62
3:AA:891:C:H2'	3:AA:892:A:C8	2.34	0.62
16:AQ:65:LEU:HB2	16:AQ:85:ILE:HD11	1.82	0.62
26:Ae:204:VAL:HG22	26:Ae:221:LEU:HD22	1.80	0.62
11:AK:179:ASP:OD1	11:AK:181:THR:OG1	2.17	0.62
32:Ak:192:LEU:HD11	32:Ak:231:LEU:HB3	1.81	0.62
28:Ag:54:ASP:HB3	28:Ag:57:LYS:HB2	1.82	0.62
1:BC:573:GLY:HA3	1:BC:595:LEU:HD23	1.82	0.62
8:AG:66:ARG:HB3	8:AG:70:LYS:HE3	1.81	0.62
3:AA:29:A:H2'	3:AA:30:A:C8	2.35	0.62
4:AB:151:ALA:HA	4:AB:167:THR:HG21	1.81	0.62
10:AJ:89:ASP:OD1	10:AJ:141:ARG:NH2	2.32	0.62
1:BC:490:SER:O	3:AA:919:A:N6	2.31	0.62
3:AA:560:C:H42	3:AA:710:G:H1	1.48	0.62
6:AE:282:ILE:HG13	6:AE:327:ILE:HD13	1.82	0.62
8:AG:77:ALA:O	9:AI:346:ARG:NH2	2.32	0.61
35:Ao:403:VAL:HG12	35:Ao:441:LEU:HD11	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Ag:101:ARG:HD2	43:Ag:500:GTP:O6	1.99	0.61
31:Aj:68:LEU:HD21	31:Aj:97:LEU:HD13	1.81	0.61
3:AA:959:U:H5'	33:Am:25:LYS:NZ	2.15	0.61
6:AE:220:THR:HB	6:AE:247:VAL:HG12	1.83	0.61
3:AA:54:A:N7	25:Ad:27:ARG:NH1	2.48	0.61
3:AA:120:A:O2'	16:AQ:22:MET:HE1	2.00	0.61
13:AN:53:ARG:NE	29:Ah:364:HIS:HD2	1.99	0.61
32:Ak:58:ARG:NH2	35:Ao:91:ASP:OD2	2.33	0.61
35:Ao:258:ASN:HD21	35:Ao:288:ASN:HD22	1.46	0.61
35:Ao:532:GLU:O	35:Ao:536:MET:HG2	2.00	0.61
1:BC:363:PHE:HB3	1:BC:524:VAL:HG13	1.83	0.61
22:Aa:287:THR:HG22	22:Aa:289:HIS:H	1.66	0.61
35:Ao:401:ASN:HA	35:Ao:404:MET:SD	2.41	0.61
7:AF:105:CYS:CB	17:AR:69:CYS:SG	2.89	0.61
22:Aa:224:ARG:NH1	22:Aa:256:GLN:O	2.32	0.61
28:Ag:272:THR:HG23	28:Ag:315:LEU:HD13	1.83	0.61
1:BC:566:THR:HG22	12:AL:84:ARG:HH11	1.65	0.61
3:AA:136:C:O2	14:AO:198:ARG:NH2	2.34	0.61
5:AC:72:HIS:HD2	5:AC:74:GLY:H	1.49	0.61
26:Ae:106:PRO:HB2	26:Ae:140:ASN:HD21	1.65	0.61
26:Ae:147:TRP:O	26:Ae:151:THR:HG23	2.00	0.61
1:BC:721:THR:HG22	1:BC:723:TRP:H	1.66	0.61
3:AA:791:G:H5''	9:AI:376:ARG:HB3	1.81	0.61
11:AK:175:ILE:HG13	11:AK:176:SER:N	2.16	0.61
29:Ah:350:LEU:HD23	30:Ai:37:PHE:HB3	1.82	0.61
6:AE:374:ARG:HG3	6:AE:374:ARG:HH11	1.65	0.60
12:AL:96:PRO:O	12:AL:127:ARG:NH1	2.34	0.60
26:Ae:83:ARG:NH2	26:Ae:416:TYR:OH	2.33	0.60
3:AA:647:A:C6	18:AU:82:ASP:HB3	2.36	0.60
3:AA:223:U:O2'	3:AA:224:U:OP1	2.18	0.60
17:AR:142:ARG:HA	18:AU:28:ARG:HH12	1.66	0.60
26:Ae:80:TRP:HB2	26:Ae:154:ARG:HH11	1.65	0.60
6:AE:427:ARG:HG2	6:AE:427:ARG:NH1	2.08	0.60
24:Ac:80:LEU:HD12	24:Ac:84:GLU:HB3	1.81	0.60
35:Ao:465:PHE:HE2	35:Ao:499:LEU:HD21	1.66	0.60
23:Ab:28:LYS:HE3	23:Ab:32:LEU:HD23	1.84	0.60
16:AQ:24:LYS:H	16:AQ:56:GLN:NE2	2.00	0.60
36:Ap:89:ARG:HB2	36:Ap:144:MET:HE3	1.83	0.60
16:AQ:29:ARG:HD3	16:AQ:46:ARG:HD3	1.83	0.60
22:Aa:279:GLY:HA2	22:Aa:281:TYR:CE1	2.37	0.60
35:Ao:343:LYS:HE2	35:Ao:347:ARG:NH2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:Ao:404:MET:SD	35:Ao:437:GLN:HB3	2.42	0.60
3:AA:882:A:H2	3:AA:886:A:N6	1.98	0.60
5:AC:123:VAL:HG21	5:AC:155:LEU:HG	1.83	0.60
3:AA:849:G:H5'	34:An:138:MET:HE3	1.83	0.60
9:AI:127:HIS:CD2	9:AI:129:GLU:HG2	2.37	0.60
9:AI:201:LEU:HD21	9:AI:245:PHE:HA	1.84	0.59
10:AJ:151:SER:HB2	32:Ak:133:THR:HG22	1.84	0.59
35:Ao:427:SER:HB3	35:Ao:463:LYS:HB3	1.84	0.59
35:Ao:382:PHE:O	35:Ao:386:GLU:HB2	2.02	0.59
35:Ao:559:LYS:HZ3	35:Ao:574:TRP:HZ2	1.49	0.59
11:AK:99:ILE:HD11	11:AK:163:ALA:HB1	1.84	0.59
3:AA:308:A:H3'	3:AA:309:A:O4'	2.02	0.59
26:Ae:327:LEU:O	26:Ae:331:THR:OG1	2.13	0.59
31:Aj:27:ARG:HH22	31:Aj:33:ARG:NH1	2.00	0.59
6:AE:132:ILE:HG22	6:AE:144:LEU:HD13	1.82	0.59
35:Ao:386:GLU:HG3	35:Ao:393:SER:HB3	1.84	0.59
9:AI:323:ARG:NH1	9:AI:327:HIS:HE1	1.97	0.59
28:Ag:178:ASP:OD1	28:Ag:178:ASP:N	2.35	0.59
35:Ao:536:MET:SD	35:Ao:581:TYR:OH	2.60	0.59
8:AG:85:VAL:HG22	28:Ag:369:LYS:HD3	1.85	0.59
3:AA:353:C:H5'	3:AA:354:C:H5'	1.84	0.59
9:AI:92:MET:HE3	9:AI:107:ALA:HB1	1.84	0.59
20:AX:8:A:H2	20:AX:9:C:H41	1.50	0.59
15:AP:108:GLU:OE2	25:Ad:59:ARG:NH2	2.36	0.59
16:AQ:95:VAL:HG12	25:Ad:120:ARG:HH12	1.68	0.59
22:Aa:311:ILE:HD13	22:Aa:368:LEU:HD13	1.84	0.59
24:Ac:12:THR:HG22	24:Ac:14:GLN:H	1.67	0.59
29:Ah:375:LYS:HD3	29:Ah:378:ILE:HD12	1.85	0.59
35:Ao:559:LYS:HG2	35:Ao:574:TRP:HE1	1.67	0.59
4:AB:238:ASN:HD21	4:AB:241:SER:HB3	1.68	0.58
8:AG:197:ARG:HG2	8:AG:197:ARG:NH1	2.15	0.58
31:Aj:30:ASP:HB2	31:Aj:34:TYR:HE1	1.68	0.58
3:AA:357:G:H21	11:AK:100:GLN:HE22	1.50	0.58
4:AB:176:THR:HG23	4:AB:214:MET:HE1	1.84	0.58
6:AE:103:LEU:HD11	6:AE:123:ARG:HB2	1.85	0.58
7:AF:105:CYS:HB3	17:AR:69:CYS:SG	2.42	0.58
35:Ao:500:LEU:HB3	35:Ao:537:LEU:HD11	1.84	0.58
3:AA:641:A:OP1	6:AE:230:ASN:HB2	2.03	0.58
25:Ad:73:GLU:O	25:Ad:76:SER:OG	2.21	0.58
26:Ae:154:ARG:NH2	26:Ae:416:TYR:OH	2.35	0.58
29:Ah:309:ASN:HD21	32:Ak:158:TYR:H	1.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AG:44:PRO:HG3	8:AG:75:LYS:O	2.04	0.58
31:Aj:95:TRP:CE2	31:Aj:131:ILE:HG23	2.39	0.58
35:Ao:392:SER:O	35:Ao:396:ILE:HG13	2.03	0.58
6:AE:120:LYS:HE2	6:AE:122:ARG:HE	1.67	0.58
1:BC:285:LEU:HD13	1:BC:304:LEU:HD11	1.85	0.58
26:Ae:74:TYR:CE1	26:Ae:413:ILE:HG12	2.38	0.58
32:Ak:300:SER:O	32:Ak:304:GLU:HB3	2.03	0.58
1:BC:168:ARG:HB2	1:BC:378:ARG:HH21	1.69	0.58
16:AQ:35:LEU:HD21	16:AQ:40:LEU:HD12	1.86	0.58
6:AE:98:LEU:HD11	30:Ai:75:HIS:CD2	2.38	0.58
14:AO:90:VAL:HG13	25:Ad:160:LEU:HD23	1.84	0.58
28:Ag:107:LEU:HD22	28:Ag:342:ILE:HD12	1.86	0.58
35:Ao:527:ARG:O	35:Ao:531:LYS:HB2	2.04	0.58
28:Ag:209:TRP:HH2	28:Ag:224:VAL:HG13	1.69	0.58
1:BC:257:LEU:HD22	1:BC:273:ILE:HD11	1.86	0.57
1:BC:566:THR:HG22	12:AL:84:ARG:NH1	2.19	0.57
3:AA:582:G:OP1	13:AN:88:ARG:NH2	2.33	0.57
3:AA:638:A:H2	6:AE:258:ILE:HG21	1.68	0.57
14:AO:69:PRO:HD2	14:AO:72:MET:HG3	1.84	0.57
26:Ae:99:LYS:HE3	26:Ae:103:ARG:HD3	1.85	0.57
27:Af:163:ILE:HG23	27:Af:165:GLU:HB2	1.86	0.57
35:Ao:259:ALA:HA	35:Ao:262:TYR:CE2	2.38	0.57
1:BC:163:LYS:HB2	1:BC:439:ARG:HH12	1.68	0.57
3:AA:667:C:H3'	3:AA:668:A:H8	1.69	0.57
16:AQ:74:THR:HG22	16:AQ:75:LYS:H	1.68	0.57
26:Ae:325:ARG:NH1	26:Ae:379:ARG:NH1	2.52	0.57
28:Ag:77:VAL:HG11	28:Ag:142:HIS:HB2	1.85	0.57
3:AA:54:A:C5	25:Ad:27:ARG:NH1	2.71	0.57
29:Ah:288:ASN:HD21	32:Ak:73:PRO:HG3	1.69	0.57
1:BC:381:LEU:HG	1:BC:399:MET:HE1	1.86	0.57
1:BC:397:ARG:HH12	3:AA:177:U:P	2.27	0.57
1:BC:635:THR:O	19:AV:70:C:N4	2.32	0.57
4:AB:149:GLN:HG3	18:AU:84:TRP:CZ2	2.39	0.57
3:AA:59:C:N3	31:Aj:54:ALA:HB1	2.19	0.57
25:Ad:189:TRP:HZ3	25:Ad:191:ILE:HG23	1.70	0.57
3:AA:58:U:OP1	31:Aj:53:ARG:NH1	2.38	0.57
5:AC:84:GLU:HB2	5:AC:85:ARG:NH1	2.19	0.57
8:AG:62:GLU:HG2	8:AG:66:ARG:HE	1.70	0.57
14:AO:137:ILE:HD13	14:AO:161:ILE:HG13	1.86	0.57
19:AV:16:A:H4'	19:AV:17:U:OP1	2.04	0.57
32:Ak:192:LEU:O	32:Ak:196:VAL:HG23	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AA:65:C:OP2	25:Ad:30:ARG:HB2	2.04	0.57
10:Aj:128:LYS:HG2	10:Aj:131:ARG:HH21	1.68	0.57
26:Ae:318:GLU:OE2	26:Ae:383:GLN:NE2	2.37	0.57
31:Aj:63:ARG:NH1	31:Aj:111:HIS:CE1	2.73	0.57
32:Ak:183:ASN:HB3	32:Ak:232:TYR:OH	2.05	0.57
35:Ao:306:LEU:HA	35:Ao:348:PHE:HZ	1.69	0.57
1:BC:350:ASP:HB3	1:BC:378:ARG:HD2	1.85	0.57
13:AN:58:ARG:HD3	13:AN:72:ASP:HA	1.86	0.57
23:Ab:134:ARG:HG2	23:Ab:135:VAL:H	1.69	0.57
10:Aj:179:GLN:O	32:Ak:150:PRO:HD2	2.04	0.57
15:AP:102:MET:HE1	25:Ad:56:LEU:HD11	1.86	0.57
1:BC:388:VAL:HG11	1:BC:443:VAL:HG11	1.87	0.57
26:Ae:148:THR:O	26:Ae:151:THR:OG1	2.21	0.57
35:Ao:376:HIS:CD2	35:Ao:417:MET:HB3	2.40	0.57
3:AA:648:A:OP1	4:AB:148:ARG:HD2	2.04	0.56
17:AR:128:PRO:HA	17:AR:131:LEU:HD22	1.85	0.56
28:Ag:265:ASN:OD1	28:Ag:265:ASN:N	2.30	0.56
1:BC:188:HIS:HA	1:BC:268:GLN:HB2	1.87	0.56
24:Ac:47:PHE:HA	24:Ac:51:ASN:ND2	2.19	0.56
3:AA:825:C:H5'	33:Am:38:ARG:HH12	1.70	0.56
3:AA:942:G:N1	3:AA:945:A:OP2	2.38	0.56
5:AC:69:LEU:HD23	32:Ak:109:LYS:HE2	1.86	0.56
8:AG:139:ARG:NH2	28:Ag:363:ASN:OD1	2.38	0.56
10:Aj:80:VAL:HG23	10:Aj:141:ARG:HB2	1.86	0.56
17:AR:56:GLU:CD	17:AR:56:GLU:H	2.14	0.56
26:Ae:276:LEU:HD13	26:Ae:328:LYS:HD2	1.86	0.56
35:Ao:423:MET:HE2	35:Ao:460:TYR:HA	1.87	0.56
3:AA:256:G:H3'	3:AA:257:U:H5'	1.86	0.56
15:AP:19:ILE:HB	15:AP:83:LEU:HD23	1.87	0.56
26:Ae:272:GLY:HA3	26:Ae:296:LEU:HD21	1.87	0.56
19:AV:49:G:H1	19:AV:56:C:H42	1.54	0.56
35:Ao:126:LYS:HE3	35:Ao:127:TYR:CE2	2.41	0.56
35:Ao:285:LEU:HD21	35:Ao:292:ALA:HB2	1.87	0.56
1:BC:184:THR:OG1	1:BC:252:THR:HG21	2.06	0.56
9:AI:115:GLY:HA3	10:Aj:84:ASP:HB2	1.86	0.56
6:AE:304:LYS:NZ	6:AE:410:ASP:OD1	2.37	0.56
17:AR:53:VAL:HG21	23:Ab:66:HIS:CE1	2.41	0.56
26:Ae:117:ASP:OD2	26:Ae:427:ARG:NH2	2.37	0.56
1:BC:673:LEU:HD23	1:BC:696:LEU:HD23	1.88	0.56
29:Ah:284:ARG:HG3	35:Ao:448:TRP:HB3	1.87	0.56
1:BC:674:THR:HG22	1:BC:695:SER:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Ak:118:PRO:O	32:Ak:122:LYS:HG2	2.05	0.56
3:AA:308:A:H2	24:Ac:68:LYS:NZ	2.03	0.56
4:AB:238:ASN:ND2	4:AB:241:SER:HB3	2.21	0.56
15:AP:119:LEU:O	15:AP:123:GLN:HG2	2.05	0.56
26:Ae:70:LEU:O	26:Ae:74:TYR:HB2	2.06	0.56
3:AA:531:U:H2'	3:AA:532:G:C8	2.41	0.55
6:AE:93:LEU:H	30:Ai:75:HIS:CD2	2.25	0.55
35:Ao:440:GLY:O	35:Ao:444:THR:OG1	2.22	0.55
12:AL:77:ASN:O	12:AL:79:LYS:NZ	2.38	0.55
28:Ag:215:THR:HG23	28:Ag:219:ARG:HG3	1.88	0.55
24:Ac:139:CYS:HB2	24:Ac:141:CYS:H	1.71	0.55
26:Ae:86:GLU:HG2	26:Ae:114:ARG:HG2	1.89	0.55
26:Ae:120:ALA:HA	26:Ae:158:LYS:NZ	2.21	0.55
35:Ao:375:TYR:O	35:Ao:379:ILE:HG13	2.06	0.55
13:AN:29:TYR:HD2	13:AN:34:MET:HE3	1.71	0.55
22:Aa:285:ARG:HH11	22:Aa:285:ARG:HG3	1.71	0.55
28:Ag:82:LEU:HD12	28:Ag:83:PRO:HD2	1.88	0.55
28:Ag:246:LEU:O	28:Ag:250:SER:OG	2.21	0.55
31:Aj:38:TYR:OH	31:Aj:63:ARG:NH2	2.39	0.55
1:BC:309:VAL:HG13	1:BC:318:VAL:HG21	1.89	0.55
17:AR:116:GLN:HG2	17:AR:123:VAL:HG22	1.88	0.55
35:Ao:647:GLY:O	35:Ao:651:ARG:HG2	2.07	0.55
36:Ap:181:HIS:CD2	36:Ap:183:ALA:H	2.24	0.55
1:BC:182:VAL:HG12	1:BC:252:THR:HG22	1.89	0.55
1:BC:397:ARG:NH1	3:AA:176:G:O3'	2.40	0.55
3:AA:663:A:H1'	13:AN:127:MET:HE2	1.89	0.55
7:AF:32:ARG:HB2	7:AF:78:MET:HE3	1.88	0.55
11:AK:190:PRO:HG2	18:AU:45:TYR:HB2	1.89	0.55
15:AP:25:GLY:C	15:AP:26:CYS:SG	2.88	0.55
1:BC:567:PHE:CZ	12:AL:105:HIS:HD2	2.25	0.55
11:AK:167:LEU:HD22	11:AK:172:LEU:HD23	1.89	0.55
20:AX:6:C:H2'	20:AX:7:C:H5''	1.89	0.55
23:Ab:67:GLU:OE2	27:Af:86:ARG:NE	2.34	0.55
12:AL:116:GLN:OE1	12:AL:116:GLN:N	2.35	0.55
17:AR:125:TYR:HB3	18:AU:9:ALA:HB2	1.88	0.55
35:Ao:469:CYS:SG	35:Ao:470:PHE:N	2.80	0.55
1:BC:567:PHE:CE1	12:AL:105:HIS:HD2	2.25	0.55
22:Aa:183:ILE:HG12	22:Aa:183:ILE:O	2.07	0.54
31:Aj:90:ASP:CG	36:Ap:215:ARG:HH22	2.15	0.54
4:AB:252:PHE:O	4:AB:256:ILE:HG12	2.07	0.54
9:AI:71:VAL:HG12	9:AI:75:LYS:HE3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Aj:41:MET:HG2	31:Aj:55:TRP:CD1	2.42	0.54
32:Ak:165:ILE:HG13	35:Ao:135:PRO:HD3	1.88	0.54
3:AA:13:U:OP1	6:AE:226:ARG:HD3	2.07	0.54
3:AA:349:A:H2'	3:AA:350:A:C8	2.42	0.54
18:AU:72:ILE:HD12	33:Am:104:LEU:HD22	1.88	0.54
35:Ao:447:ASN:N	35:Ao:447:ASN:OD1	2.40	0.54
3:AA:250:A:H2'	3:AA:251:C:C6	2.41	0.54
11:AK:192:LYS:HZ2	11:AK:196:LEU:HD11	1.72	0.54
11:AK:195:ARG:HG2	11:AK:195:ARG:NH1	2.21	0.54
12:AL:57:GLN:HB3	12:AL:109:LEU:HD11	1.89	0.54
26:Ae:80:TRP:HE3	26:Ae:83:ARG:HD2	1.73	0.54
26:Ae:126:ASP:OD1	26:Ae:164:LYS:NZ	2.39	0.54
26:Ae:205:PHE:CZ	26:Ae:243:ASN:HB3	2.42	0.54
26:Ae:312:ASP:O	26:Ae:388:VAL:HB	2.08	0.54
36:Ap:72:PRO:HD2	36:Ap:75:ALA:HB2	1.89	0.54
1:BC:686:VAL:HG11	1:BC:692:CYS:HB3	1.89	0.54
5:AC:105:ALA:HB3	5:AC:122:LEU:HB3	1.88	0.54
6:AE:124:LYS:HZ2	30:Ai:81:GLU:CD	2.15	0.54
6:AE:308:GLN:HG3	6:AE:312:TYR:CD1	2.42	0.54
13:AN:54:ILE:HG21	13:AN:75:ILE:HB	1.90	0.54
23:Ab:73:LYS:HZ2	23:Ab:114:GLU:HG3	1.72	0.54
3:AA:918:A:O2'	3:AA:919:A:H3'	2.08	0.54
24:Ac:23:PHE:H	24:Ac:59:ASN:ND2	2.04	0.54
26:Ae:224:TYR:HA	26:Ae:227:TYR:HD1	1.72	0.54
35:Ao:353:LYS:NZ	35:Ao:385:HIS:HD2	2.05	0.54
8:AG:175:ALA:O	8:AG:179:ARG:HG3	2.07	0.54
11:AK:192:LYS:NZ	11:AK:196:LEU:HD11	2.23	0.54
3:AA:344:G:H2'	3:AA:345:U:C6	2.42	0.54
6:AE:291:TYR:H	6:AE:356:GLN:NE2	2.04	0.54
26:Ae:223:LEU:HD21	26:Ae:398:THR:HA	1.90	0.54
30:Ai:26:THR:HG22	30:Ai:30:SER:HB2	1.89	0.54
35:Ao:382:PHE:HB3	35:Ao:396:ILE:HD11	1.90	0.54
1:BC:364:THR:HG23	1:BC:370:LEU:HD23	1.90	0.54
4:AB:270:TYR:HA	4:AB:273:GLN:CD	2.33	0.54
8:AG:103:ASN:HB3	8:AG:106:LEU:HB3	1.89	0.54
12:AL:58:LEU:O	12:AL:109:LEU:HD12	2.08	0.54
14:AO:127:GLU:HG2	14:AO:178:VAL:HG11	1.89	0.54
26:Ae:312:ASP:C	26:Ae:314:GLN:HB2	2.33	0.54
1:BC:255:VAL:HG13	1:BC:281:VAL:HG11	1.90	0.54
6:AE:305:MET:CE	6:AE:332:LEU:HD21	2.38	0.54
9:AI:197:GLY:O	9:AI:249:ILE:HG12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AN:29:TYR:HB3	13:AN:34:MET:HG2	1.90	0.54
1:BC:387:LEU:HD13	1:BC:431:ILE:HG21	1.89	0.53
3:AA:873:A:H4'	14:AO:225:LYS:NZ	2.23	0.53
8:AG:196:HIS:HD2	8:AG:198:ARG:HB2	1.72	0.53
26:Ae:311:GLU:HA	26:Ae:388:VAL:HG21	1.89	0.53
32:Ak:199:ARG:HB3	32:Ak:208:THR:O	2.07	0.53
13:AN:60:ASN:HD21	13:AN:62:ILE:HB	1.73	0.53
26:Ae:80:TRP:CH2	26:Ae:151:THR:HG22	2.42	0.53
3:AA:142:G:OP2	31:Aj:5:LYS:NZ	2.41	0.53
9:AI:123:PRO:N	32:Ak:89:MET:HG3	2.23	0.53
28:Ag:201:ILE:HG12	28:Ag:255:PHE:HE1	1.74	0.53
1:BC:647:ARG:HG3	1:BC:691:ASP:OD1	2.08	0.53
3:AA:127:A:H2'	3:AA:128:C:C6	2.43	0.53
3:AA:736:A:O2'	28:Ag:165:ARG:NH2	2.41	0.53
5:AC:75:ASN:HD21	13:AN:104:TRP:NE1	2.06	0.53
26:Ae:166:LEU:HD13	26:Ae:199:ASP:HB2	1.90	0.53
3:AA:386:U:H2'	3:AA:387:C:C6	2.43	0.53
3:AA:745:C:H3'	3:AA:746:A:C8	2.43	0.53
8:AG:176:ASP:O	8:AG:180:ARG:HG2	2.09	0.53
9:AI:104:ILE:O	9:AI:108:ILE:HG13	2.08	0.53
23:Ab:62:ASP:OD1	23:Ab:62:ASP:N	2.41	0.53
26:Ae:228:HIS:O	26:Ae:232:GLU:HG3	2.08	0.53
28:Ag:264:VAL:HG11	28:Ag:307:LEU:HD13	1.91	0.53
3:AA:524:U:H2'	3:AA:525:U:C6	2.42	0.53
4:AB:161:CYS:SG	4:AB:253:GLN:HA	2.49	0.53
6:AE:154:VAL:HG22	35:Ao:108:LEU:HD21	1.91	0.53
9:AI:288:GLY:HA2	9:AI:327:HIS:CD2	2.44	0.53
14:AO:172:ARG:HG2	14:AO:172:ARG:HH11	1.74	0.53
26:Ae:69:LEU:HB2	26:Ae:405:LEU:HD23	1.89	0.53
29:Ah:323:HIS:CD2	29:Ah:361:LYS:HZ2	2.26	0.53
3:AA:841:C:H1'	20:AX:7:C:H42	1.73	0.53
8:AG:155:VAL:H	8:AG:227:HIS:CE1	2.27	0.53
17:AR:87:PRO:HA	17:AR:126:LYS:HB3	1.90	0.53
22:Aa:285:ARG:HH11	22:Aa:285:ARG:CG	2.20	0.53
23:Ab:8:THR:HG23	23:Ab:46:PHE:CD2	2.44	0.53
31:Aj:31:SER:HA	31:Aj:111:HIS:HD2	1.72	0.53
32:Ak:136:PRO:HG2	32:Ak:139:LEU:HD12	1.90	0.53
35:Ao:520:LYS:HG3	35:Ao:527:ARG:NH2	2.24	0.53
3:AA:640:A:H5''	6:AE:228:VAL:HG11	1.90	0.53
24:Ac:160:THR:HG22	24:Ac:162:LYS:H	1.74	0.53
31:Aj:64:LEU:HB3	31:Aj:134:VAL:HG13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BC:215:GLN:HE21	1:BC:599:ILE:HG22	1.73	0.53
3:AA:54:A:OP2	25:Ad:27:ARG:HG2	2.07	0.53
22:Aa:166:GLU:OE1	36:Ap:193:LEU:HD21	2.09	0.53
31:Aj:31:SER:HA	31:Aj:111:HIS:CD2	2.44	0.53
35:Ao:267:ARG:HH21	35:Ao:295:TYR:HB2	1.74	0.53
3:AA:739:A:H5'	3:AA:740:U:O4'	2.08	0.52
4:AB:58:ARG:O	4:AB:61:ILE:HG22	2.08	0.52
6:AE:289:THR:HG23	6:AE:331:ASP:O	2.08	0.52
26:Ae:188:MET:HG3	26:Ae:221:LEU:HD21	1.91	0.52
32:Ak:191:LYS:HD3	32:Ak:235:SER:HA	1.91	0.52
35:Ao:342:LEU:O	35:Ao:346:ARG:HG2	2.09	0.52
35:Ao:600:GLY:HA2	35:Ao:603:ARG:NE	2.24	0.52
9:AI:323:ARG:NH1	9:AI:327:HIS:CE1	2.76	0.52
35:Ao:432:LEU:HD23	35:Ao:472:GLU:HG2	1.90	0.52
35:Ao:653:MET:SD	35:Ao:665:ALA:HB1	2.49	0.52
1:BC:197:LEU:HD11	1:BC:234:ASP:HB2	1.90	0.52
1:BC:486:TRP:CD1	3:AA:256:G:HO2'	2.28	0.52
3:AA:498:U:OP1	34:An:161:ARG:HD3	2.08	0.52
6:AE:117:ARG:HG3	20:AX:10:C:H5'	1.91	0.52
18:AU:78:LYS:HE2	33:Am:111:PHE:HZ	1.73	0.52
24:Ac:139:CYS:HB2	24:Ac:141:CYS:HB2	1.90	0.52
32:Ak:166:ARG:NE	35:Ao:134:GLU:OE1	2.37	0.52
35:Ao:265:MET:HE2	35:Ao:281:LEU:HD11	1.90	0.52
3:AA:308:A:H2	24:Ac:68:LYS:HZ1	1.57	0.52
3:AA:752:A:H3'	3:AA:753:A:H5'	1.91	0.52
26:Ae:216:PRO:HB2	26:Ae:219:GLN:CD	2.34	0.52
28:Ag:80:HIS:HB3	28:Ag:155:PRO:HG3	1.91	0.52
35:Ao:160:ARG:HA	35:Ao:163:LEU:HD12	1.91	0.52
35:Ao:634:VAL:HG11	35:Ao:652:VAL:HG21	1.91	0.52
3:AA:182:A:N7	12:AL:55:ARG:NH1	2.57	0.52
26:Ae:80:TRP:HH2	26:Ae:151:THR:HG22	1.75	0.52
26:Ae:173:VAL:HG13	31:Aj:69:ASN:HB2	1.91	0.52
32:Ak:89:MET:HG2	32:Ak:90:GLY:N	2.23	0.52
32:Ak:246:THR:HG22	32:Ak:248:ALA:H	1.74	0.52
35:Ao:432:LEU:HB2	35:Ao:471:MET:HG2	1.92	0.52
1:BC:562:ASN:OD1	1:BC:589:LYS:NZ	2.40	0.52
3:AA:124:A:H2'	3:AA:125:U:N1	2.25	0.52
3:AA:870:G:O5'	3:AA:870:G:H8	1.93	0.52
26:Ae:377:ALA:O	26:Ae:380:SER:OG	2.19	0.52
35:Ao:147:PRO:HG3	35:Ao:160:ARG:HG2	1.89	0.52
35:Ao:602:PHE:HD1	35:Ao:609:PRO:HG3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Aa:353:PHE:CE2	22:Aa:358:ALA:HB2	2.45	0.52
24:Ac:94:SER:HB2	24:Ac:97:GLU:HG3	1.90	0.52
26:Ae:329:ALA:O	26:Ae:333:PRO:HD2	2.10	0.52
31:Aj:30:ASP:HB2	31:Aj:34:TYR:CE1	2.43	0.52
3:AA:635:C:H5''	4:AB:213:LYS:HE2	1.92	0.52
10:AJ:126:ILE:HD12	10:AJ:126:ILE:O	2.10	0.52
12:AL:93:CYS:SG	12:AL:125:VAL:HG23	2.50	0.52
16:AQ:96:THR:HG23	25:Ad:120:ARG:HH11	1.75	0.52
29:Ah:314:ASP:OD1	32:Ak:218:ARG:NH1	2.34	0.52
1:BC:285:LEU:HD22	1:BC:304:LEU:HD12	1.91	0.52
3:AA:353:C:C5'	3:AA:354:C:H5'	2.40	0.52
3:AA:561:U:H2'	3:AA:562:A:H5'	1.92	0.52
8:AG:155:VAL:H	8:AG:227:HIS:HE1	1.57	0.52
26:Ae:74:TYR:OH	26:Ae:416:TYR:HB3	2.09	0.52
32:Ak:69:PRO:HB3	32:Ak:120:ALA:HB2	1.92	0.52
9:AI:275:GLY:H	9:AI:348:ALA:HB2	1.75	0.52
22:Aa:298:VAL:HA	22:Aa:303:ILE:HD11	1.91	0.52
35:Ao:292:ALA:HB3	35:Ao:297:PHE:CE2	2.44	0.52
3:AA:804:A:C8	13:AN:85:VAL:HG12	2.45	0.51
9:AI:397:ARG:NH1	19:AV:32:A:P	2.84	0.51
13:AN:91:CYS:SG	13:AN:94:THR:HG22	2.49	0.51
26:Ae:147:TRP:HB3	26:Ae:423:TRP:CE3	2.45	0.51
35:Ao:390:LYS:O	35:Ao:393:SER:OG	2.24	0.51
6:AE:291:TYR:CZ	6:AE:358:THR:HG23	2.45	0.51
26:Ae:216:PRO:O	26:Ae:219:GLN:HG2	2.10	0.51
30:AI:60:ALA:O	30:AI:64:THR:HG23	2.10	0.51
35:Ao:129:GLN:NE2	35:Ao:144:TYR:OH	2.35	0.51
36:Ap:110:ASP:HB3	36:Ap:113:LEU:HD22	1.93	0.51
2:BT:60:PRO:HB3	26:Ae:127:HIS:ND1	2.25	0.51
5:AC:154:HIS:CG	32:Ak:77:PRO:HG3	2.45	0.51
7:AF:119:SER:OG	7:AF:120:THR:N	2.43	0.51
9:AI:264:ASP:HB2	9:AI:270:PHE:CE2	2.45	0.51
11:AK:135:ILE:HD11	11:AK:169:MET:HE2	1.92	0.51
24:Ac:156:PRO:HG2	24:Ac:159:MET:HG2	1.91	0.51
28:Ag:332:GLY:O	28:Ag:336:LEU:HB2	2.10	0.51
29:Ah:341:HIS:CE1	30:AI:24:ARG:HD2	2.46	0.51
35:Ao:617:PHE:CD2	35:Ao:633:LEU:HD11	2.39	0.51
3:AA:174:C:H2'	3:AA:175:A:O4'	2.10	0.51
3:AA:203:G:H2'	3:AA:204:U:C6	2.45	0.51
6:AE:317:HIS:HD2	6:AE:319:ALA:N	2.00	0.51
14:AO:96:LEU:HD13	14:AO:104:LYS:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AR:95:ARG:HH12	17:AR:102:GLY:CA	2.23	0.51
17:AR:133:ASP:HB3	17:AR:134:PRO:HD2	1.93	0.51
35:Ao:80:ARG:NH2	35:Ao:488:VAL:HG22	2.25	0.51
35:Ao:423:MET:HE1	35:Ao:463:LYS:HD2	1.91	0.51
35:Ao:565:GLN:HB2	35:Ao:572:PRO:HG3	1.92	0.51
3:AA:209:C:H2'	3:AA:210:U:C6	2.46	0.51
3:AA:344:G:N1	11:AK:121:ASN:HB3	2.22	0.51
5:AC:129:PRO:HB2	35:Ao:106:PHE:CE1	2.45	0.51
6:AE:131:ILE:HG13	6:AE:134:GLU:HB2	1.92	0.51
32:Ak:89:MET:HE3	32:Ak:106:GLU:HB3	1.91	0.51
35:Ao:412:ASP:HB3	35:Ao:413:PRO:HD2	1.93	0.51
6:AE:317:HIS:HB3	6:AE:320:ILE:HG13	1.93	0.51
3:AA:26:A:H2'	3:AA:27:U:C6	2.45	0.51
5:AC:72:HIS:CD2	5:AC:74:GLY:H	2.28	0.51
5:AC:138:TYR:CE1	30:Ai:70:LEU:HD13	2.46	0.51
6:AE:304:LYS:HZ3	6:AE:410:ASP:CG	2.19	0.51
28:Ag:386:ASN:HD22	28:Ag:389:GLN:H	1.58	0.51
32:Ak:88:ARG:HB3	32:Ak:98:PRO:HB2	1.92	0.51
3:AA:750:G:N1	3:AA:776:A:OP2	2.31	0.51
7:AF:92:ASN:CG	17:AR:118:LEU:HD22	2.36	0.51
9:AI:382:LYS:HD2	9:AI:388:ALA:HA	1.93	0.51
17:AR:112:ILE:HA	17:AR:121:MET:HE1	1.92	0.51
26:Ae:94:ALA:HA	26:Ae:131:TYR:HE2	1.76	0.51
3:AA:125:U:H2'	3:AA:126:A:O4'	2.11	0.51
3:AA:588:A:H5''	3:AA:589:C:OP2	2.11	0.51
11:AK:76:ARG:HH11	11:AK:81:LYS:HG2	1.72	0.51
17:AR:89:THR:OG1	18:AU:33:ASP:OD2	2.24	0.51
35:Ao:326:MET:HG3	35:Ao:331:VAL:HB	1.92	0.51
35:Ao:366:ILE:HG13	35:Ao:368:ILE:HG13	1.93	0.51
6:AE:219:ASP:OD1	6:AE:220:THR:N	2.44	0.51
6:AE:400:GLU:HG2	6:AE:401:VAL:H	1.76	0.51
11:AK:62:PHE:CE2	18:AU:15:GLN:HB2	2.46	0.51
13:AN:33:LYS:HD2	13:AN:36:ARG:HH21	1.75	0.51
13:AN:60:ASN:ND2	29:Ah:342:PHE:HD1	2.09	0.51
22:Aa:128:MET:HB3	22:Aa:132:GLN:HB2	1.93	0.51
29:Ah:287:GLN:HG3	35:Ao:448:TRP:CD1	2.46	0.51
29:Ah:343:MET:HE2	29:Ah:343:MET:HA	1.93	0.51
35:Ao:342:LEU:HD21	35:Ao:359:THR:HB	1.93	0.51
6:AE:289:THR:HG22	6:AE:290:ILE:H	1.76	0.50
35:Ao:538:MET:HE3	35:Ao:551:PHE:HD2	1.76	0.50
3:AA:876:A:N6	31:Aj:17:ARG:HH12	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AB:87:ARG:HB3	4:AB:90:LEU:HD12	1.93	0.50
19:AV:40:A:H2'	19:AV:41:A:C8	2.46	0.50
35:Ao:159:GLU:O	35:Ao:163:LEU:HG	2.10	0.50
28:Ag:111:LEU:HA	28:Ag:114:THR:HG23	1.93	0.50
35:Ao:543:HIS:CD2	35:Ao:588:ARG:HG3	2.44	0.50
1:BC:516:LEU:HG	1:BC:518:VAL:HG23	1.93	0.50
3:AA:740:U:H2'	3:AA:741:C:H5''	1.93	0.50
14:AO:210:LEU:HD22	34:An:173:LEU:HD13	1.92	0.50
1:BC:361:GLU:HB3	1:BC:524:VAL:HG11	1.93	0.50
3:AA:432:A:H4'	3:AA:433:U:H5''	1.93	0.50
3:AA:878:A:H2'	3:AA:879:A:O4'	2.12	0.50
1:BC:677:LYS:HE3	1:BC:680:LYS:HA	1.93	0.50
6:AE:368:LEU:HD12	22:Aa:127:LEU:HB3	1.93	0.50
15:AP:81:ALA:O	25:Ad:71:ARG:NH2	2.44	0.50
24:Ac:74:PRO:HD2	24:Ac:91:GLU:OE1	2.11	0.50
26:Ae:191:PHE:HE2	26:Ae:203:VAL:HG21	1.75	0.50
26:Ae:218:THR:O	26:Ae:222:SER:N	2.30	0.50
31:Aj:41:MET:HG2	31:Aj:55:TRP:NE1	2.27	0.50
35:Ao:302:GLU:HA	35:Ao:344:CYS:SG	2.52	0.50
35:Ao:509:LEU:HD23	35:Ao:547:LEU:HD13	1.94	0.50
1:BC:257:LEU:HD11	1:BC:269:THR:HG23	1.94	0.50
3:AA:561:U:H1'	3:AA:711:A:H62	1.75	0.50
3:AA:857:C:H2'	3:AA:858:C:C6	2.46	0.50
13:AN:125:ARG:HG2	13:AN:125:ARG:NH1	2.18	0.50
26:Ae:119:ILE:HG23	26:Ae:124:ASP:HB2	1.93	0.50
35:Ao:580:ASN:HA	35:Ao:613:LEU:HD13	1.94	0.50
1:BC:179:ARG:HG2	1:BC:180:SER:H	1.77	0.50
17:AR:128:PRO:HA	17:AR:131:LEU:CD2	2.42	0.50
22:Aa:150:MET:HE1	22:Aa:291:GLY:CA	2.41	0.50
26:Ae:409:GLU:O	26:Ae:413:ILE:HG13	2.12	0.50
28:Ag:188:LYS:HE2	28:Ag:229:ILE:HG23	1.93	0.50
31:Aj:145:HIS:CD2	31:Aj:146:GLU:HG2	2.47	0.50
35:Ao:262:TYR:CD1	35:Ao:262:TYR:C	2.90	0.50
35:Ao:372:LEU:O	35:Ao:418:PHE:HB2	2.12	0.50
36:Ap:93:MET:HE2	36:Ap:145:LYS:HD3	1.94	0.50
4:AB:123:HIS:CE1	23:Ab:41:LEU:HD12	2.47	0.50
6:AE:296:LEU:HD11	6:AE:303:ILE:HD12	1.94	0.50
35:Ao:469:CYS:SG	35:Ao:498:ASP:HB3	2.52	0.50
35:Ao:538:MET:HE3	35:Ao:551:PHE:CD2	2.47	0.50
4:AB:151:ALA:HB3	18:AU:87:CYS:SG	2.52	0.49
6:AE:304:LYS:NZ	6:AE:410:ASP:CG	2.70	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Ag:275:ARG:HE	28:Ag:281:ILE:HG22	1.76	0.49
35:Ao:335:LEU:HB2	35:Ao:368:ILE:HG21	1.94	0.49
1:BC:392:CYS:HB3	1:BC:423:ASP:HB2	1.94	0.49
1:BC:559:ASN:HB2	3:AA:180:U:OP1	2.12	0.49
4:AB:81:ARG:HD2	27:Af:84:MET:HE3	1.93	0.49
16:AQ:35:LEU:HB2	16:AQ:42:TYR:CE1	2.47	0.49
26:Ae:122:ARG:HB2	26:Ae:159:TYR:CE2	2.47	0.49
32:Ak:255:TRP:CD1	32:Ak:295:ARG:HG2	2.47	0.49
33:Am:95:GLU:OE2	33:Am:101:PRO:HD3	2.12	0.49
3:AA:916:A:H2'	3:AA:917:C:O4'	2.12	0.49
4:AB:166:HIS:CE1	9:AI:153:THR:HA	2.47	0.49
18:AU:78:LYS:HE2	33:Am:111:PHE:CZ	2.47	0.49
22:Aa:211:ARG:O	22:Aa:215:ILE:HG13	2.12	0.49
3:AA:512:A:H2'	3:AA:513:A:C8	2.48	0.49
8:AG:112:THR:HG23	28:Ag:396:TYR:HB3	1.94	0.49
9:AI:284:VAL:HG22	9:AI:331:CYS:SG	2.53	0.49
15:AP:67:ALA:HB1	22:Aa:183:ILE:HD12	1.93	0.49
26:Ae:185:ASN:OD1	26:Ae:220:LEU:HD22	2.12	0.49
30:AI:19:PHE:CZ	32:Ak:199:ARG:NH1	2.81	0.49
1:BC:215:GLN:NE2	1:BC:599:ILE:H	2.11	0.49
21:AZ:695:ALA:HB2	30:AI:10:ARG:NH1	2.26	0.49
26:Ae:257:ASN:HD22	26:Ae:260:GLY:H	1.60	0.49
26:Ae:286:ASN:O	31:Aj:70:ARG:NH2	2.46	0.49
29:Ah:324:ILE:HD12	32:Ak:213:ARG:HH11	1.78	0.49
34:An:163:ARG:HH11	34:An:163:ARG:HB2	1.78	0.49
5:AC:50:PRO:HB3	5:AC:167:ILE:HG13	1.95	0.49
24:Ac:23:PHE:HZ	24:Ac:30:MET:HE3	1.77	0.49
26:Ae:434:GLU:O	26:Ae:438:ARG:HG3	2.12	0.49
3:AA:195:G:H5''	15:AP:20:ARG:HB2	1.94	0.49
4:AB:131:THR:HG22	4:AB:256:ILE:HD11	1.95	0.49
8:AG:238:HIS:CE1	11:AK:128:ILE:HG13	2.46	0.49
10:AJ:158:GLU:HG2	35:Ao:70:ILE:HG21	1.92	0.49
28:Ag:243:LEU:HG	28:Ag:295:MET:HE3	1.95	0.49
35:Ao:421:SER:HA	35:Ao:424:ARG:HB3	1.94	0.49
35:Ao:587:LEU:HD12	35:Ao:620:SER:HB2	1.95	0.49
6:AE:400:GLU:H	6:AE:400:GLU:CD	2.19	0.49
25:Ad:159:GLN:O	25:Ad:163:GLU:HG2	2.13	0.49
29:Ah:343:MET:HE1	29:Ah:368:PHE:CD2	2.47	0.49
35:Ao:417:MET:HA	35:Ao:420:GLN:HB3	1.95	0.49
1:BC:184:THR:OG1	1:BC:255:VAL:HG12	2.12	0.49
1:BC:394:ALA:HB2	1:BC:421:TRP:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AA:53:A:OP1	25:Ad:38:LYS:HE3	2.12	0.49
3:AA:285:C:H1'	3:AA:488:A:C2	2.47	0.49
5:AC:73:THR:HG23	10:AJ:169:ALA:HB2	1.95	0.49
11:AK:167:LEU:O	11:AK:172:LEU:HB3	2.13	0.49
15:AP:59:ASN:ND2	24:Ac:146:GLN:HE22	2.08	0.49
26:Ae:378:LEU:O	26:Ae:382:LEU:HG	2.12	0.49
36:Ap:55:PRO:HD2	36:Ap:56:TRP:CE3	2.47	0.49
3:AA:87:U:H2'	3:AA:88:C:H6	1.77	0.49
3:AA:887:U:H2'	3:AA:888:A:H8	1.78	0.49
27:Af:155:LEU:HD11	33:Am:27:LEU:HB3	1.95	0.49
29:Ah:340:ARG:O	29:Ah:344:GLU:HB2	2.13	0.49
35:Ao:342:LEU:HD22	35:Ao:356:ALA:HB1	1.94	0.49
35:Ao:468:LEU:O	35:Ao:477:THR:HG22	2.13	0.49
3:AA:928:A:O2'	3:AA:929:A:H5'	2.12	0.48
6:AE:305:MET:HE2	6:AE:332:LEU:HD11	1.94	0.48
10:AJ:178:GLU:O	32:Ak:151:ILE:HB	2.12	0.48
13:AN:71:ALA:O	13:AN:74:GLU:HB2	2.13	0.48
17:AR:68:LEU:HB2	17:AR:104:LYS:HG3	1.95	0.48
18:AU:83:PRO:HG2	18:AU:84:TRP:CD1	2.47	0.48
24:Ac:10:ARG:HA	24:Ac:15:TYR:CD2	2.48	0.48
32:Ak:199:ARG:H	32:Ak:199:ARG:HD2	1.77	0.48
35:Ao:86:PRO:HG2	35:Ao:89:PHE:CD2	2.47	0.48
35:Ao:559:LYS:HE2	35:Ao:578:SER:HB3	1.96	0.48
35:Ao:582:VAL:HG11	35:Ao:598:MET:HG3	1.95	0.48
3:AA:128:C:H2'	3:AA:129:G:O4'	2.13	0.48
3:AA:922:C:H2'	3:AA:923:G:O4'	2.13	0.48
8:AG:82:THR:HA	9:AI:316:PHE:CD2	2.48	0.48
9:AI:73:PHE:O	9:AI:77:GLN:HG2	2.12	0.48
28:Ag:294:LYS:HG2	28:Ag:297:LYS:NZ	2.27	0.48
29:Ah:324:ILE:CD1	32:Ak:213:ARG:HD3	2.43	0.48
1:BC:394:ALA:HB2	1:BC:421:TRP:CD2	2.48	0.48
3:AA:115:A:OP2	14:AO:201:HIS:HE1	1.96	0.48
4:AB:102:GLU:N	4:AB:103:PRO:HD2	2.28	0.48
22:Aa:104:MET:HB3	22:Aa:290:PHE:HE1	1.78	0.48
26:Ae:228:HIS:HA	26:Ae:231:ALA:HB3	1.94	0.48
35:Ao:478:LEU:HD21	35:Ao:511:MET:HG3	1.94	0.48
35:Ao:503:LEU:HD22	35:Ao:508:ARG:HB2	1.95	0.48
5:AC:113:ARG:O	5:AC:116:GLN:HG2	2.14	0.48
6:AE:122:ARG:HB2	6:AE:183:ARG:HH21	1.78	0.48
7:AF:113:LEU:HD21	27:Af:155:LEU:HA	1.94	0.48
13:AN:58:ARG:NH1	13:AN:58:ARG:HB3	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Ab:8:THR:HG23	23:Ab:46:PHE:HD2	1.78	0.48
28:Ag:111:LEU:HD23	28:Ag:114:THR:HG21	1.95	0.48
29:Ah:334:PRO:HG2	29:Ah:339:ILE:HB	1.94	0.48
3:AA:561:U:H1'	3:AA:711:A:N6	2.28	0.48
3:AA:562:A:C2'	3:AA:708:A:H61	2.25	0.48
3:AA:577:C:O3'	10:AJ:128:LYS:HD2	2.13	0.48
6:AE:278:TYR:HB3	23:Ab:6:LEU:HD21	1.96	0.48
10:AJ:83:HIS:CE1	13:AN:122:GLY:HA3	2.48	0.48
15:AP:27:THR:O	15:AP:28:ASN:HB2	2.13	0.48
26:Ae:248:LEU:HD22	26:Ae:266:TYR:HB3	1.95	0.48
27:Af:162:THR:HB	27:Af:164:LEU:HD23	1.95	0.48
28:Ag:330:LYS:O	28:Ag:334:ASP:HB2	2.13	0.48
30:Ai:19:PHE:HZ	32:Ak:196:VAL:HG13	1.77	0.48
6:AE:122:ARG:HB2	6:AE:183:ARG:NH2	2.29	0.48
8:AG:70:LYS:HB3	8:AG:72:GLN:HG3	1.95	0.48
25:Ad:48:VAL:HG21	36:Ap:220:TYR:CD2	2.49	0.48
26:Ae:80:TRP:CD1	26:Ae:154:ARG:HB3	2.48	0.48
27:Af:115:ILE:HG21	27:Af:143:LEU:HD11	1.94	0.48
27:Af:150:LEU:HB2	27:Af:163:ILE:HG21	1.95	0.48
31:Aj:171:ARG:HH11	31:Aj:171:ARG:HG3	1.77	0.48
3:AA:87:U:H2'	3:AA:88:C:C6	2.48	0.48
6:AE:216:ASP:OD1	6:AE:216:ASP:N	2.46	0.48
16:AQ:94:PRO:HB3	24:Ac:77:ARG:NH2	2.28	0.48
26:Ae:113:SER:HA	26:Ae:148:THR:HG23	1.95	0.48
26:Ae:266:TYR:CE2	26:Ae:316:CYS:HB3	2.49	0.48
35:Ao:559:LYS:NZ	35:Ao:578:SER:O	2.46	0.48
1:BC:396:VAL:HG13	1:BC:418:ILE:HG23	1.96	0.48
6:AE:112:LYS:HB3	6:AE:114:ARG:HG3	1.95	0.48
35:Ao:372:LEU:HD13	35:Ao:419:PHE:HZ	1.78	0.48
5:AC:128:PRO:HD2	5:AC:131:LYS:HD2	1.95	0.48
16:AQ:57:GLN:O	16:AQ:87:LYS:NZ	2.47	0.48
24:Ac:24:LYS:HG3	24:Ac:107:GLY:O	2.13	0.48
24:Ac:27:VAL:HG21	24:Ac:106:LEU:HD13	1.95	0.48
26:Ae:110:LEU:HD11	26:Ae:430:LEU:HB3	1.96	0.48
28:Ag:265:ASN:HD21	28:Ag:310:SER:H	1.62	0.48
28:Ag:379:LEU:O	28:Ag:383:SER:OG	2.27	0.48
1:BC:179:ARG:HD3	1:BC:347:LEU:HB3	1.94	0.48
9:AI:88:LEU:HD11	9:AI:107:ALA:HB1	1.96	0.48
9:AI:387:GLY:O	9:AI:388:ALA:HB3	2.14	0.48
10:AJ:52:VAL:HG13	35:Ao:479:LYS:HD3	1.96	0.48
22:Aa:282:ASP:OD1	22:Aa:282:ASP:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Ae:265:LEU:HD21	26:Ae:302:VAL:HB	1.96	0.48
28:Ag:203:VAL:HG13	28:Ag:245:GLU:HG2	1.95	0.48
3:AA:551:G:C2	3:AA:552:A:C8	3.02	0.47
10:AJ:136:MET:HE3	13:AN:123:VAL:HG22	1.95	0.47
21:AZ:708:ALA:HB2	32:Ak:226:TYR:CE2	2.49	0.47
26:Ae:281:ARG:HA	26:Ae:284:TYR:CE2	2.49	0.47
28:Ag:123:TYR:HE1	28:Ag:340:ILE:HD12	1.79	0.47
35:Ao:378:VAL:O	35:Ao:382:PHE:HB2	2.14	0.47
1:BC:239:ALA:HB3	1:BC:727:PHE:HB2	1.96	0.47
1:BC:370:LEU:HB2	1:BC:421:TRP:HB2	1.97	0.47
1:BC:669:TRP:CZ3	1:BC:696:LEU:HD22	2.49	0.47
3:AA:327:U:O2'	3:AA:328:A:N7	2.40	0.47
6:AE:93:LEU:H	30:Ai:75:HIS:HD2	1.60	0.47
6:AE:198:TRP:HB2	6:AE:225:VAL:CG1	2.45	0.47
19:AV:24:U:H2'	19:AV:25:C:C6	2.50	0.47
35:Ao:455:HIS:HA	35:Ao:458:ASN:ND2	2.29	0.47
4:AB:262:LYS:O	4:AB:266:VAL:HG23	2.14	0.47
7:AF:32:ARG:HD2	7:AF:77:SER:OG	2.14	0.47
8:AG:46:ILE:HG12	9:AI:316:PHE:HZ	1.78	0.47
9:AI:316:PHE:HB3	9:AI:317:PRO:HD3	1.97	0.47
28:Ag:123:TYR:CE1	28:Ag:340:ILE:HD12	2.49	0.47
28:Ag:386:ASN:HD22	28:Ag:389:GLN:HB2	1.78	0.47
1:BC:213:ILE:HG23	1:BC:238:HIS:CE1	2.50	0.47
6:AE:296:LEU:HD22	6:AE:352:GLY:HA3	1.96	0.47
26:Ae:322:VAL:HG22	26:Ae:325:ARG:CZ	2.44	0.47
9:AI:207:GLU:HG3	9:AI:212:GLU:O	2.15	0.47
13:AN:62:ILE:HG21	29:Ah:341:HIS:HB3	1.96	0.47
14:AO:116:VAL:HG21	14:AO:186:LEU:HD21	1.96	0.47
22:Aa:197:ARG:HH11	22:Aa:197:ARG:HG3	1.78	0.47
26:Ae:130:TYR:HD2	26:Ae:131:TYR:CD1	2.33	0.47
28:Ag:216:GLU:O	28:Ag:219:ARG:HG2	2.13	0.47
3:AA:866:U:H2'	3:AA:867:G:C8	2.49	0.47
10:AJ:52:VAL:HG21	35:Ao:479:LYS:CB	2.43	0.47
28:Ag:209:TRP:CH2	28:Ag:224:VAL:HG13	2.49	0.47
1:BC:198:ASP:OD1	1:BC:205:VAL:HG22	2.15	0.47
1:BC:467:ARG:NH2	3:AA:246:A:O2'	2.48	0.47
3:AA:283:U:OP1	6:AE:419:ARG:NH1	2.47	0.47
3:AA:394:U:H4'	3:AA:395:C:H5''	1.95	0.47
4:AB:81:ARG:HD2	27:Af:84:MET:CE	2.45	0.47
4:AB:146:ARG:NH1	4:AB:146:ARG:HG3	2.29	0.47
4:AB:168:ARG:HG3	9:AI:159:TYR:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AE:427:ARG:NH1	6:AE:427:ARG:CG	2.76	0.47
7:AF:6:LEU:HB3	7:AF:66:VAL:HB	1.96	0.47
9:AI:101:GLN:HA	9:AI:104:ILE:HD12	1.96	0.47
9:AI:311:ARG:NH1	28:Ag:382:LEU:O	2.47	0.47
9:AI:358:THR:HG23	9:AI:360:ASP:H	1.79	0.47
10:AJ:68:GLU:HB2	35:Ao:62:LYS:HE2	1.96	0.47
11:AK:67:PRO:HB3	11:AK:73:ASN:HD22	1.80	0.47
11:AK:75:LEU:O	11:AK:76:ARG:HD3	2.15	0.47
11:AK:175:ILE:O	18:AU:14:VAL:HG13	2.15	0.47
26:Ae:188:MET:O	26:Ae:192:ILE:HG13	2.15	0.47
26:Ae:254:LYS:HB2	26:Ae:260:GLY:HA3	1.95	0.47
31:Aj:42:MET:HE2	31:Aj:42:MET:HB2	1.75	0.47
32:Ak:164:SER:HA	35:Ao:134:GLU:HB2	1.97	0.47
32:Ak:268:LEU:O	32:Ak:272:LYS:HG2	2.15	0.47
35:Ao:419:PHE:CZ	35:Ao:450:LEU:HD22	2.50	0.47
7:AF:94:VAL:HG12	7:AF:95:LYS:O	2.15	0.47
9:AI:286:VAL:HB	9:AI:329:MET:HE3	1.96	0.47
18:AU:52:ARG:CG	18:AU:52:ARG:NH1	2.78	0.47
32:Ak:89:MET:HE2	32:Ak:89:MET:HB3	1.72	0.47
3:AA:59:C:C2	31:Aj:54:ALA:HB1	2.50	0.47
3:AA:244:C:H5''	3:AA:245:C:C6	2.50	0.47
6:AE:290:ILE:HD12	6:AE:294:ILE:HD12	1.95	0.47
8:AG:40:GLU:H	8:AG:40:GLU:HG3	1.41	0.47
14:AO:171:LEU:HB3	14:AO:179:PHE:HB2	1.97	0.47
16:AQ:93:ASP:OD2	16:AQ:96:THR:OG1	2.33	0.47
3:AA:308:A:H3'	3:AA:309:A:C5'	2.45	0.47
6:AE:198:TRP:HB2	6:AE:225:VAL:HG11	1.97	0.47
14:AO:150:ASP:OD2	14:AO:153:HIS:HD2	1.98	0.47
17:AR:66:CYS:HB3	17:AR:101:CYS:H	1.80	0.47
28:Ag:122:ARG:HA	28:Ag:305:ILE:HG13	1.97	0.47
28:Ag:160:TRP:N	28:Ag:160:TRP:CD1	2.83	0.47
29:Ah:289:GLY:HA3	32:Ak:74:VAL:HG21	1.97	0.47
32:Ak:85:LEU:H	32:Ak:85:LEU:HG	1.45	0.47
32:Ak:218:ARG:HG3	32:Ak:219:GLN:N	2.30	0.47
3:AA:841:C:H1'	20:AX:7:C:N4	2.30	0.46
10:AJ:161:GLN:CG	10:AJ:170:MET:HE1	2.45	0.46
12:AL:62:VAL:HG21	12:AL:102:LEU:HD22	1.98	0.46
28:Ag:137:LEU:HD11	28:Ag:260:ALA:HB1	1.97	0.46
32:Ak:165:ILE:CG1	35:Ao:135:PRO:HD3	2.44	0.46
1:BC:253:ASP:O	1:BC:281:VAL:HG13	2.16	0.46
3:AA:287:C:C2	24:Ac:11:ARG:NH2	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AA:334:U:H2'	3:AA:335:A:C8	2.50	0.46
3:AA:729:A:H2'	3:AA:730:C:O4'	2.16	0.46
3:AA:873:A:H4'	14:AO:225:LYS:HZ2	1.80	0.46
4:AB:130:PHE:HE1	4:AB:191:LEU:HD13	1.81	0.46
6:AE:206:PRO:HG2	6:AE:215:TYR:HD2	1.80	0.46
12:AL:78:ARG:HH12	12:AL:117:ASP:CG	2.23	0.46
14:AO:112:LEU:HD23	14:AO:131:VAL:HG13	1.97	0.46
24:Ac:32:VAL:HB	24:Ac:66:MET:HG3	1.96	0.46
26:Ae:149:ILE:O	26:Ae:153:ILE:HG13	2.14	0.46
26:Ae:405:LEU:O	26:Ae:409:GLU:HG3	2.14	0.46
3:AA:275:U:H2'	3:AA:276:U:C6	2.50	0.46
3:AA:490:A:H2'	3:AA:491:G:O4'	2.15	0.46
3:AA:622:U:H2'	3:AA:623:C:C6	2.51	0.46
3:AA:703:U:H2'	3:AA:704:U:H6	1.81	0.46
3:AA:706:G:H3'	3:AA:707:A:H5''	1.96	0.46
3:AA:723:U:O4	3:AA:738:U:O2'	2.30	0.46
4:AB:70:ASP:O	4:AB:72:PHE:N	2.48	0.46
6:AE:396:GLU:CD	6:AE:397:PRO:HD2	2.41	0.46
8:AG:70:LYS:HD2	8:AG:72:GLN:HE21	1.81	0.46
8:AG:180:ARG:HB3	8:AG:180:ARG:NH1	2.23	0.46
23:Ab:67:GLU:H	23:Ab:67:GLU:HG3	1.37	0.46
25:Ad:88:GLY:O	25:Ad:92:GLU:HG2	2.16	0.46
30:Ai:5:SER:OG	30:Ai:6:GLU:N	2.48	0.46
31:Aj:95:TRP:CE3	31:Aj:131:ILE:HG12	2.49	0.46
35:Ao:292:ALA:HB1	35:Ao:296:THR:HB	1.98	0.46
35:Ao:596:TRP:HB2	35:Ao:617:PHE:CZ	2.49	0.46
3:AA:225:A:N1	3:AA:272:A:O2'	2.43	0.46
3:AA:959:U:H5'	33:Am:25:LYS:HZ2	1.77	0.46
5:AC:49:LYS:O	5:AC:166:TYR:HB2	2.15	0.46
19:AV:15:A:O2'	19:AV:16:A:O4'	2.32	0.46
22:Aa:245:GLN:O	22:Aa:248:ASP:N	2.46	0.46
26:Ae:80:TRP:CE3	26:Ae:83:ARG:HD2	2.50	0.46
27:Af:173:LEU:HD23	27:Af:173:LEU:H	1.81	0.46
28:Ag:211:LYS:HE3	28:Ag:212:ARG:HE	1.80	0.46
35:Ao:379:ILE:HG23	35:Ao:396:ILE:HG21	1.96	0.46
3:AA:168:A:H2'	3:AA:169:A:C8	2.51	0.46
6:AE:180:ASP:O	6:AE:184:LYS:HG2	2.15	0.46
6:AE:358:THR:HB	6:AE:361:GLN:HG3	1.97	0.46
8:AG:88:ASP:HA	8:AG:89:PRO:HD2	1.76	0.46
9:AI:316:PHE:CD1	9:AI:370:LEU:HD21	2.51	0.46
22:Aa:285:ARG:CG	22:Aa:285:ARG:NH1	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Ah:334:PRO:O	29:Ah:340:ARG:HG2	2.14	0.46
35:Ao:434:LEU:O	35:Ao:438:VAL:HG23	2.16	0.46
36:Ap:79:ARG:NH1	36:Ap:86:PRO:HB2	2.31	0.46
6:AE:122:ARG:NH1	20:AX:13:U:O2'	2.49	0.46
9:AI:150:LEU:HD23	9:AI:150:LEU:HA	1.65	0.46
9:AI:379:GLU:OE2	9:AI:389:ARG:NH2	2.48	0.46
10:AJ:92:GLU:HG3	10:AJ:108:VAL:HG11	1.96	0.46
11:AK:181:THR:H	18:AU:10:ARG:HH12	1.64	0.46
12:AL:82:ARG:NE	12:AL:90:GLU:OE2	2.31	0.46
15:AP:41:CYS:HB2	15:AP:42:PRO:HD2	1.98	0.46
16:AQ:32:ARG:NH2	16:AQ:49:TYR:OH	2.49	0.46
22:Aa:88:ARG:HD3	22:Aa:88:ARG:HA	1.71	0.46
22:Aa:148:LEU:HA	22:Aa:148:LEU:HD23	1.63	0.46
24:Ac:30:MET:HG3	24:Ac:78:PHE:CE2	2.51	0.46
26:Ae:100:THR:HG22	26:Ae:103:ARG:NH2	2.30	0.46
28:Ag:296:VAL:HG12	28:Ag:305:ILE:HD12	1.98	0.46
35:Ao:86:PRO:HG2	35:Ao:89:PHE:HD2	1.81	0.46
35:Ao:423:MET:CE	35:Ao:460:TYR:HA	2.45	0.46
14:AO:171:LEU:HA	14:AO:171:LEU:HD23	1.74	0.46
17:AR:68:LEU:O	17:AR:69:CYS:C	2.59	0.46
32:Ak:153:ILE:HG12	32:Ak:221:TYR:HE1	1.81	0.46
3:AA:739:A:C6	8:AG:197:ARG:NH1	2.84	0.46
3:AA:942:G:O6	34:An:145:LYS:HE3	2.16	0.46
4:AB:87:ARG:HD3	27:Af:118:GLY:O	2.15	0.46
6:AE:163:GLU:HA	6:AE:166:GLU:HG2	1.98	0.46
10:AJ:170:MET:HB3	32:Ak:159:VAL:CG1	2.46	0.46
22:Aa:245:GLN:HE22	36:Ap:164:ARG:NE	2.13	0.46
22:Aa:281:TYR:CD2	22:Aa:306:LEU:HD13	2.51	0.46
24:Ac:7:PHE:O	24:Ac:10:ARG:HG2	2.16	0.46
31:Aj:78:ARG:HE	31:Aj:78:ARG:HB3	1.49	0.46
1:BC:439:ARG:NH1	1:BC:442:GLU:OE1	2.48	0.46
6:AE:197:THR:HG22	6:AE:199:GLY:N	2.20	0.46
9:AI:265:GLU:C	9:AI:267:GLY:H	2.23	0.46
22:Aa:108:ASP:O	22:Aa:112:ILE:HG12	2.16	0.46
26:Ae:239:GLU:HA	26:Ae:242:ARG:HD3	1.98	0.46
26:Ae:327:LEU:HD23	26:Ae:327:LEU:HA	1.84	0.46
29:Ah:324:ILE:HD12	32:Ak:213:ARG:NH1	2.31	0.46
1:BC:655:LYS:HZ1	1:BC:674:THR:C	2.23	0.46
3:AA:724:U:OP1	8:AG:195:LYS:NZ	2.49	0.46
8:AG:96:ASN:OD1	8:AG:104:LYS:HE3	2.16	0.46
9:AI:382:LYS:HB2	9:AI:385:GLN:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AR:79:GLN:HB2	25:Ad:188:ASN:OD1	2.15	0.46
22:Aa:230:VAL:HG13	22:Aa:233:LYS:NZ	2.31	0.46
32:Ak:165:ILE:H	35:Ao:134:GLU:HB2	1.81	0.46
35:Ao:442:LEU:HD22	35:Ao:460:TYR:CZ	2.51	0.46
1:BC:555:ASP:OD1	1:BC:555:ASP:N	2.49	0.45
3:AA:91:A:H2'	3:AA:92:A:O4'	2.16	0.45
3:AA:498:U:H5'	3:AA:499:C:OP2	2.16	0.45
3:AA:667:C:H5'	3:AA:668:A:OP2	2.16	0.45
5:AC:92:LEU:HD13	5:AC:119:ILE:HD11	1.97	0.45
11:AK:155:GLY:H	11:AK:181:THR:HG23	1.80	0.45
13:AN:53:ARG:HE	29:Ah:364:HIS:CD2	2.23	0.45
25:Ad:54:PHE:CD2	36:Ap:208:PRO:HB3	2.50	0.45
31:Aj:84:SER:HB2	31:Aj:138:ASP:OD2	2.16	0.45
35:Ao:484:LEU:O	35:Ao:488:VAL:HG23	2.15	0.45
2:BT:59:LYS:HA	2:BT:60:PRO:HD3	1.77	0.45
3:AA:258:C:C5	6:AE:119:LYS:HE3	2.52	0.45
3:AA:307:A:H2'	3:AA:308:A:H4'	1.99	0.45
3:AA:491:G:H5''	3:AA:492:U:OP2	2.17	0.45
3:AA:625:U:H5	3:AA:659:A:OP1	1.99	0.45
9:AI:386:GLU:HB3	9:AI:390:ARG:HG2	1.98	0.45
11:AK:102:VAL:HG12	11:AK:106:HIS:HA	1.98	0.45
22:Aa:293:MET:HE2	22:Aa:293:MET:HB2	1.92	0.45
24:Ac:29:VAL:HB	24:Ac:79:TYR:HB2	1.97	0.45
30:AI:86:LYS:HG3	30:AI:89:ARG:NH2	2.31	0.45
35:Ao:527:ARG:O	35:Ao:531:LYS:HE3	2.16	0.45
3:AA:262:C:H2'	3:AA:263:G:C8	2.52	0.45
3:AA:677:C:H2'	3:AA:678:G:O4'	2.16	0.45
5:AC:80:ASP:HB3	5:AC:81:HIS:CD2	2.50	0.45
9:AI:86:ARG:NH1	9:AI:96:PRO:HB2	2.30	0.45
19:AV:54:A:O2'	19:AV:55:C:H6	2.00	0.45
35:Ao:419:PHE:CE2	35:Ao:450:LEU:HD13	2.51	0.45
35:Ao:596:TRP:HB2	35:Ao:617:PHE:HZ	1.81	0.45
36:Ap:136:HIS:HD2	36:Ap:139:TYR:H	1.64	0.45
1:BC:335:ALA:O	1:BC:339:VAL:HG23	2.17	0.45
1:BC:628:ILE:HD13	1:BC:704:GLN:O	2.17	0.45
6:AE:124:LYS:HD3	6:AE:183:ARG:NH1	2.31	0.45
13:AN:70:VAL:HG21	29:Ah:378:ILE:HD13	1.99	0.45
14:AO:144:MET:HE3	14:AO:153:HIS:HB2	1.97	0.45
18:AU:25:THR:O	18:AU:29:ILE:HG12	2.16	0.45
26:Ae:230:LEU:HD22	26:Ae:394:LEU:HD22	1.98	0.45
30:AI:85:LEU:HD23	30:AI:85:LEU:HA	1.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AA:800:G:H2'	3:AA:801:A:C8	2.51	0.45
6:AE:124:LYS:HZ3	30:Ai:85:LEU:HD11	1.82	0.45
8:AG:180:ARG:HG2	8:AG:180:ARG:H	1.41	0.45
12:AL:59:LYS:HE3	12:AL:130:TYR:CZ	2.52	0.45
18:AU:50:ARG:HD2	18:AU:50:ARG:HA	1.66	0.45
29:Ah:278:LEU:HD11	35:Ao:411:ARG:HA	1.98	0.45
33:Am:6:LEU:HD12	33:Am:6:LEU:HA	1.66	0.45
3:AA:371:A:H8	3:AA:371:A:OP1	1.98	0.45
3:AA:960:A:H5'	3:AA:961:C:OP1	2.16	0.45
8:AG:121:LYS:NZ	8:AG:207:GLN:HA	2.32	0.45
22:Aa:189:HIS:CD2	36:Ap:173:ARG:HD3	2.52	0.45
25:Ad:171:GLU:CD	25:Ad:171:GLU:H	2.25	0.45
28:Ag:116:PHE:HB3	28:Ag:302:GLY:HA2	1.98	0.45
1:BC:322:PRO:O	1:BC:330:ASN:HB2	2.16	0.45
3:AA:131:U:H1'	16:AQ:23:GLN:HE21	1.82	0.45
5:AC:99:THR:C	5:AC:101:PRO:HD3	2.41	0.45
10:AJ:79:LEU:HD12	10:AJ:141:ARG:O	2.17	0.45
22:Aa:91:THR:H	22:Aa:94:ASP:CG	2.25	0.45
22:Aa:197:ARG:HH11	22:Aa:197:ARG:CG	2.29	0.45
26:Ae:358:LEU:HB2	26:Ae:361:GLU:HB2	1.97	0.45
29:Ah:323:HIS:CD2	29:Ah:361:LYS:HZ1	2.20	0.45
35:Ao:314:GLU:O	35:Ao:318:ASN:ND2	2.50	0.45
35:Ao:376:HIS:NE2	35:Ao:417:MET:HB3	2.32	0.45
3:AA:767:U:H2'	3:AA:768:A:C8	2.52	0.45
3:AA:846:C:H2'	3:AA:847:C:O4'	2.17	0.45
6:AE:173:VAL:O	6:AE:177:GLU:HG2	2.17	0.45
9:AI:274:GLU:HG2	9:AI:283:GLU:HG2	1.99	0.45
16:AQ:96:THR:HG22	25:Ad:117:HIS:CE1	2.51	0.45
24:Ac:28:LYS:O	24:Ac:62:VAL:HG13	2.17	0.45
28:Ag:173:ASN:HB2	28:Ag:176:ARG:HB2	1.98	0.45
31:Aj:63:ARG:NH1	31:Aj:111:HIS:HE1	2.13	0.45
1:BC:407:ILE:HD11	1:BC:416:VAL:HG22	1.99	0.45
3:AA:532:G:O2'	3:AA:533:C:H5'	2.16	0.45
3:AA:709:A:H8	3:AA:709:A:OP2	1.99	0.45
3:AA:740:U:H2'	3:AA:741:C:O4'	2.17	0.45
22:Aa:245:GLN:HE22	36:Ap:164:ARG:HE	1.65	0.45
26:Ae:136:ARG:HG3	26:Ae:176:GLY:HA3	1.98	0.45
29:Ah:288:ASN:ND2	29:Ah:289:GLY:H	2.15	0.45
31:Aj:98:THR:HG22	31:Aj:99:ARG:HG2	1.99	0.45
1:BC:180:SER:OG	1:BC:229:LYS:O	2.34	0.45
6:AE:162:LYS:O	6:AE:166:GLU:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AE:243:VAL:HG11	6:AE:268:PHE:CE1	2.52	0.45
16:AQ:22:MET:HG3	16:AQ:25:THR:HB	1.99	0.45
28:Ag:223:GLU:O	28:Ag:227:GLN:HB2	2.17	0.45
30:AI:62:MET:HE2	30:AI:62:MET:HA	1.99	0.45
35:Ao:531:LYS:HB2	35:Ao:531:LYS:HE3	1.68	0.45
35:Ao:586:PHE:HA	35:Ao:589:ALA:HB3	1.98	0.45
1:BC:426:SER:O	1:BC:429:GLU:HB2	2.17	0.44
3:AA:202:A:H5'	15:AP:102:MET:HE3	1.99	0.44
6:AE:292:HIS:CE1	6:AE:357:GLU:H	2.24	0.44
8:AG:182:LEU:HA	8:AG:182:LEU:HD23	1.85	0.44
11:AK:195:ARG:NH1	11:AK:195:ARG:CG	2.78	0.44
19:AV:19:A:H2'	19:AV:20:G:H8	1.82	0.44
23:Ab:98:ARG:HB3	23:Ab:125:LEU:HD21	1.98	0.44
24:Ac:106:LEU:H	24:Ac:106:LEU:HG	1.61	0.44
26:Ae:101:TYR:HE1	26:Ae:138:SER:OG	1.99	0.44
7:AF:2:PRO:HB2	7:AF:96:HIS:CD2	2.52	0.44
14:AO:144:MET:HE2	14:AO:144:MET:HA	1.99	0.44
25:Ad:70:LEU:O	25:Ad:73:GLU:HB3	2.16	0.44
28:Ag:56:ALA:C	28:Ag:112:LYS:HZ1	2.22	0.44
35:Ao:527:ARG:C	35:Ao:531:LYS:HE3	2.42	0.44
1:BC:435:GLU:OE1	1:BC:439:ARG:HG2	2.18	0.44
3:AA:285:C:N4	12:AL:45:PRO:HD3	2.32	0.44
3:AA:460:A:H4'	3:AA:461:A:OP2	2.15	0.44
3:AA:532:G:O2'	3:AA:959:U:C4	2.70	0.44
6:AE:109:GLY:HA2	6:AE:114:ARG:HB2	1.99	0.44
17:AR:104:LYS:HD3	17:AR:104:LYS:HA	1.86	0.44
22:Aa:307:LEU:HD23	22:Aa:307:LEU:HA	1.89	0.44
22:Aa:348:HIS:O	22:Aa:352:VAL:HG23	2.17	0.44
22:Aa:368:LEU:HD12	22:Aa:368:LEU:HA	1.67	0.44
3:AA:879:A:H2'	3:AA:880:U:C6	2.53	0.44
3:AA:884:C:H5''	26:Ae:143:TYR:HE2	1.81	0.44
6:AE:412:LYS:HG2	6:AE:417:MET:HB2	1.98	0.44
9:AI:91:MET:H	9:AI:91:MET:HG2	1.57	0.44
13:AN:35:LEU:HD13	13:AN:39:LYS:HE3	1.99	0.44
16:AQ:55:LEU:H	16:AQ:55:LEU:HG	1.63	0.44
19:AV:12:C:H2'	19:AV:13:U:O4'	2.17	0.44
22:Aa:150:MET:HE1	22:Aa:291:GLY:HA3	1.99	0.44
24:Ac:2:PRO:O	24:Ac:8:PRO:HB3	2.17	0.44
1:BC:424:LEU:HD12	1:BC:553:VAL:HG21	1.98	0.44
3:AA:739:A:C5	8:AG:197:ARG:NH1	2.85	0.44
8:AG:161:ILE:HD12	8:AG:170:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AV:3:U:H3	19:AV:65:A:N6	2.11	0.44
26:Ae:258:SER:HB3	26:Ae:311:GLU:CB	2.37	0.44
26:Ae:270:LEU:O	26:Ae:274:VAL:HG23	2.18	0.44
31:Aj:169:LEU:HD21	31:Aj:173:MET:HE3	2.00	0.44
32:Ak:68:TRP:N	32:Ak:69:PRO:HD2	2.32	0.44
33:Am:69:GLU:OE1	33:Am:69:GLU:N	2.46	0.44
3:AA:838:A:C4	34:An:131:LEU:HD11	2.52	0.44
4:AB:203:GLU:HG3	33:Am:114:LYS:NZ	2.32	0.44
12:AL:50:GLY:HA3	12:AL:51:PRO:HD2	1.82	0.44
15:AP:99:LEU:HD23	22:Aa:169:ILE:HD11	2.00	0.44
17:AR:74:ASP:OD2	17:AR:76:LYS:HE3	2.17	0.44
17:AR:142:ARG:HA	18:AU:28:ARG:NH1	2.31	0.44
26:Ae:75:VAL:HG12	26:Ae:78:HIS:HB2	2.00	0.44
26:Ae:223:LEU:CD2	26:Ae:398:THR:HA	2.47	0.44
28:Ag:338:PRO:HA	32:Ak:314:TYR:OH	2.17	0.44
29:Ah:284:ARG:HH21	35:Ao:451:ILE:HB	1.83	0.44
35:Ao:116:ALA:O	35:Ao:120:ILE:HG12	2.16	0.44
35:Ao:457:ARG:NH1	35:Ao:489:PHE:CE1	2.86	0.44
1:BC:298:GLU:O	1:BC:302:LYS:HG2	2.18	0.44
4:AB:164:TYR:N	4:AB:164:TYR:CD2	2.86	0.44
7:AF:65:LEU:HD21	17:AR:76:LYS:CD	2.46	0.44
8:AG:168:TYR:CD2	8:AG:239:TYR:HE2	2.36	0.44
12:AL:31:ALA:O	24:Ac:4:LYS:HE2	2.18	0.44
13:AN:101:LYS:HD3	13:AN:101:LYS:HA	1.85	0.44
19:AV:19:A:H2'	19:AV:20:G:C8	2.52	0.44
22:Aa:157:ARG:HB3	22:Aa:260:ASP:OD2	2.17	0.44
35:Ao:371:SER:HB3	35:Ao:412:ASP:OD2	2.17	0.44
35:Ao:645:CYS:HA	35:Ao:648:LEU:HB2	1.99	0.44
1:BC:401:ASP:OD1	1:BC:402:GLU:N	2.50	0.44
1:BC:471:LYS:HA	1:BC:471:LYS:HD3	1.79	0.44
3:AA:391:U:H4'	14:AO:156:PHE:CZ	2.53	0.44
3:AA:675:A:OP2	5:AC:37:ASN:ND2	2.51	0.44
3:AA:815:U:H2'	3:AA:816:U:C6	2.52	0.44
6:AE:147:PRO:O	6:AE:155:GLN:NE2	2.51	0.44
13:AN:30:VAL:HG13	13:AN:95:SER:HB2	2.00	0.44
24:Ac:125:HIS:HA	24:Ac:126:PRO:HD3	1.81	0.44
35:Ao:459:PHE:HD2	35:Ao:463:LYS:HE3	1.83	0.44
35:Ao:559:LYS:NZ	35:Ao:574:TRP:HZ2	2.16	0.44
3:AA:254:C:N4	12:AL:74:ASN:OD1	2.50	0.44
3:AA:279:U:O2'	12:AL:54:GLY:O	2.36	0.44
3:AA:303:U:OP2	3:AA:398:G:N1	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AC:165:LYS:HG2	5:AC:166:TYR:H	1.82	0.44
9:AI:168:LYS:HD2	9:AI:241:PHE:CD1	2.52	0.44
13:AN:83:CYS:HA	13:AN:84:PRO:HD3	1.76	0.44
22:Aa:147:ARG:HH11	36:Ap:169:GLN:NE2	2.15	0.44
24:Ac:44:ALA:O	24:Ac:47:PHE:HB3	2.18	0.44
28:Ag:55:PRO:HD2	28:Ag:146:LYS:NZ	2.33	0.44
35:Ao:524:HIS:HA	35:Ao:527:ARG:NE	2.33	0.44
1:BC:183:VAL:HA	1:BC:254:ILE:O	2.17	0.43
3:AA:262:C:H2'	3:AA:263:G:H8	1.82	0.43
3:AA:560:C:N4	3:AA:710:G:H1	2.15	0.43
3:AA:649:U:H3'	3:AA:650:A:H5''	1.98	0.43
4:AB:177:ASN:C	4:AB:177:ASN:HD22	2.25	0.43
8:AG:108:ARG:NH2	9:AI:312:GLU:OE2	2.51	0.43
14:AO:144:MET:HE1	14:AO:150:ASP:O	2.18	0.43
15:AP:31:PHE:CE1	24:Ac:140:MET:HB2	2.53	0.43
26:Ae:110:LEU:HD12	26:Ae:434:GLU:CD	2.43	0.43
26:Ae:152:TRP:HZ3	26:Ae:165:ALA:HA	1.82	0.43
35:Ao:370:PRO:HB2	35:Ao:375:TYR:CE2	2.53	0.43
35:Ao:608:ILE:HD12	35:Ao:640:PHE:HB3	2.00	0.43
35:Ao:618:LEU:O	35:Ao:622:LYS:HB3	2.18	0.43
3:AA:407:U:H2'	3:AA:408:A:O4'	2.17	0.43
3:AA:708:A:H5'	3:AA:709:A:OP2	2.19	0.43
4:AB:152:HIS:CE1	9:AI:163:HIS:CE1	3.06	0.43
4:AB:166:HIS:ND1	9:AI:153:THR:HA	2.33	0.43
19:AV:49:G:H1	19:AV:56:C:N4	2.15	0.43
22:Aa:281:TYR:OH	22:Aa:305:GLY:HA3	2.18	0.43
26:Ae:223:LEU:HD22	26:Ae:223:LEU:HA	1.91	0.43
27:Af:174:GLN:HA	27:Af:174:GLN:NE2	2.33	0.43
35:Ao:400:MET:O	35:Ao:404:MET:HE3	2.18	0.43
1:BC:686:VAL:HG12	1:BC:690:MET:HG2	2.01	0.43
5:AC:145:HIS:CD2	35:Ao:121:ILE:HD13	2.53	0.43
6:AE:362:LEU:HD21	22:Aa:127:LEU:HD21	2.00	0.43
10:AJ:166:GLU:CD	10:AJ:166:GLU:H	2.26	0.43
11:AK:68:ILE:HG22	11:AK:69:PRO:HD2	2.00	0.43
13:AN:28:TYR:O	30:AI:55:HIS:HB3	2.18	0.43
23:Ab:89:ASN:HB3	23:Ab:92:PHE:HB2	2.00	0.43
28:Ag:55:PRO:HG3	28:Ag:142:HIS:CE1	2.54	0.43
31:AJ:34:TYR:CD2	31:AJ:135:MET:HG2	2.53	0.43
35:Ao:336:GLN:HA	35:Ao:339:ASN:HB3	2.00	0.43
35:Ao:443:ASN:HA	35:Ao:447:ASN:HB3	2.00	0.43
1:BC:191:HIS:HB3	1:BC:258:VAL:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BC:531:ILE:O	1:BC:535:ILE:HD12	2.19	0.43
3:AA:365:A:H2'	3:AA:366:A:C8	2.53	0.43
3:AA:930:G:OP1	3:AA:933:A:H4'	2.18	0.43
4:AB:188:LEU:HD23	4:AB:188:LEU:HA	1.82	0.43
6:AE:314:LEU:HA	6:AE:314:LEU:HD23	1.68	0.43
9:AI:349:MET:O	9:AI:353:LEU:HG	2.18	0.43
10:AJ:148:LEU:HD23	10:AJ:148:LEU:HA	1.81	0.43
15:AP:99:LEU:HB2	36:Ap:203:TYR:CZ	2.53	0.43
25:Ad:79:ARG:HA	25:Ad:79:ARG:HH11	1.83	0.43
26:Ae:112:ILE:O	26:Ae:116:VAL:HG23	2.18	0.43
26:Ae:273:LYS:HB3	26:Ae:273:LYS:HE2	1.74	0.43
28:Ag:66:HIS:CD2	28:Ag:99:MET:HB2	2.53	0.43
31:Aj:83:LYS:HE2	31:Aj:87:TRP:CZ2	2.52	0.43
32:Ak:89:MET:CE	32:Ak:106:GLU:HB3	2.48	0.43
32:Ak:211:THR:HG23	32:Ak:223:TYR:HD2	1.84	0.43
34:An:130:ILE:O	34:An:134:ARG:HG3	2.19	0.43
3:AA:76:U:H3'	3:AA:77:G:O4'	2.19	0.43
3:AA:708:A:C3'	3:AA:709:A:H5'	2.48	0.43
6:AE:320:ILE:HD11	6:AE:345:LEU:HD11	2.01	0.43
8:AG:97:MET:HB3	8:AG:97:MET:HE2	1.74	0.43
10:AJ:94:PHE:HZ	10:AJ:163:ASN:HD22	1.67	0.43
28:Ag:181:LEU:H	28:Ag:181:LEU:HG	1.55	0.43
30:Ai:36:LEU:HD12	30:Ai:36:LEU:HA	1.87	0.43
3:AA:59:C:C6	31:Aj:136:TYR:CG	3.07	0.43
3:AA:176:G:H5''	3:AA:176:G:H8	1.84	0.43
3:AA:368:A:P	11:AK:186:ASN:HD22	2.42	0.43
10:AJ:111:PRO:HA	10:AJ:112:PRO:HD3	1.86	0.43
22:Aa:285:ARG:NH2	22:Aa:310:GLN:HG3	2.34	0.43
31:Aj:118:LEU:HD11	31:Aj:120:PHE:HB2	2.01	0.43
5:AC:84:GLU:CB	5:AC:85:ARG:NH1	2.82	0.43
9:AI:370:LEU:HD23	9:AI:370:LEU:HA	1.75	0.43
9:AI:374:ASP:OD1	9:AI:376:ARG:NH1	2.51	0.43
12:AL:33:LEU:HD23	12:AL:33:LEU:HA	1.75	0.43
14:AO:133:LEU:HD23	14:AO:133:LEU:HA	1.76	0.43
15:AP:99:LEU:HD12	15:AP:99:LEU:HA	1.80	0.43
23:Ab:48:ARG:NH1	23:Ab:48:ARG:HG2	2.34	0.43
24:Ac:167:LEU:HD23	24:Ac:167:LEU:HA	1.81	0.43
35:Ao:397:TYR:CG	35:Ao:434:LEU:HD13	2.54	0.43
3:AA:65:C:H6	3:AA:65:C:H2'	1.60	0.43
3:AA:124:A:HO2'	3:AA:127:A:N6	2.17	0.43
11:AK:102:VAL:CG1	11:AK:106:HIS:HA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AK:177:ILE:HD11	18:AU:23:TYR:CD2	2.49	0.43
31:Aj:171:ARG:NE	36:Ap:190:ALA:HB2	2.34	0.43
32:Ak:115:HIS:CD2	32:Ak:116:LEU:HG	2.53	0.43
35:Ao:258:ASN:HD21	35:Ao:288:ASN:HB2	1.82	0.43
35:Ao:382:PHE:HB3	35:Ao:396:ILE:CD1	2.49	0.43
3:AA:85:G:H2'	3:AA:86:A:C8	2.54	0.43
3:AA:858:C:O5'	3:AA:858:C:H6	2.02	0.43
3:AA:925:A:H5'	3:AA:925:A:H8	1.83	0.43
4:AB:196:HIS:CD2	4:AB:239:ASP:HB2	2.54	0.43
9:AI:275:GLY:N	9:AI:348:ALA:HB2	2.33	0.43
9:AI:302:LEU:HD22	28:Ag:384:ASN:HB3	2.01	0.43
13:AN:58:ARG:HB3	13:AN:58:ARG:HH11	1.84	0.43
14:AO:150:ASP:CG	14:AO:153:HIS:HD2	2.27	0.43
22:Aa:121:LYS:HB2	22:Aa:121:LYS:HE3	1.83	0.43
22:Aa:167:ASP:OD2	22:Aa:197:ARG:NH2	2.51	0.43
31:Aj:116:GLY:O	31:Aj:128:ALA:HA	2.18	0.43
35:Ao:636:LEU:O	35:Ao:640:PHE:HD2	2.01	0.43
1:BC:398:LEU:HD23	1:BC:398:LEU:HA	1.79	0.43
1:BC:436:SER:OG	1:BC:438:PRO:HD2	2.19	0.43
1:BC:592:LYS:HD2	1:BC:594:LYS:HE3	1.99	0.43
1:BC:693:GLY:HA3	19:AV:71:A:H1'	2.01	0.43
6:AE:395:PRO:HB3	22:Aa:132:GLN:NE2	2.34	0.43
31:Aj:27:ARG:HD2	31:Aj:28:PRO:HD2	2.01	0.43
32:Ak:166:ARG:HA	32:Ak:166:ARG:HD3	1.73	0.43
35:Ao:407:ARG:HG2	35:Ao:444:THR:CG2	2.49	0.43
3:AA:111:A:C2	3:AA:114:A:C8	3.07	0.42
3:AA:889:U:O2'	3:AA:890:U:H5'	2.19	0.42
6:AE:325:ARG:NH1	6:AE:325:ARG:HG3	2.34	0.42
8:AG:180:ARG:HH11	8:AG:180:ARG:CB	2.24	0.42
14:AO:195:PRO:HB2	14:AO:196:TYR:CD2	2.54	0.42
26:Ae:74:TYR:CD1	26:Ae:413:ILE:HG12	2.54	0.42
26:Ae:298:ARG:O	26:Ae:302:VAL:HG23	2.18	0.42
28:Ag:93:PHE:C	28:Ag:95:GLU:H	2.27	0.42
28:Ag:227:GLN:HE21	28:Ag:231:ARG:NH2	2.16	0.42
32:Ak:69:PRO:HG2	32:Ak:123:ARG:NH2	2.33	0.42
32:Ak:76:ALA:HA	32:Ak:77:PRO:HD2	1.78	0.42
1:BC:179:ARG:HG3	1:BC:349:ALA:HB2	2.00	0.42
1:BC:462:ILE:O	1:BC:466:LYS:HG3	2.18	0.42
3:AA:82:C:H2'	3:AA:83:C:O4'	2.19	0.42
5:AC:113:ARG:HH21	5:AC:118:GLU:CD	2.23	0.42
17:AR:128:PRO:O	17:AR:131:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Ab:41:LEU:HD23	23:Ab:41:LEU:HA	1.86	0.42
23:Ab:73:LYS:HZ3	23:Ab:114:GLU:HG3	1.80	0.42
25:Ad:169:THR:HG22	25:Ad:170:ARG:H	1.84	0.42
35:Ao:610:ARG:HD3	35:Ao:610:ARG:HA	1.86	0.42
36:Ap:235:MET:HA	36:Ap:236:PRO:HD3	1.72	0.42
1:BC:325:ALA:HB3	37:BC:901:GSP:N7	2.35	0.42
9:Al:122:ARG:C	32:Ak:89:MET:HG3	2.43	0.42
9:Al:155:LYS:HB3	9:Al:212:GLU:OE2	2.19	0.42
10:AJ:136:MET:HE2	10:AJ:136:MET:HB3	1.76	0.42
18:Au:47:LYS:HE2	18:Au:47:LYS:HB3	1.75	0.42
18:Au:67:GLU:OE1	18:Au:70:ARG:NH1	2.52	0.42
28:Ag:160:TRP:CE3	28:Ag:288:LEU:HB3	2.54	0.42
28:Ag:201:ILE:O	28:Ag:220:PRO:HA	2.20	0.42
35:Ao:305:ALA:O	35:Ao:308:VAL:HG23	2.19	0.42
1:BC:310:VAL:O	1:BC:318:VAL:HB	2.19	0.42
7:AF:89:ILE:HG23	7:AF:89:ILE:HD12	1.68	0.42
10:AJ:188:ILE:HG12	32:Ak:236:TRP:CE3	2.54	0.42
12:AL:62:VAL:HG23	12:AL:106:HIS:O	2.20	0.42
22:Aa:237:LEU:HD23	22:Aa:237:LEU:HA	1.76	0.42
24:Ac:130:GLY:O	24:Ac:138:GLU:HG2	2.19	0.42
26:Ae:172:LYS:HB3	26:Ae:173:VAL:H	1.57	0.42
36:Ap:91:ARG:NH2	36:Ap:103:ASN:O	2.51	0.42
1:BC:183:VAL:HG22	1:BC:254:ILE:HB	2.01	0.42
1:BC:305:LEU:HD11	1:BC:314:TYR:CE1	2.54	0.42
4:AB:101:MET:CE	4:AB:222:VAL:HB	2.49	0.42
4:AB:146:ARG:HG3	4:AB:146:ARG:HH11	1.84	0.42
6:AE:312:TYR:HD1	6:AE:312:TYR:O	2.03	0.42
6:AE:374:ARG:HG3	6:AE:374:ARG:NH1	2.31	0.42
8:AG:81:LYS:HE3	8:AG:81:LYS:HB2	1.75	0.42
16:AQ:8:VAL:HG12	16:AQ:10:ALA:H	1.84	0.42
16:AQ:36:ASP:HA	16:AQ:37:PRO:HD3	1.61	0.42
28:Ag:63:GLU:CD	28:Ag:102:LYS:HG3	2.45	0.42
29:Ah:352:LYS:HG2	32:Ak:213:ARG:HH21	1.85	0.42
29:Ah:353:ASN:HA	29:Ah:354:PRO:HD3	1.86	0.42
31:Aj:59:ARG:HB2	31:Aj:60:HIS:CD2	2.55	0.42
35:Ao:381:LEU:HD23	35:Ao:381:LEU:HA	1.86	0.42
1:BC:217:ILE:HG13	1:BC:244:MET:SD	2.59	0.42
3:AA:137:A:OP2	14:AO:196:TYR:OH	2.22	0.42
3:AA:719:U:HO2'	3:AA:752:A:H2	1.62	0.42
5:AC:142:LEU:HD12	5:AC:142:LEU:HA	1.80	0.42
8:AG:154:PRO:O	8:AG:179:ARG:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AI:123:PRO:HG3	32:Ak:89:MET:SD	2.58	0.42
10:AJ:96:VAL:HA	10:AJ:106:ILE:HD11	2.01	0.42
22:Aa:283:LEU:HD23	22:Aa:283:LEU:HA	1.81	0.42
23:Ab:126:LEU:HD23	23:Ab:130:VAL:O	2.20	0.42
27:Af:101:VAL:HG12	27:Af:102:ILE:N	2.35	0.42
28:Ag:122:ARG:HH11	28:Ag:336:LEU:HD22	1.82	0.42
1:BC:372:THR:HG21	1:BC:425:PRO:HG2	2.01	0.42
3:AA:689:G:H2'	3:AA:690:U:O4'	2.19	0.42
4:AB:93:LYS:HG2	27:Af:149:GLU:OE1	2.19	0.42
5:AC:76:LEU:HD22	10:AJ:138:THR:HG23	2.02	0.42
6:AE:425:LEU:HD13	36:Ap:85:ILE:HG21	2.01	0.42
11:AK:64:ILE:HD11	17:AR:142:ARG:HD2	2.02	0.42
17:AR:53:VAL:HA	17:AR:54:PRO:HD3	1.86	0.42
1:BC:439:ARG:HA	1:BC:439:ARG:HD2	1.87	0.42
6:AE:203:LEU:HD11	6:AE:222:ILE:HD11	2.01	0.42
8:AG:41:TYR:CE1	8:AG:73:LEU:HD13	2.55	0.42
9:AI:176:HIS:CD2	9:AI:180:ARG:HH21	2.37	0.42
16:AQ:96:THR:HG22	25:Ad:117:HIS:HE1	1.83	0.42
22:Aa:284:LEU:HD12	22:Aa:293:MET:HG2	2.00	0.42
23:Ab:125:LEU:O	23:Ab:130:VAL:HG22	2.20	0.42
23:Ab:125:LEU:HD23	23:Ab:125:LEU:HA	1.86	0.42
26:Ae:182:TYR:CE2	26:Ae:186:LEU:HD12	2.54	0.42
26:Ae:200:ALA:O	26:Ae:204:VAL:HG23	2.20	0.42
27:Af:96:ALA:HB2	27:Af:148:LEU:HD22	2.01	0.42
32:Ak:213:ARG:HD2	32:Ak:223:TYR:CE2	2.55	0.42
33:Am:66:CYS:HB2	33:Am:69:GLU:OE1	2.18	0.42
33:Am:104:LEU:HA	33:Am:104:LEU:HD23	1.63	0.42
35:Ao:126:LYS:HA	35:Ao:129:GLN:HG2	2.02	0.42
35:Ao:442:LEU:HD21	35:Ao:451:ILE:HD11	2.02	0.42
35:Ao:542:GLN:O	35:Ao:544:PRO:HD3	2.20	0.42
6:AE:358:THR:HG22	6:AE:360:GLN:H	1.85	0.42
7:AF:92:ASN:OD1	17:AR:118:LEU:HD22	2.20	0.42
11:AK:184:PRO:C	11:AK:186:ASN:H	2.28	0.42
13:AN:96:ARG:HG2	13:AN:97:PRO:HD2	2.01	0.42
14:AO:127:GLU:H	14:AO:127:GLU:HG3	1.41	0.42
31:Aj:171:ARG:NH1	31:Aj:171:ARG:HG3	2.35	0.42
35:Ao:306:LEU:HD21	35:Ao:347:ARG:NH1	2.35	0.42
3:AA:621:A:H5''	10:AJ:130:HIS:CD2	2.54	0.42
3:AA:924:U:OP2	20:AX:1:A:O2'	2.38	0.42
6:AE:372:GLU:HB2	22:Aa:125:TYR:CE2	2.55	0.42
11:AK:183:ILE:O	11:AK:183:ILE:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AN:114:LEU:HB3	13:AN:120:LEU:HD13	2.00	0.42
26:Ae:80:TRP:CH2	26:Ae:151:THR:HA	2.55	0.42
26:Ae:84:ASP:OD1	26:Ae:84:ASP:N	2.52	0.42
26:Ae:147:TRP:H	26:Ae:147:TRP:CD1	2.37	0.42
28:Ag:152:LEU:HD21	28:Ag:243:LEU:HD11	2.02	0.42
32:Ak:164:SER:HB3	35:Ao:134:GLU:HG2	2.02	0.42
35:Ao:292:ALA:O	35:Ao:331:VAL:HG21	2.19	0.42
35:Ao:442:LEU:HA	35:Ao:450:LEU:HD12	2.02	0.42
35:Ao:543:HIS:HB3	35:Ao:551:PHE:HE1	1.85	0.42
1:BC:223:SER:CB	1:BC:229:LYS:HZ3	2.29	0.41
1:BC:490:SER:C	3:AA:919:A:H61	2.24	0.41
1:BC:673:LEU:HD21	1:BC:694:LEU:HB3	2.02	0.41
8:AG:73:LEU:HG	9:AI:254:LYS:HZ1	1.79	0.41
9:AI:108:ILE:HD11	9:AI:125:MET:HB3	2.01	0.41
11:AK:194:ARG:HD2	18:AU:44:TYR:OH	2.20	0.41
12:AL:137:LYS:HD3	12:AL:137:LYS:HA	1.73	0.41
19:AV:50:U:H3	19:AV:54:A:H62	1.68	0.41
22:Aa:334:GLN:H	22:Aa:334:GLN:HG2	1.59	0.41
24:Ac:60:PRO:HG2	24:Ac:61:TRP:HD1	1.84	0.41
26:Ae:425:GLY:O	26:Ae:429:ARG:HG3	2.20	0.41
28:Ag:77:VAL:C	28:Ag:79:PRO:HD3	2.45	0.41
35:Ao:263:CYS:O	35:Ao:267:ARG:HG2	2.19	0.41
35:Ao:355:PRO:O	35:Ao:358:GLN:HB3	2.20	0.41
35:Ao:530:LEU:O	35:Ao:534:ILE:HG13	2.20	0.41
4:AB:179:PRO:HA	4:AB:183:GLY:O	2.20	0.41
8:AG:240:ARG:O	33:Am:43:ALA:HB2	2.20	0.41
19:AV:41:A:H2'	19:AV:42:A:O4'	2.20	0.41
22:Aa:189:HIS:HD2	36:Ap:173:ARG:HD3	1.85	0.41
28:Ag:264:VAL:HG12	28:Ag:267:LEU:HD12	2.02	0.41
35:Ao:509:LEU:HD21	35:Ao:551:PHE:HZ	1.86	0.41
3:AA:439:A:H2'	3:AA:440:C:O4'	2.20	0.41
12:AL:70:PRO:HD3	12:AL:76:ALA:O	2.20	0.41
19:AV:15:A:H2'	19:AV:16:A:N3	2.35	0.41
26:Ae:324:ASP:O	26:Ae:328:LYS:HG2	2.21	0.41
32:Ak:139:LEU:HD23	32:Ak:139:LEU:HA	1.93	0.41
32:Ak:167:ASN:HA	32:Ak:168:PRO:HD2	1.84	0.41
33:Am:62:ARG:HG3	33:Am:65:ALA:HB2	2.01	0.41
3:AA:254:C:H41	12:AL:74:ASN:CG	2.29	0.41
3:AA:562:A:H8	3:AA:708:A:N1	2.18	0.41
3:AA:619:C:H5'	3:AA:620:C:OP2	2.20	0.41
3:AA:653:A:H5'	3:AA:654:A:OP1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AA:719:U:H2'	3:AA:720:A:O4'	2.20	0.41
9:AI:264:ASP:HB2	9:AI:270:PHE:HE2	1.84	0.41
9:AI:341:GLN:O	9:AI:345:VAL:HG23	2.21	0.41
9:AI:381:LYS:HE2	9:AI:386:GLU:O	2.21	0.41
11:AK:109:LEU:HD13	11:AK:146:VAL:HG11	2.02	0.41
22:Aa:117:LEU:HD23	22:Aa:117:LEU:HA	1.86	0.41
22:Aa:299:ASN:HD21	22:Aa:329:LEU:HD13	1.86	0.41
22:Aa:347:LEU:HD13	22:Aa:347:LEU:HA	1.87	0.41
26:Ae:137:HIS:O	31:Aj:104:TYR:HB2	2.21	0.41
27:Af:151:THR:HG23	27:Af:160:ASP:HB3	2.02	0.41
35:Ao:131:ASP:OD1	35:Ao:132:ILE:N	2.52	0.41
1:BC:341:LEU:O	1:BC:345:LEU:HG	2.20	0.41
4:AB:128:LEU:HA	4:AB:128:LEU:HD23	1.74	0.41
8:AG:82:THR:HA	9:AI:316:PHE:CE2	2.56	0.41
9:AI:157:SER:HB3	9:AI:210:LEU:HB3	2.03	0.41
9:AI:261:LEU:HG	9:AI:355:SER:HB3	2.01	0.41
10:AJ:52:VAL:HG21	35:Ao:479:LYS:C	2.45	0.41
12:AL:45:PRO:HA	12:AL:46:PRO:HD3	1.93	0.41
16:AQ:110:ILE:O	16:AQ:112:PRO:HD3	2.20	0.41
28:Ag:122:ARG:HG2	28:Ag:305:ILE:HD11	2.02	0.41
28:Ag:150:LEU:HB3	28:Ag:257:LEU:HD12	2.02	0.41
31:Aj:95:TRP:CZ3	31:Aj:131:ILE:HG12	2.56	0.41
34:An:163:ARG:HA	34:An:196:LEU:HD21	2.00	0.41
3:AA:872:A:H2'	3:AA:873:A:C8	2.55	0.41
3:AA:882:A:C6	3:AA:883:C:C4	3.08	0.41
6:AE:408:TRP:NE1	6:AE:412:LYS:HE2	2.36	0.41
7:AF:8:LEU:HA	7:AF:8:LEU:HD23	1.81	0.41
14:AO:119:ASN:HA	14:AO:120:PRO:HD2	1.92	0.41
22:Aa:97:VAL:HG11	22:Aa:295:TRP:HE1	1.85	0.41
26:Ae:157:LEU:HD23	26:Ae:161:ALA:HB1	2.01	0.41
3:AA:901:A:O3'	34:An:171:ARG:NH1	2.54	0.41
5:AC:127:LEU:HB3	5:AC:131:LYS:HB2	2.02	0.41
9:AI:291:SER:OG	9:AI:292:GLY:N	2.53	0.41
15:AP:90:LEU:HD12	15:AP:90:LEU:HA	1.82	0.41
18:AU:49:CYS:SG	18:AU:50:ARG:N	2.94	0.41
22:Aa:258:GLU:HG3	22:Aa:259:PRO:HD2	2.03	0.41
23:Ab:89:ASN:HA	23:Ab:90:PRO:HD3	1.89	0.41
31:Aj:83:LYS:HE2	31:Aj:87:TRP:CE2	2.55	0.41
32:Ak:89:MET:HE1	32:Ak:106:GLU:C	2.45	0.41
1:BC:599:ILE:O	1:BC:602:LEU:HB3	2.21	0.41
3:AA:209:C:H2'	3:AA:210:U:H6	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AA:277:A:H2'	3:AA:278:A:H8	1.86	0.41
11:AK:183:ILE:HD12	11:AK:183:ILE:HG23	1.78	0.41
13:AN:30:VAL:HG12	13:AN:34:MET:CE	2.51	0.41
15:AP:52:GLY:HA3	15:AP:67:ALA:O	2.21	0.41
17:AR:141:TYR:CD1	18:AU:32:MET:HE3	2.56	0.41
26:Ae:416:TYR:O	26:Ae:420:LEU:HG	2.21	0.41
28:Ag:55:PRO:HA	28:Ag:58:HIS:CD2	2.56	0.41
1:BC:180:SER:HA	1:BC:181:PRO:HD3	1.87	0.41
1:BC:288:ASN:HA	1:BC:323:VAL:O	2.20	0.41
3:AA:958:U:H2'	18:AU:57:TYR:OH	2.21	0.41
4:AB:230:LEU:HD23	4:AB:230:LEU:HA	1.88	0.41
5:AC:62:ILE:C	5:AC:64:HIS:H	2.29	0.41
5:AC:100:PHE:HB3	5:AC:103:CYS:SG	2.60	0.41
7:AF:29:LEU:HA	7:AF:29:LEU:HD12	1.87	0.41
7:AF:106:GLU:CD	7:AF:106:GLU:H	2.29	0.41
7:AF:117:LEU:HD23	7:AF:117:LEU:HA	1.85	0.41
8:AG:172:VAL:HA	8:AG:173:PRO:HD2	1.94	0.41
12:AL:32:THR:HG23	12:AL:35:GLN:NE2	2.36	0.41
14:AO:116:VAL:HG22	14:AO:185:GLU:CB	2.50	0.41
22:Aa:164:LEU:HD21	22:Aa:205:LYS:HE3	2.03	0.41
29:Ah:285:PRO:HB3	35:Ao:88:VAL:HG21	2.02	0.41
29:Ah:298:LYS:CE	35:Ao:68:VAL:HG21	2.51	0.41
29:Ah:324:ILE:HD12	32:Ak:213:ARG:HD3	2.03	0.41
30:Ai:11:MET:HE3	32:Ak:241:TRP:HH2	1.86	0.41
31:Aj:63:ARG:HB3	31:Aj:137:HIS:HD2	1.86	0.41
31:Aj:142:VAL:HA	31:Aj:143:PRO:HD3	1.86	0.41
5:AC:140:GLU:OE2	5:AC:152:HIS:HA	2.20	0.41
9:AI:397:ARG:HH21	19:AV:30:C:P	2.43	0.41
11:AK:183:ILE:HD13	11:AK:183:ILE:HA	1.77	0.41
12:AL:61:VAL:HG12	12:AL:107:VAL:HG12	2.03	0.41
26:Ae:178:PHE:HB3	31:Aj:72:PRO:HA	2.03	0.41
29:Ah:341:HIS:CG	30:Ai:24:ARG:HD2	2.55	0.41
29:Ah:384:ILE:HG12	29:Ah:386:LEU:HG	2.03	0.41
32:Ak:151:ILE:HG23	32:Ak:175:LEU:HD21	2.03	0.41
36:Ap:136:HIS:CD2	36:Ap:139:TYR:H	2.39	0.41
1:BC:213:ILE:HD12	1:BC:238:HIS:CE1	2.55	0.40
1:BC:596:HIS:CD2	1:BC:602:LEU:HA	2.56	0.40
3:AA:59:C:H2'	31:Aj:136:TYR:CE2	2.55	0.40
3:AA:136:C:C2	14:AO:198:ARG:NH2	2.88	0.40
3:AA:182:A:H5'	12:AL:59:LYS:HB2	2.02	0.40
3:AA:580:U:OP1	10:AJ:128:LYS:NZ	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AA:883:C:H5''	3:AA:884:C:OP1	2.21	0.40
4:AB:175:LEU:HD23	4:AB:175:LEU:HA	1.86	0.40
15:AP:51:LEU:HD23	15:AP:51:LEU:HA	1.85	0.40
16:AQ:33:LEU:HB2	24:Ac:56:GLN:HE21	1.85	0.40
17:AR:67:ILE:HG21	25:Ad:191:ILE:HD12	2.03	0.40
17:AR:81:LEU:HD13	17:AR:112:ILE:HA	2.03	0.40
22:Aa:345:GLU:O	22:Aa:349:LEU:N	2.51	0.40
27:Af:149:GLU:OE2	27:Af:162:THR:HG21	2.21	0.40
27:Af:150:LEU:HB2	27:Af:163:ILE:CG2	2.51	0.40
31:Aj:65:LEU:HD22	31:Aj:65:LEU:HA	1.90	0.40
32:Ak:59:THR:HG23	32:Ak:84:PRO:HA	2.02	0.40
33:Am:18:ARG:HG3	33:Am:19:PRO:HD2	2.03	0.40
35:Ao:509:LEU:HD21	35:Ao:551:PHE:CZ	2.56	0.40
1:BC:645:GLY:HA3	42:AV:101:FME:HE2	2.04	0.40
3:AA:665:A:H2'	3:AA:665:A:N3	2.36	0.40
4:AB:72:PHE:CE1	4:AB:259:ALA:HA	2.56	0.40
8:AG:190:GLU:HG3	8:AG:194:LYS:HD2	2.03	0.40
9:AI:129:GLU:HG3	9:AI:130:GLU:HG3	2.04	0.40
13:AN:28:TYR:N	30:Ai:56:ASN:HD22	2.18	0.40
16:AQ:80:GLU:HG2	16:AQ:81:LEU:N	2.34	0.40
26:Ae:199:ASP:OD1	26:Ae:200:ALA:N	2.54	0.40
26:Ae:266:TYR:CD1	26:Ae:320:LEU:HD22	2.57	0.40
28:Ag:108:LEU:O	28:Ag:112:LYS:HG2	2.21	0.40
31:Aj:134:VAL:HA	31:Aj:139:TRP:HE1	1.85	0.40
1:BC:424:LEU:HD23	1:BC:424:LEU:HA	1.72	0.40
1:BC:535:ILE:HG23	1:BC:546:LEU:HD23	2.03	0.40
1:BC:562:ASN:O	1:BC:566:THR:HG23	2.21	0.40
3:AA:390:A:O2'	14:AO:153:HIS:HE1	2.05	0.40
3:AA:959:U:H5'	33:Am:25:LYS:HZ1	1.82	0.40
7:AF:8:LEU:HD13	7:AF:10:LEU:HD21	2.04	0.40
7:AF:105:CYS:HB2	17:AR:69:CYS:SG	2.57	0.40
14:AO:76:ASP:HB3	25:Ad:153:LYS:HD2	2.02	0.40
14:AO:117:LEU:HD21	14:AO:127:GLU:HB2	2.04	0.40
19:AV:15:A:H2'	19:AV:16:A:C2	2.56	0.40
20:AX:5:C:H2'	20:AX:6:C:O4'	2.21	0.40
26:Ae:129:GLU:HG2	26:Ae:175:TYR:CE1	2.56	0.40
27:Af:163:ILE:HD12	27:Af:163:ILE:HA	1.79	0.40
28:Ag:191:LYS:HA	28:Ag:191:LYS:HD2	1.93	0.40
28:Ag:392:ARG:HA	28:Ag:392:ARG:HD3	1.85	0.40
32:Ak:117:THR:HG22	32:Ak:118:PRO:HD2	2.04	0.40
33:Am:40:LYS:HD3	33:Am:40:LYS:HA	1.71	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:Ao:423:MET:SD	35:Ao:463:LYS:HB2	2.62	0.40
1:BC:599:ILE:O	1:BC:603:VAL:HG23	2.21	0.40
1:BC:614:LEU:HD12	1:BC:614:LEU:HA	1.89	0.40
1:BC:676:LEU:CD1	1:BC:692:CYS:HB2	2.52	0.40
3:AA:85:G:H2'	3:AA:86:A:H8	1.87	0.40
3:AA:708:A:H3'	3:AA:709:A:H5'	2.04	0.40
4:AB:57:LEU:H	4:AB:57:LEU:HD12	1.85	0.40
6:AE:196:ASN:HD22	6:AE:196:ASN:HA	1.61	0.40
6:AE:211:ASN:HB2	6:AE:213:GLU:HG2	2.03	0.40
6:AE:223:LEU:HD23	6:AE:223:LEU:HA	1.90	0.40
22:Aa:334:GLN:HB2	22:Aa:356:THR:HG21	2.03	0.40
23:Ab:19:LEU:HD12	23:Ab:19:LEU:HA	1.89	0.40
24:Ac:82:SER:OG	24:Ac:84:GLU:HB2	2.20	0.40
28:Ag:338:PRO:HD3	32:Ak:294:TYR:OH	2.21	0.40
30:Ai:65:LEU:HD21	35:Ao:120:ILE:HG21	2.03	0.40
31:Aj:58:VAL:HG13	31:Aj:137:HIS:CE1	2.57	0.40
33:Am:29:LEU:HD12	33:Am:29:LEU:HA	1.68	0.40
35:Ao:644:VAL:O	35:Ao:644:VAL:HG12	2.21	0.40
35:Ao:644:VAL:O	35:Ao:647:GLY:N	2.54	0.40
36:Ap:126:PHE:CE2	36:Ap:140:THR:HG21	2.47	0.40
3:AA:882:A:C5	3:AA:883:C:C4	3.10	0.40
6:AE:321:MET:HE2	6:AE:325:ARG:NH2	2.37	0.40
9:AI:176:HIS:O	9:AI:180:ARG:HG3	2.21	0.40
11:AK:155:GLY:N	11:AK:181:THR:HG23	2.36	0.40
16:AQ:87:LYS:HD2	16:AQ:87:LYS:HA	1.96	0.40
19:AV:54:A:HO2'	19:AV:55:C:P	2.40	0.40
20:AX:10:C:O2	20:AX:10:C:H2'	2.21	0.40
23:Ab:48:ARG:HG2	23:Ab:48:ARG:HH11	1.86	0.40
23:Ab:71:ARG:HG2	23:Ab:96:CYS:SG	2.61	0.40
28:Ag:209:TRP:HB3	28:Ag:231:ARG:NH1	2.36	0.40
35:Ao:531:LYS:HD3	35:Ao:562:TYR:OH	2.21	0.40
35:Ao:574:TRP:HH2	35:Ao:579:LEU:CB	2.30	0.40
36:Ap:95:ILE:HG22	36:Ap:100:VAL:HG22	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	
1	BC	569/657 (87%)	549 (96%)	19 (3%)	1 (0%)	43	73
2	BT	15/292 (5%)	14 (93%)	0	1 (7%)	1	6
4	AB	218/289 (75%)	210 (96%)	8 (4%)	0	100	100
5	AC	130/167 (78%)	121 (93%)	9 (7%)	0	100	100
6	AE	341/430 (79%)	330 (97%)	11 (3%)	0	100	100
7	AF	120/124 (97%)	119 (99%)	1 (1%)	0	100	100
8	AG	206/242 (85%)	204 (99%)	2 (1%)	0	100	100
9	AI	326/397 (82%)	312 (96%)	14 (4%)	0	100	100
10	AJ	138/201 (69%)	129 (94%)	7 (5%)	2 (1%)	9	34
11	AK	135/196 (69%)	129 (96%)	5 (4%)	1 (1%)	18	49
12	AL	107/139 (77%)	104 (97%)	3 (3%)	0	100	100
13	AN	99/128 (77%)	99 (100%)	0	0	100	100
14	AO	173/239 (72%)	167 (96%)	6 (4%)	0	100	100
15	AP	115/135 (85%)	113 (98%)	2 (2%)	0	100	100
16	AQ	110/130 (85%)	107 (97%)	3 (3%)	0	100	100
17	AR	95/143 (66%)	95 (100%)	0	0	100	100
18	AU	84/87 (97%)	84 (100%)	0	0	100	100
21	AZ	16/18 (89%)	15 (94%)	1 (6%)	0	100	100
22	Aa	290/382 (76%)	284 (98%)	6 (2%)	0	100	100
23	Ab	133/190 (70%)	128 (96%)	5 (4%)	0	100	100
24	Ac	167/173 (96%)	161 (96%)	5 (3%)	1 (1%)	21	52
25	Ad	175/205 (85%)	169 (97%)	6 (3%)	0	100	100
26	Ae	386/390 (99%)	350 (91%)	33 (8%)	3 (1%)	16	47
27	Af	97/188 (52%)	92 (95%)	5 (5%)	0	100	100
28	Ag	351/397 (88%)	339 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	Ah	118/387 (30%)	115 (98%)	3 (2%)	0	100	100
30	Ai	97/106 (92%)	91 (94%)	6 (6%)	0	100	100
31	Aj	211/218 (97%)	207 (98%)	4 (2%)	0	100	100
32	Ak	273/325 (84%)	267 (98%)	6 (2%)	0	100	100
33	Am	114/118 (97%)	109 (96%)	5 (4%)	0	100	100
34	An	70/199 (35%)	68 (97%)	2 (3%)	0	100	100
35	Ao	532/692 (77%)	505 (95%)	27 (5%)	0	100	100
36	Ap	188/258 (73%)	181 (96%)	7 (4%)	0	100	100
All	All	6199/8242 (75%)	5967 (96%)	223 (4%)	9 (0%)	49	78

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	BT	68	PRO
10	AJ	185	ARG
10	AJ	179	GLN
26	Ae	344	GLU
1	BC	502	PRO
26	Ae	161	ALA
26	Ae	342	PRO
11	AK	160	ARG
24	Ac	105	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BC	464/556 (84%)	440 (95%)	24 (5%)	21	51
2	BT	8/258 (3%)	7 (88%)	1 (12%)	4	19
4	AB	187/233 (80%)	172 (92%)	15 (8%)	11	37
5	AC	115/142 (81%)	97 (84%)	18 (16%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	AE	282/351 (80%)	244 (86%)	38 (14%)	4	16
7	AF	107/109 (98%)	92 (86%)	15 (14%)	3	15
8	AG	181/205 (88%)	164 (91%)	17 (9%)	8	31
9	AI	273/333 (82%)	248 (91%)	25 (9%)	8	31
10	AJ	130/181 (72%)	117 (90%)	13 (10%)	7	29
11	AK	103/151 (68%)	84 (82%)	19 (18%)	1	8
12	AL	92/116 (79%)	80 (87%)	12 (13%)	4	18
13	AN	92/114 (81%)	80 (87%)	12 (13%)	4	18
14	AO	159/205 (78%)	142 (89%)	17 (11%)	6	25
15	AP	97/113 (86%)	91 (94%)	6 (6%)	16	46
16	AQ	97/114 (85%)	83 (86%)	14 (14%)	3	14
17	AR	89/127 (70%)	82 (92%)	7 (8%)	11	37
18	AU	77/78 (99%)	63 (82%)	14 (18%)	2	8
22	Aa	258/330 (78%)	233 (90%)	25 (10%)	8	30
23	Ab	113/162 (70%)	103 (91%)	10 (9%)	9	33
24	Ac	152/155 (98%)	136 (90%)	16 (10%)	6	26
25	Ad	149/168 (89%)	139 (93%)	10 (7%)	15	43
26	Ae	325/342 (95%)	297 (91%)	28 (9%)	10	34
27	Af	86/160 (54%)	74 (86%)	12 (14%)	3	15
28	Ag	312/350 (89%)	289 (93%)	23 (7%)	13	40
29	Ah	109/346 (32%)	103 (94%)	6 (6%)	19	50
30	Ai	86/93 (92%)	78 (91%)	8 (9%)	8	31
31	Aj	188/190 (99%)	176 (94%)	12 (6%)	16	44
32	Ak	249/289 (86%)	224 (90%)	25 (10%)	7	29
33	Am	100/102 (98%)	88 (88%)	12 (12%)	5	21
34	An	66/174 (38%)	55 (83%)	11 (17%)	2	10
35	Ao	478/538 (89%)	450 (94%)	28 (6%)	18	48
36	Ap	170/225 (76%)	146 (86%)	24 (14%)	3	15
All	All	5394/7010 (77%)	4877 (90%)	517 (10%)	10	30

All (517) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BC	184	THR
1	BC	215	GLN
1	BC	251	VAL
1	BC	283	ILE
1	BC	304	LEU
1	BC	310	VAL
1	BC	330	ASN
1	BC	373	THR
1	BC	398	LEU
1	BC	424	LEU
1	BC	426	SER
1	BC	471	LYS
1	BC	472	GLU
1	BC	494	PHE
1	BC	515	VAL
1	BC	519	ILE
1	BC	520	ILE
1	BC	524	VAL
1	BC	544	CYS
1	BC	566	THR
1	BC	575	ASN
1	BC	674	THR
1	BC	679	HIS
1	BC	727	PHE
2	BT	61	VAL
4	AB	57	LEU
4	AB	125	GLN
4	AB	141	ILE
4	AB	167	THR
4	AB	176	THR
4	AB	186	VAL
4	AB	197	THR
4	AB	206	VAL
4	AB	218	THR
4	AB	221	ILE
4	AB	222	VAL
4	AB	224	THR
4	AB	235	VAL
4	AB	241	SER
4	AB	261	GLU
5	AC	38	ARG
5	AC	41	ARG
5	AC	44	VAL

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Mol	Chain	Res	Type
5	AC	71	LEU
5	AC	80	ASP
5	AC	89	ASP
5	AC	103	CYS
5	AC	104	LEU
5	AC	108	LEU
5	AC	115	ASN
5	AC	117	LEU
5	AC	123	VAL
5	AC	124	LEU
5	AC	125	ARG
5	AC	127	LEU
5	AC	153	LEU
5	AC	166	TYR
5	AC	167	ILE
6	AE	124	LYS
6	AE	137	HIS
6	AE	154	VAL
6	AE	156	THR
6	AE	191	ARG
6	AE	194	SER
6	AE	196	ASN
6	AE	203	LEU
6	AE	215	TYR
6	AE	216	ASP
6	AE	220	THR
6	AE	228	VAL
6	AE	239	ARG
6	AE	240	SER
6	AE	241	VAL
6	AE	242	ARG
6	AE	245	VAL
6	AE	283	GLU
6	AE	289	THR
6	AE	290	ILE
6	AE	296	LEU
6	AE	312	TYR
6	AE	320	ILE
6	AE	336	VAL
6	AE	337	SER
6	AE	340	VAL
6	AE	346	THR

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Mol	Chain	Res	Type
6	AE	355	ARG
6	AE	370	VAL
6	AE	374	ARG
6	AE	376	GLU
6	AE	400	GLU
6	AE	401	VAL
6	AE	404	ILE
6	AE	417	MET
6	AE	420	SER
6	AE	427	ARG
6	AE	430	THR
7	AF	13	MET
7	AF	17	GLU
7	AF	29	LEU
7	AF	39	LEU
7	AF	45	ARG
7	AF	46	MET
7	AF	57	ARG
7	AF	65	LEU
7	AF	67	ASP
7	AF	78	MET
7	AF	79	MET
7	AF	83	SER
7	AF	89	ILE
7	AF	106	GLU
7	AF	120	THR
8	AG	40	GLU
8	AG	46	ILE
8	AG	57	GLU
8	AG	82	THR
8	AG	85	VAL
8	AG	88	ASP
8	AG	109	SER
8	AG	118	VAL
8	AG	153	GLU
8	AG	159	VAL
8	AG	180	ARG
8	AG	187	MET
8	AG	197	ARG
8	AG	200	LEU
8	AG	205	LEU
8	AG	219	VAL

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Mol	Chain	Res	Type
8	AG	226	MET
9	AI	70	THR
9	AI	91	MET
9	AI	98	THR
9	AI	100	THR
9	AI	153	THR
9	AI	161	LEU
9	AI	172	VAL
9	AI	199	ARG
9	AI	201	LEU
9	AI	202	ILE
9	AI	206	LEU
9	AI	217	GLN
9	AI	224	ARG
9	AI	229	LEU
9	AI	230	SER
9	AI	237	THR
9	AI	256	GLN
9	AI	261	LEU
9	AI	277	ARG
9	AI	314	LEU
9	AI	329	MET
9	AI	338	ARG
9	AI	357	VAL
9	AI	366	ARG
9	AI	390	ARG
10	AJ	52	VAL
10	AJ	64	THR
10	AJ	80	VAL
10	AJ	81	LYS
10	AJ	126	ILE
10	AJ	133	GLN
10	AJ	136	MET
10	AJ	145	LEU
10	AJ	148	LEU
10	AJ	166	GLU
10	AJ	168	VAL
10	AJ	176	LYS
10	AJ	184	ILE
11	AK	64	ILE
11	AK	68	ILE
11	AK	83	GLU

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Mol	Chain	Res	Type
11	AK	85	ILE
11	AK	87	ILE
11	AK	97	THR
11	AK	121	ASN
11	AK	123	LYS
11	AK	147	THR
11	AK	150	ARG
11	AK	153	VAL
11	AK	161	LEU
11	AK	164	ILE
11	AK	169	MET
11	AK	177	ILE
11	AK	181	THR
11	AK	183	ILE
11	AK	188	CYS
11	AK	195	ARG
12	AL	32	THR
12	AL	55	ARG
12	AL	67	ILE
12	AL	74	ASN
12	AL	84	ARG
12	AL	93	CYS
12	AL	95	ILE
12	AL	101	SER
12	AL	102	LEU
12	AL	107	VAL
12	AL	124	THR
12	AL	129	LYS
13	AN	30	VAL
13	AN	34	MET
13	AN	35	LEU
13	AN	43	MET
13	AN	80	ARG
13	AN	92	VAL
13	AN	93	MET
13	AN	94	THR
13	AN	102	ARG
13	AN	106	LEU
13	AN	107	SER
13	AN	125	ARG
14	AO	72	MET
14	AO	73	LEU

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Mol	Chain	Res	Type
14	AO	74	LEU
14	AO	78	GLN
14	AO	80	VAL
14	AO	83	ILE
14	AO	105	LEU
14	AO	116	VAL
14	AO	122	ASP
14	AO	127	GLU
14	AO	130	ILE
14	AO	133	LEU
14	AO	158	LEU
14	AO	159	MET
14	AO	161	ILE
14	AO	171	LEU
14	AO	208	LYS
15	AP	35	VAL
15	AP	90	LEU
15	AP	94	SER
15	AP	99	LEU
15	AP	102	MET
15	AP	119	LEU
16	AQ	6	SER
16	AQ	22	MET
16	AQ	31	THR
16	AQ	40	LEU
16	AQ	55	LEU
16	AQ	56	GLN
16	AQ	59	THR
16	AQ	62	ASP
16	AQ	64	VAL
16	AQ	69	LEU
16	AQ	81	LEU
16	AQ	90	GLN
16	AQ	96	THR
16	AQ	104	THR
17	AR	56	GLU
17	AR	83	GLN
17	AR	86	SER
17	AR	89	THR
17	AR	117	ILE
17	AR	124	THR
17	AR	131	LEU

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Mol	Chain	Res	Type
18	AU	10	ARG
18	AU	13	MET
18	AU	14	VAL
18	AU	18	ASN
18	AU	32	MET
18	AU	35	LEU
18	AU	47	LYS
18	AU	50	ARG
18	AU	52	ARG
18	AU	66	MET
18	AU	76	MET
18	AU	77	ARG
18	AU	82	ASP
18	AU	85	GLN
22	Aa	124	THR
22	Aa	126	LYS
22	Aa	128	MET
22	Aa	129	THR
22	Aa	147	ARG
22	Aa	150	MET
22	Aa	167	ASP
22	Aa	177	LYS
22	Aa	183	ILE
22	Aa	195	VAL
22	Aa	197	ARG
22	Aa	202	THR
22	Aa	204	ARG
22	Aa	222	GLU
22	Aa	226	ILE
22	Aa	239	THR
22	Aa	240	MET
22	Aa	247	VAL
22	Aa	276	ASP
22	Aa	285	ARG
22	Aa	293	MET
22	Aa	295	TRP
22	Aa	325	LEU
22	Aa	347	LEU
22	Aa	356	THR
23	Ab	6	LEU
23	Ab	7	GLU
23	Ab	12	ILE

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Mol	Chain	Res	Type
23	Ab	14	SER
23	Ab	17	ARG
23	Ab	30	LEU
23	Ab	45	VAL
23	Ab	57	LYS
23	Ab	67	GLU
23	Ab	112	THR
24	Ac	3	MET
24	Ac	4	LYS
24	Ac	9	ILE
24	Ac	25	ASP
24	Ac	30	MET
24	Ac	31	THR
24	Ac	33	ASN
24	Ac	39	GLU
24	Ac	51	ASN
24	Ac	84	GLU
24	Ac	102	ILE
24	Ac	104	LYS
24	Ac	106	LEU
24	Ac	124	SER
24	Ac	139	CYS
24	Ac	140	MET
25	Ad	41	ARG
25	Ad	56	LEU
25	Ad	62	GLN
25	Ad	71	ARG
25	Ad	161	GLN
25	Ad	166	THR
25	Ad	169	THR
25	Ad	173	LEU
25	Ad	192	THR
25	Ad	196	LEU
26	Ae	84	ASP
26	Ae	102	GLU
26	Ae	107	VAL
26	Ae	112	ILE
26	Ae	122	ARG
26	Ae	136	ARG
26	Ae	138	SER
26	Ae	150	HIS
26	Ae	159	TYR

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Mol	Chain	Res	Type
26	Ae	171	ASN
26	Ae	180	ASP
26	Ae	186	LEU
26	Ae	201	LEU
26	Ae	206	GLU
26	Ae	208	MET
26	Ae	220	LEU
26	Ae	223	LEU
26	Ae	230	LEU
26	Ae	249	LEU
26	Ae	250	LEU
26	Ae	253	LEU
26	Ae	255	GLN
26	Ae	257	ASN
26	Ae	281	ARG
26	Ae	315	LEU
26	Ae	322	VAL
26	Ae	388	VAL
26	Ae	421	GLN
27	Af	84	MET
27	Af	85	LEU
27	Af	88	SER
27	Af	90	LEU
27	Af	108	ILE
27	Af	109	VAL
27	Af	111	ASP
27	Af	145	LEU
27	Af	148	LEU
27	Af	151	THR
27	Af	155	LEU
27	Af	162	THR
28	Ag	50	THR
28	Ag	88	MET
28	Ag	101	ARG
28	Ag	135	LEU
28	Ag	138	CYS
28	Ag	142	HIS
28	Ag	172	TYR
28	Ag	178	ASP
28	Ag	181	LEU
28	Ag	194	ASN
28	Ag	215	THR

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Mol	Chain	Res	Type
28	Ag	243	LEU
28	Ag	246	LEU
28	Ag	252	LEU
28	Ag	264	VAL
28	Ag	265	ASN
28	Ag	296	VAL
28	Ag	305	ILE
28	Ag	334	ASP
28	Ag	336	LEU
28	Ag	337	ASP
28	Ag	372	THR
28	Ag	397	LEU
29	Ah	302	LEU
29	Ah	308	ASN
29	Ah	323	HIS
29	Ah	328	LYS
29	Ah	359	LYS
29	Ah	384	ILE
30	Ai	11	MET
30	Ai	26	THR
30	Ai	31	MET
30	Ai	36	LEU
30	Ai	50	ASP
30	Ai	61	LEU
30	Ai	62	MET
30	Ai	72	ARG
31	Aj	21	LEU
31	Aj	40	THR
31	Aj	42	MET
31	Aj	52	MET
31	Aj	65	LEU
31	Aj	80	VAL
31	Aj	99	ARG
31	Aj	101	ARG
31	Aj	118	LEU
31	Aj	135	MET
31	Aj	138	ASP
31	Aj	170	LEU
32	Ak	53	LYS
32	Ak	79	LYS
32	Ak	85	LEU
32	Ak	89	MET

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Mol	Chain	Res	Type
32	Ak	93	VAL
32	Ak	102	GLU
32	Ak	108	LEU
32	Ak	117	THR
32	Ak	125	CYS
32	Ak	134	GLU
32	Ak	152	GLU
32	Ak	154	ASP
32	Ak	159	VAL
32	Ak	165	ILE
32	Ak	166	ARG
32	Ak	175	LEU
32	Ak	196	VAL
32	Ak	204	THR
32	Ak	213	ARG
32	Ak	249	ASP
32	Ak	264	ILE
32	Ak	269	LEU
32	Ak	288	THR
32	Ak	298	VAL
32	Ak	309	ASN
33	Am	6	LEU
33	Am	13	LEU
33	Am	17	ARG
33	Am	29	LEU
33	Am	33	VAL
33	Am	46	ILE
33	Am	48	GLU
33	Am	49	MET
33	Am	53	MET
33	Am	63	ASP
33	Am	72	ASP
33	Am	113	ASN
34	An	130	ILE
34	An	144	ARG
34	An	145	LYS
34	An	146	LEU
34	An	154	ARG
34	An	158	ARG
34	An	163	ARG
34	An	164	GLN
34	An	176	ILE

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Mol	Chain	Res	Type
34	An	191	THR
34	An	199	GLN
35	Ao	59	ILE
35	Ao	71	LEU
35	Ao	96	ILE
35	Ao	101	VAL
35	Ao	243	THR
35	Ao	256	GLU
35	Ao	262	TYR
35	Ao	285	LEU
35	Ao	296	THR
35	Ao	363	MET
35	Ao	372	LEU
35	Ao	387	SER
35	Ao	414	ASP
35	Ao	416	ASP
35	Ao	432	LEU
35	Ao	441	LEU
35	Ao	442	LEU
35	Ao	446	ASP
35	Ao	447	ASN
35	Ao	488	VAL
35	Ao	537	LEU
35	Ao	538	MET
35	Ao	582	VAL
35	Ao	608	ILE
35	Ao	622	LYS
35	Ao	645	CYS
35	Ao	652	VAL
35	Ao	661	GLU
36	Ap	53	ASP
36	Ap	89	ARG
36	Ap	91	ARG
36	Ap	95	ILE
36	Ap	103	ASN
36	Ap	107	ILE
36	Ap	108	CYS
36	Ap	113	LEU
36	Ap	127	VAL
36	Ap	140	THR
36	Ap	149	LYS
36	Ap	155	GLN

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Mol	Chain	Res	Type
36	Ap	167	ILE
36	Ap	170	VAL
36	Ap	175	LEU
36	Ap	177	PHE
36	Ap	184	VAL
36	Ap	186	SER
36	Ap	193	LEU
36	Ap	204	SER
36	Ap	213	LEU
36	Ap	216	LEU
36	Ap	219	LEU
36	Ap	235	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (139) such sidechains are listed below:

Mol	Chain	Res	Type
1	BC	215	GLN
1	BC	238	HIS
1	BC	330	ASN
1	BC	470	HIS
1	BC	575	ASN
1	BC	596	HIS
1	BC	652	GLN
4	AB	68	HIS
4	AB	125	GLN
4	AB	133	HIS
4	AB	149	GLN
4	AB	152	HIS
4	AB	200	ASN
4	AB	253	GLN
5	AC	72	HIS
5	AC	75	ASN
5	AC	115	ASN
5	AC	145	HIS
6	AE	137	HIS
6	AE	151	ASN
6	AE	196	ASN
6	AE	292	HIS
6	AE	317	HIS
6	AE	356	GLN
6	AE	360	GLN
8	AG	140	ASN

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Mol	Chain	Res	Type
8	AG	146	HIS
8	AG	196	HIS
8	AG	227	HIS
8	AG	233	ASN
8	AG	238	HIS
9	AI	87	HIS
9	AI	101	GLN
9	AI	127	HIS
9	AI	156	GLN
9	AI	163	HIS
9	AI	176	HIS
9	AI	327	HIS
9	AI	367	GLN
10	AJ	109	HIS
10	AJ	130	HIS
11	AK	100	GLN
11	AK	131	GLN
11	AK	186	ASN
12	AL	35	GLN
12	AL	77	ASN
12	AL	100	HIS
12	AL	105	HIS
12	AL	106	HIS
13	AN	60	ASN
13	AN	119	GLN
14	AO	84	HIS
14	AO	119	ASN
14	AO	139	ASN
14	AO	147	HIS
14	AO	153	HIS
14	AO	197	HIS
14	AO	201	HIS
15	AP	100	HIS
16	AQ	9	HIS
16	AQ	23	GLN
16	AQ	56	GLN
16	AQ	76	HIS
16	AQ	79	HIS
17	AR	77	ASN
17	AR	116	GLN
18	AU	3	ASN
18	AU	79	ASN

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Mol	Chain	Res	Type
22	Aa	236	ASN
22	Aa	245	GLN
22	Aa	246	HIS
22	Aa	251	ASN
22	Aa	299	ASN
22	Aa	310	GLN
22	Aa	327	HIS
22	Aa	337	GLN
22	Aa	348	HIS
23	Ab	36	ASN
24	Ac	14	GLN
24	Ac	35	ASN
24	Ac	56	GLN
24	Ac	59	ASN
24	Ac	63	GLN
24	Ac	69	ASN
24	Ac	118	GLN
24	Ac	122	GLN
24	Ac	125	HIS
24	Ac	146	GLN
25	Ad	117	HIS
25	Ad	161	GLN
26	Ae	140	ASN
26	Ae	185	ASN
26	Ae	196	ASN
26	Ae	243	ASN
26	Ae	257	ASN
26	Ae	301	GLN
26	Ae	314	GLN
26	Ae	421	GLN
26	Ae	422	GLN
27	Af	87	HIS
27	Af	92	GLN
27	Af	122	HIS
27	Af	174	GLN
28	Ag	58	HIS
28	Ag	62	HIS
28	Ag	113	ASN
28	Ag	115	ASN
28	Ag	118	HIS
28	Ag	142	HIS
28	Ag	311	GLN

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Mol	Chain	Res	Type
28	Ag	386	ASN
29	Ah	288	ASN
29	Ah	309	ASN
29	Ah	323	HIS
29	Ah	341	HIS
29	Ah	364	HIS
30	Ai	56	ASN
30	Ai	75	HIS
31	Aj	60	HIS
31	Aj	111	HIS
32	Ak	263	ASN
32	Ak	303	ASN
33	Am	32	HIS
33	Am	113	ASN
34	An	164	GLN
35	Ao	258	ASN
35	Ao	272	HIS
35	Ao	288	ASN
35	Ao	318	ASN
35	Ao	329	GLN
35	Ao	385	HIS
35	Ao	443	ASN
35	Ao	455	HIS
35	Ao	543	HIS
36	Ap	81	HIS
36	Ap	136	HIS
36	Ap	147	HIS
36	Ap	169	GLN
36	Ap	181	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
19	AV	70/71 (98%)	28 (40%)	0
20	AX	16/201 (7%)	10 (62%)	1 (6%)
3	AA	959/962 (99%)	249 (25%)	4 (0%)
All	All	1045/1234 (84%)	287 (27%)	5 (0%)

All (287) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	AA	5	A
3	AA	10	U
3	AA	11	G
3	AA	18	G
3	AA	27	U
3	AA	32	U
3	AA	34	U
3	AA	36	A
3	AA	42	A
3	AA	44	U
3	AA	49	A
3	AA	54	A
3	AA	55	G
3	AA	58	U
3	AA	61	G
3	AA	65	C
3	AA	66	C
3	AA	67	C
3	AA	75	A
3	AA	77	G
3	AA	83	C
3	AA	89	U
3	AA	90	U
3	AA	93	A
3	AA	98	A
3	AA	102	G
3	AA	103	G
3	AA	104	A
3	AA	111	A
3	AA	115	A
3	AA	120	A
3	AA	124	A
3	AA	125	U
3	AA	131	U
3	AA	147	G
3	AA	152	A
3	AA	161	C
3	AA	168	A
3	AA	170	A
3	AA	171	C
3	AA	173	G
3	AA	176	G
3	AA	178	G

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Mol	Chain	Res	Type
3	AA	186	U
3	AA	187	U
3	AA	191	C
3	AA	192	C
3	AA	193	A
3	AA	203	G
3	AA	212	A
3	AA	216	A
3	AA	217	U
3	AA	222	A
3	AA	223	U
3	AA	224	U
3	AA	225	A
3	AA	231	G
3	AA	238	C
3	AA	244	C
3	AA	253	G
3	AA	257	U
3	AA	258	C
3	AA	273	A
3	AA	280	A
3	AA	281	G
3	AA	288	G
3	AA	294	A
3	AA	297	A
3	AA	306	G
3	AA	308	A
3	AA	309	A
3	AA	310	A
3	AA	312	A
3	AA	314	A
3	AA	315	U
3	AA	317	A
3	AA	320	A
3	AA	328	A
3	AA	330	A
3	AA	335	A
3	AA	340	A
3	AA	345	U
3	AA	353	C
3	AA	354	C
3	AA	355	U

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Mol	Chain	Res	Type
3	AA	361	A
3	AA	362	A
3	AA	367	A
3	AA	368	A
3	AA	381	G
3	AA	392	A
3	AA	395	C
3	AA	396	C
3	AA	399	A
3	AA	407	U
3	AA	417	C
3	AA	421	A
3	AA	426	G
3	AA	432	A
3	AA	433	U
3	AA	434	A
3	AA	439	A
3	AA	450	C
3	AA	455	A
3	AA	456	A
3	AA	457	C
3	AA	465	G
3	AA	471	U
3	AA	472	A
3	AA	477	A
3	AA	479	C
3	AA	480	U
3	AA	483	U
3	AA	488	A
3	AA	489	G
3	AA	491	G
3	AA	497	C
3	AA	498	U
3	AA	502	A
3	AA	503	A
3	AA	518	A
3	AA	523	C
3	AA	530	G
3	AA	531	U
3	AA	536	C
3	AA	538	C
3	AA	540	U

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Mol	Chain	Res	Type
3	AA	554	C
3	AA	560	C
3	AA	561	U
3	AA	564	A
3	AA	566	U
3	AA	571	A
3	AA	574	C
3	AA	576	C
3	AA	578	G
3	AA	579	A
3	AA	580	U
3	AA	581	A
3	AA	588	A
3	AA	589	C
3	AA	593	C
3	AA	594	C
3	AA	596	U
3	AA	597	U
3	AA	598	G
3	AA	604	U
3	AA	616	C
3	AA	618	G
3	AA	619	C
3	AA	620	C
3	AA	625	U
3	AA	628	G
3	AA	633	C
3	AA	638	A
3	AA	639	A
3	AA	641	A
3	AA	644	A
3	AA	645	A
3	AA	646	C
3	AA	647	A
3	AA	648	A
3	AA	649	U
3	AA	650	A
3	AA	651	G
3	AA	665	A
3	AA	666	G
3	AA	681	A
3	AA	682	G

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Mol	Chain	Res	Type
3	AA	687	A
3	AA	695	C
3	AA	696	U
3	AA	698	A
3	AA	699	U
3	AA	702	G
3	AA	707	A
3	AA	709	A
3	AA	711	A
3	AA	712	A
3	AA	722	A
3	AA	731	A
3	AA	732	U
3	AA	734	A
3	AA	739	A
3	AA	741	C
3	AA	742	C
3	AA	743	A
3	AA	744	C
3	AA	745	C
3	AA	746	A
3	AA	749	C
3	AA	751	A
3	AA	753	A
3	AA	766	C
3	AA	775	A
3	AA	778	G
3	AA	786	U
3	AA	790	A
3	AA	791	G
3	AA	803	U
3	AA	807	G
3	AA	823	G
3	AA	825	C
3	AA	826	C
3	AA	838	A
3	AA	841	C
3	AA	842	A
3	AA	850	U
3	AA	854	C
3	AA	860	C
3	AA	862	A

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Mol	Chain	Res	Type
3	AA	863	G
3	AA	869	A
3	AA	870	G
3	AA	871	U
3	AA	874	U
3	AA	876	A
3	AA	877	A
3	AA	878	A
3	AA	880	U
3	AA	883	C
3	AA	885	U
3	AA	886	A
3	AA	887	U
3	AA	892	A
3	AA	893	A
3	AA	894	U
3	AA	897	C
3	AA	899	C
3	AA	900	A
3	AA	902	C
3	AA	905	U
3	AA	910	G
3	AA	917	C
3	AA	918	A
3	AA	920	G
3	AA	923	G
3	AA	925	A
3	AA	928	A
3	AA	930	G
3	AA	932	U
3	AA	933	A
3	AA	943	G
3	AA	945	A
3	AA	946	A
3	AA	955	G
3	AA	956	G
3	AA	959	U
3	AA	962	C
19	AV	6	G
19	AV	7	G
19	AV	9	C
19	AV	13	U

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Mol	Chain	Res	Type
19	AV	14	A
19	AV	15	A
19	AV	16	A
19	AV	17	U
19	AV	18	A
19	AV	22	U
19	AV	33	U
19	AV	43	A
19	AV	44	U
19	AV	45	G
19	AV	46	U
19	AV	51	U
19	AV	52	A
19	AV	53	U
19	AV	54	A
19	AV	55	C
19	AV	56	C
19	AV	62	C
19	AV	63	G
19	AV	64	U
19	AV	65	A
19	AV	67	U
19	AV	68	A
19	AV	71	A
20	AX	3	G
20	AX	4	A
20	AX	7	C
20	AX	8	A
20	AX	9	C
20	AX	10	C
20	AX	11	A
20	AX	13	U
20	AX	14	C
20	AX	15	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	AA	65	C
3	AA	395	C
3	AA	587	U
3	AA	743	A

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Mol	Chain	Res	Type
20	AX	12	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 119 ligands modelled in this entry, 115 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
42	FME	AV	101	19	8,9,10	0.97	0	8,9,11	1.00	1 (12%)
43	GTP	Ag	500	38	33,34,34	0.95	1 (3%)	50,54,54	1.51	10 (20%)
37	GSP	BC	901	38	33,34,34	1.89	4 (12%)	47,54,54	1.66	9 (19%)
40	SPM	AA	3001	-	13,13,13	0.34	0	12,12,12	1.03	1 (8%)

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
42	FME	AV	101	19	-	4/7/9/11	-
43	GTP	Ag	500	38	-	7/22/38/38	0/3/3/3
37	GSP	BC	901	38	-	0/21/38/38	0/3/3/3
40	SPM	AA	3001	-	-	5/11/11/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	BC	901	GSP	PG-S1G	-9.21	1.70	1.90
37	BC	901	GSP	C2-N3	2.28	1.38	1.33
37	BC	901	GSP	PB-O3B	2.13	1.61	1.59
43	Ag	500	GTP	C2-N3	2.07	1.38	1.33
37	BC	901	GSP	PA-O3A	2.01	1.61	1.59

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	BC	901	GSP	C5-C4-N3	-5.07	120.33	128.39
43	Ag	500	GTP	C5-C4-N3	-4.79	120.77	128.39
37	BC	901	GSP	C2-N3-C4	4.57	120.17	112.30
43	Ag	500	GTP	C2-N3-C4	4.32	119.74	112.30
37	BC	901	GSP	PB-O3B-PG	-3.28	121.17	133.17
37	BC	901	GSP	N9-C4-N3	3.14	132.23	125.95
43	Ag	500	GTP	N9-C4-N3	2.96	131.88	125.95
43	Ag	500	GTP	C2-N1-C6	-2.78	120.07	125.11
37	BC	901	GSP	C2-N1-C6	-2.73	120.15	125.11
37	BC	901	GSP	C8-N7-C5	2.69	109.06	104.26
37	BC	901	GSP	N9-C8-N7	-2.65	108.49	113.40
43	Ag	500	GTP	O2G-PG-O3B	2.61	113.40	104.64
43	Ag	500	GTP	O6-C6-C5	-2.42	120.14	126.53
43	Ag	500	GTP	C5-C6-N1	2.35	119.24	113.25
37	BC	901	GSP	C5-C6-N1	2.30	119.11	113.25
43	Ag	500	GTP	C2'-C1'-N9	-2.28	106.91	113.25
37	BC	901	GSP	O6-C6-C5	-2.28	120.53	126.53
43	Ag	500	GTP	N9-C8-N7	-2.15	109.42	113.40
40	AA	3001	SPM	C11-C12-C13	-2.11	106.65	114.17
43	Ag	500	GTP	C8-N7-C5	2.10	108.01	104.26
42	AV	101	FME	CB-CA-N	2.05	114.25	110.52

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
42	AV	101	FME	C-CA-CB-CG
40	AA	3001	SPM	C2-C3-C4-N5
40	AA	3001	SPM	C7-C8-C9-N10
42	AV	101	FME	CA-CB-CG-SD
43	Ag	500	GTP	O4'-C4'-C5'-O5'
42	AV	101	FME	N-CA-CB-CG

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Continued from previous page...

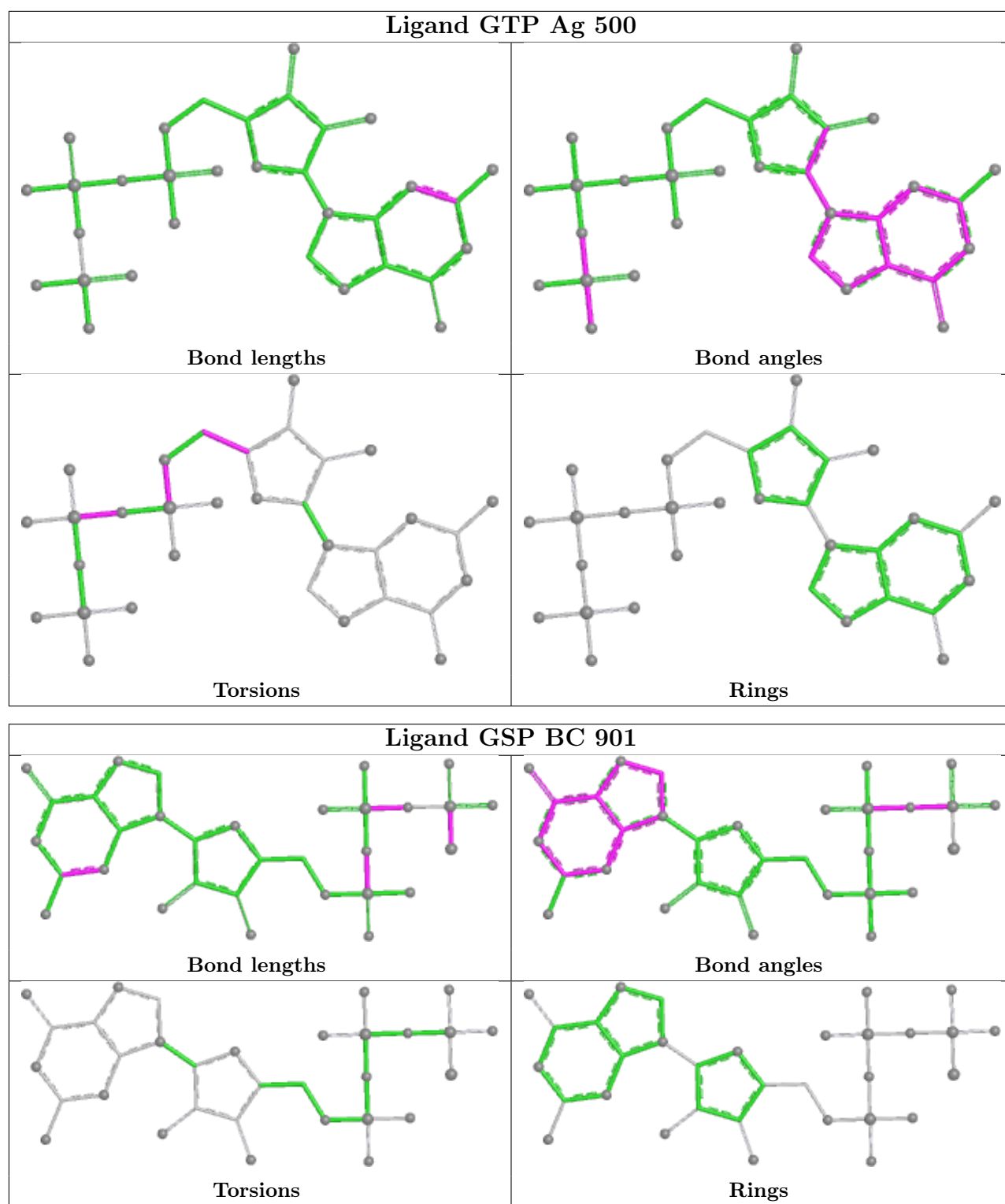
Mol	Chain	Res	Type	Atoms
40	AA	3001	SPM	C8-C9-N10-C11
40	AA	3001	SPM	C12-C11-N10-C9
43	Ag	500	GTP	C3'-C4'-C5'-O5'
42	AV	101	FME	CB-CG-SD-CE
40	AA	3001	SPM	N1-C2-C3-C4
43	Ag	500	GTP	C5'-O5'-PA-O3A
43	Ag	500	GTP	C5'-O5'-PA-O1A
43	Ag	500	GTP	C5'-O5'-PA-O2A
43	Ag	500	GTP	PA-O3A-PB-O2B
43	Ag	500	GTP	PA-O3A-PB-O1B

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	AV	101	FME	1	0
43	Ag	500	GTP	3	0
37	BC	901	GSP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
35	Ao	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Ao	234:UNK	C	240:THR	N	8.66

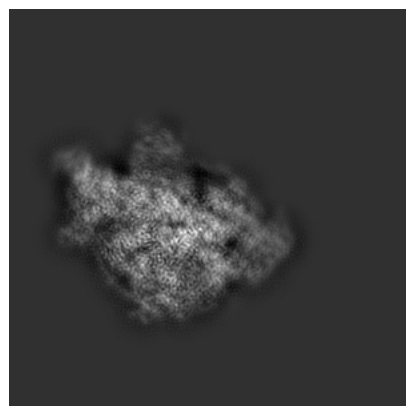
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4369. These allow visual inspection of the internal detail of the map and identification of artifacts.

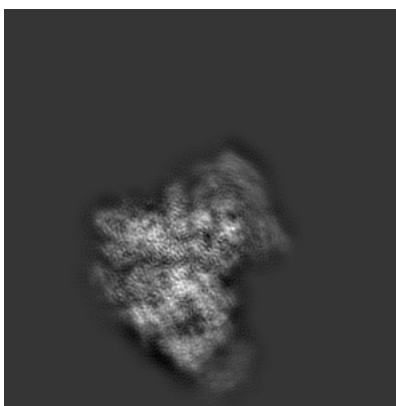
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

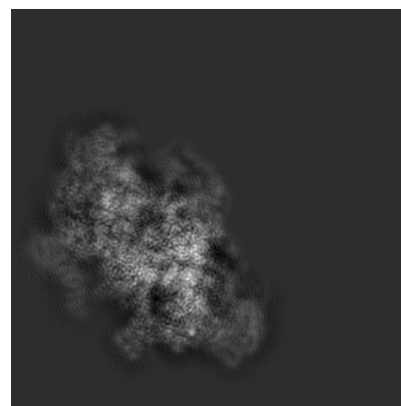
6.1.1 Primary map



X

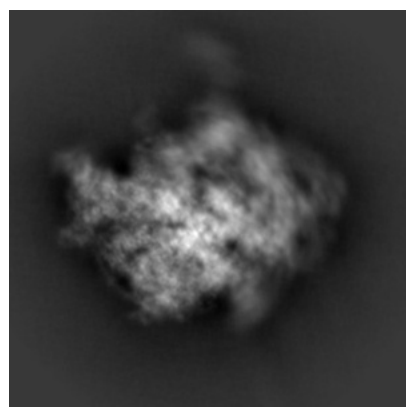


Y

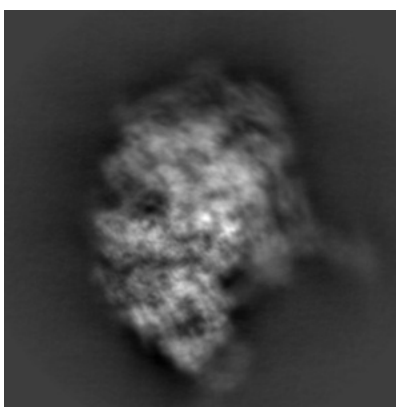


Z

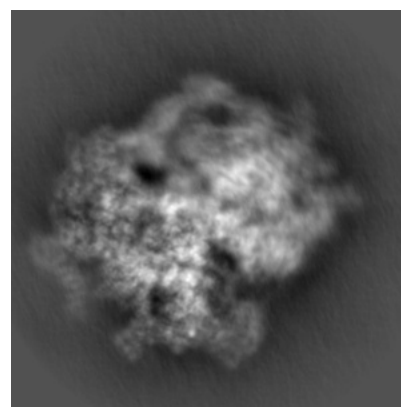
6.1.2 Raw map



X



Y

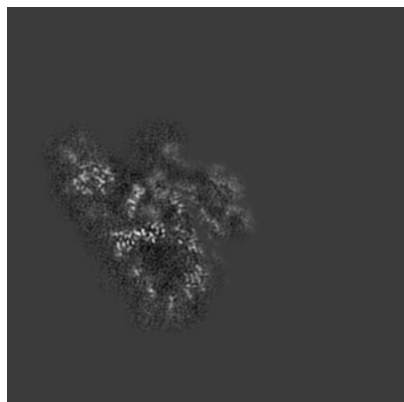


Z

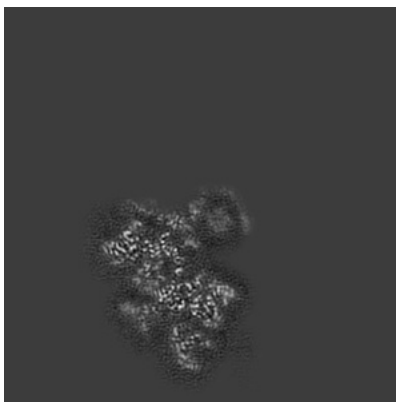
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

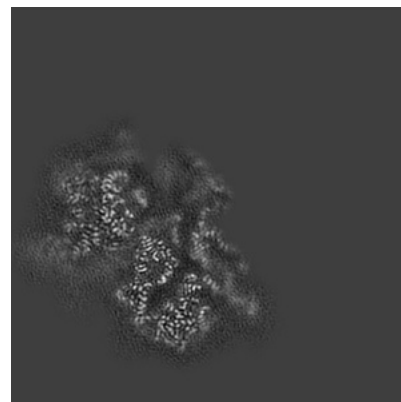
6.2.1 Primary map



X Index: 140

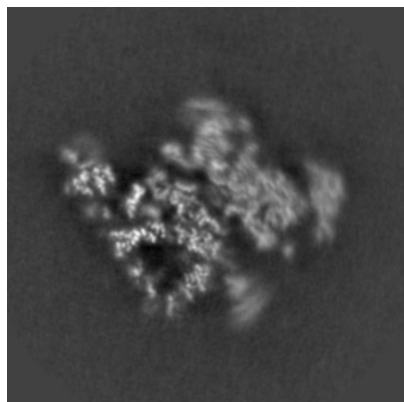


Y Index: 140

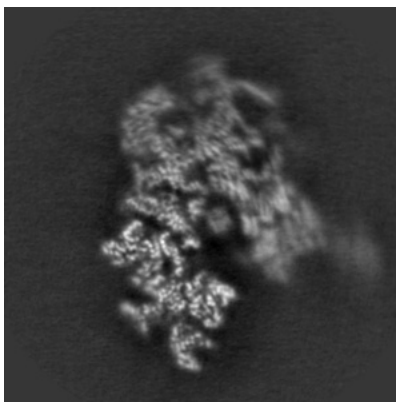


Z Index: 140

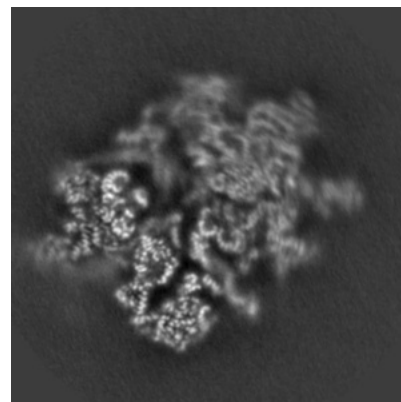
6.2.2 Raw map



X Index: 140



Y Index: 140

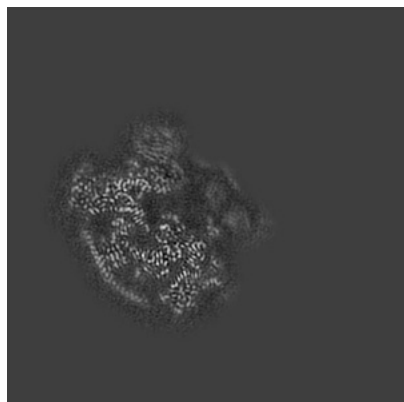


Z Index: 140

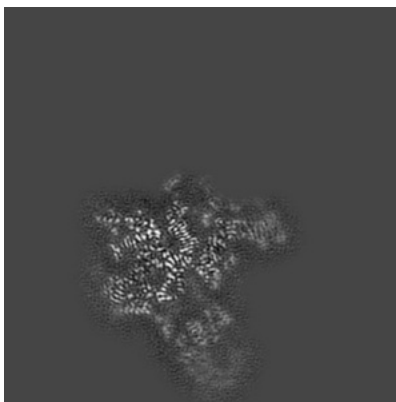
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

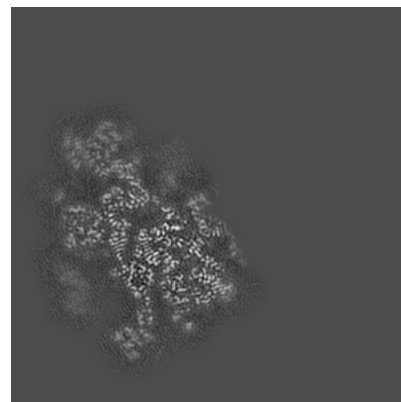
6.3.1 Primary map



X Index: 123

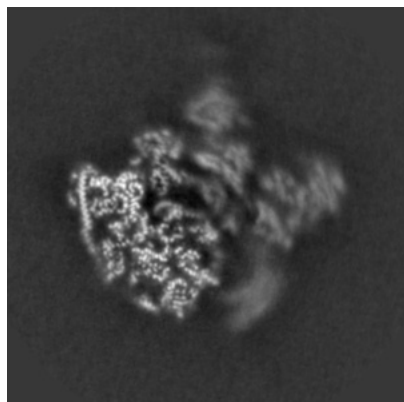


Y Index: 108

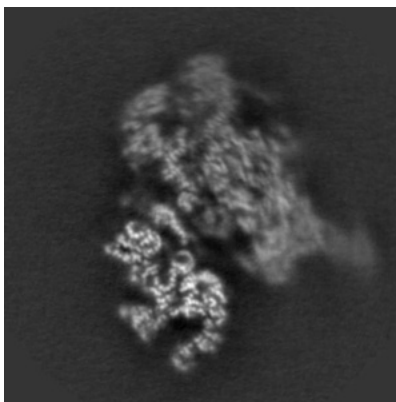


Z Index: 118

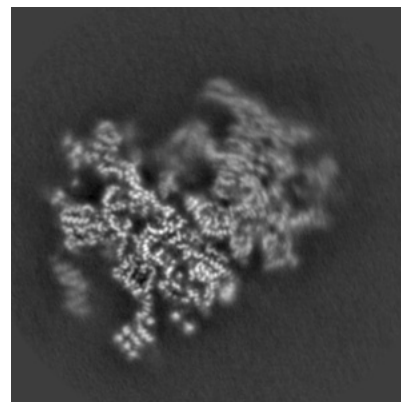
6.3.2 Raw map



X Index: 127



Y Index: 145

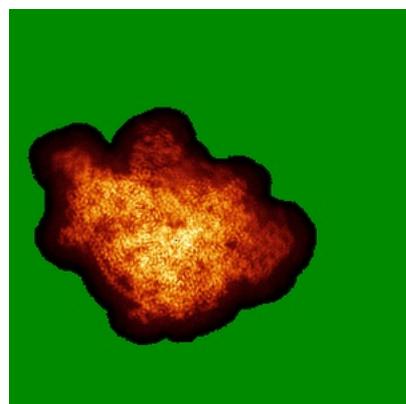


Z Index: 120

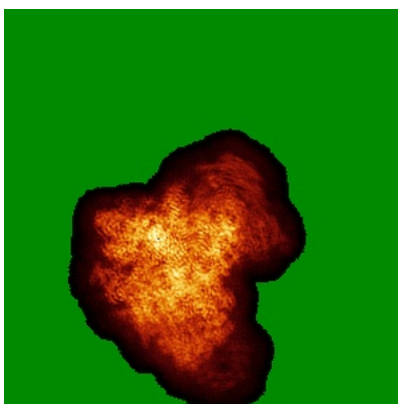
The images above show the largest variance slices of the map in three orthogonal directions.

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

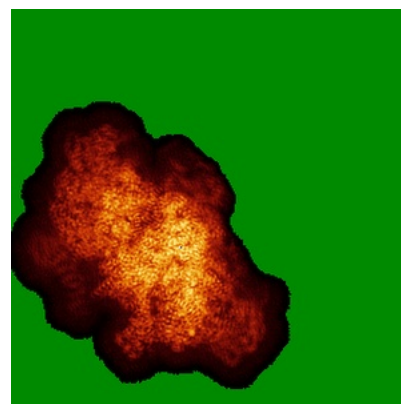
6.4.1 Primary map



X



Y



Z

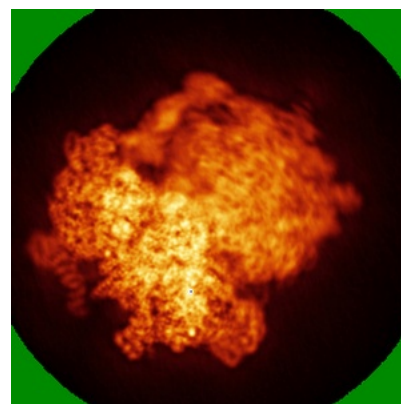
6.4.2 Raw map



X



Y

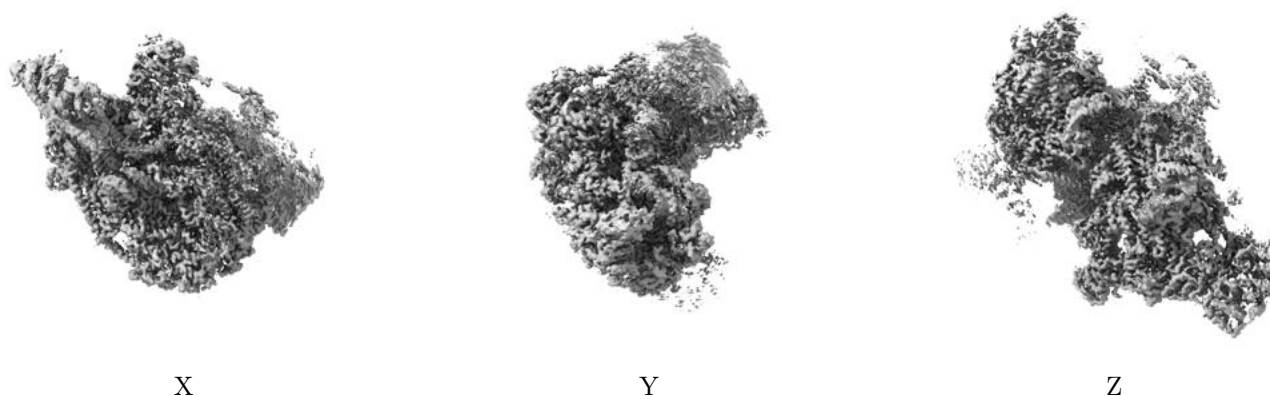


Z

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 0.085. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

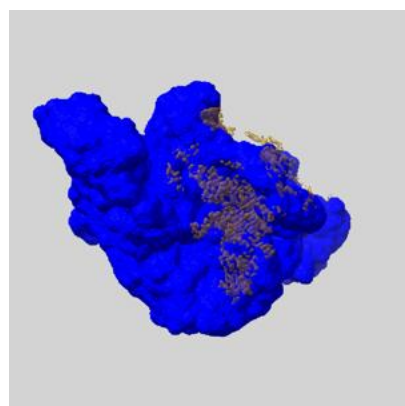
6.6 Mask visualisation [i](#)

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

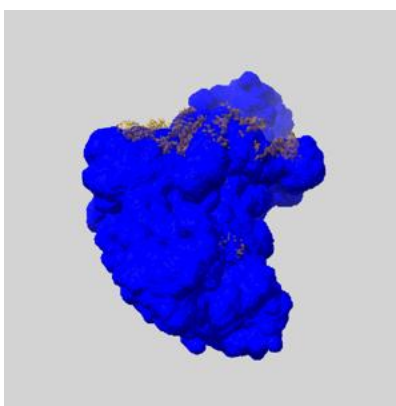
A mask typically either:

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

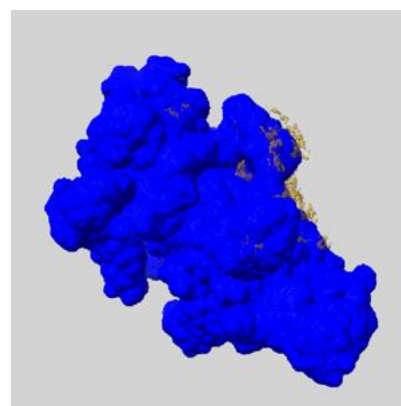
6.6.1 emd_4369_msk_1.map [i](#)



X



Y

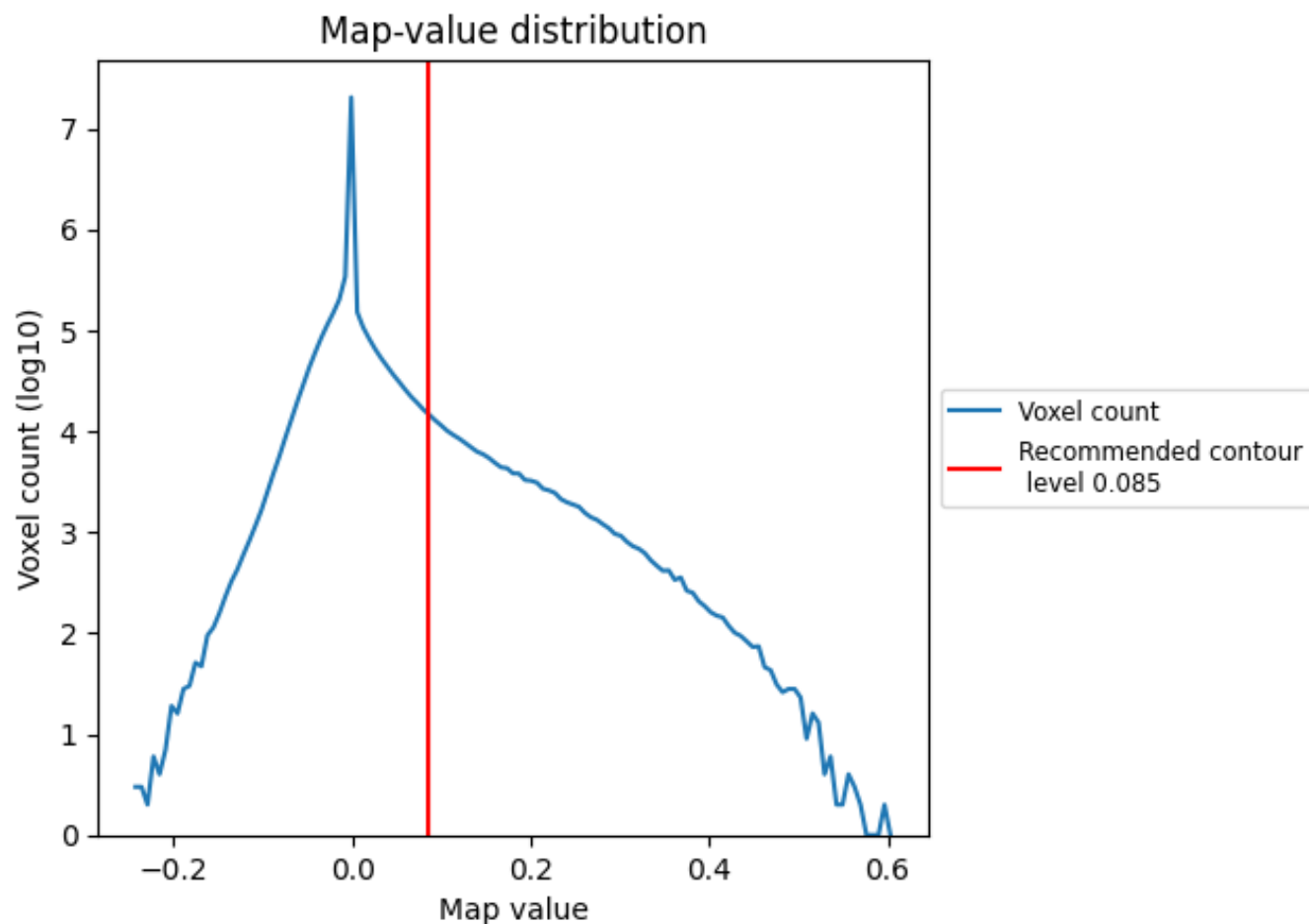


Z

7 Map analysis [i](#)

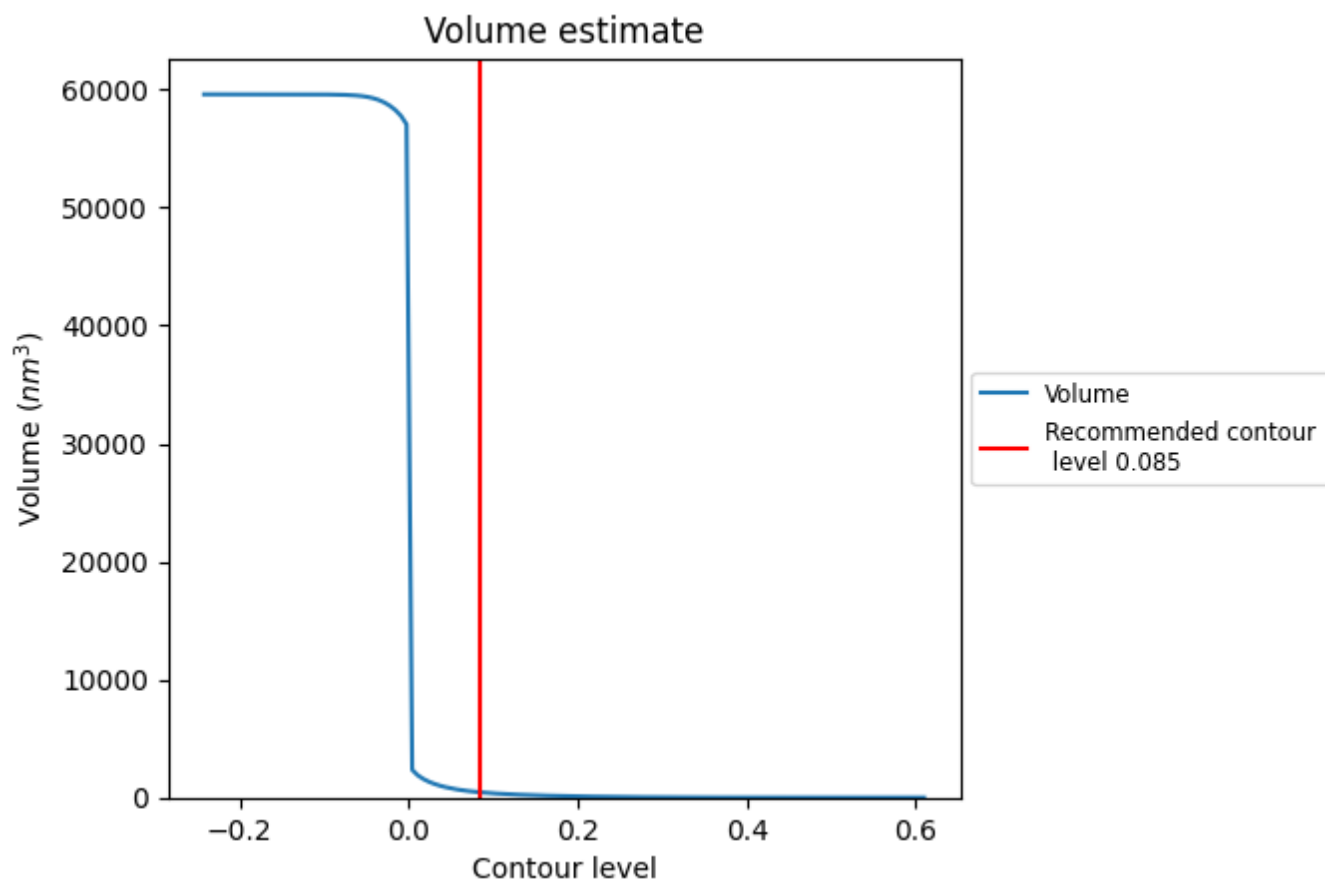
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

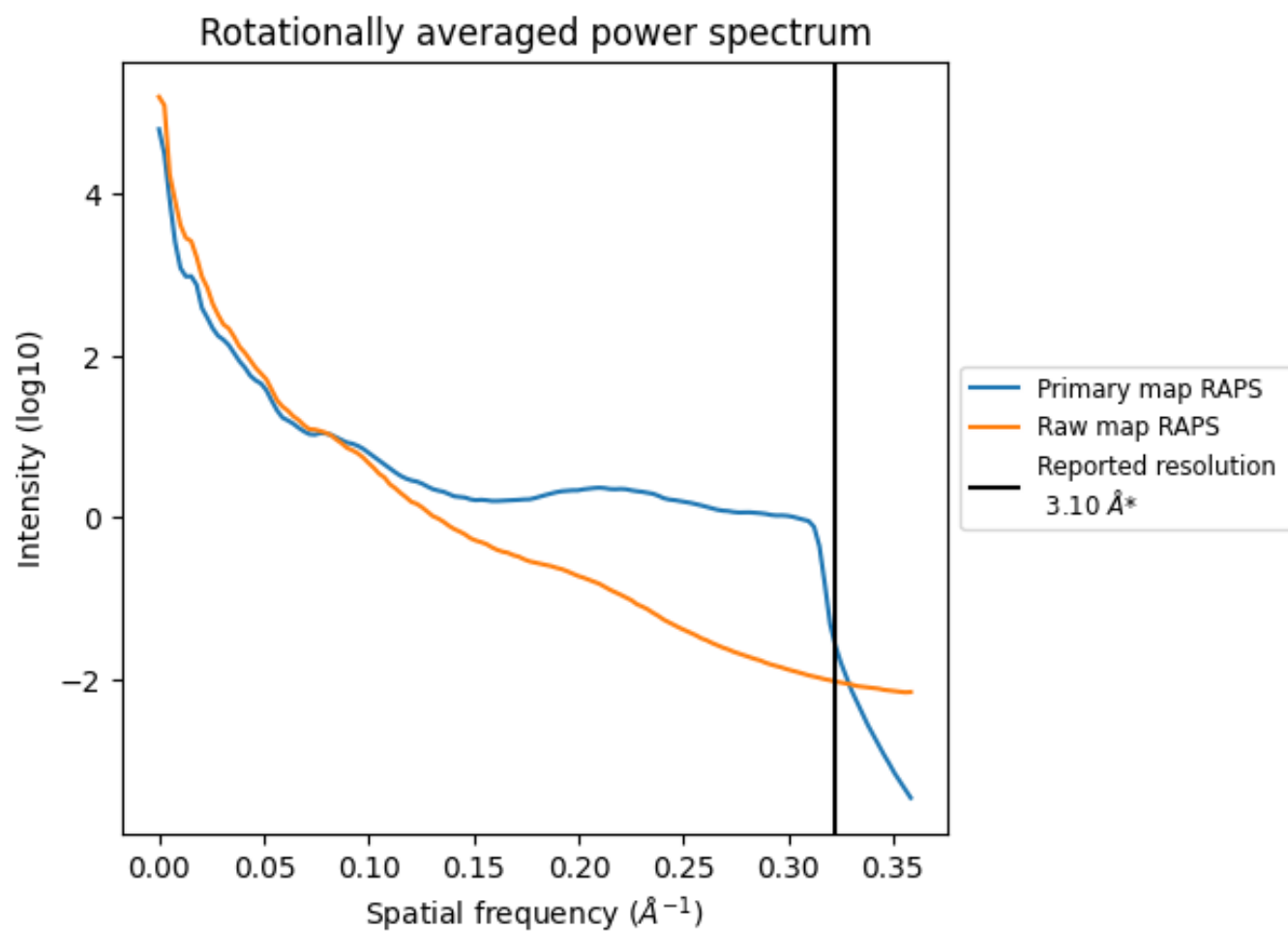
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 442 nm^3 ; this corresponds to an approximate mass of 399 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

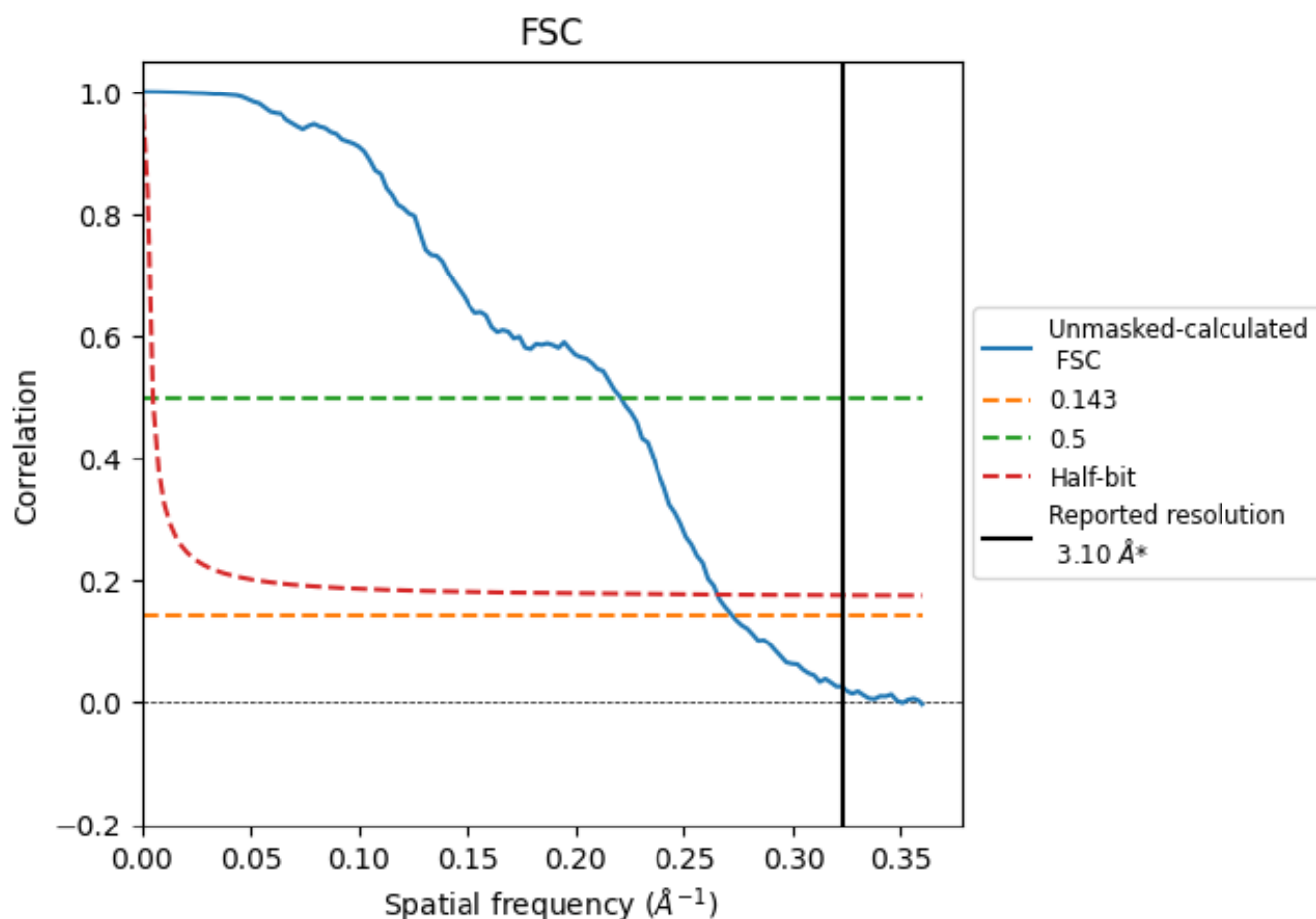


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 $0.323 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

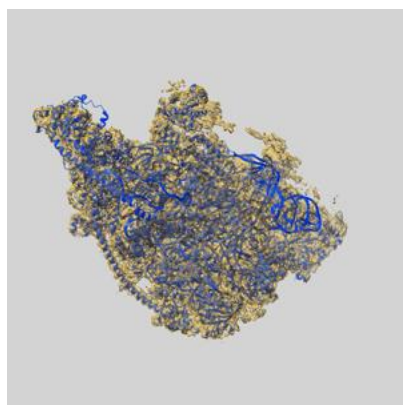
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.68	4.54	3.77

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.68 differs from the reported value 3.1 by more than 10 %

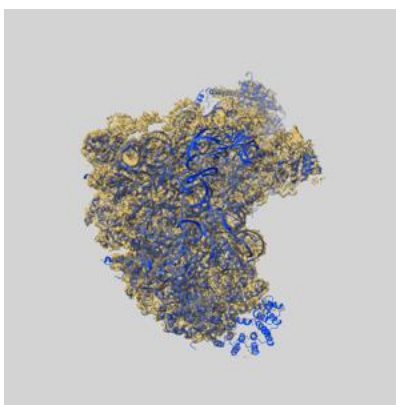
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4369 and PDB model 6GAZ. Per-residue inclusion information can be found in section 3 on page 15.

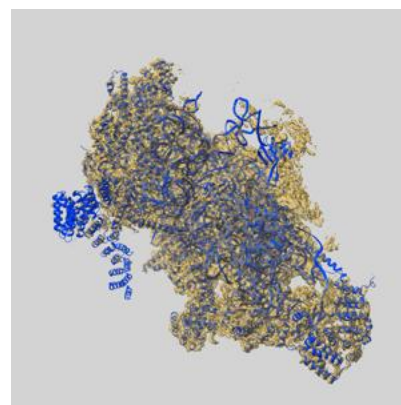
9.1 Map-model overlay [i](#)



X



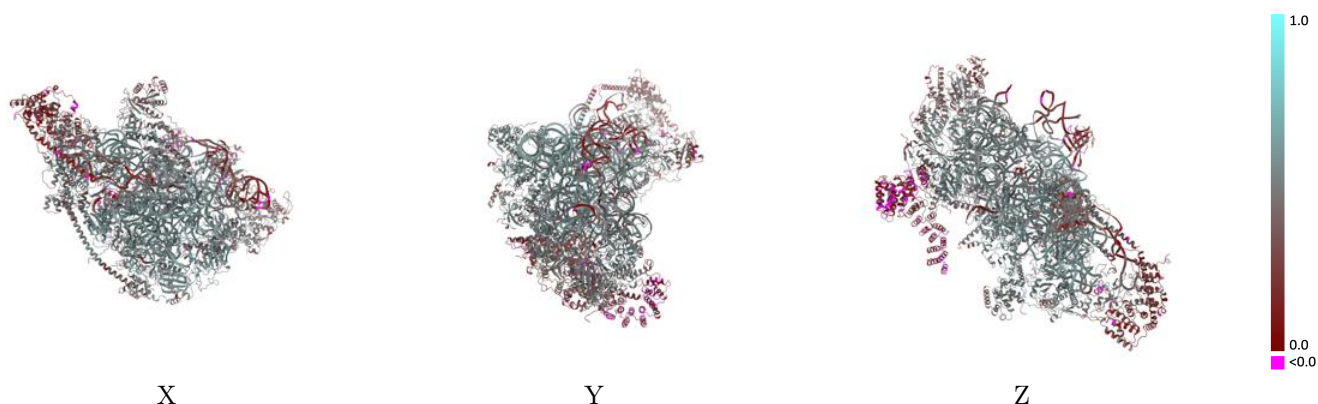
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.085 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

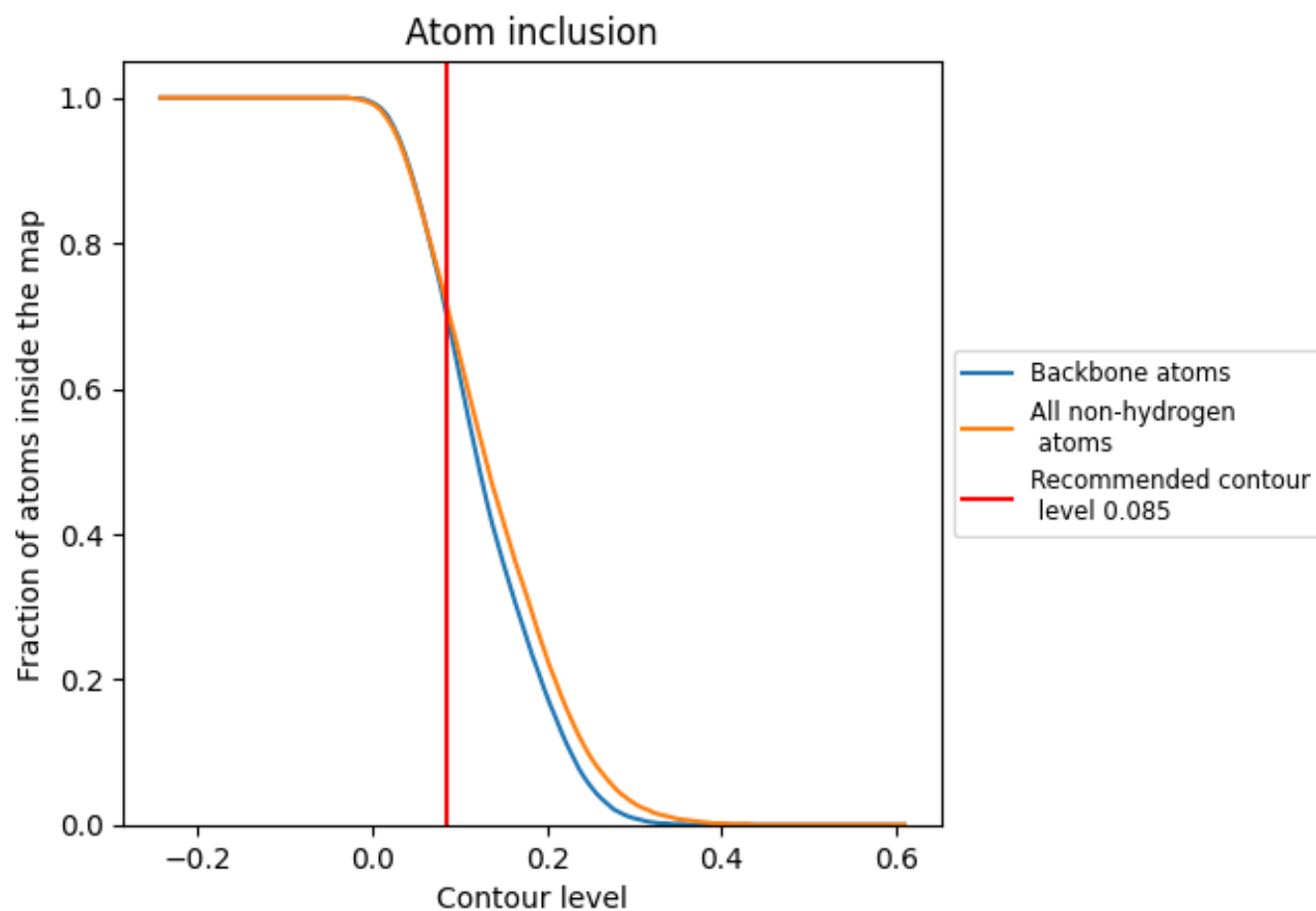


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 72% 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 (0.085) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7170	 0.4620
AA	 0.9250	 0.5370
AB	 0.8750	 0.5380
AC	 0.7650	 0.5360
AE	 0.7400	 0.5130
AF	 0.8300	 0.5300
AG	 0.7600	 0.4660
AI	 0.7310	 0.4680
AJ	 0.7070	 0.4650
AK	 0.8700	 0.5250
AL	 0.8220	 0.5530
AN	 0.8690	 0.5450
AO	 0.7620	 0.4980
AP	 0.8690	 0.5380
AQ	 0.8480	 0.5410
AR	 0.8620	 0.5400
AU	 0.8880	 0.5510
AV	 0.4190	 0.3250
AX	 0.2060	 0.2840
AZ	 0.5220	 0.3510
Aa	 0.7920	 0.4970
Ab	 0.7890	 0.4920
Ac	 0.8490	 0.5310
Ad	 0.7870	 0.4710
Ae	 0.4260	 0.2420
Af	 0.8520	 0.5230
Ag	 0.5640	 0.3850
Ah	 0.6360	 0.4240
Ai	 0.7280	 0.4890
Aj	 0.6670	 0.4430
Ak	 0.6360	 0.4190
Am	 0.6980	 0.4870
An	 0.7390	 0.5210
Ao	 0.1400	 0.1860
Ap	 0.8320	 0.5220



Continued on next page...

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Chain	Atom inclusion	Q-score
BC	 0.4670	 0.3780
BT	 0.2380	 0.3100