Full wwPDB EM Validation Report ⓘ

Aug 23, 2026 – 04:43 am BST

PDB ID	:	8OIP / pdb_00008oip
EMDB ID	:	EMD-16895
Title	:	28S mammalian mitochondrial small ribosomal subunit with mtRF1 and P-site tRNA
Authors	:	Saurer, M.; Leibundgut, M.; Scaiola, A.; Schoenhut, T.; Ban, N.
Deposited on	:	2023-03-23
Resolution	:	3.60 Å(reported)
Based on initial models	:	., 7NQH, 7QI4

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:

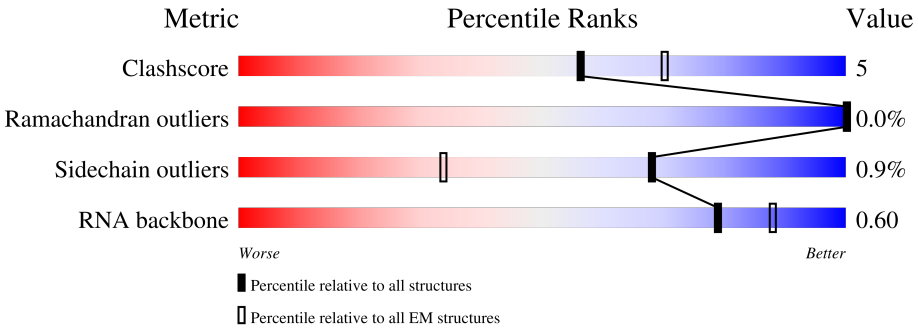
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.50

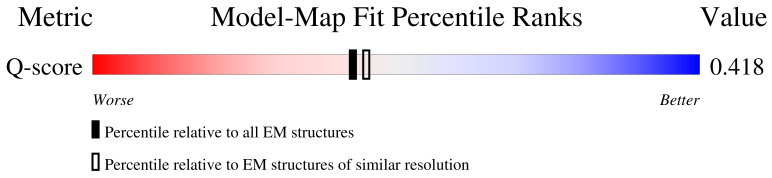
1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 Å.

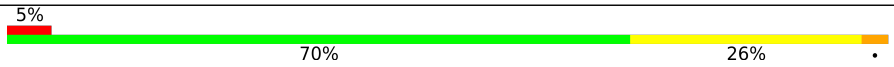
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





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	12797 (3.10 - 4.10)

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 <=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	BX	303	
2	Bd	126	
3	AA	962	

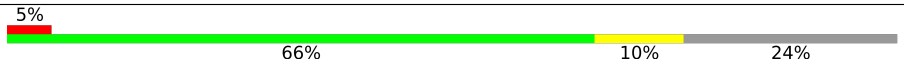
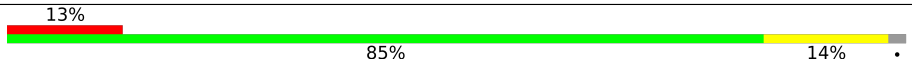
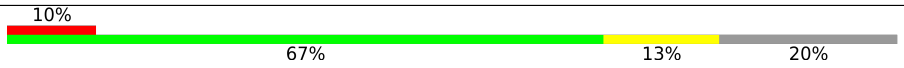
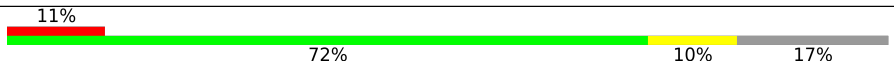
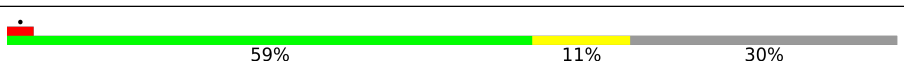
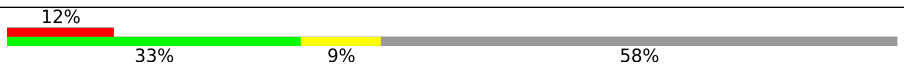
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Mol	Chain	Length	Quality of chain
4	AB	366	9% 59% 16% 25%
5	AC	167	59% 19% 21%
6	AD	199	33% 64%
7	AE	376	27% 6% 68%
8	AF	242	7% 74% 12% 14%
9	AG	72	44% 60% 36%
10	AH	200	9% 57% 12% 30%
11	AI	9	11% 44% 56%
12	AJ	139	65% 13% 22%
13	AK	128	66% 13% 21%
14	AL	259	9% 57% 10% 32%
15	AM	135	75% 12% 13%
16	AN	130	6% 70% 16% 14%
17	AO	258	6% 64% 10% 26%
18	AP	143	6% 59% 9% 32%
19	AQ	87	86% 13%
20	AR	382	12% 66% 11% 24%
21	AS	190	16% 64% 7% 29%
22	AT	173	81% 17%
23	AU	205	9% 80% 7% 14%
24	AV	395	64% 80% 18%
25	AW	188	44% 9% 47%
26	AX	410	10% 67% 19% 14%
27	AY	381	14% 34% 5% 61%
28	AZ	148	61% 5% 33%

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Mol	Chain	Length	Quality of chain
29	Aa	474	
30	Ab	289	
31	Ac	118	
32	Ad	430	
33	Ae	692	
34	Ag	397	
35	Ai	196	
36	Aj	505	

2 Entry composition

There are 45 unique types of molecules in this entry. The entry contains 72369 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 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	BX	15	99	66	17	16	0	0

- Molecule 2 is a protein called bL31m.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	Bd	23	192	124	31	37	0	0

- Molecule 3 is a RNA chain called 12S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	AA	960	20418	9169	3708	6581	960	0	0

- Molecule 4 is a protein called 28S ribosomal protein S35, mitochondrial isoform 1.

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

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

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

- Molecule 6 is a protein called Aurora kinase A interacting protein 1.

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

- Molecule 7 is a protein called bS6m,Mitochondrial ribosomal protein S6.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	-22	SER	PRO	conflict	UNP A0A4X1TSM9

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AF	208	Total	C	N	O	S	0	0
			1722	1097	314	300	11		

- Molecule 9 is a RNA chain called P-site Met-tRNA(fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
9	AG	72	Total	C	N	O	P	S	0	0
			1512	679	265	496	71	1		

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

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

- Molecule 11 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AI	9	Total	C	N	O	P	0	0
			193	88	40	57	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AJ	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	AK	101	Total	C	N	O	S	0	0
			858	534	174	144	6		

- Molecule 14 is a protein called 28S ribosomal protein S15, mitochondrial.

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

- Molecule 15 is a protein called 28S ribosomal protein S16, mitochondrial.

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

- Molecule 16 is a protein called uS17m.

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

- Molecule 17 is a protein called 28S ribosomal protein S18b, mitochondrial.

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

- Molecule 18 is a protein called Mitochondrial ribosomal protein S18C.

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

- Molecule 19 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AQ	86	Total	C	N	O	S	0	0
			737	455	148	126	8		

- Molecule 20 is a protein called Mitochondrial ribosomal protein S22.

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

- Molecule 21 is a protein called mS23.

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

- Molecule 22 is a protein called Mitochondrial ribosomal protein S25.

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

- Molecule 23 is a protein called Mitochondrial ribosomal protein S26.

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

- Molecule 24 is a protein called Mitochondrial ribosomal protein S27.

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

- Molecule 25 is a protein called Mitoribosomal protein ms28, mrps28.

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

- Molecule 26 is a protein called Death associated protein 3.

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

- Molecule 27 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AY	149	Total	C	N	O	S	0	0
			1250	807	211	229	3		

- Molecule 28 is a protein called Mitochondrial ribosomal protein S33.

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

- Molecule 29 is a protein called Peptide chain release factor 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Aa	381	Total	C	N	O	S	1	0
			3120	1943	572	592	13		

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Aa	446	GLY	-	expression tag	UNP O75570
Aa	447	GLY	-	expression tag	UNP O75570
Aa	448	SER	-	expression tag	UNP O75570
Aa	449	GLY	-	expression tag	UNP O75570
Aa	450	GLY	-	expression tag	UNP O75570
Aa	451	SER	-	expression tag	UNP O75570
Aa	452	GLY	-	expression tag	UNP O75570
Aa	453	ASP	-	expression tag	UNP O75570
Aa	454	TYR	-	expression tag	UNP O75570
Aa	455	LYS	-	expression tag	UNP O75570
Aa	456	ASP	-	expression tag	UNP O75570
Aa	457	HIS	-	expression tag	UNP O75570
Aa	458	ASP	-	expression tag	UNP O75570
Aa	459	GLY	-	expression tag	UNP O75570
Aa	460	ASP	-	expression tag	UNP O75570
Aa	461	TYR	-	expression tag	UNP O75570
Aa	462	LYS	-	expression tag	UNP O75570
Aa	463	ASP	-	expression tag	UNP O75570
Aa	464	HIS	-	expression tag	UNP O75570
Aa	465	ASP	-	expression tag	UNP O75570
Aa	466	ILE	-	expression tag	UNP O75570
Aa	467	ASP	-	expression tag	UNP O75570
Aa	468	TYR	-	expression tag	UNP O75570
Aa	469	LYS	-	expression tag	UNP O75570
Aa	470	ASP	-	expression tag	UNP O75570

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Chain	Residue	Modelled	Actual	Comment	Reference
Aa	471	ASP	-	expression tag	UNP O75570
Aa	472	ASP	-	expression tag	UNP O75570
Aa	473	ASP	-	expression tag	UNP O75570
Aa	474	LYS	-	expression tag	UNP O75570

- Molecule 30 is a protein called Mitochondrial ribosomal protein S2.

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

- Molecule 31 is a protein called Coiled-coil-helix-coiled-coil-helix domain containing 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Ac	116	Total	C	N	O	S	0	0
			933	579	185	161	8		

- Molecule 32 is a protein called 28S ribosomal protein S5, mitochondrial isoform X2.

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

- Molecule 33 is a protein called mS39.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Ae	588	Total	C	N	O	S	0	0
			4748	3039	804	879	26		

- Molecule 34 is a protein called uS9m.

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

- Molecule 35 is a protein called Mitochondrial ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Ai	137	Total	C	N	O	S	0	0
			1008	632	192	181	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ai	186	5F0	ASN	variant	UNP A0A286ZJJ6

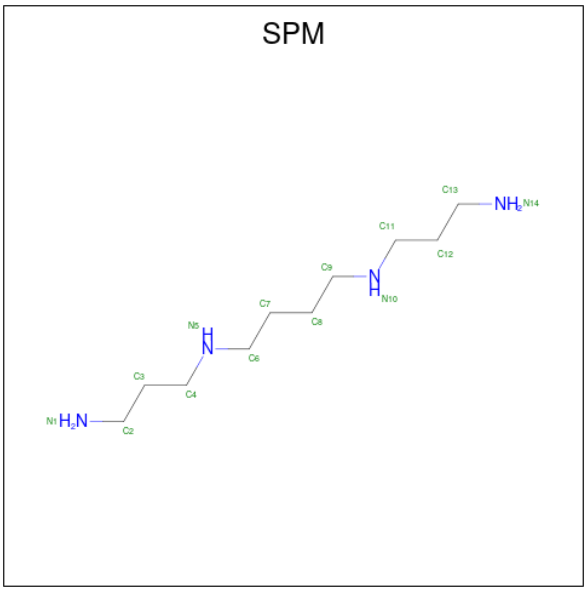
- Molecule 36 is a protein called Mitochondrial ribosomal protein S34.

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

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

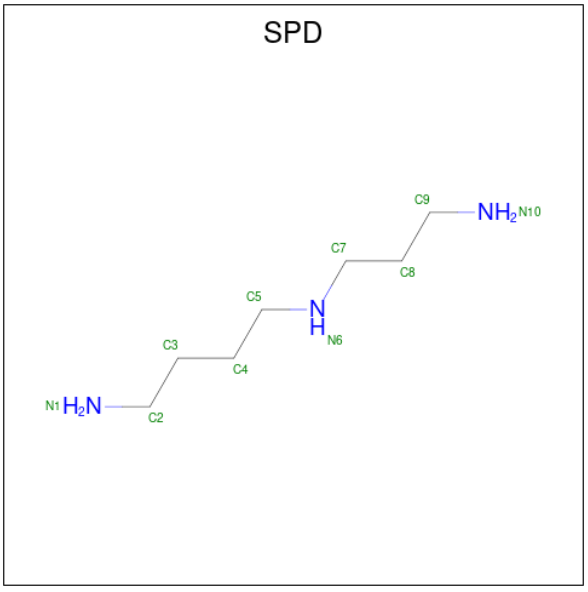
Mol	Chain	Residues	Atoms		AltConf
37	AA	120	Total	Mg	0
			120	120	
37	AD	1	Total	Mg	0
			1	1	
37	AG	1	Total	Mg	0
			1	1	
37	AI	1	Total	Mg	0
			1	1	
37	AJ	2	Total	Mg	0
			2	2	
37	AX	1	Total	Mg	0
			1	1	
37	Ab	1	Total	Mg	0
			1	1	

- Molecule 38 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



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

- Molecule 39 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms			AltConf
39	AA	1	Total	C	N	0
			10	7	3	

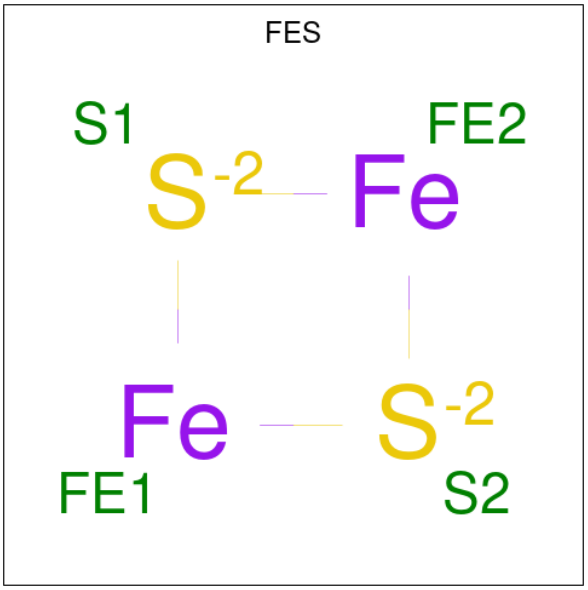
- Molecule 40 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
40	AA	11	Total K 11 11	0

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

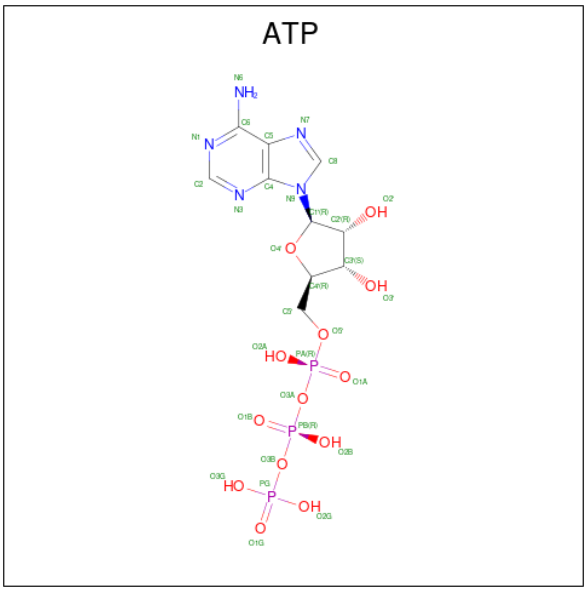
Mol	Chain	Residues	Atoms	AltConf
41	AO	1	Total Zn 1 1	0

- Molecule 42 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



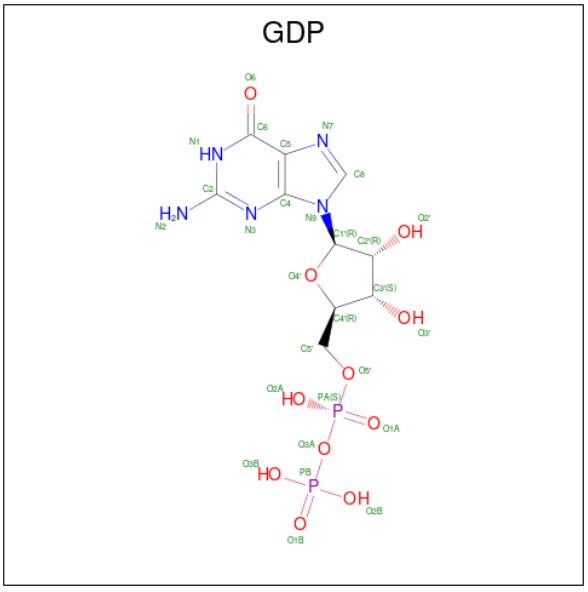
Mol	Chain	Residues	Atoms	AltConf
42	AP	1	Total Fe S 4 2 2	0
42	AT	1	Total Fe S 4 2 2	0

- Molecule 43 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
43	AX	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 44 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 45 is water.

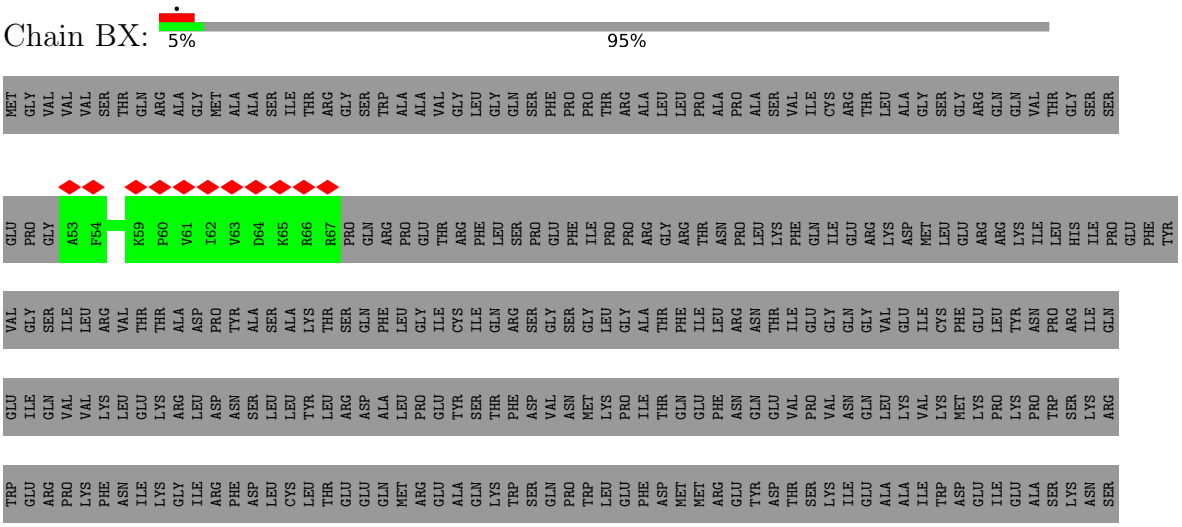
Mol	Chain	Residues	Atoms		AltConf
45	AX	3	Total	O	0
			3	3	

3 Residue-property plots (i)

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

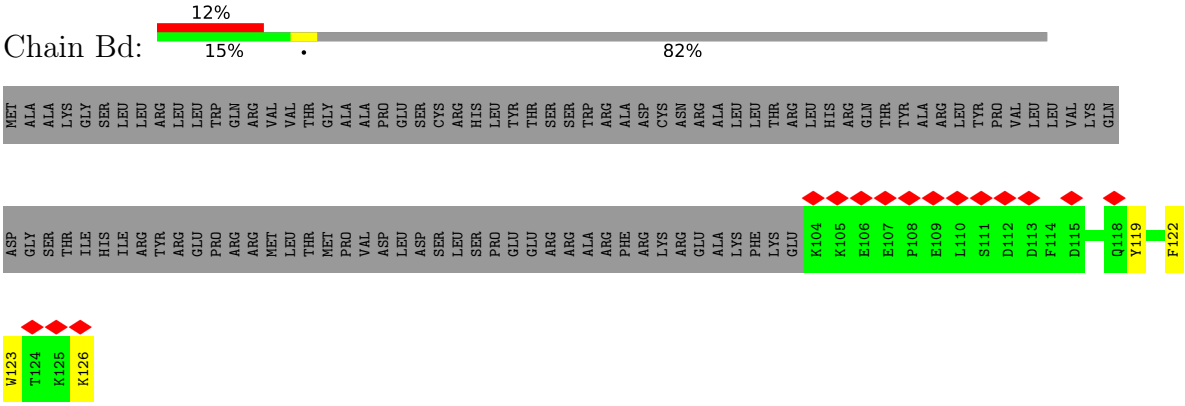
• Molecule 1: 39S ribosomal protein L19, mitochondrial

Chain BX:



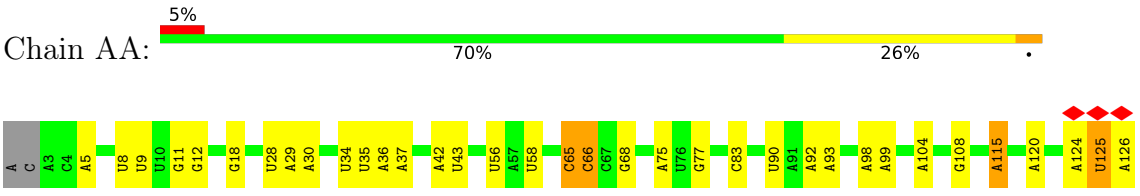
• Molecule 2: bL31m

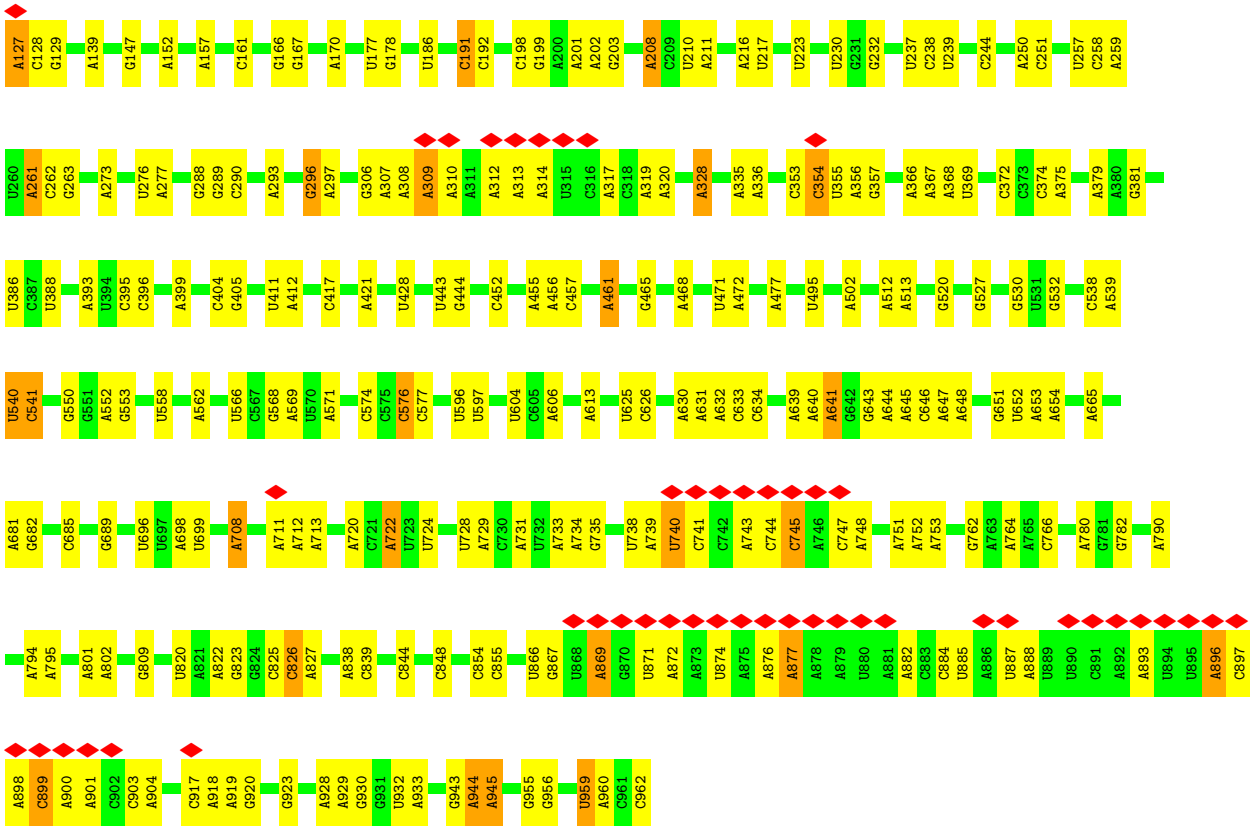
Chain Bd:



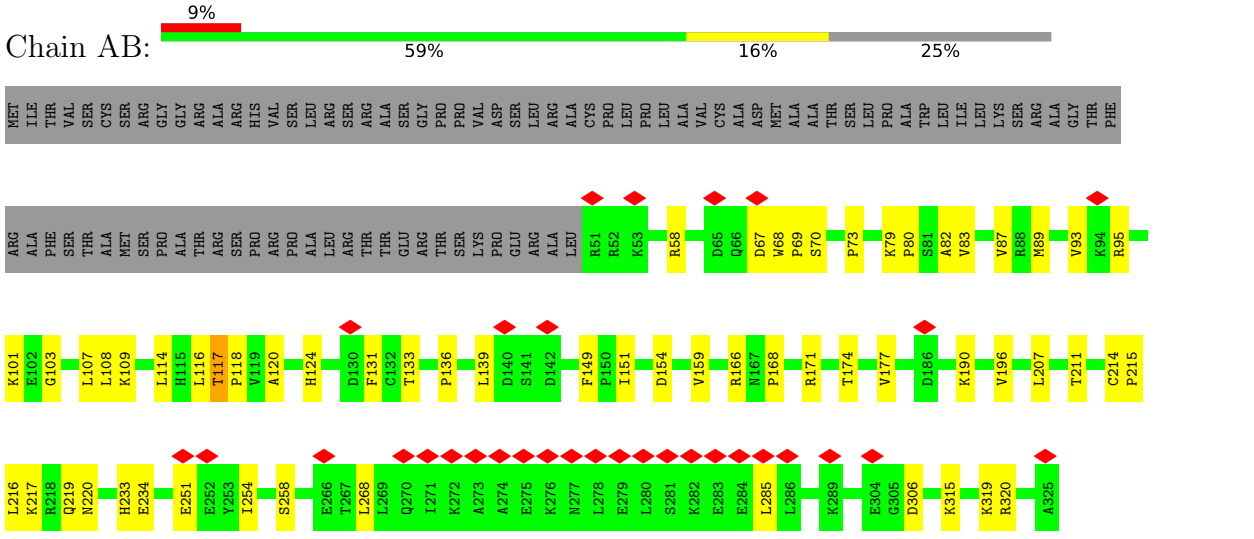
• Molecule 3: 12S rRNA

Chain AA:

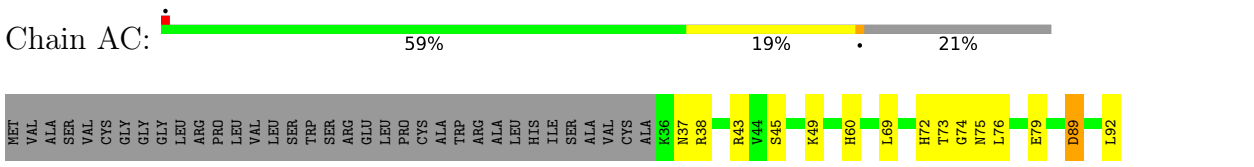


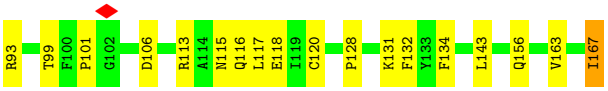


• Molecule 4: 28S ribosomal protein S35, mitochondrial isoform 1



• Molecule 5: Mitochondrial ribosomal protein S24

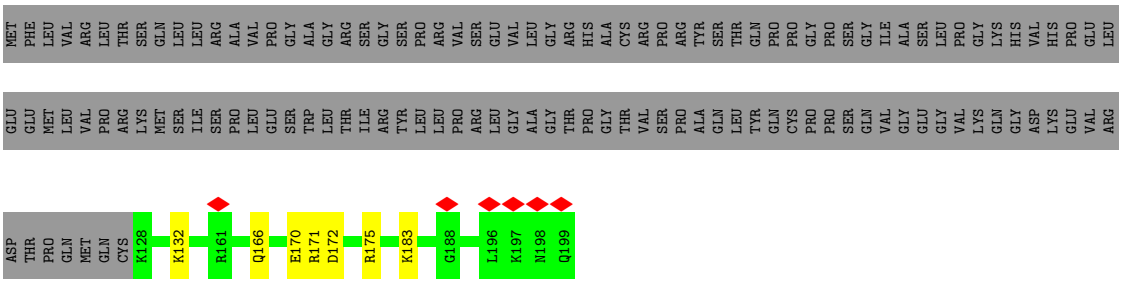




• Molecule 6: Aurora kinase A interacting protein 1

Chain AD:

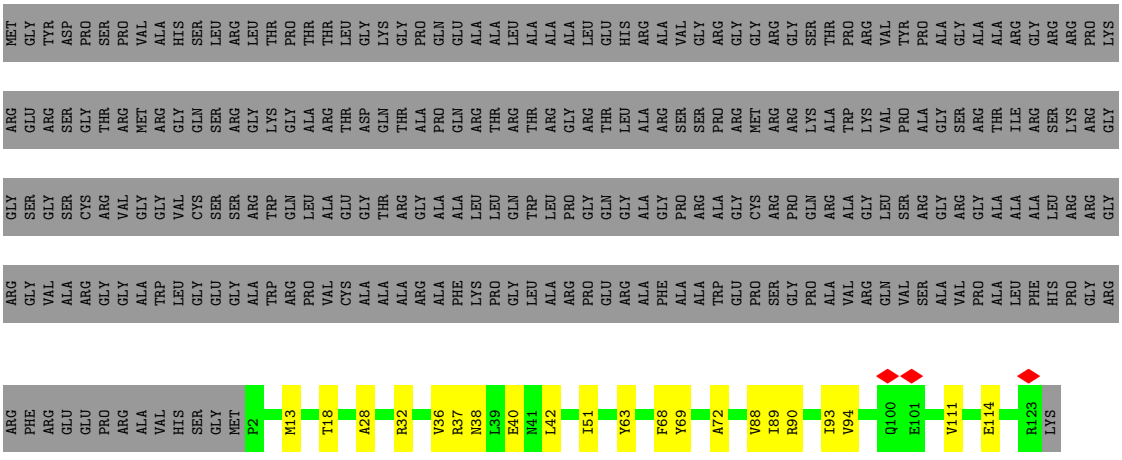




• Molecule 7: bS6m,Mitochondrial ribosomal protein S6

Chain AE:

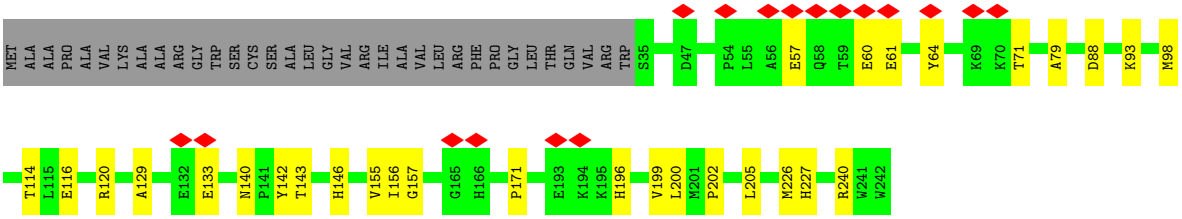




• Molecule 8: Mitochondrial ribosomal protein S7

Chain AF:

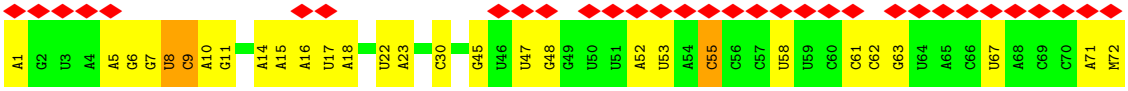




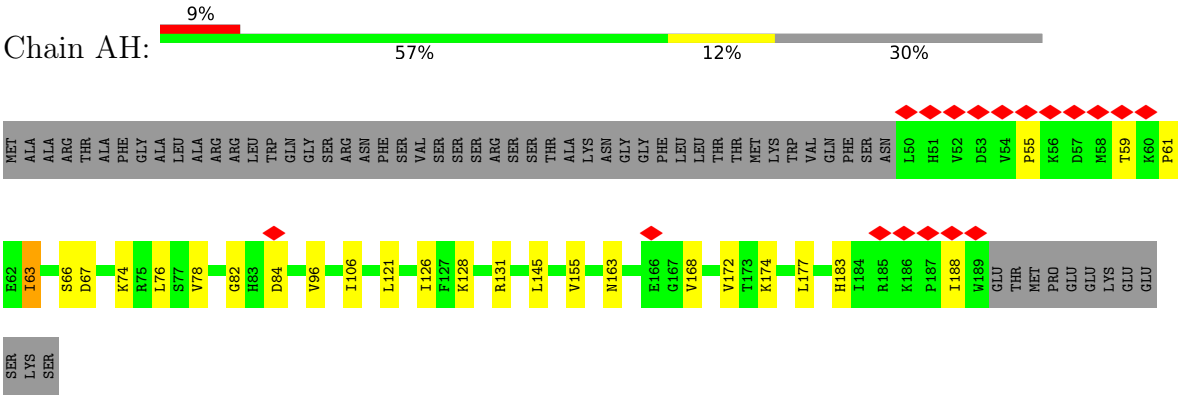
• Molecule 9: P-site Met-tRNA(fMet)

Chain AG:

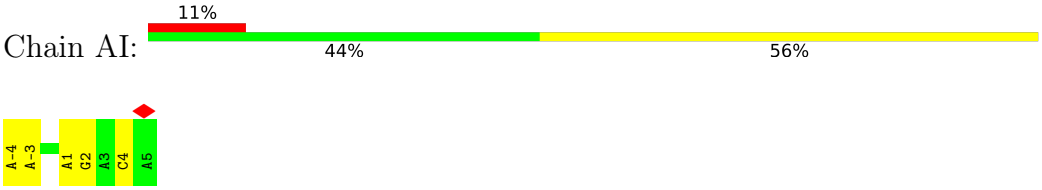




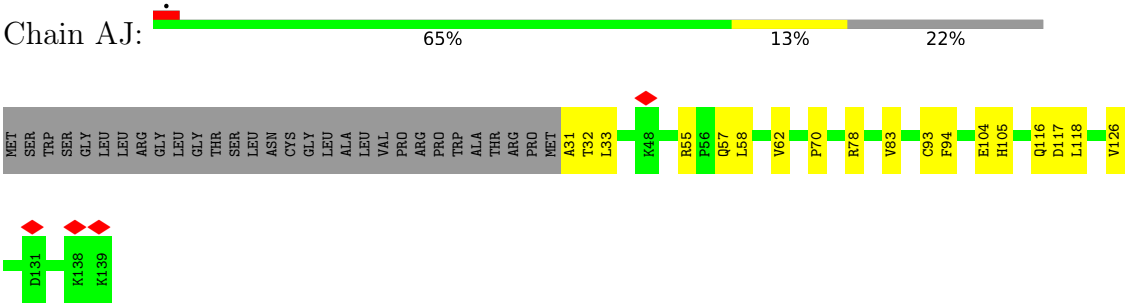
• Molecule 10: Mitochondrial ribosomal protein S10



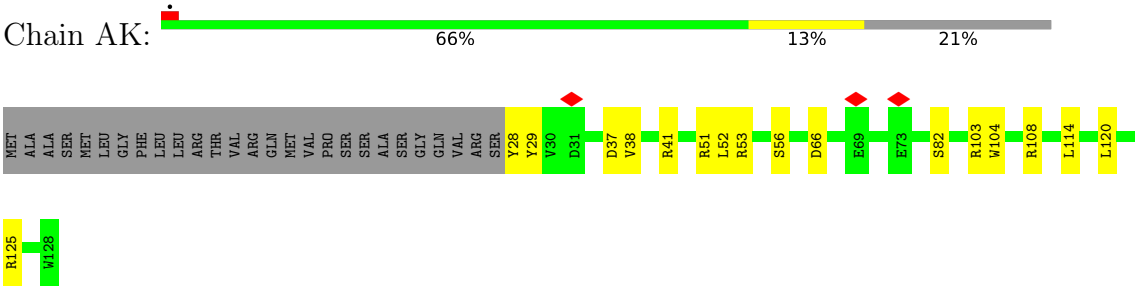
• Molecule 11: mRNA



• Molecule 12: Mitochondrial ribosomal protein S12

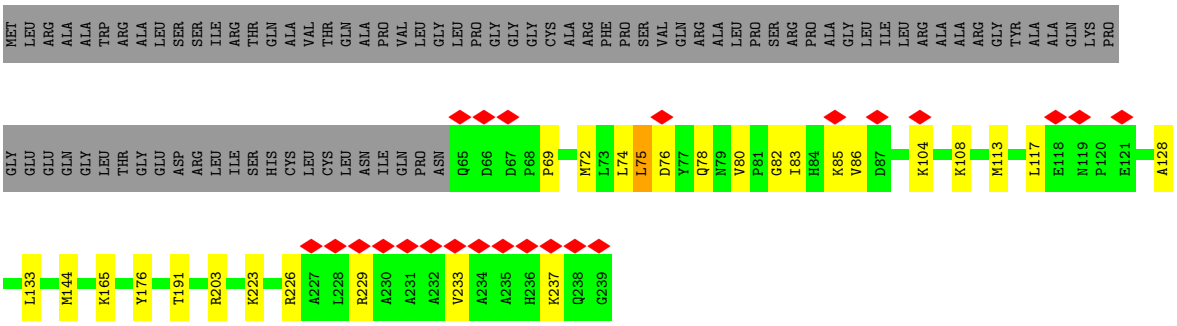


• Molecule 13: Mitochondrial ribosomal protein S14



• Molecule 14: 28S ribosomal protein S15, mitochondrial

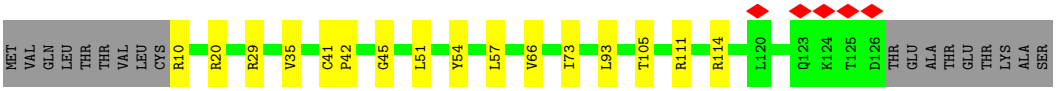




• Molecule 15: 28S ribosomal protein S16, mitochondrial

Chain AM:

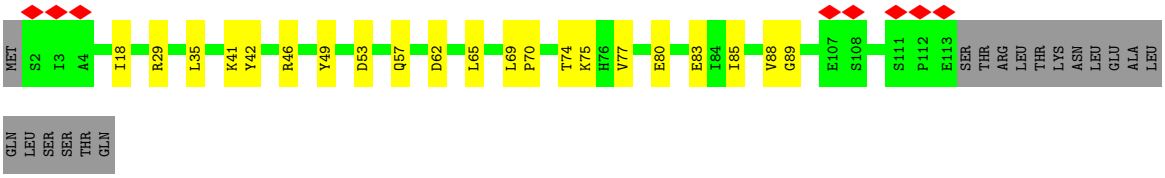




• Molecule 16: uS17m

Chain AN:

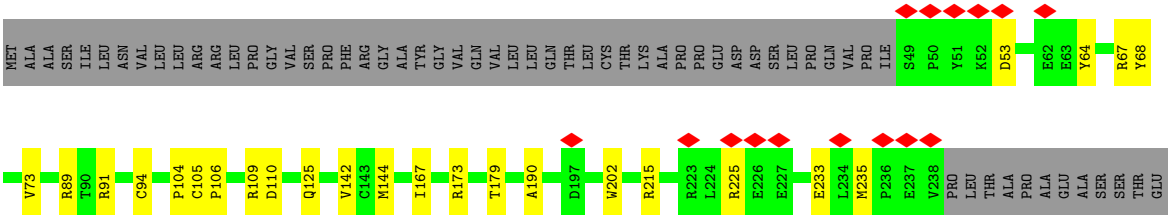




• Molecule 17: 28S ribosomal protein S18b, mitochondrial

Chain AO:

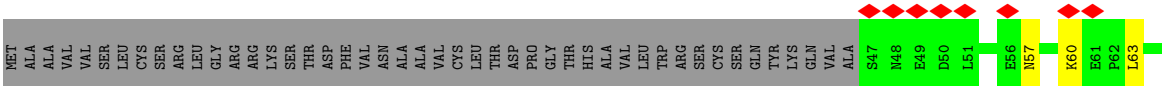




• Molecule 18: Mitochondrial ribosomal protein S18C

Chain AP:



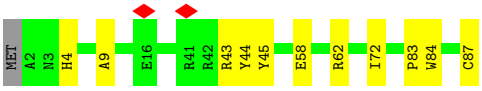




• Molecule 19: 28S ribosomal protein S21, mitochondrial

Chain AQ:

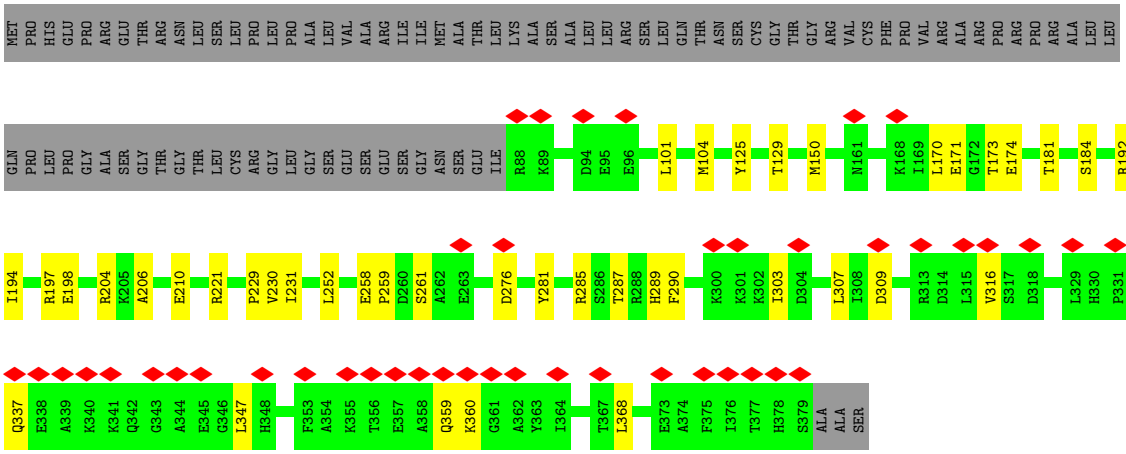




• Molecule 20: Mitochondrial ribosomal protein S22

Chain AR:

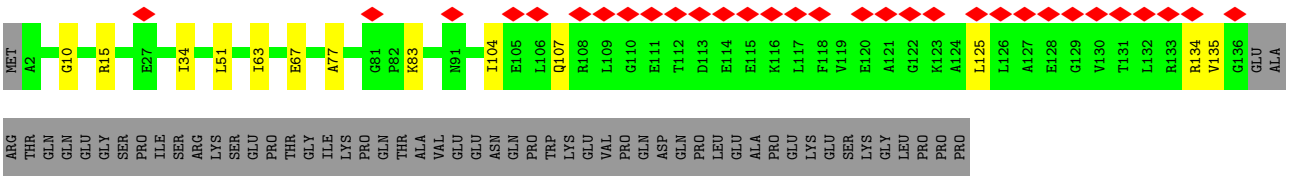




• Molecule 21: mS23

Chain AS:

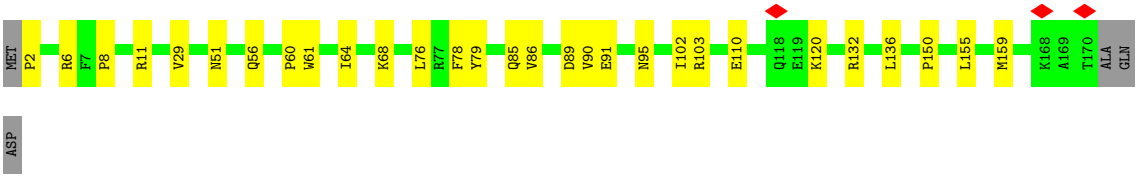




• Molecule 22: Mitochondrial ribosomal protein S25

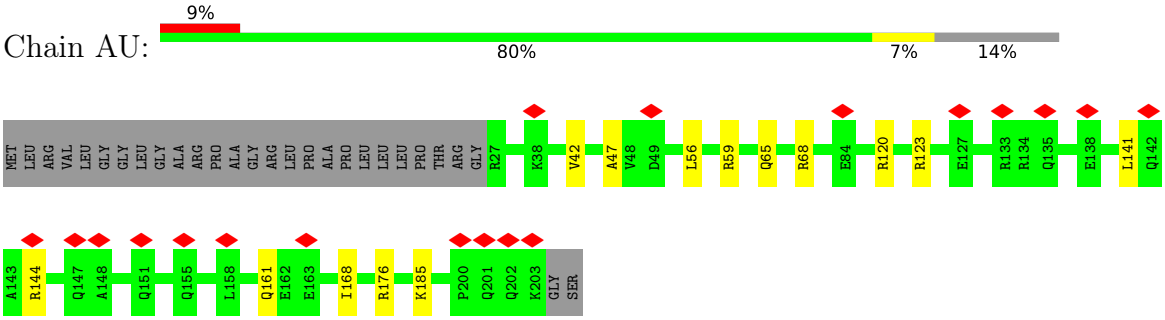
Chain AT:





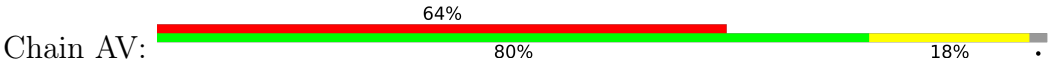
• Molecule 23: Mitochondrial ribosomal protein S26

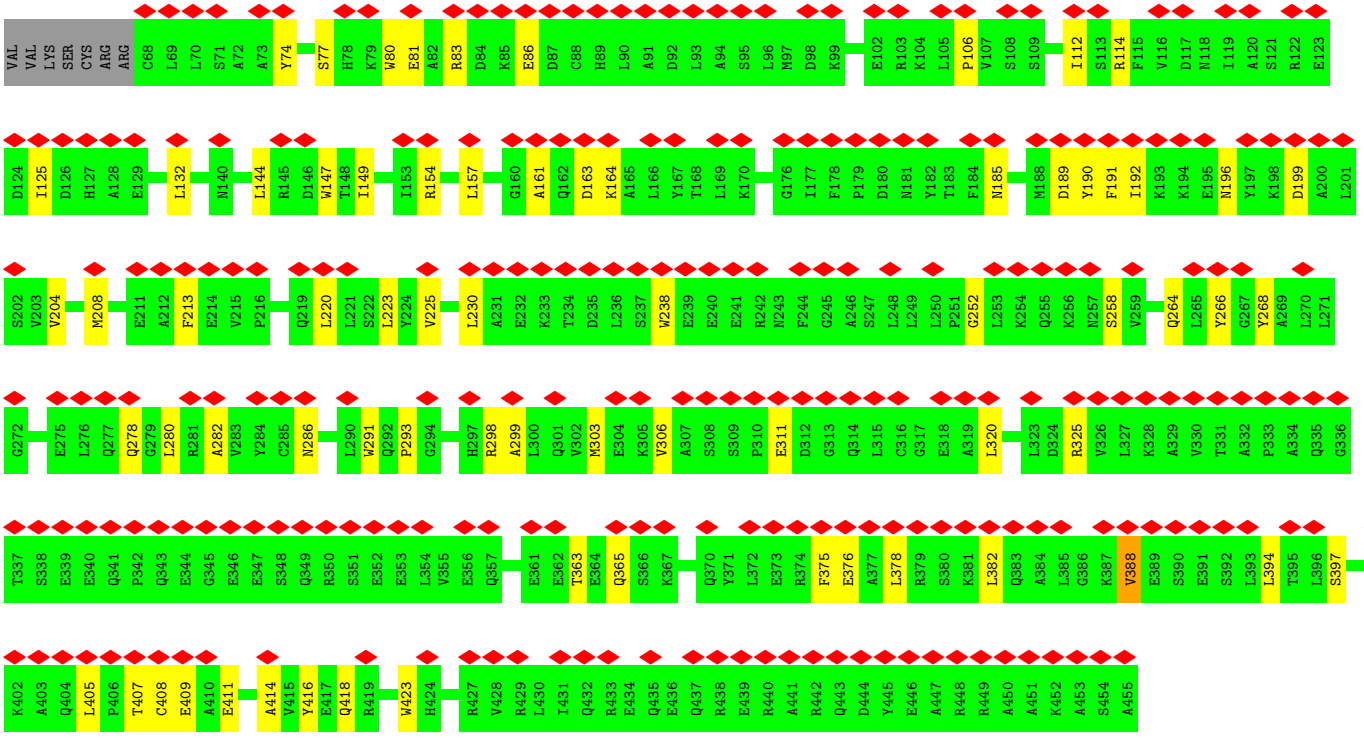
Chain AU:



• Molecule 24: Mitochondrial ribosomal protein S27

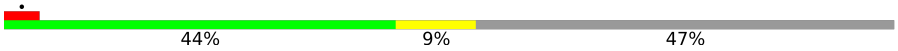
Chain AV:

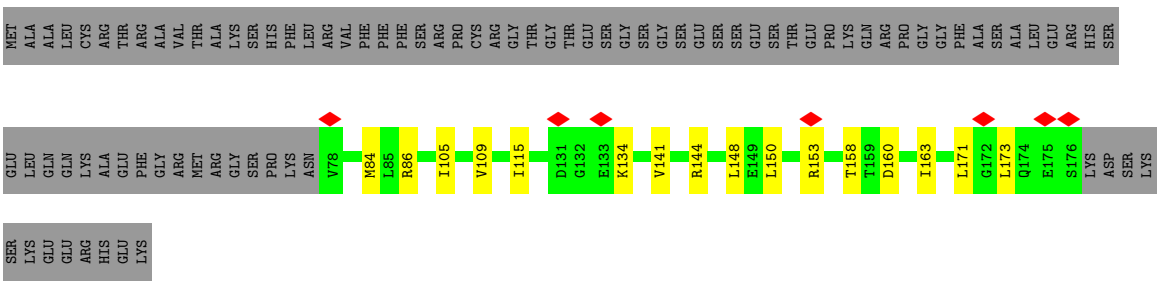




• Molecule 25: Mitoribosomal protein ms28, mrps28

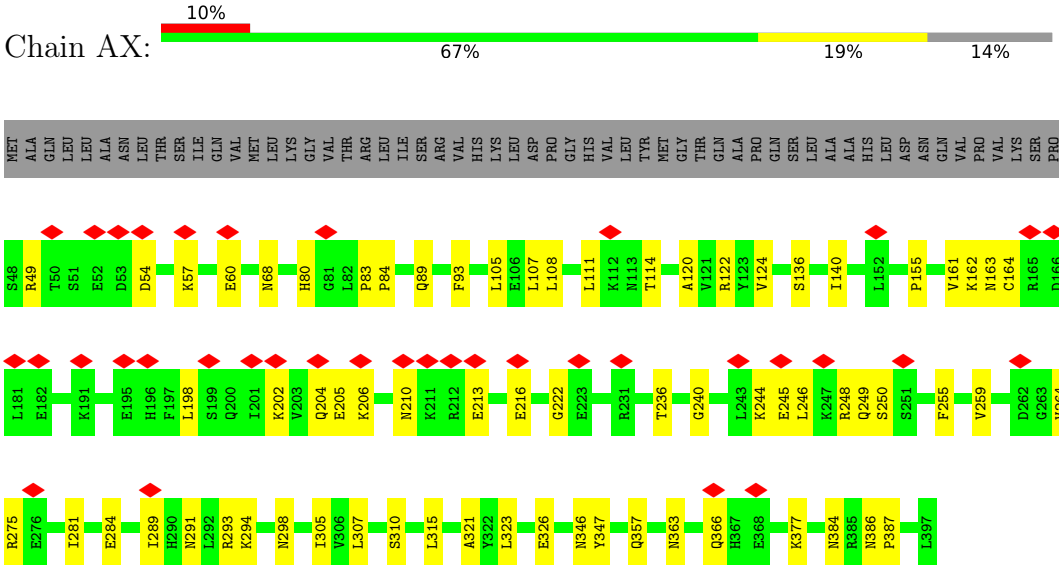
Chain AW:





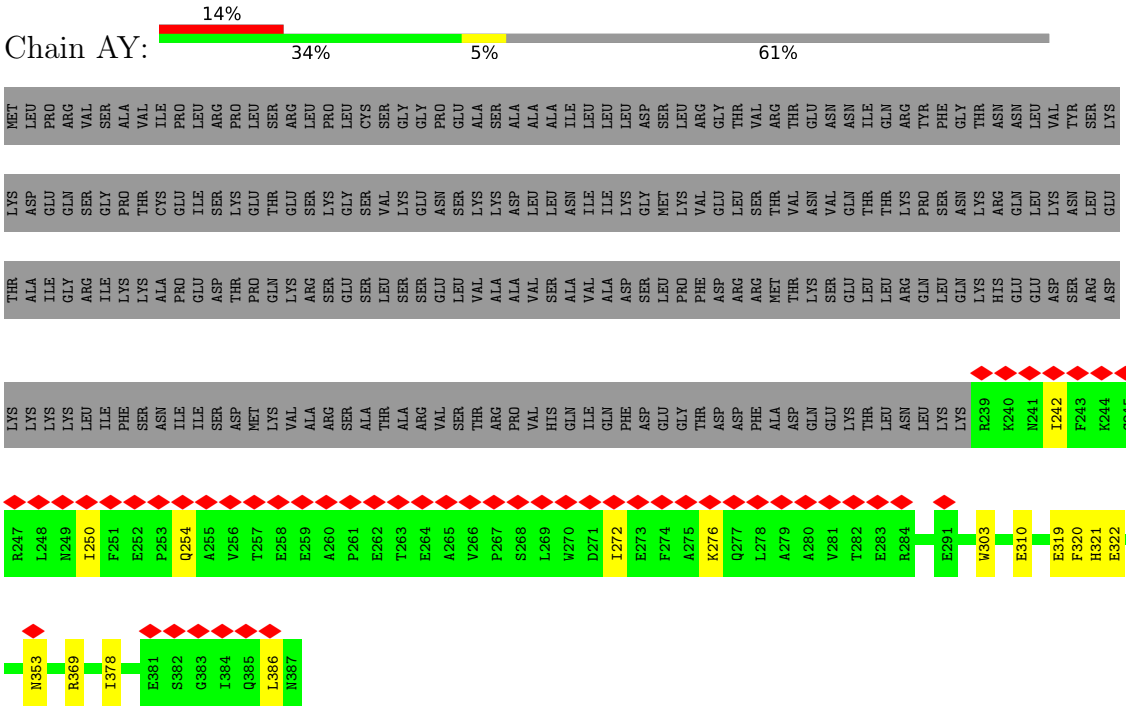
• Molecule 26: Death associated protein 3

Chain AX:



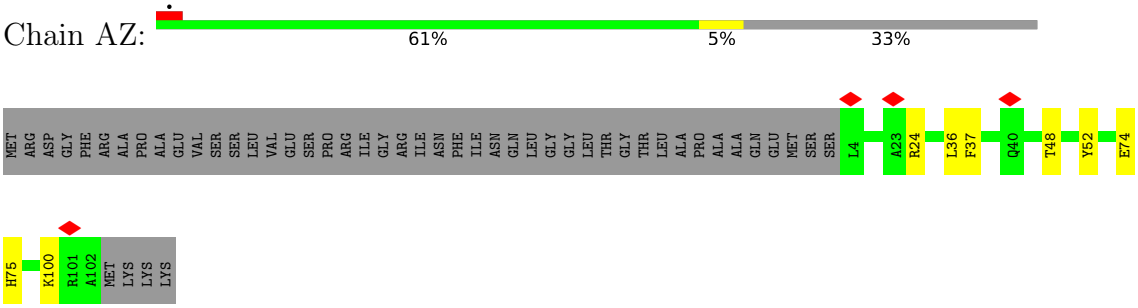
• Molecule 27: 28S ribosomal protein S31, mitochondrial

Chain AY:



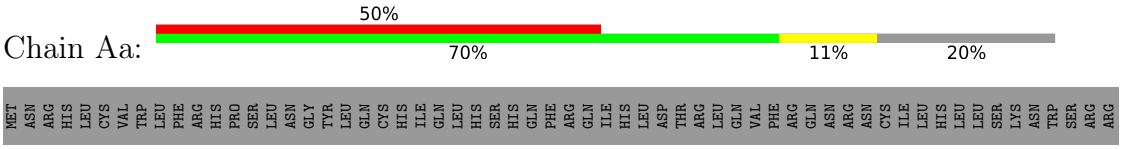
• Molecule 28: Mitochondrial ribosomal protein S33

Chain AZ:



• Molecule 29: Peptide chain release factor 1, mitochondrial

Chain Aa:



• Molecule 30: Mitochondrial ribosomal protein S2

Chain Ab:



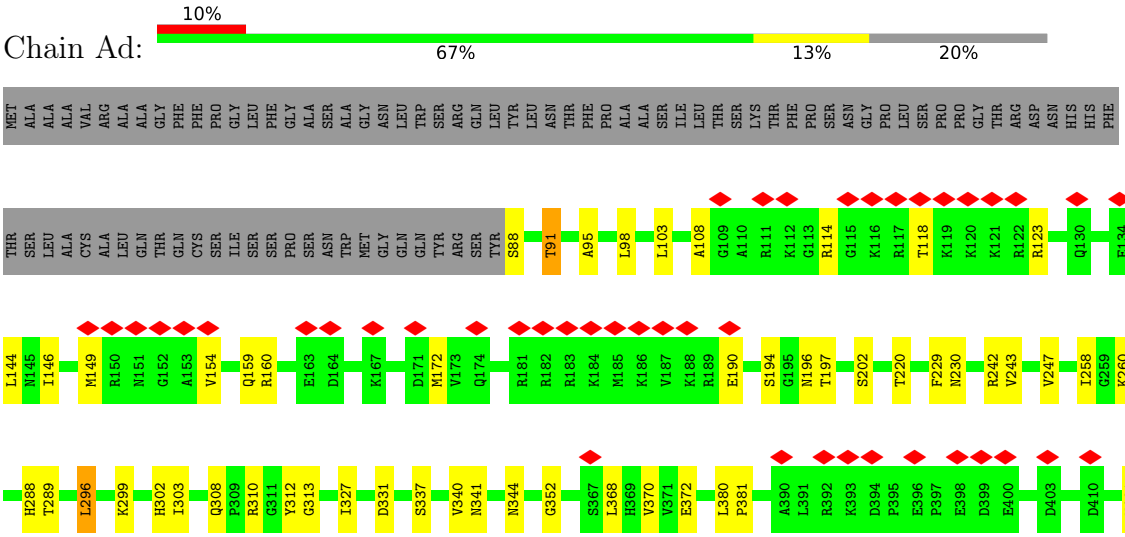
• Molecule 31: Coiled-coil-helix-coiled-coil-helix domain containing 1

Chain Ac:



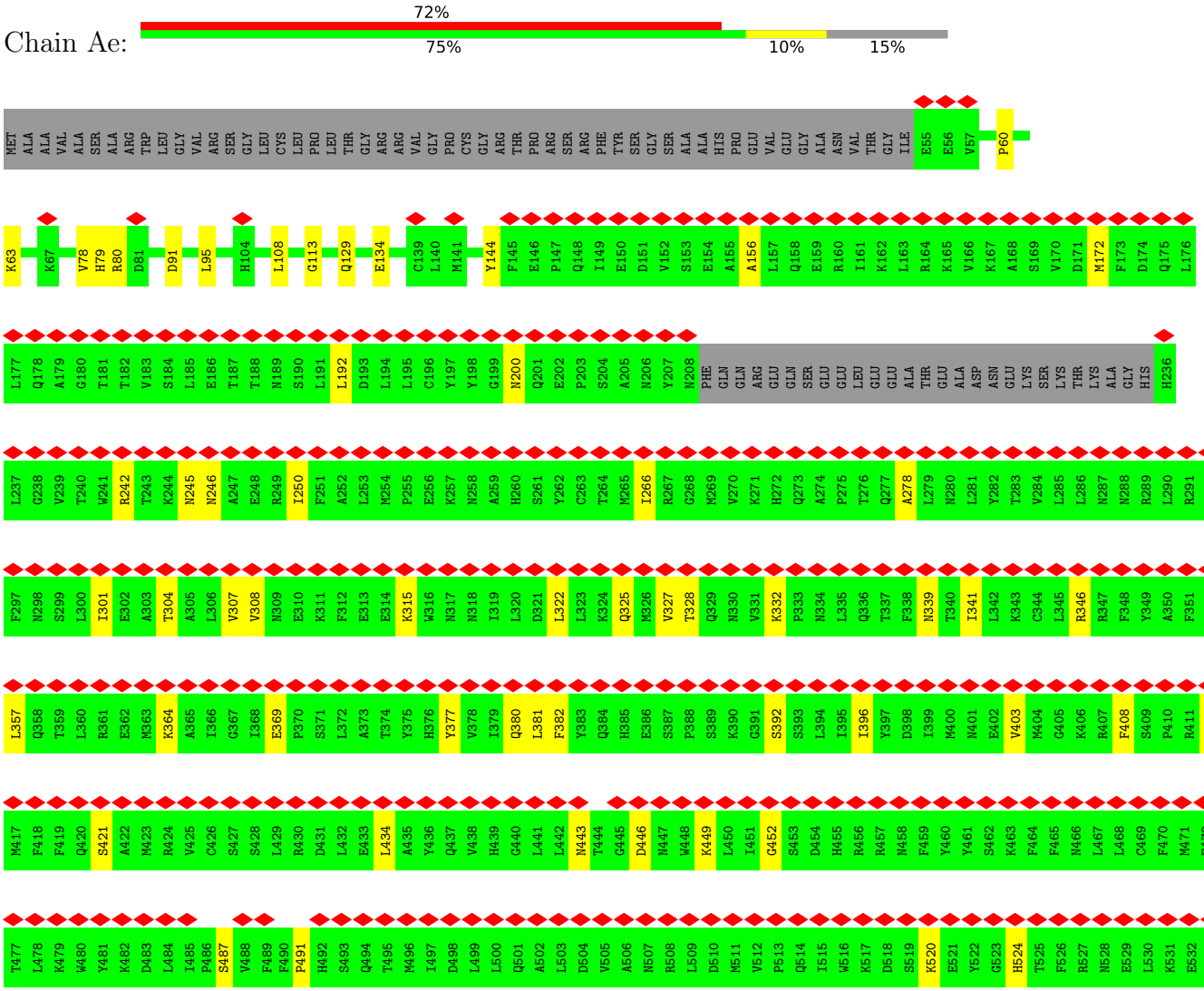
• Molecule 32: 28S ribosomal protein S5, mitochondrial isoform X2

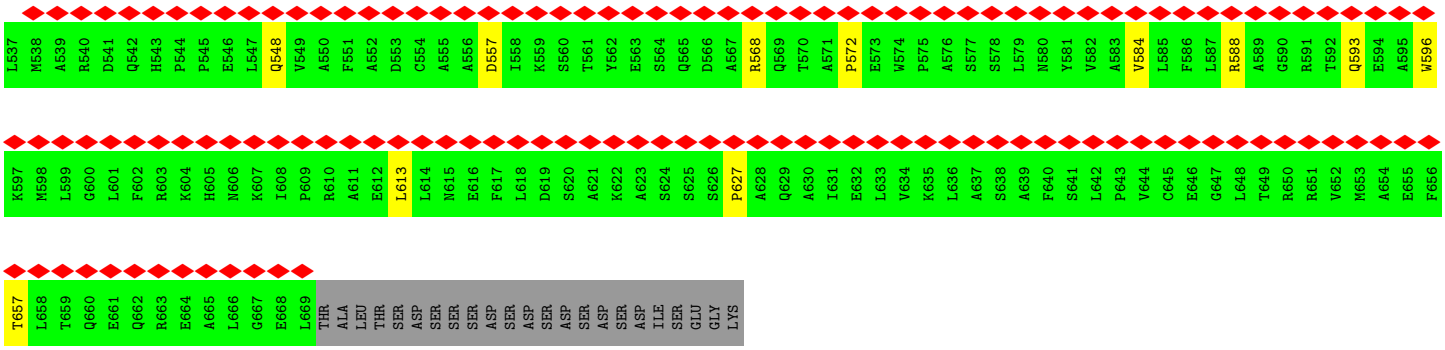
Chain Ad:



• Molecule 33: mS39

Chain Ae:

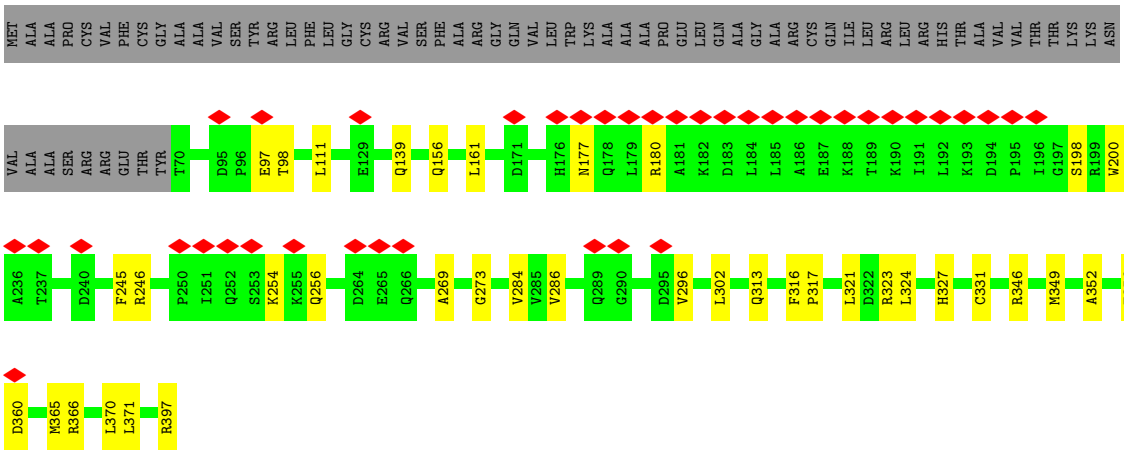




• Molecule 34: uS9m

Chain Ag:

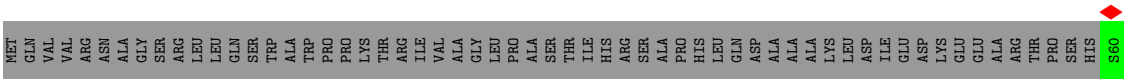


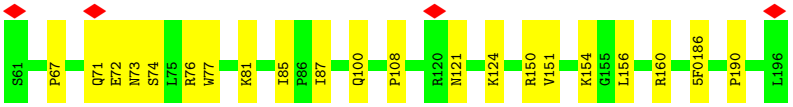


• Molecule 35: Mitochondrial ribosomal protein S11

Chain Ai:



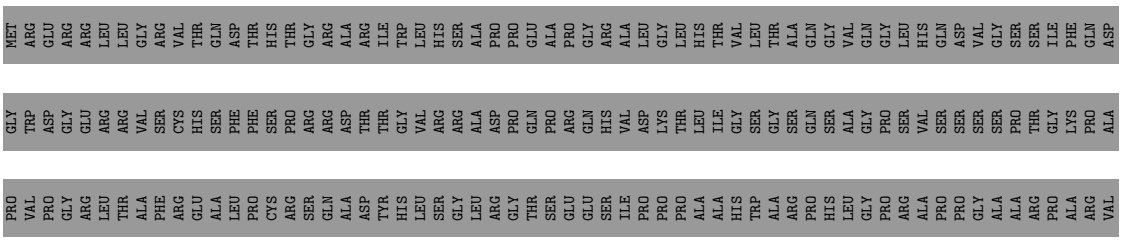


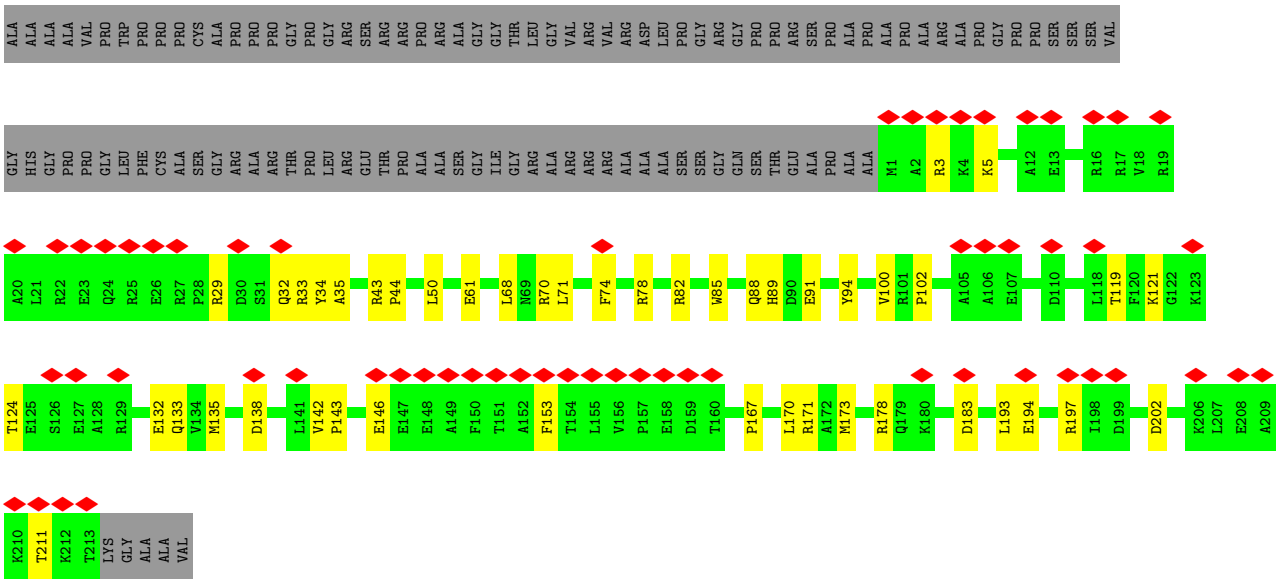


• Molecule 36: Mitochondrial ribosomal protein S34

Chain Aj:






ALA ALA ALA ALA VAL PRO TRP PRO PRO PRO CYS ALA PRO PRO PRO GLY PRO GLY ARG SER ARG ARG PRO ARG ALA GLY GLY THR LEU GLY VAL ARG VAL ARG ASP LEU PRO GLY ARG GLY PRO PRO ARG SER PRO ALA PRO ALA PRO ALA ARG ALA PRO GLY PRO PRO SER SER VAL
GLY HIS GLY PRO PRO GLY LEU PHE CYS ALA SER GLY ARG ALA ARG THR PRO LEU ARG GLU THR PRO ALA ALA SER GLY ILE GLY ARG ALA ARG ARG ARG ALA ALA ALA SER SER GLY GLN SER THR GLU ALA PRO ALA ALA M1 A2 R3 K4 K5 A12 E13 R16 R17 V18 R19
A20 L21 R22 E23 Q24 R25 E26 R27 P28 R29 D30 S31 Q32 R33 Y34 A35 R43 P44 L50 E61 L68 N69 R70 L71 F74 R78 R82 W85 Q88 H89 D90 E91 Y94 V100 R101 P102 A105 A106 E107 D110 L118 T119 F120 K121 G122 K123
T124 E125 S126 E127 A128 R129 E132 Q133 V134 M135 D138 L141 V142 P143 E146 E147 E148 A149 F150 T151 A152 F153 T154 L155 V156 P157 E158 D159 T160 P167 L170 R171 A172 M173 R178 Q179 K180 D183 L193 E194 R197 I198 D199 D202 K206 L207 E208 A209
K210 T211 K212 T213 LYS GLY ALA ALA VAL

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50622	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.185	Depositor
Minimum map value	-1.749	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.102	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	532.5, 532.5, 532.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.065, 1.065, 1.065	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SPM, GDP, ATP, B8T, FME, 5F0, K, AYA, FES, ZN, SPD, MG, MA6, 5MC, 5MU

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	BX	0.13	0/103	0.29	0/143
2	Bd	0.14	0/197	0.36	0/265
3	AA	0.09	0/22734	0.14	0/35392
4	AB	0.09	0/2268	0.22	0/3069
5	AC	0.10	0/1105	0.27	0/1496
6	AD	0.10	0/650	0.21	0/858
7	AE	0.09	0/999	0.23	0/1347
8	AF	0.08	0/1764	0.22	0/2368
9	AG	0.07	0/1677	0.14	0/2606
10	AH	0.12	0/1181	0.28	0/1597
11	AI	0.08	0/217	0.15	0/337
12	AJ	0.10	0/858	0.23	0/1152
13	AK	0.10	0/874	0.20	0/1171
14	AL	0.09	0/1473	0.19	0/1970
15	AM	0.10	0/954	0.24	0/1284
16	AN	0.10	0/894	0.22	0/1213
17	AO	0.11	0/1616	0.24	0/2195
18	AP	0.10	0/802	0.22	0/1079
19	AQ	0.09	0/740	0.21	0/986
20	AR	0.09	0/2428	0.22	0/3279
21	AS	0.09	0/1126	0.20	0/1514
22	AT	0.10	0/1399	0.22	0/1881
23	AU	0.09	0/1490	0.20	0/2005
24	AV	0.08	0/3171	0.23	0/4292
25	AW	0.10	0/790	0.21	0/1064
26	AX	0.08	0/2945	0.22	0/3984
27	AY	0.08	0/1285	0.20	0/1734
28	AZ	0.07	0/841	0.18	0/1121
29	Aa	0.08	0/3171	0.19	0/4263
30	Ab	0.10	0/1804	0.22	0/2445
31	Ac	0.09	0/942	0.25	0/1261
32	Ad	0.09	0/2785	0.21	0/3735

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
33	Ae	0.07	0/4856	0.18	0/6579
34	Ag	0.08	0/2707	0.21	0/3636
35	Ai	0.10	0/1018	0.24	0/1375
36	Aj	0.08	0/1835	0.22	0/2484
All	All	0.09	0/75699	0.19	0/107180

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BX	99	0	83	0	0
2	Bd	192	0	167	6	0
3	AA	20418	0	10344	117	0
4	AB	2222	0	2270	40	0
5	AC	1075	0	1087	28	0
6	AD	639	0	709	6	0
7	AE	981	0	1012	14	0
8	AF	1722	0	1747	20	0
9	AG	1512	0	774	12	0
10	AH	1155	0	1193	18	0
11	AI	193	0	100	2	0
12	AJ	840	0	890	10	0
13	AK	858	0	883	13	0
14	AL	1448	0	1536	18	0
15	AM	932	0	951	9	0
16	AN	875	0	931	15	0
17	AO	1564	0	1531	20	0
18	AP	784	0	813	10	0
19	AQ	737	0	749	9	0
20	AR	2378	0	2392	23	0
21	AS	1101	0	1118	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	AT	1367	0	1385	18	0
23	AU	1467	0	1466	12	0
24	AV	3109	0	3029	47	0
25	AW	778	0	791	9	0
26	AX	2875	0	2885	49	0
27	AY	1250	0	1206	21	0
28	AZ	824	0	842	8	0
29	Aa	3120	0	3124	26	0
30	Ab	1762	0	1774	20	0
31	Ac	933	0	963	11	0
32	Ad	2732	0	2774	37	0
33	Ae	4748	0	4733	45	0
34	Ag	2650	0	2613	25	0
35	Ai	1008	0	1036	13	0
36	Aj	1788	0	1799	31	0
37	AA	120	0	0	0	0
37	AD	1	0	0	0	0
37	AG	1	0	0	0	0
37	AI	1	0	0	0	0
37	AJ	2	0	0	0	0
37	AX	1	0	0	0	0
37	Ab	1	0	0	0	0
38	AA	14	0	26	2	0
39	AA	10	0	19	0	0
40	AA	11	0	0	0	0
41	AO	1	0	0	0	0
42	AP	4	0	0	0	0
42	AT	4	0	0	0	0
43	AX	31	0	12	0	0
44	AX	28	0	12	3	0
45	AX	3	0	0	0	0
All	All	72369	0	61769	641	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (641) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bd:123:TRP:HE1	27:AY:321:HIS:HB3	1.20	1.03
2:Bd:119:TYR:OH	4:AB:234:GLU:OE1	2.00	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bd:123:TRP:NE1	27:AY:321:HIS:HB3	1.99	0.76
3:AA:65:C:N4	3:AA:157:A:O2'	2.18	0.76
24:AV:258:SER:HB3	24:AV:311:GLU:HB3	1.70	0.74
26:AX:259:VAL:HB	26:AX:305:ILE:HG22	1.71	0.73
26:AX:80:HIS:HB3	26:AX:155:PRO:HG3	1.71	0.72
12:AJ:78:ARG:HG3	12:AJ:118:LEU:HD11	1.72	0.70
10:AH:74:LYS:HB2	10:AH:177:LEU:HD23	1.74	0.70
24:AV:74:TYR:HD2	24:AV:409:GLU:HG2	1.56	0.69
3:AA:115:A:OP1	14:AL:203:ARG:NH2	2.25	0.69
7:AE:51:ILE:HB	7:AE:89:ILE:HD11	1.74	0.69
7:AE:37:ARG:NH2	7:AE:69:TYR:OH	2.26	0.69
36:Aj:43:ARG:HH21	36:Aj:50:LEU:HD21	1.59	0.67
18:AP:125:TYR:HB3	19:AQ:9:ALA:HB2	1.76	0.67
29:Aa:194:THR:HG21	29:Aa:381:GLN:HG3	1.76	0.67
26:AX:284:GLU:OE2	26:AX:293:ARG:NH2	2.29	0.66
26:AX:264:VAL:HG21	26:AX:307:LEU:HB3	1.77	0.66
24:AV:86:GLU:HG3	24:AV:114:ARG:HG2	1.78	0.66
24:AV:405:LEU:O	24:AV:409:GLU:N	2.25	0.65
35:Ai:76:ARG:HH21	35:Ai:81:LYS:HE2	1.60	0.65
3:AA:375:A:H62	31:Ac:17:ARG:HH22	1.42	0.65
24:AV:298:ARG:NH2	36:Aj:146:GLU:OE2	2.29	0.65
8:AF:240:ARG:NH2	31:Ac:44:THR:O	2.30	0.65
3:AA:353:C:H5"	3:AA:354:C:H5"	1.78	0.65
4:AB:168:PRO:O	4:AB:171:ARG:NH1	2.30	0.65
35:Ai:67:PRO:HB3	35:Ai:73:ASN:HD22	1.62	0.65
36:Aj:178:ARG:HB2	36:Aj:183:ASP:HB3	1.79	0.65
14:AL:176:TYR:HB2	16:AN:89:GLY:HA3	1.79	0.64
10:AH:59:THR:HG22	10:AH:61:PRO:HD3	1.78	0.64
33:Ae:242:ARG:O	33:Ae:245:ASN:ND2	2.28	0.64
29:Aa:183:ASN:ND2	29:Aa:289:ASP:OD1	2.31	0.64
24:AV:80:TRP:HA	24:AV:83:ARG:HG3	1.80	0.64
26:AX:120:ALA:O	26:AX:298:ASN:ND2	2.30	0.64
29:Aa:394[B]:ARG:NH1	29:Aa:403:GLU:OE1	2.31	0.64
34:Ag:321:LEU:HD11	34:Ag:365:MET:HE1	1.80	0.64
26:AX:122:ARG:HG2	26:AX:305:ILE:HD11	1.80	0.63
3:AA:468:A:OP2	30:Ab:99:ARG:NH2	2.27	0.63
3:AA:648:A:OP1	30:Ab:200:ASN:ND2	2.31	0.63
22:AT:51:ASN:OD1	22:AT:95:ASN:ND2	2.31	0.63
3:AA:869:A:N6	3:AA:899:C:O2'	2.32	0.63
3:AA:83:C:O2'	3:AA:99:A:N6	2.32	0.62
5:AC:60:HIS:HA	13:AK:125:ARG:HG3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AV:238:TRP:HZ2	24:AV:282:ALA:HB3	1.64	0.62
29:Aa:202:GLN:NE2	29:Aa:233:GLY:O	2.33	0.62
15:AM:114:ARG:HD3	17:AO:235:MET:HB3	1.82	0.62
3:AA:90:U:OP1	23:AU:68:ARG:NH1	2.33	0.62
12:AJ:62:VAL:HA	12:AJ:83:VAL:HG12	1.82	0.62
29:Aa:189:VAL:HG12	29:Aa:282:VAL:HG22	1.82	0.62
24:AV:125:ILE:HG21	24:AV:164:LYS:HD3	1.82	0.62
3:AA:328:A:N6	3:AA:366:A:N1	2.48	0.61
15:AM:51:LEU:HD13	15:AM:73:ILE:HG12	1.83	0.61
17:AO:190:ALA:HB2	36:Aj:171:ARG:HH22	1.65	0.61
30:Ab:238:ASN:ND2	30:Ab:241:SER:OG	2.33	0.61
15:AM:42:PRO:HG2	15:AM:45:GLY:HA3	1.81	0.61
17:AO:68:TYR:OH	17:AO:110:ASP:OD2	2.17	0.61
10:AH:55:PRO:HA	33:Ae:443:ASN:HB3	1.80	0.61
4:AB:315:LYS:HB3	4:AB:319:LYS:HZ3	1.65	0.61
16:AN:29:ARG:HD3	16:AN:46:ARG:HD2	1.83	0.61
9:AG:5:A:H2	9:AG:63:G:H1	1.49	0.60
20:AR:129:THR:HG22	32:Ad:368:LEU:HD22	1.83	0.60
36:Aj:3:ARG:HG3	36:Aj:5:LYS:H	1.65	0.60
36:Aj:194:GLU:OE2	36:Aj:197:ARG:NH2	2.32	0.60
19:AQ:43:ARG:NH2	19:AQ:44:TYR:OH	2.34	0.60
29:Aa:70:TRP:HA	29:Aa:75:LEU:HD23	1.82	0.60
4:AB:120:ALA:O	4:AB:124:HIS:ND1	2.34	0.60
3:AA:689:G:H5'	32:Ad:91:THR:HG22	1.84	0.60
8:AF:156:ILE:HD11	8:AF:171:PRO:HB2	1.83	0.60
14:AL:104:LYS:HE2	14:AL:108:LYS:HE3	1.82	0.60
13:AK:66:ASP:HB3	27:AY:378:ILE:HD11	1.82	0.60
27:AY:330:LEU:HD11	27:AY:347:THR:HG21	1.83	0.60
3:AA:104:A:OP2	16:AN:49:TYR:OH	2.17	0.60
24:AV:154:ARG:NH2	24:AV:416:TYR:OH	2.34	0.60
3:AA:289:G:O6	12:AJ:31:ALA:N	2.35	0.59
4:AB:151:ILE:HG12	4:AB:177:VAL:HG22	1.84	0.59
13:AK:28:TYR:O	32:Ad:88:SER:N	2.36	0.59
21:AS:134:ARG:NH1	21:AS:135:VAL:O	2.36	0.59
31:Ac:36:ARG:NH2	31:Ac:92:ASN:OD1	2.35	0.59
32:Ad:140:LEU:HB3	32:Ad:146:ILE:HD13	1.85	0.59
3:AA:357:G:H21	35:Ai:100:GLN:HE22	1.51	0.59
3:AA:532:G:O2'	3:AA:959:U:N3	2.36	0.59
4:AB:73:PRO:HB3	33:Ae:78:VAL:HG11	1.83	0.59
2:Bd:123:TRP:HE1	27:AY:321:HIS:CB	2.06	0.59
26:AX:124:VAL:HG12	26:AX:307:LEU:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AV:189:ASP:HA	24:AV:192:ILE:HD12	1.85	0.59
36:Aj:135:MET:SD	36:Aj:135:MET:N	2.76	0.59
3:AA:306:G:H2'	3:AA:307:A:H8	1.68	0.59
8:AF:155:VAL:HG11	31:Ac:70:ILE:HD12	1.84	0.59
34:Ag:97:GLU:HG3	34:Ag:98:THR:HG23	1.83	0.59
20:AR:347:LEU:HD22	20:AR:368:LEU:HD11	1.84	0.59
5:AC:38:ARG:HG2	5:AC:43:ARG:HH21	1.68	0.58
27:AY:250:ILE:HG22	33:Ae:327:VAL:HG21	1.85	0.58
3:AA:29:A:H1'	12:AJ:57:GLN:HE22	1.69	0.58
26:AX:161:VAL:HG22	26:AX:289:ILE:HD11	1.86	0.58
3:AA:562:A:H8	3:AA:708:A:H61	1.51	0.58
17:AO:235:MET:SD	17:AO:235:MET:N	2.77	0.58
20:AR:173:THR:OG1	20:AR:174:GLU:OE1	2.21	0.57
27:AY:329:TYR:O	27:AY:369:ARG:NH2	2.37	0.57
3:AA:290:C:OP1	38:AA:1120:SPM:N1	2.38	0.57
26:AX:294:LYS:NZ	44:AX:503:GDP:O1B	2.37	0.57
15:AM:105:THR:HG21	23:AU:56:LEU:HD13	1.86	0.57
26:AX:60:GLU:HA	26:AX:105:LEU:HD13	1.87	0.57
22:AT:78:PHE:HB2	22:AT:86:VAL:HB	1.86	0.57
24:AV:191:PHE:HA	24:AV:196:ASN:HD22	1.70	0.57
3:AA:887:U:H2'	3:AA:888:A:H8	1.70	0.56
4:AB:196:VAL:HG21	4:AB:207:LEU:HD11	1.87	0.56
5:AC:163:VAL:HG21	5:AC:167:ILE:HD12	1.87	0.56
6:AD:166:GLN:NE2	6:AD:170:GLU:OE2	2.38	0.56
34:Ag:256:GLN:HE22	34:Ag:371:LEU:HB3	1.70	0.56
4:AB:217:LYS:NZ	27:AY:310:GLU:OE1	2.39	0.56
5:AC:128:PRO:HD2	5:AC:131:LYS:HD2	1.87	0.56
3:AA:632:A:OP1	32:Ad:269:ARG:NH2	2.39	0.56
6:AD:172:ASP:OD1	6:AD:175:ARG:NH2	2.37	0.56
9:AG:30:C:OP2	34:Ag:397:ARG:NH2	2.34	0.56
11:AI:-4:A:O2'	11:AI:-3:A:N7	2.39	0.56
27:AY:344:GLU:OE2	28:AZ:24:ARG:NE	2.31	0.56
36:Aj:68:LEU:HD12	36:Aj:71:LEU:HD12	1.88	0.56
17:AO:89:ARG:HG3	17:AO:144:MET:HE3	1.88	0.56
20:AR:104:MET:HG3	20:AR:290:PHE:HE2	1.71	0.56
33:Ae:380:GLN:HE21	33:Ae:421:SER:HB3	1.69	0.56
4:AB:154:ASP:HB2	4:AB:174:THR:HB	1.88	0.55
3:AA:237:U:O2'	3:AA:238:C:O4'	2.21	0.55
4:AB:114:LEU:HD23	34:Ag:111:LEU:HD12	1.88	0.55
33:Ae:80:ARG:NH2	33:Ae:487:SER:OG	2.39	0.55
5:AC:113:ARG:NH1	5:AC:118:GLU:OE2	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Ad:194:SER:HB2	32:Ad:197:THR:HG22	1.88	0.55
3:AA:735:G:N3	26:AX:163:ASN:ND2	2.54	0.55
21:AS:10:GLY:O	21:AS:15:ARG:NH1	2.39	0.55
26:AX:265:ASN:ND2	26:AX:310:SER:O	2.39	0.55
27:AY:254:GLN:HE22	33:Ae:332:LYS:HB3	1.70	0.55
32:Ad:313:GLY:HA2	32:Ad:331:ASP:HA	1.88	0.55
3:AA:66:C:OP2	15:AM:10:ARG:NH2	2.40	0.55
14:AL:223:LYS:HA	14:AL:226:ARG:HE	1.71	0.55
24:AV:223:LEU:HD22	24:AV:397:SER:HB2	1.89	0.55
32:Ad:380:LEU:HD12	32:Ad:381:PRO:HD2	1.88	0.55
20:AR:206:ALA:HB1	20:AR:210:GLU:HG3	1.89	0.55
26:AX:46:ALA:HB3	26:AX:357:GLN:HG3	1.89	0.55
29:Aa:395:VAL:HG23	29:Aa:407:ILE:HG12	1.89	0.55
33:Ae:192:LEU:HD21	33:Ae:250:ILE:HB	1.89	0.55
24:AV:230:LEU:HD22	24:AV:394:LEU:HD13	1.89	0.55
30:Ab:177:ASN:HD21	30:Ab:180:LEU:HD22	1.72	0.55
26:AX:264:VAL:HG12	26:AX:268:TRP:HZ3	1.72	0.55
3:AA:874:U:H4'	14:AL:229:ARG:HH22	1.72	0.54
5:AC:73:THR:HG22	5:AC:79:GLU:HG2	1.88	0.54
20:AR:276:ASP:OD1	20:AR:281:TYR:OH	2.24	0.54
26:AX:107:LEU:HD23	26:AX:140:ILE:HG13	1.88	0.54
33:Ae:307:VAL:HG12	33:Ae:308:VAL:HG13	1.88	0.54
3:AA:643:G:O2'	3:AA:651:G:OP2	2.21	0.54
20:AR:184:SER:H	20:AR:192:ARG:HH12	1.55	0.54
22:AT:91:GLU:OE2	23:AU:123:ARG:NH2	2.39	0.54
33:Ae:129:GLN:OE1	33:Ae:144:TYR:OH	2.25	0.54
24:AV:306:VAL:HB	24:AV:382:LEU:HD22	1.89	0.54
34:Ag:161:LEU:HD22	34:Ag:210:LEU:HD21	1.89	0.54
17:AO:105:CYS:HB2	17:AO:142:VAL:HA	1.90	0.54
33:Ae:584:VAL:HG22	33:Ae:613:LEU:HD13	1.88	0.54
26:AX:245:GLU:OE2	26:AX:249:GLN:NE2	2.40	0.54
3:AA:568:G:N2	3:AA:577:C:O2	2.41	0.54
3:AA:888:A:H1'	24:AV:106:PRO:HD3	1.90	0.54
33:Ae:446:ASP:HB3	33:Ae:449:LYS:HE2	1.89	0.54
34:Ag:366:ARG:HG3	34:Ag:371:LEU:HD12	1.89	0.54
25:AW:84:MET:HE1	30:Ab:81:ARG:HA	1.89	0.54
32:Ad:140:LEU:HD11	32:Ad:160:ARG:HE	1.72	0.53
15:AM:111:ARG:NH2	17:AO:233:GLU:O	2.38	0.53
24:AV:147:TRP:HB3	24:AV:423:TRP:CD2	2.43	0.53
36:Aj:82:ARG:NH1	36:Aj:133:GLN:OE1	2.39	0.53
36:Aj:91:GLU:OE2	36:Aj:121:LYS:NZ	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AA:923:G:H1'	3:AA:944:MA6:H2	1.90	0.53
7:AE:36:VAL:HG23	23:AU:168:ILE:HB	1.88	0.53
17:AO:104:PRO:HB2	17:AO:109:ARG:HB3	1.90	0.53
22:AT:155:LEU:HD13	22:AT:159:MET:HE3	1.90	0.53
29:Aa:67:LYS:HG2	29:Aa:71:LYS:HE3	1.89	0.53
3:AA:230:U:H2'	3:AA:237:U:H5	1.72	0.53
33:Ae:396:ILE:HG12	33:Ae:434:LEU:HD21	1.91	0.53
5:AC:132:PHE:HD2	33:Ae:95:LEU:HD21	1.73	0.53
28:AZ:74:GLU:HB3	32:Ad:95:ALA:HB2	1.90	0.53
32:Ad:154:VAL:HG21	33:Ae:108:LEU:HD13	1.91	0.53
33:Ae:491:PRO:O	33:Ae:524:HIS:NE2	2.37	0.52
4:AB:83:VAL:O	4:AB:101:LYS:NZ	2.41	0.52
36:Aj:88:GLN:NE2	36:Aj:202:ASP:OD2	2.42	0.52
36:Aj:132:GLU:HG2	36:Aj:133:GLN:HG3	1.92	0.52
3:AA:127:A:H2'	3:AA:128:C:O4'	2.10	0.52
22:AT:89:ASP:OD2	23:AU:120:ARG:NH2	2.42	0.52
34:Ag:296:VAL:HG22	34:Ag:331:CYS:HB2	1.91	0.52
3:AA:374:C:OP2	31:Ac:9:ARG:NH2	2.31	0.52
26:AX:210:ASN:ND2	26:AX:213:GLU:OE2	2.42	0.52
30:Ab:219:VAL:HG22	30:Ab:233:TYR:HB2	1.92	0.52
33:Ae:346:ARG:HA	33:Ae:381:LEU:HD13	1.91	0.52
4:AB:233:HIS:HE1	10:AH:188:ILE:HB	1.74	0.52
5:AC:115:ASN:HB3	27:AY:303:TRP:CE2	2.44	0.52
10:AH:78:VAL:HG22	10:AH:172:VAL:HG12	1.91	0.52
3:AA:801:A:N6	3:AA:802:A:N1	2.57	0.52
9:AG:47:U:H3	9:AG:58:U:H3	1.57	0.52
33:Ae:308:VAL:HG23	33:Ae:315:LYS:HE2	1.89	0.52
5:AC:134:PHE:CD2	32:Ad:144:LEU:HG	2.45	0.52
16:AN:62:ASP:OD1	16:AN:88:VAL:N	2.43	0.52
26:AX:164:CYS:SG	26:AX:179:GLN:NE2	2.83	0.52
4:AB:70:SER:HA	33:Ae:78:VAL:HG13	1.91	0.52
35:Ai:77:TRP:HB2	35:Ai:85:ILE:HD11	1.92	0.52
18:AP:125:TYR:HE1	19:AQ:4:HIS:HB3	1.75	0.52
26:AX:162:LYS:HB3	26:AX:315:LEU:HD11	1.92	0.52
26:AX:198:LEU:HD12	26:AX:222:GLY:HA2	1.91	0.52
31:Ac:11:ALA:O	31:Ac:12:ARG:NH1	2.42	0.52
3:AA:259:A:O2'	3:AA:261:A:OP1	2.27	0.51
8:AF:200:LEU:HB3	8:AF:202:PRO:HD2	1.92	0.51
3:AA:826:C:H2'	3:AA:827:A:H8	1.75	0.51
19:AQ:87:CYS:O	30:Ab:168:ARG:NH1	2.42	0.51
3:AA:386:U:O2'	7:AE:93:ILE:O	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AN:41:LYS:HB2	22:AT:11:ARG:HD2	1.93	0.51
33:Ae:364:LYS:NZ	33:Ae:369:GLU:OE1	2.44	0.51
26:AX:294:LYS:NZ	44:AX:503:GDP:O1A	2.44	0.51
34:Ag:269:ALA:HB1	34:Ag:356:PHE:HE2	1.76	0.51
36:Aj:85:TRP:HD1	36:Aj:89:HIS:HD2	1.56	0.51
3:AA:201:A:H2'	3:AA:202:A:C8	2.46	0.51
23:AU:168:ILE:HG12	23:AU:176:ARG:HG3	1.92	0.51
26:AX:178:ASP:HB3	26:AX:236:THR:HG21	1.92	0.51
33:Ae:416:ASP:HB2	33:Ae:452:GLY:HA2	1.92	0.51
34:Ag:365:MET:HG3	34:Ag:370:LEU:HB2	1.92	0.51
3:AA:443:U:H2'	3:AA:444:G:H8	1.76	0.51
3:AA:129:G:OP2	14:AL:226:ARG:NH1	2.44	0.51
3:AA:844:C:O2'	11:AI:1:A:N6	2.36	0.51
3:AA:386:U:H4'	7:AE:94:VAL:HG12	1.93	0.51
15:AM:54:TYR:HD1	15:AM:66:VAL:HG22	1.75	0.51
3:AA:896:A:O2'	6:AD:183:LYS:NZ	2.44	0.50
14:AL:74:LEU:HD12	14:AL:76:ASP:H	1.74	0.50
20:AR:198:GLU:OE2	20:AR:204:ARG:NH1	2.43	0.50
24:AV:238:TRP:CZ3	24:AV:278:GLN:HB2	2.46	0.50
29:Aa:122:GLU:HB3	29:Aa:162:LYS:HZ3	1.77	0.50
30:Ab:134:VAL:HG11	30:Ab:191:LEU:HD13	1.92	0.50
16:AN:65:LEU:HB2	16:AN:85:ILE:HD11	1.92	0.50
20:AR:181:THR:HG22	20:AR:194:ILE:HG23	1.94	0.50
22:AT:132:ARG:NH1	22:AT:136:LEU:O	2.44	0.50
26:AX:205:GLU:HG2	26:AX:248:ARG:HH22	1.75	0.50
4:AB:103:GLY:H	5:AC:156:GLN:HE22	1.59	0.50
27:AY:353:ASN:ND2	28:AZ:37:PHE:O	2.42	0.50
29:Aa:258:HIS:HB3	29:Aa:388:TYR:HE1	1.76	0.50
21:AS:77:ALA:O	21:AS:134:ARG:NH1	2.45	0.50
30:Ab:182:LEU:HB2	30:Ab:186:VAL:HG21	1.93	0.50
3:AA:722:A:N6	3:AA:738:U:O2'	2.44	0.50
24:AV:268:TYR:HB3	24:AV:299:ALA:HB2	1.94	0.50
7:AE:13:MET:HE3	7:AE:18:THR:HA	1.94	0.50
36:Aj:91:GLU:HG3	36:Aj:121:LYS:HA	1.94	0.50
24:AV:157:LEU:HD22	24:AV:190:TYR:HD2	1.76	0.50
8:AF:61:GLU:HA	8:AF:64:TYR:CE2	2.47	0.50
9:AG:22:U:H2'	9:AG:23:A:H8	1.77	0.50
10:AH:96:VAL:HG22	10:AH:106:ILE:HD11	1.94	0.50
24:AV:363:THR:HG22	24:AV:365:GLN:H	1.77	0.50
26:AX:250:SER:HA	26:AX:255:PHE:HD2	1.75	0.50
13:AK:52:LEU:HD11	28:AZ:36:LEU:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AV:286:ASN:HA	36:Aj:70:ARG:HH22	1.76	0.49
26:AX:164:CYS:H	26:AX:273:LEU:HD21	1.77	0.49
32:Ad:149:MET:HG2	32:Ad:154:VAL:HG22	1.94	0.49
36:Aj:143:PRO:HD2	36:Aj:146:GLU:HB2	1.94	0.49
24:AV:83:ARG:HH12	24:AV:154:ARG:HG3	1.77	0.49
31:Ac:17:ARG:HE	31:Ac:20:ILE:HD11	1.76	0.49
36:Aj:119:THR:HG22	36:Aj:124:THR:HG22	1.94	0.49
3:AA:210:U:O4	3:AA:211:A:N6	2.45	0.49
3:AA:740:U:H3	3:AA:747:C:H42	1.61	0.49
3:AA:876:A:H4'	3:AA:877:A:C5	2.48	0.49
22:AT:103:ARG:NH2	22:AT:110:GLU:OE2	2.45	0.49
32:Ad:242:ARG:HD2	32:Ad:258:ILE:HD11	1.92	0.49
29:Aa:93:LEU:HD21	29:Aa:106:LEU:HB2	1.94	0.49
4:AB:117:THR:HG22	4:AB:118:PRO:HD2	1.95	0.49
15:AM:20:ARG:NH2	15:AM:41:CYS:SG	2.86	0.49
29:Aa:190:THR:OG1	29:Aa:281:SER:OG	2.30	0.49
3:AA:869:A:OP2	3:AA:900:A:N6	2.38	0.49
24:AV:147:TRP:HB3	24:AV:423:TRP:CG	2.48	0.49
30:Ab:140:ILE:HG13	30:Ab:187:ARG:HH21	1.77	0.49
3:AA:56:U:O2'	3:AA:198:C:O2	2.30	0.49
20:AR:285:ARG:NH2	20:AR:309:ASP:OD2	2.46	0.49
20:AR:303:ILE:HG22	20:AR:307:LEU:HG	1.95	0.49
3:AA:328:A:OP1	7:AE:90:ARG:NH2	2.23	0.49
3:AA:379:A:N1	3:AA:404:C:O2'	2.45	0.49
3:AA:962:C:O2	31:Ac:37:ARG:NH1	2.46	0.49
33:Ae:382:PHE:O	33:Ae:392:SER:OG	2.30	0.49
33:Ae:520:LYS:NZ	33:Ae:557:ASP:OD2	2.43	0.49
3:AA:820:U:OP2	8:AF:93:LYS:NZ	2.43	0.48
13:AK:114:LEU:HB3	13:AK:120:LEU:HD13	1.95	0.48
24:AV:325:ARG:NH2	24:AV:376:GLU:OE2	2.46	0.48
3:AA:826:C:H2'	3:AA:827:A:C8	2.48	0.48
5:AC:92:LEU:HD11	5:AC:117:LEU:HD21	1.94	0.48
21:AS:67:GLU:OE2	25:AW:86:ARG:NH2	2.38	0.48
32:Ad:190:GLU:OE1	32:Ad:202:SER:OG	2.29	0.48
32:Ad:341:ASN:HD22	32:Ad:344:ASN:HD22	1.62	0.48
3:AA:654:A:H5'	4:AB:95:ARG:HH12	1.78	0.48
12:AJ:32:THR:OG1	12:AJ:33:LEU:N	2.47	0.48
16:AN:69:LEU:HD13	16:AN:80:GLU:HB2	1.94	0.48
20:AR:229:PRO:HB2	20:AR:231:ILE:HG22	1.96	0.48
16:AN:74:THR:HG23	16:AN:77:VAL:H	1.78	0.48
35:Ai:100:GLN:HE21	35:Ai:108:PRO:HB3	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AO:110:ASP:OD1	17:AO:110:ASP:N	2.46	0.48
3:AA:35:U:H2'	3:AA:36:A:H8	1.79	0.48
3:AA:903:C:H2'	3:AA:904:A:C8	2.48	0.48
4:AB:109:LYS:HE2	5:AC:69:LEU:HD23	1.95	0.48
8:AF:155:VAL:H	8:AF:227:HIS:HE1	1.61	0.48
13:AK:51:ARG:NH1	13:AK:82:SER:O	2.47	0.48
32:Ad:220:THR:HB	32:Ad:247:VAL:HG12	1.94	0.48
33:Ae:266:ILE:HG23	33:Ae:278:ALA:HB1	1.94	0.48
36:Aj:167:PRO:HG2	36:Aj:170:LEU:HB3	1.95	0.48
4:AB:131:PHE:HB2	10:AH:155:VAL:HG11	1.96	0.48
9:AG:8:U:H3	9:AG:14:A:H62	1.61	0.48
22:AT:60:PRO:HG2	22:AT:61:TRP:HD1	1.78	0.48
32:Ad:288:HIS:CE1	32:Ad:310:ARG:HG2	2.49	0.48
33:Ae:301:ILE:HG21	33:Ae:341:ILE:HG12	1.96	0.48
7:AE:40:GLU:OE2	23:AU:185:LYS:NZ	2.31	0.47
24:AV:163:ASP:OD1	24:AV:163:ASP:N	2.46	0.47
24:AV:204:VAL:HG11	24:AV:225:VAL:HG22	1.96	0.47
33:Ae:339:ASN:ND2	33:Ae:412:ASP:OD2	2.47	0.47
8:AF:114:THR:HG21	8:AF:205:LEU:HD22	1.96	0.47
18:AP:95:ARG:HH12	18:AP:102:GLY:HA2	1.78	0.47
32:Ad:140:LEU:HD23	32:Ad:146:ILE:HG21	1.96	0.47
4:AB:306:ASP:HB2	26:AX:323:LEU:HD13	1.96	0.47
16:AN:18:ILE:HD11	16:AN:29:ARG:HB2	1.96	0.47
8:AF:57:GLU:OE1	8:AF:60:GLU:N	2.33	0.47
8:AF:142:TYR:O	8:AF:146:HIS:ND1	2.47	0.47
26:AX:384:ASN:HB3	34:Ag:302:LEU:HD22	1.96	0.47
27:AY:319:GLU:HG3	27:AY:320:PHE:H	1.80	0.47
3:AA:11:G:H21	32:Ad:230:ASN:HA	1.79	0.47
3:AA:124:A:H2'	3:AA:125:U:O4'	2.14	0.47
3:AA:712:A:H2'	3:AA:713:A:H8	1.79	0.47
26:AX:244:LYS:HD2	44:AX:503:GDP:H5'	1.97	0.47
26:AX:347:TYR:CZ	26:AX:387:PRO:HB3	2.49	0.47
29:Aa:126:THR:HG22	29:Aa:159:ILE:HG23	1.95	0.47
8:AF:155:VAL:H	8:AF:227:HIS:CE1	2.33	0.47
32:Ad:296:LEU:HD22	32:Ad:352:GLY:HA3	1.97	0.47
4:AB:116:LEU:HD11	10:AH:163:ASN:HB3	1.96	0.47
7:AE:36:VAL:HG12	7:AE:68:PHE:HB3	1.97	0.47
29:Aa:259:ARG:HH21	29:Aa:387:THR:HG21	1.80	0.47
34:Ag:177:ASN:HA	34:Ag:180:ARG:HE	1.80	0.47
35:Ai:71:GLN:HG3	35:Ai:72:GLU:H	1.80	0.47
3:AA:405:G:N1	3:AA:452:C:O2'	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AE:37:ARG:HG2	7:AE:38:ASN:HD22	1.80	0.47
19:AQ:83:PRO:HG2	19:AQ:84:TRP:CD1	2.50	0.47
3:AA:540:U:H1'	3:AA:541:C:H5	1.80	0.46
32:Ad:282:ILE:HG13	32:Ad:327:ILE:HD13	1.96	0.46
26:AX:202:LYS:O	26:AX:204:GLN:NE2	2.48	0.46
34:Ag:358:THR:OG1	34:Ag:360:ASP:OD1	2.27	0.46
35:Ai:87:ILE:HD11	35:Ai:150:ARG:NH2	2.30	0.46
3:AA:871:U:H2'	3:AA:872:A:C8	2.51	0.46
14:AL:165:LYS:NZ	14:AL:191:THR:H	2.13	0.46
18:AP:81:LEU:HB3	18:AP:112:ILE:HG12	1.97	0.46
31:Ac:100:PRO:HD2	31:Ac:103:LYS:HD2	1.96	0.46
33:Ae:325:GLN:O	33:Ae:328:THR:OG1	2.28	0.46
3:AA:191:C:H42	3:AA:208:A:H62	1.63	0.46
3:AA:901:A:O3'	6:AD:171:ARG:NH1	2.48	0.46
29:Aa:419:GLN:OE1	29:Aa:423:ARG:NH1	2.49	0.46
3:AA:28:U:H2'	3:AA:29:A:H8	1.80	0.46
3:AA:68:G:H4'	3:AA:208:A:H4'	1.98	0.46
3:AA:356:A:H2'	3:AA:357:G:H8	1.81	0.46
25:AW:105:ILE:HG12	25:AW:115:ILE:HG12	1.97	0.46
28:AZ:75:HIS:CD2	32:Ad:98:LEU:HD11	2.51	0.46
32:Ad:308:GLN:NE2	32:Ad:312:TYR:O	2.49	0.46
5:AC:72:HIS:HD2	5:AC:74:GLY:H	1.63	0.46
21:AS:34:ILE:HD11	30:Ab:137:ARG:HD3	1.98	0.46
21:AS:63:ILE:HD11	30:Ab:107:GLY:HA3	1.98	0.46
24:AV:280:LEU:HD22	24:AV:293:PRO:HB3	1.98	0.46
19:AQ:45:TYR:HB2	35:Ai:190:PRO:HG2	1.96	0.46
24:AV:414:ALA:O	24:AV:418:GLN:HG2	2.15	0.46
3:AA:512:A:H2'	3:AA:513:A:H8	1.80	0.46
3:AA:794:A:H2'	3:AA:795:A:C8	2.50	0.46
12:AJ:70:PRO:HB3	12:AJ:117:ASP:HB3	1.97	0.46
29:Aa:393:ASP:OD1	29:Aa:407:ILE:HG13	2.16	0.46
35:Ai:74:SER:HA	35:Ai:76:ARG:HH11	1.80	0.46
12:AJ:104:GLU:HG2	12:AJ:105:HIS:ND1	2.31	0.45
13:AK:41:ARG:NH1	28:AZ:48:THR:O	2.48	0.45
17:AO:235:MET:HE1	20:AR:171:GLU:HB3	1.97	0.45
24:AV:185:ASN:HD22	24:AV:220:LEU:HD23	1.80	0.45
24:AV:291:TRP:HH2	36:Aj:142:VAL:HG12	1.82	0.45
3:AA:262:C:N4	3:AA:263:G:O6	2.49	0.45
3:AA:296:G:O2'	3:AA:461:A:OP2	2.26	0.45
10:AH:76:LEU:HB3	10:AH:145:LEU:HB2	1.99	0.45
26:AX:377:LYS:HB3	34:Ag:324:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Aa:224:LEU:HD11	29:Aa:227:TYR:HB2	1.98	0.45
36:Aj:29:ARG:H	36:Aj:32:GLN:HE21	1.64	0.45
3:AA:199:G:N2	3:AA:202:A:OP2	2.49	0.45
3:AA:312:A:H2'	3:AA:313:A:C8	2.51	0.45
3:AA:630:A:H2'	3:AA:631:A:C8	2.52	0.45
3:AA:901:A:O2'	6:AD:171:ARG:NH1	2.49	0.45
4:AB:133:THR:HG21	33:Ae:60:PRO:HB2	1.98	0.45
24:AV:144:LEU:HD13	24:AV:149:ILE:HD11	1.99	0.45
4:AB:89:MET:HG2	4:AB:107:LEU:HG	1.98	0.45
17:AO:202:TRP:O	23:AU:59:ARG:NH1	2.50	0.45
24:AV:311:GLU:HA	24:AV:388:VAL:HG11	1.98	0.45
34:Ag:139:GLN:OE1	34:Ag:156:GLN:NE2	2.43	0.45
34:Ag:323:ARG:HD2	34:Ag:327:HIS:NE2	2.32	0.45
3:AA:552:A:H2'	3:AA:553:G:C8	2.52	0.45
26:AX:162:LYS:HD3	26:AX:315:LEU:HD21	1.99	0.45
35:Ai:121:ASN:O	35:Ai:124:LYS:HG2	2.16	0.45
25:AW:144:ARG:HB2	25:AW:171:LEU:HD11	1.98	0.45
26:AX:161:VAL:HG21	26:AX:266:ALA:HB1	1.97	0.45
27:AY:242:ILE:HB	33:Ae:357:LEU:HD22	1.97	0.45
3:AA:166:G:H2'	3:AA:167:G:H8	1.81	0.45
7:AE:42:LEU:HB2	7:AE:63:TYR:HB2	1.99	0.45
4:AB:79:LYS:HB2	4:AB:82:ALA:HB3	1.99	0.45
22:AT:56:GLN:HB2	22:AT:64:ILE:HD12	1.98	0.45
27:AY:339:ILE:HG12	27:AY:386:LEU:HD13	1.98	0.45
3:AA:576:C:O2'	3:AA:809:G:O2'	2.26	0.44
4:AB:214:CYS:HB3	4:AB:219:GLN:HB2	1.99	0.44
10:AH:63:ILE:HG22	33:Ae:63:LYS:HB3	1.99	0.44
36:Aj:94:TYR:O	36:Aj:119:THR:OG1	2.32	0.44
3:AA:887:U:H2'	3:AA:888:A:C8	2.49	0.44
4:AB:268:LEU:HD13	4:AB:285:LEU:HD12	1.98	0.44
20:AR:287:THR:HG22	20:AR:289:HIS:H	1.83	0.44
26:AX:54:ASP:HB3	26:AX:57:LYS:HG2	1.99	0.44
33:Ae:627:PRO:HB3	33:Ae:657:THR:HA	1.99	0.44
5:AC:75:ASN:OD1	13:AK:104:TRP:NE1	2.44	0.44
10:AH:128:LYS:HE2	10:AH:131:ARG:NH2	2.32	0.44
14:AL:69:PRO:HB2	14:AL:72:MET:HG3	1.99	0.44
14:AL:117:LEU:HD11	14:AL:128:ALA:HA	1.99	0.44
23:AU:65:GLN:HG2	36:Aj:193:LEU:HD22	1.99	0.44
29:Aa:307:ALA:HB2	29:Aa:321:ALA:HB2	1.99	0.44
32:Ad:289:THR:HG23	32:Ad:331:ASP:O	2.17	0.44
4:AB:68:TRP:N	4:AB:69:PRO:HD2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:AX:168:LEU:O	26:AX:178:ASP:N	2.47	0.44
3:AA:641:A:N7	32:Ad:260:LYS:NZ	2.62	0.44
5:AC:37:ASN:O	5:AC:43:ARG:NH2	2.48	0.44
5:AC:73:THR:HG23	5:AC:76:LEU:HD12	1.98	0.44
3:AA:917:C:H2'	3:AA:918:A:H2'	1.98	0.44
19:AQ:58:GLU:HG2	19:AQ:62:ARG:HH12	1.82	0.44
33:Ae:548:GLN:HG2	33:Ae:588:ARG:HB2	2.00	0.44
22:AT:29:VAL:HB	22:AT:79:TYR:HB2	2.00	0.44
32:Ad:159:GLN:HG2	32:Ad:160:ARG:H	1.81	0.44
3:AA:897:C:H2'	3:AA:898:A:H8	1.83	0.44
5:AC:45:SER:HB2	5:AC:49:LYS:HD2	2.00	0.44
17:AO:67:ARG:HD2	17:AO:68:TYR:CE2	2.53	0.44
17:AO:225:ARG:HB2	23:AU:47:ALA:HB1	2.00	0.44
30:Ab:218:THR:H	30:Ab:232:THR:HG22	1.82	0.44
33:Ae:79:HIS:ND1	33:Ae:80:ARG:O	2.48	0.44
3:AA:550:G:N1	3:AA:782:G:OP2	2.51	0.44
16:AN:74:THR:OG1	16:AN:75:LYS:N	2.51	0.44
24:AV:157:LEU:HA	24:AV:161:ALA:HB2	2.00	0.44
29:Aa:389:ASN:HB3	29:Aa:394[A]:ARG:HG3	1.98	0.44
3:AA:388:U:H5"	7:AE:72:ALA:HB1	2.00	0.43
3:AA:794:A:H2'	3:AA:795:A:H8	1.81	0.43
8:AF:140:ASN:OD1	8:AF:143:THR:N	2.44	0.43
25:AW:153:ARG:NH1	25:AW:158:THR:O	2.51	0.43
26:AX:246:LEU:O	26:AX:250:SER:OG	2.26	0.43
3:AA:520:G:H4'	6:AD:132:LYS:HE3	1.99	0.43
14:AL:75:LEU:HA	14:AL:78:GLN:HE21	1.83	0.43
14:AL:144:MET:HE2	14:AL:144:MET:HA	1.99	0.43
27:AY:321:HIS:CE1	27:AY:322:GLU:HG3	2.53	0.43
29:Aa:188:GLU:OE1	29:Aa:372:ARG:NH2	2.50	0.43
32:Ad:302:HIS:HB2	32:Ad:337:SER:HB2	1.99	0.43
33:Ae:412:ASP:N	33:Ae:415:ASP:OD2	2.51	0.43
3:AA:728:U:H2'	3:AA:729:A:C8	2.53	0.43
17:AO:73:VAL:HG12	17:AO:106:PRO:HB3	2.00	0.43
22:AT:150:PRO:HB3	22:AT:155:LEU:HG	2.00	0.43
23:AU:141:LEU:HD23	23:AU:144:ARG:NH1	2.33	0.43
3:AA:411:U:H2'	3:AA:412:A:C8	2.54	0.43
5:AC:76:LEU:O	13:AK:103:ARG:NH2	2.46	0.43
9:AG:16:A:H5'	9:AG:55:C:N3	2.33	0.43
21:AS:104:ILE:O	21:AS:107:GLN:HG3	2.18	0.43
24:AV:252:GLY:O	24:AV:264:GLN:NE2	2.40	0.43
36:Aj:82:ARG:HB3	36:Aj:85:TRP:CE3	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AA:558:U:H4'	3:AA:569:A:H61	1.84	0.43
8:AF:196:HIS:HB3	8:AF:199:VAL:HG12	2.00	0.43
10:AH:66:SER:OG	10:AH:67:ASP:N	2.48	0.43
10:AH:121:LEU:HB2	13:AK:108:ARG:NE	2.34	0.43
24:AV:401:ALA:HA	24:AV:405:LEU:HB2	1.99	0.43
17:AO:167:ILE:HD12	20:AR:252:LEU:HD21	2.00	0.43
30:Ab:242:PRO:N	30:Ab:243:PRO:HD2	2.34	0.43
32:Ad:299:LYS:HD2	32:Ad:344:ASN:OD1	2.18	0.43
36:Aj:33:ARG:HD2	36:Aj:34:TYR:CE1	2.53	0.43
3:AA:335:A:H2'	3:AA:336:A:C8	2.54	0.43
5:AC:89:ASP:O	5:AC:93:ARG:HG2	2.18	0.43
27:AY:319:GLU:HB3	27:AY:321:HIS:CD2	2.54	0.43
3:AA:866:U:H2'	3:AA:867:G:C8	2.53	0.43
18:AP:63:LEU:HD12	18:AP:63:LEU:H	1.84	0.43
26:AX:89:GLN:HE21	26:AX:93:PHE:HE2	1.66	0.43
35:Ai:154:LYS:HE2	35:Ai:154:LYS:HB2	1.90	0.43
7:AE:114:GLU:HG3	31:Ac:7:ARG:HA	2.00	0.43
9:AG:47:U:H2'	9:AG:48:G:C8	2.53	0.43
24:AV:405:LEU:HD12	24:AV:408:CYS:HB2	2.00	0.43
3:AA:527:G:N2	3:AA:839:C:O2	2.52	0.43
4:AB:69:PRO:HB3	4:AB:120:ALA:HB2	2.01	0.43
5:AC:99:THR:O	5:AC:101:PRO:HD3	2.19	0.43
13:AK:53:ARG:O	13:AK:56:SER:OG	2.30	0.43
16:AN:53:ASP:OD2	16:AN:57:GLN:N	2.42	0.43
17:AO:173:ARG:HA	20:AR:221:ARG:NH1	2.34	0.43
32:Ad:103:LEU:HD11	32:Ad:123:ARG:HB2	2.00	0.43
5:AC:115:ASN:HB3	27:AY:303:TRP:CZ2	2.54	0.42
18:AP:57:ASN:HB3	18:AP:60:LYS:HG3	2.01	0.42
29:Aa:274:ARG:NH2	32:Ad:114:ARG:HE	2.17	0.42
36:Aj:78:ARG:NH2	36:Aj:142:VAL:O	2.52	0.42
3:AA:8:U:H2'	3:AA:9:U:H5"	2.00	0.42
3:AA:276:U:H2'	3:AA:277:A:H8	1.84	0.42
4:AB:166:ARG:HD3	33:Ae:134:GLU:HB3	2.01	0.42
4:AB:190:LYS:NZ	4:AB:251:GLU:OE1	2.44	0.42
9:AG:1:A:H61	9:AG:67:U:H3	1.65	0.42
9:AG:9:C:O2'	9:AG:10:A:N7	2.42	0.42
20:AR:170:LEU:HD12	20:AR:197:ARG:NH2	2.35	0.42
26:AX:206:LYS:HE2	26:AX:216:GLU:HG2	2.00	0.42
26:AX:321:ALA:HB1	26:AX:326:GLU:HG3	2.00	0.42
30:Ab:161:CYS:SG	30:Ab:253:GLN:HA	2.59	0.42
33:Ae:593:GLN:HA	33:Ae:596:TRP:HD1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:Ag:273:GLY:HA3	34:Ag:352:ALA:HB2	2.00	0.42
5:AC:106:ASP:OD1	5:AC:106:ASP:N	2.52	0.42
8:AF:88:ASP:OD2	8:AF:146:HIS:NE2	2.44	0.42
14:AL:80:VAL:HG23	14:AL:83:ILE:HD11	2.01	0.42
18:AP:68:LEU:HD21	18:AP:80:LEU:HD11	2.01	0.42
22:AT:2:PRO:HB3	22:AT:11:ARG:NH2	2.33	0.42
36:Aj:35:ALA:O	36:Aj:44:PRO:HD2	2.18	0.42
2:Bd:126:LYS:H	2:Bd:126:LYS:HD2	1.85	0.42
3:AA:309:A:H62	22:AT:6:ARG:NH1	2.18	0.42
4:AB:58:ARG:NH1	33:Ae:91:ASP:OD2	2.52	0.42
36:Aj:74:PHE:CZ	36:Aj:102:PRO:HG3	2.54	0.42
38:AA:1120:SPM:H91	38:AA:1120:SPM:H62	1.81	0.42
4:AB:67:ASP:OD1	4:AB:67:ASP:N	2.52	0.42
4:AB:149:PHE:CG	10:AH:177:LEU:HD13	2.55	0.42
10:AH:84:ASP:OD1	10:AH:84:ASP:N	2.45	0.42
26:AX:49:ARG:HH21	26:AX:68:ASN:HB2	1.84	0.42
32:Ad:243:VAL:HG11	32:Ad:268:PHE:HE1	1.84	0.42
34:Ag:198:SER:HB2	34:Ag:246:ARG:HD2	2.01	0.42
36:Aj:61:GLU:HG2	36:Aj:138:ASP:HA	2.00	0.42
8:AF:71:THR:HB	34:Ag:254:LYS:HG2	2.02	0.42
26:AX:136:SER:O	26:AX:140:ILE:HG12	2.20	0.42
3:AA:762:G:N2	3:AA:764:A:H3'	2.34	0.42
8:AF:140:ASN:ND2	26:AX:366:GLN:O	2.53	0.42
10:AH:82:GLY:HA3	10:AH:168:VAL:HG12	2.01	0.42
16:AN:35:LEU:HB2	16:AN:42:TYR:CE1	2.55	0.42
21:AS:125:LEU:HD23	21:AS:125:LEU:HA	1.92	0.42
24:AV:407:THR:O	24:AV:411:GLU:HG3	2.20	0.42
26:AX:363:ASN:O	26:AX:366:GLN:NE2	2.40	0.42
36:Aj:91:GLU:HB2	36:Aj:153:PHE:HE1	1.85	0.42
4:AB:108:LEU:HD21	5:AC:120:CYS:HB3	2.02	0.42
5:AC:134:PHE:CE1	33:Ae:113:GLY:HA2	2.55	0.42
9:AG:15:A:H2	9:AG:18:A:H1'	1.84	0.42
20:AR:258:GLU:CD	20:AR:259:PRO:HD2	2.44	0.42
25:AW:150:LEU:HB2	25:AW:163:ILE:HG21	2.02	0.42
26:AX:240:GLY:HA3	26:AX:291:ASN:HD22	1.84	0.42
27:AY:272:ILE:HG22	27:AY:276:LYS:HE3	2.01	0.42
33:Ae:377:TYR:OH	33:Ae:414:ASP:OD2	2.38	0.42
34:Ag:284:VAL:HG11	34:Ag:349:MET:HG2	2.02	0.42
14:AL:233:VAL:HG12	14:AL:237:LYS:HE3	2.02	0.42
24:AV:208:MET:HA	24:AV:213:PHE:HE2	1.84	0.42
29:Aa:162:LYS:HE2	29:Aa:166:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Ad:108:ALA:O	32:Ad:114:ARG:NH1	2.52	0.42
3:AA:308:A:N1	22:AT:68:LYS:NZ	2.59	0.42
3:AA:369:U:O2	18:AP:92:ILE:N	2.53	0.42
3:AA:696:U:OP1	28:AZ:100:LYS:HB2	2.20	0.42
17:AO:91:ARG:HE	17:AO:94:CYS:HB3	1.85	0.42
20:AR:258:GLU:O	20:AR:261:SER:OG	2.37	0.42
24:AV:378:LEU:O	24:AV:382:LEU:HG	2.20	0.42
26:AX:111:LEU:HA	26:AX:114:THR:HG23	2.02	0.42
26:AX:275:ARG:HH21	26:AX:281:ILE:HG22	1.84	0.42
35:Ai:87:ILE:HD11	35:Ai:150:ARG:HH21	1.84	0.42
3:AA:12:G:H5'	32:Ad:229:PHE:HB2	2.02	0.41
13:AK:37:ASP:HB3	28:AZ:52:TYR:HE2	1.85	0.41
20:AR:359:GLN:HG3	20:AR:360:LYS:HD3	2.01	0.41
27:AY:319:GLU:HB3	27:AY:321:HIS:NE2	2.35	0.41
33:Ae:156:ALA:HB3	33:Ae:172:MET:HE1	2.02	0.41
3:AA:393:A:H5'	14:AL:133:LEU:HD21	2.02	0.41
16:AN:69:LEU:HD12	16:AN:70:PRO:HD2	2.02	0.41
20:AR:101:LEU:HB3	20:AR:150:MET:HE1	2.01	0.41
27:AY:321:HIS:ND1	27:AY:322:GLU:HG3	2.35	0.41
34:Ag:200:TRP:NE1	34:Ag:227:GLU:OE2	2.54	0.41
3:AA:251:C:OP2	12:AJ:116:GLN:NE2	2.54	0.41
3:AA:411:U:H2'	3:AA:412:A:H8	1.85	0.41
3:AA:652:U:H2'	3:AA:653:A:C8	2.55	0.41
3:AA:944:MA6:O5'	3:AA:944:MA6:H8	2.20	0.41
14:AL:86:VAL:HG13	23:AU:161:GLN:HE22	1.85	0.41
18:AP:112:ILE:O	18:AP:116:GLN:HG2	2.21	0.41
33:Ae:403:VAL:HG13	33:Ae:408:PHE:HE1	1.85	0.41
3:AA:232:G:H5"	32:Ad:196:ASN:HD22	1.84	0.41
4:AB:320:ARG:NH1	4:AB:320:ARG:HA	2.35	0.41
17:AO:53:ASP:OD1	17:AO:53:ASP:N	2.53	0.41
20:AR:125:TYR:OH	32:Ad:372:GLU:OE2	2.34	0.41
25:AW:160:ASP:HB2	30:Ab:96:CYS:SG	2.60	0.41
35:Ai:156:LEU:HA	35:Ai:160:ARG:HD2	2.03	0.41
4:AB:254:ILE:O	4:AB:258:SER:OG	2.39	0.41
8:AF:157:GLY:HA2	8:AF:226:MET:HE2	2.02	0.41
20:AR:184:SER:H	20:AR:192:ARG:NH1	2.19	0.41
3:AA:166:G:H2'	3:AA:167:G:C8	2.56	0.41
4:AB:171:ARG:O	4:AB:220:ASN:ND2	2.53	0.41
15:AM:29:ARG:NH1	15:AM:57:LEU:HB2	2.35	0.41
17:AO:215:ARG:HD3	36:Aj:88:GLN:HA	2.02	0.41
24:AV:77:SER:O	24:AV:81:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AV:196:ASN:HB3	24:AV:199:ASP:OD1	2.21	0.41
36:Aj:193:LEU:HD23	36:Aj:193:LEU:HA	1.89	0.41
12:AJ:93:CYS:SG	12:AJ:94:PHE:N	2.94	0.41
14:AL:82:GLY:HA3	14:AL:85:LYS:HE3	2.01	0.41
22:AT:2:PRO:HB2	22:AT:8:PRO:HB3	2.03	0.41
22:AT:76:LEU:HD22	22:AT:102:ILE:HD11	2.02	0.41
24:AV:303:MET:HE1	24:AV:375:PHE:HD1	1.84	0.41
25:AW:115:ILE:HD13	25:AW:141:VAL:HG21	2.01	0.41
29:Aa:280:MET:HE2	29:Aa:280:MET:HB2	1.78	0.41
3:AA:29:A:H2'	3:AA:30:A:C8	2.56	0.41
3:AA:238:C:H2'	3:AA:239:U:C6	2.55	0.41
3:AA:740:U:H2'	3:AA:741:C:C6	2.55	0.41
3:AA:854:C:H2'	3:AA:855:C:C6	2.56	0.41
8:AF:79:ALA:HA	34:Ag:313:GLN:HE22	1.86	0.41
24:AV:266:TYR:CZ	24:AV:320:LEU:HD22	2.56	0.41
26:AX:271:THR:HG22	26:AX:273:LEU:H	1.85	0.41
29:Aa:349:PHE:HB3	29:Aa:353:ARG:HH12	1.85	0.41
34:Ag:316:PHE:HD2	34:Ag:346:ARG:HH11	1.69	0.41
3:AA:35:U:H2'	3:AA:36:A:C8	2.55	0.41
3:AA:128:C:H2'	3:AA:129:G:O4'	2.21	0.41
4:AB:120:ALA:HB1	4:AB:124:HIS:CE1	2.55	0.41
4:AB:215:PRO:HB2	4:AB:216:LEU:HD12	2.03	0.41
5:AC:134:PHE:HE1	33:Ae:113:GLY:HA2	1.86	0.41
7:AE:28:ALA:O	7:AE:32:ARG:HG2	2.21	0.41
17:AO:64:TYR:OH	17:AO:125:GLN:NE2	2.43	0.41
26:AX:346:ASN:OD1	26:AX:386:ASN:ND2	2.50	0.41
29:Aa:369:GLN:HB3	29:Aa:373:LYS:HE2	2.02	0.41
30:Ab:94:ALA:N	30:Ab:111:GLY:O	2.54	0.41
33:Ae:200:ASN:ND2	33:Ae:246:ASN:H	2.19	0.41
34:Ag:161:LEU:HD11	34:Ag:245:PHE:HZ	1.85	0.41
34:Ag:317:PRO:HG2	34:Ag:349:MET:HE3	2.03	0.41
3:AA:744:C:H2'	3:AA:745:C:O4'	2.21	0.41
5:AC:113:ARG:O	5:AC:116:GLN:HG2	2.20	0.41
8:AF:129:ALA:HB1	8:AF:133:GLU:HB2	2.01	0.41
12:AJ:55:ARG:HD3	12:AJ:58:LEU:HD21	2.02	0.41
24:AV:157:LEU:HD13	24:AV:190:TYR:CE2	2.56	0.41
26:AX:83:PRO:HA	26:AX:84:PRO:HD3	1.94	0.41
8:AF:116:GLU:O	8:AF:120:ARG:HG2	2.21	0.40
9:AG:61:C:H2'	9:AG:62:C:C6	2.55	0.40
2:Bd:122:PHE:HA	10:AH:183:HIS:NE2	2.36	0.40
13:AK:29:TYR:CZ	13:AK:38:VAL:HG21	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AL:113:MET:HB2	14:AL:117:LEU:HD12	2.03	0.40
16:AN:83:GLU:OE2	22:AT:85:GLN:NE2	2.53	0.40
19:AQ:72:ILE:HD12	31:Ac:104:LEU:HD22	2.03	0.40
19:AQ:84:TRP:O	30:Ab:148:ARG:NH2	2.54	0.40
30:Ab:182:LEU:HD12	30:Ab:186:VAL:HG11	2.03	0.40
33:Ae:568:ARG:HG2	33:Ae:572:PRO:HB3	2.02	0.40
4:AB:136:PRO:HG2	4:AB:139:LEU:HD12	2.03	0.40
10:AH:76:LEU:HG	10:AH:174:LYS:HG2	2.03	0.40
24:AV:112:ILE:HD11	24:AV:132:LEU:HD23	2.02	0.40
24:AV:401:ALA:O	24:AV:405:LEU:HB3	2.22	0.40
32:Ad:243:VAL:HG11	32:Ad:268:PHE:CE1	2.57	0.40
33:Ae:304:THR:HG21	33:Ae:322:LEU:HD11	2.03	0.40
3:AA:36:A:H2'	3:AA:37:A:C8	2.56	0.40
5:AC:143:LEU:HD13	5:AC:143:LEU:HA	1.90	0.40
16:AN:18:ILE:HD11	16:AN:29:ARG:NE	2.36	0.40
18:AP:124:THR:HG23	18:AP:125:TYR:HD1	1.85	0.40
24:AV:238:TRP:CZ2	24:AV:282:ALA:HB3	2.51	0.40
30:Ab:92:HIS:HD2	30:Ab:224:THR:HG22	1.87	0.40
3:AA:177:U:H2'	3:AA:178:G:H8	1.86	0.40
3:AA:633:C:H2'	3:AA:634:C:C6	2.57	0.40
4:AB:80:PRO:HG2	5:AC:156:GLN:NE2	2.36	0.40
9:AG:5:A:H2'	9:AG:6:G:C8	2.57	0.40
25:AW:134:LYS:HB3	25:AW:134:LYS:HE2	1.87	0.40
29:Aa:70:TRP:CE2	29:Aa:123:ILE:HG21	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	BX	13/303 (4%)	12 (92%)	1 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Bd	21/126 (17%)	20 (95%)	1 (5%)	0	100	100
4	AB	273/366 (75%)	268 (98%)	5 (2%)	0	100	100
5	AC	130/167 (78%)	125 (96%)	5 (4%)	0	100	100
6	AD	70/199 (35%)	70 (100%)	0	0	100	100
7	AE	120/376 (32%)	118 (98%)	2 (2%)	0	100	100
8	AF	206/242 (85%)	201 (98%)	5 (2%)	0	100	100
10	AH	138/200 (69%)	129 (94%)	8 (6%)	1 (1%)	18	51
12	AJ	107/139 (77%)	105 (98%)	2 (2%)	0	100	100
13	AK	99/128 (77%)	99 (100%)	0	0	100	100
14	AL	173/259 (67%)	169 (98%)	4 (2%)	0	100	100
15	AM	115/135 (85%)	112 (97%)	3 (3%)	0	100	100
16	AN	110/130 (85%)	106 (96%)	4 (4%)	0	100	100
17	AO	188/258 (73%)	185 (98%)	3 (2%)	0	100	100
18	AP	95/143 (66%)	95 (100%)	0	0	100	100
19	AQ	84/87 (97%)	84 (100%)	0	0	100	100
20	AR	290/382 (76%)	283 (98%)	7 (2%)	0	100	100
21	AS	133/190 (70%)	130 (98%)	3 (2%)	0	100	100
22	AT	167/173 (96%)	165 (99%)	2 (1%)	0	100	100
23	AU	175/205 (85%)	174 (99%)	1 (1%)	0	100	100
24	AV	386/395 (98%)	369 (96%)	17 (4%)	0	100	100
25	AW	97/188 (52%)	96 (99%)	1 (1%)	0	100	100
26	AX	351/410 (86%)	341 (97%)	10 (3%)	0	100	100
27	AY	147/381 (39%)	146 (99%)	1 (1%)	0	100	100
28	AZ	97/148 (66%)	95 (98%)	2 (2%)	0	100	100
29	Aa	380/474 (80%)	372 (98%)	8 (2%)	0	100	100
30	Ab	218/289 (75%)	209 (96%)	9 (4%)	0	100	100
31	Ac	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
32	Ad	341/430 (79%)	331 (97%)	10 (3%)	0	100	100
33	Ae	584/692 (84%)	576 (99%)	8 (1%)	0	100	100
34	Ag	326/397 (82%)	323 (99%)	3 (1%)	0	100	100
35	Ai	134/196 (68%)	130 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	Aj	211/505 (42%)	208 (99%)	3 (1%)	0	100	100
All	All	6093/8831 (69%)	5957 (98%)	135 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	AH	126	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BX	8/266 (3%)	8 (100%)	0	100	100
2	Bd	19/114 (17%)	19 (100%)	0	100	100
4	AB	249/322 (77%)	244 (98%)	5 (2%)	48	66
5	AC	115/142 (81%)	113 (98%)	2 (2%)	53	69
6	AD	66/174 (38%)	66 (100%)	0	100	100
7	AE	107/283 (38%)	105 (98%)	2 (2%)	50	67
8	AF	181/205 (88%)	180 (99%)	1 (1%)	78	79
10	AH	130/180 (72%)	129 (99%)	1 (1%)	73	77
12	AJ	92/116 (79%)	91 (99%)	1 (1%)	65	74
13	AK	92/114 (81%)	92 (100%)	0	100	100
14	AL	159/222 (72%)	158 (99%)	1 (1%)	78	79
15	AM	97/113 (86%)	95 (98%)	2 (2%)	47	65
16	AN	97/114 (85%)	97 (100%)	0	100	100
17	AO	170/225 (76%)	169 (99%)	1 (1%)	78	79
18	AP	89/127 (70%)	89 (100%)	0	100	100
19	AQ	77/78 (99%)	77 (100%)	0	100	100
20	AR	258/330 (78%)	255 (99%)	3 (1%)	63	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	AS	113/162 (70%)	111 (98%)	2 (2%)	51	68
22	AT	152/155 (98%)	150 (99%)	2 (1%)	61	72
23	AU	149/168 (89%)	148 (99%)	1 (1%)	76	78
24	AV	325/347 (94%)	324 (100%)	1 (0%)	86	83
25	AW	86/160 (54%)	83 (96%)	3 (4%)	32	57
26	AX	312/361 (86%)	311 (100%)	1 (0%)	86	83
27	AY	134/342 (39%)	134 (100%)	0	100	100
28	AZ	86/125 (69%)	86 (100%)	0	100	100
29	Aa	339/424 (80%)	335 (99%)	4 (1%)	63	73
30	Ab	187/233 (80%)	187 (100%)	0	100	100
31	Ac	100/102 (98%)	98 (98%)	2 (2%)	48	66
32	Ad	282/351 (80%)	274 (97%)	8 (3%)	38	60
33	Ae	521/604 (86%)	521 (100%)	0	100	100
34	Ag	273/333 (82%)	272 (100%)	1 (0%)	84	81
35	Ai	102/150 (68%)	101 (99%)	1 (1%)	68	75
36	Aj	188/404 (46%)	185 (98%)	3 (2%)	55	69
All	All	5355/7546 (71%)	5307 (99%)	48 (1%)	68	76

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	AB	87	VAL
4	AB	93	VAL
4	AB	117	THR
4	AB	159	VAL
4	AB	211	THR
5	AC	89	ASP
5	AC	167	ILE
7	AE	88	VAL
7	AE	111	VAL
8	AF	98	MET
10	AH	63	ILE
12	AJ	126	VAL
14	AL	75	LEU
15	AM	35	VAL
15	AM	93	LEU

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Mol	Chain	Res	Type
17	AO	179	THR
20	AR	230	VAL
20	AR	316	VAL
20	AR	337	GLN
21	AS	51	LEU
21	AS	83	LYS
22	AT	90	VAL
22	AT	120	LYS
23	AU	42	VAL
24	AV	388	VAL
25	AW	109	VAL
25	AW	148	LEU
25	AW	173	LEU
26	AX	108	LEU
29	Aa	147	GLN
29	Aa	207	ILE
29	Aa	275	ILE
29	Aa	284	VAL
31	Ac	95	GLU
31	Ac	117	VAL
32	Ad	91	THR
32	Ad	118	THR
32	Ad	172	MET
32	Ad	296	LEU
32	Ad	303	ILE
32	Ad	340	VAL
32	Ad	370	VAL
32	Ad	421	VAL
34	Ag	286	VAL
35	Ai	151	VAL
36	Aj	100	VAL
36	Aj	173	MET
36	Aj	211	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
4	AB	115	HIS
5	AC	57	HIS
5	AC	81	HIS
5	AC	156	GLN
6	AD	141	HIS

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Mol	Chain	Res	Type
6	AD	198	ASN
7	AE	38	ASN
7	AE	92	ASN
8	AF	127	HIS
8	AF	224	HIS
8	AF	227	HIS
12	AJ	57	GLN
13	AK	68	GLN
13	AK	124	GLN
14	AL	78	GLN
14	AL	139	ASN
14	AL	143	HIS
14	AL	153	HIS
14	AL	213	GLN
15	AM	16	HIS
16	AN	76	HIS
16	AN	90	GLN
18	AP	83	GLN
20	AR	189	HIS
20	AR	216	GLN
22	AT	63	GLN
22	AT	95	ASN
22	AT	146	GLN
23	AU	135	GLN
23	AU	161	GLN
24	AV	118	ASN
24	AV	137	HIS
24	AV	162	GLN
24	AV	185	ASN
24	AV	196	ASN
24	AV	228	HIS
24	AV	301	GLN
24	AV	399	GLN
25	AW	104	GLN
25	AW	174	GLN
26	AX	89	GLN
26	AX	109	HIS
26	AX	115	ASN
26	AX	169	GLN
26	AX	175	GLN
26	AX	179	GLN
26	AX	301	GLN

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Mol	Chain	Res	Type
28	AZ	75	HIS
29	Aa	124	GLN
29	Aa	183	ASN
29	Aa	202	GLN
29	Aa	258	HIS
29	Aa	341	GLN
29	Aa	381	GLN
29	Aa	392	GLN
30	Ab	133	HIS
30	Ab	152	HIS
30	Ab	166	HIS
30	Ab	177	ASN
32	Ad	130	GLN
32	Ad	155	GLN
32	Ad	196	ASN
32	Ad	341	ASN
32	Ad	360	GLN
33	Ae	380	GLN
33	Ae	473	GLN
33	Ae	494	GLN
33	Ae	543	HIS
34	Ag	127	HIS
34	Ag	163	HIS
34	Ag	256	GLN
35	Ai	73	ASN
35	Ai	98	GLN
35	Ai	100	GLN
35	Ai	106	HIS
35	Ai	107	GLN
36	Aj	32	GLN
36	Aj	111	HIS
36	Aj	137	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	AI	8/9 (88%)	2 (25%)	0
3	AA	959/962 (99%)	144 (15%)	0
9	AG	70/72 (97%)	10 (14%)	0
All	All	1037/1043 (99%)	156 (15%)	0

All (156) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	AA	5	A
3	AA	18	G
3	AA	34	U
3	AA	42	A
3	AA	43	U
3	AA	58	U
3	AA	65	C
3	AA	66	C
3	AA	75	A
3	AA	77	G
3	AA	92	A
3	AA	93	A
3	AA	98	A
3	AA	108	G
3	AA	115	A
3	AA	120	A
3	AA	125	U
3	AA	126	A
3	AA	127	A
3	AA	139	A
3	AA	147	G
3	AA	152	A
3	AA	161	C
3	AA	170	A
3	AA	186	U
3	AA	191	C
3	AA	192	C
3	AA	203	G
3	AA	208	A
3	AA	216	A
3	AA	217	U
3	AA	223	U
3	AA	244	C
3	AA	250	A
3	AA	257	U
3	AA	258	C
3	AA	261	A
3	AA	273	A
3	AA	288	G
3	AA	293	A
3	AA	296	G
3	AA	297	A
3	AA	309	A

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Mol	Chain	Res	Type
3	AA	310	A
3	AA	314	A
3	AA	317	A
3	AA	319	A
3	AA	320	A
3	AA	328	A
3	AA	354	C
3	AA	355	U
3	AA	367	A
3	AA	368	A
3	AA	372	C
3	AA	381	G
3	AA	395	C
3	AA	396	C
3	AA	399	A
3	AA	417	C
3	AA	421	A
3	AA	455	A
3	AA	456	A
3	AA	457	C
3	AA	461	A
3	AA	465	G
3	AA	471	U
3	AA	472	A
3	AA	477	A
3	AA	495	U
3	AA	502	A
3	AA	530	G
3	AA	538	C
3	AA	539	A
3	AA	540	U
3	AA	541	C
3	AA	566	U
3	AA	571	A
3	AA	574	C
3	AA	576	C
3	AA	596	U
3	AA	597	U
3	AA	604	U
3	AA	606	A
3	AA	613	A
3	AA	625	U

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Mol	Chain	Res	Type
3	AA	626	C
3	AA	639	A
3	AA	640	A
3	AA	641	A
3	AA	644	A
3	AA	645	A
3	AA	646	C
3	AA	647	A
3	AA	665	A
3	AA	681	A
3	AA	682	G
3	AA	685	C
3	AA	698	A
3	AA	699	U
3	AA	708	A
3	AA	711	A
3	AA	720	A
3	AA	722	A
3	AA	724	U
3	AA	731	A
3	AA	733	A
3	AA	734	A
3	AA	739	A
3	AA	740	U
3	AA	743	A
3	AA	745	C
3	AA	748	A
3	AA	751	A
3	AA	752	A
3	AA	753	A
3	AA	766	C
3	AA	780	A
3	AA	790	A
3	AA	822	A
3	AA	823	G
3	AA	825	C
3	AA	826	C
3	AA	838	A
3	AA	869	A
3	AA	877	A
3	AA	882	A
3	AA	884	C

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Mol	Chain	Res	Type
3	AA	885	U
3	AA	893	A
3	AA	896	A
3	AA	899	C
3	AA	919	A
3	AA	920	G
3	AA	928	A
3	AA	929	A
3	AA	930	G
3	AA	932	U
3	AA	933	A
3	AA	943	G
3	AA	945	MA6
3	AA	955	G
3	AA	956	G
3	AA	959	U
3	AA	960	A
9	AG	7	G
9	AG	8	U
9	AG	9	C
9	AG	11	G
9	AG	17	U
9	AG	45	G
9	AG	52	A
9	AG	53	U
9	AG	55	C
9	AG	71	A
11	AI	2	G
11	AI	4	C

There are no RNA pucker outliers to report.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	MA6	AA	945	3	23,26,27	2.25	5 (21%)	34,38,41	3.79	14 (41%)
9	FME	AG	72	9	8,9,10	0.55	0	7,9,11	0.98	1 (14%)
3	MA6	AA	944	3	23,26,27	2.26	5 (21%)	34,38,41	3.68	13 (38%)
3	B8T	AA	846	3	19,22,23	0.43	0	26,31,34	0.37	0
31	AYA	Ac	2	31	6,7,8	0.78	0	5,8,10	0.27	0
19	AYA	AQ	2	19	6,7,8	0.77	0	5,8,10	0.29	0
3	5MC	AA	848	3	18,22,23	0.93	2 (11%)	26,32,35	1.05	2 (7%)
3	5MU	AA	428	3	19,22,23	1.38	5 (26%)	28,32,35	1.98	6 (21%)
35	5F0	Ai	186	35	8,8,9	1.46	2 (25%)	7,9,11	1.69	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MA6	AA	945	3	-	4/11/29/30	0/3/3/3
9	FME	AG	72	9	-	1/7/9/11	-
3	MA6	AA	944	3	-	0/11/29/30	0/3/3/3
3	B8T	AA	846	3	-	0/7/27/28	0/2/2/2
31	AYA	Ac	2	31	-	2/4/6/8	-
19	AYA	AQ	2	19	-	2/4/6/8	-
3	5MC	AA	848	3	-	0/7/25/26	0/2/2/2
3	5MU	AA	428	3	-	0/7/25/26	0/2/2/2
35	5F0	Ai	186	35	-	4/9/9/10	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AA	944	MA6	C5-N7	6.78	1.51	1.39
3	AA	945	MA6	C5-N7	6.73	1.51	1.39
3	AA	945	MA6	C8-N9	-5.42	1.27	1.37
3	AA	944	MA6	C8-N9	-5.38	1.27	1.37
3	AA	944	MA6	C4-N9	-3.73	1.29	1.37
3	AA	945	MA6	C4-N9	-3.65	1.29	1.37
3	AA	945	MA6	C5-C4	3.18	1.44	1.39
3	AA	944	MA6	C5-C4	3.15	1.44	1.39
3	AA	944	MA6	C6-N6	3.04	1.45	1.36
3	AA	945	MA6	C6-N6	3.01	1.45	1.36
35	Ai	186	5F0	OD1-C1	2.92	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AA	428	5MU	C6-C5	2.66	1.39	1.34
3	AA	428	5MU	C4-N3	-2.62	1.34	1.38
3	AA	848	5MC	C6-C5	2.62	1.38	1.34
3	AA	428	5MU	C6-N1	-2.30	1.34	1.38
3	AA	428	5MU	C4-C5	2.23	1.48	1.44
3	AA	848	5MC	C6-N1	-2.23	1.34	1.38
35	Ai	186	5F0	OD1-CXT	-2.10	1.40	1.45
3	AA	428	5MU	C2-N3	-2.06	1.34	1.38

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	AA	945	MA6	C4-N9-C8	15.16	122.16	105.73
3	AA	944	MA6	C4-N9-C8	14.56	121.50	105.73
3	AA	945	MA6	N3-C4-N9	7.19	138.93	127.08
3	AA	944	MA6	N3-C4-N9	6.68	138.09	127.08
3	AA	945	MA6	N9-C8-N7	-6.09	105.59	113.91
3	AA	944	MA6	N9-C8-N7	-5.93	105.81	113.91
3	AA	944	MA6	C4-C5-N7	-5.84	103.51	110.62
3	AA	944	MA6	C5-C4-N3	-5.74	119.26	126.75
3	AA	945	MA6	C5-C4-N3	-5.73	119.28	126.75
3	AA	945	MA6	C4-C5-N7	-5.47	103.96	110.62
3	AA	428	5MU	C4-N3-C2	-4.88	121.04	127.35
3	AA	428	5MU	N3-C2-N1	4.57	120.95	114.89
3	AA	428	5MU	C5-C4-N3	4.30	118.98	115.31
3	AA	944	MA6	N1-C2-N3	-4.25	121.96	128.60
3	AA	944	MA6	C2-N1-C6	4.04	121.29	111.75
3	AA	428	5MU	O4-C4-C5	-3.99	120.28	124.90
3	AA	945	MA6	C2-N1-C6	3.97	121.14	111.75
3	AA	945	MA6	N1-C2-N3	-3.97	122.40	128.60
3	AA	428	5MU	C5-C6-N1	-3.69	119.54	123.34
3	AA	945	MA6	C1'-N9-C8	-3.55	119.11	127.14
3	AA	944	MA6	C4-N9-C1'	-3.55	118.13	126.59
3	AA	944	MA6	C2-N3-C4	3.52	120.06	111.75
3	AA	944	MA6	C6-C5-N7	3.49	139.15	133.28
3	AA	945	MA6	C5-C4-N9	-3.43	101.80	105.78
35	Ai	186	5F0	OD1-C1-CA	3.33	120.04	111.52
3	AA	945	MA6	C4-N9-C1'	-3.30	118.73	126.59
3	AA	945	MA6	C2-N3-C4	3.27	119.48	111.75
3	AA	848	5MC	C5-C6-N1	-3.21	120.03	123.34
3	AA	944	MA6	C1'-N9-C8	-3.00	120.36	127.14
3	AA	945	MA6	C6-C5-N7	2.98	138.28	133.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	AA	944	MA6	C5-C4-N9	-2.70	102.65	105.78
9	AG	72	FME	O-C-CA	-2.53	118.14	124.78
3	AA	428	5MU	O2-C2-N1	-2.52	119.43	122.79
3	AA	848	5MC	C5-C4-N3	-2.46	119.02	121.67
3	AA	945	MA6	C5-C6-N6	-2.37	121.17	125.30
3	AA	944	MA6	C5-N7-C8	2.13	106.54	103.51
3	AA	945	MA6	C5-N7-C8	2.10	106.49	103.51

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AA	945	MA6	C5-C6-N6-C9
3	AA	945	MA6	C5-C6-N6-C10
9	AG	72	FME	O1-CN-N-CA
35	Ai	186	5F0	OD1-C1-CA-CB
19	AQ	2	AYA	OT-CT-N-CA
19	AQ	2	AYA	CM-CT-N-CA
31	Ac	2	AYA	OT-CT-N-CA
31	Ac	2	AYA	CM-CT-N-CA
3	AA	945	MA6	N1-C6-N6-C9
35	Ai	186	5F0	CA-C1-OD1-CXT
35	Ai	186	5F0	O1-C1-CA-CB
35	Ai	186	5F0	O1-C1-OD1-CXT
3	AA	945	MA6	C4'-C5'-O5'-P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AA	944	MA6	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 145 ligands modelled in this entry, 139 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
39	SPD	AA	1121	-	9,9,9	0.33	0	8,8,8	0.85	0
44	GDP	AX	503	-	28,30,30	1.13	3 (10%)	44,47,47	1.85	8 (18%)
42	FES	AP	201	7,18	0,4,4	-	-	-		
42	FES	AT	201	15,22	0,4,4	-	-	-		
43	ATP	AX	501	37	29,33,33	0.29	0	44,52,52	0.45	1 (2%)
38	SPM	AA	1120	-	13,13,13	0.35	0	12,12,12	0.94	0

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
44	GDP	AX	503	-	-	3/16/32/32	0/3/3/3
39	SPD	AA	1121	-	-	0/7/7/7	-
42	FES	AP	201	7,18	-	-	0/1/1/1
42	FES	AT	201	15,22	-	-	0/1/1/1
43	ATP	AX	501	37	-	2/22/38/38	0/3/3/3
38	SPM	AA	1120	-	-	2/11/11/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	AX	503	GDP	C5-C4	3.11	1.47	1.38
44	AX	503	GDP	C6-N1	-2.37	1.34	1.38
44	AX	503	GDP	C5-N7	-2.12	1.35	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	AX	503	GDP	C5-C4-N3	-6.16	118.47	128.46
44	AX	503	GDP	C2-N3-C4	4.95	121.13	112.30
44	AX	503	GDP	N9-C4-N3	4.61	135.19	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	AX	503	GDP	PA-O3A-PB	-3.59	120.49	132.83
44	AX	503	GDP	C6-C5-N7	3.15	136.10	130.25
44	AX	503	GDP	C4-C5-N7	-2.63	106.56	110.72
44	AX	503	GDP	C3'-C2'-C1'	2.18	105.58	101.43
44	AX	503	GDP	O6-C6-C5	-2.08	121.08	126.60
43	AX	501	ATP	PB-O3B-PG	2.01	139.73	132.83

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	AX	501	ATP	O4'-C4'-C5'-O5'
44	AX	503	GDP	O4'-C4'-C5'-O5'
43	AX	501	ATP	C3'-C4'-C5'-O5'
44	AX	503	GDP	C3'-C4'-C5'-O5'
38	AA	1120	SPM	N5-C6-C7-C8
38	AA	1120	SPM	C6-C7-C8-C9
44	AX	503	GDP	C5'-O5'-PA-O3A

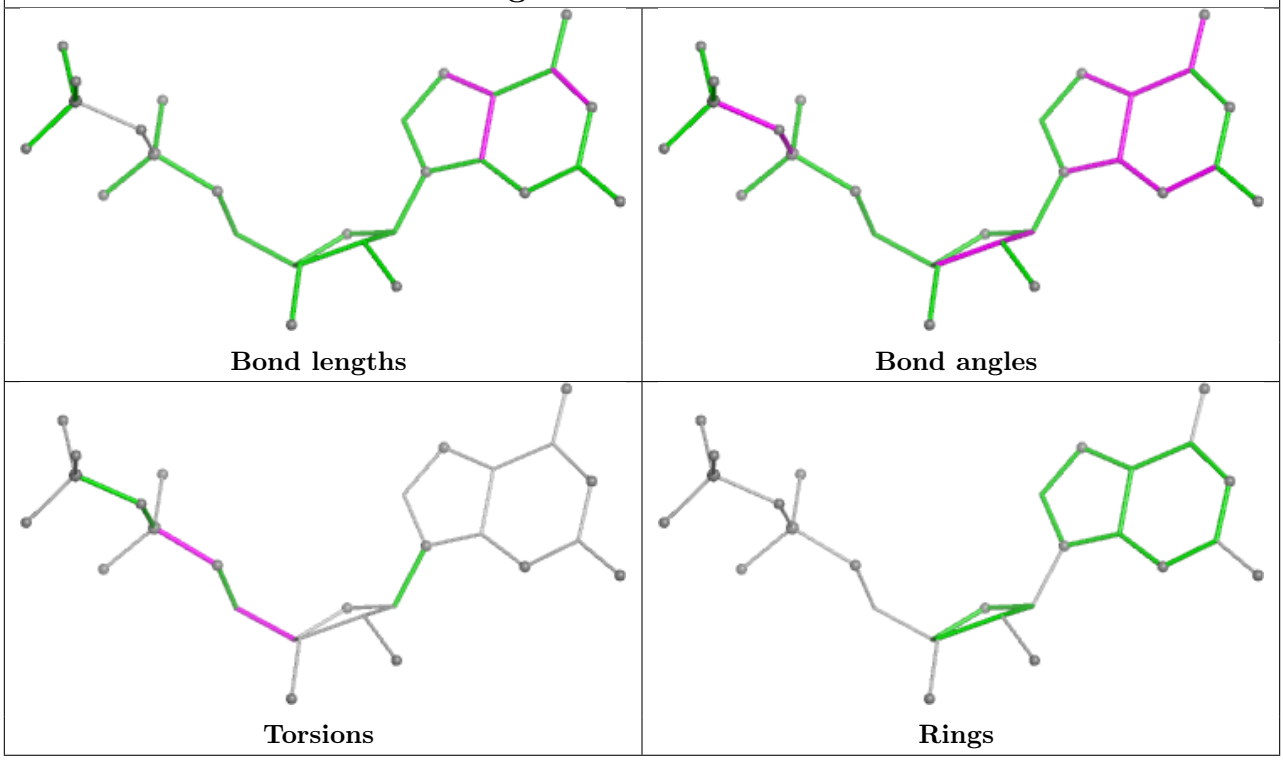
There are no ring outliers.

2 monomers are involved in 5 short contacts:

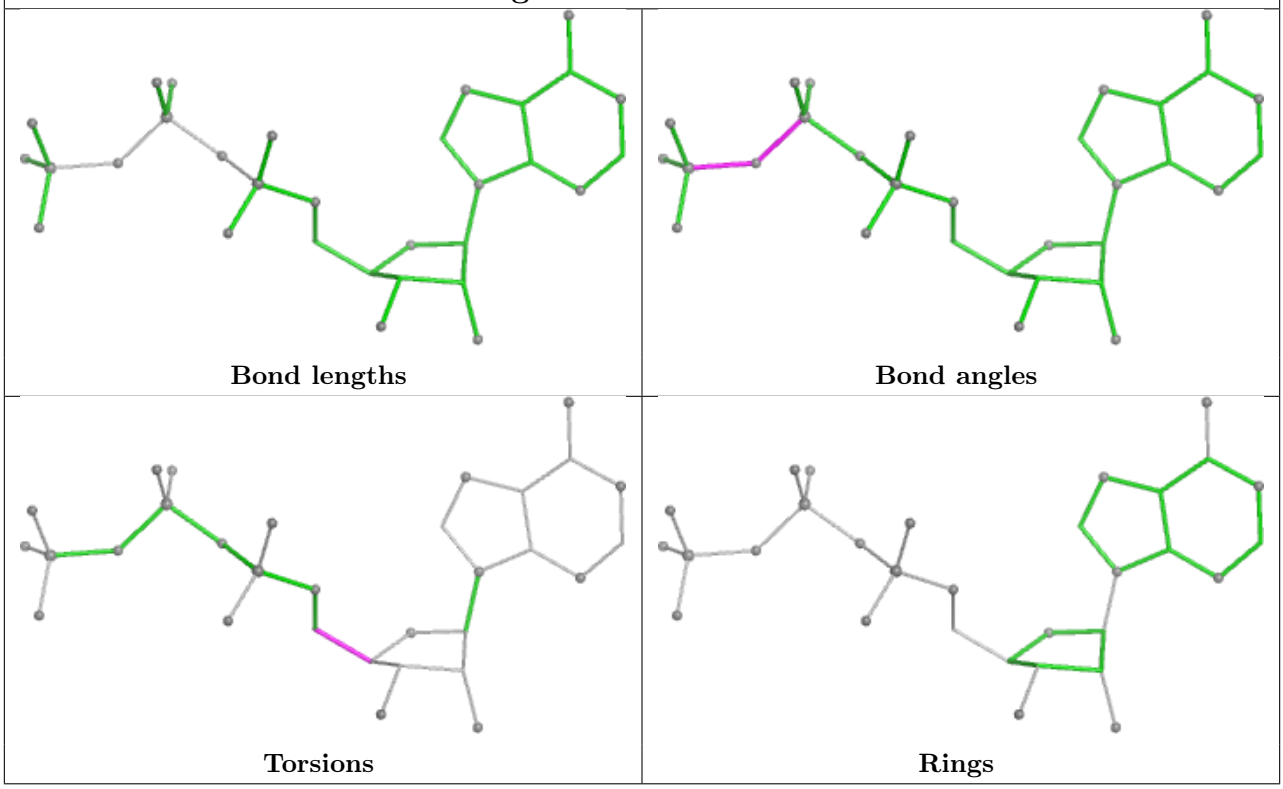
Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	AX	503	GDP	3	0
38	AA	1120	SPM	2	0

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 then 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.

Ligand GDP AX 503



Ligand ATP AX 501



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

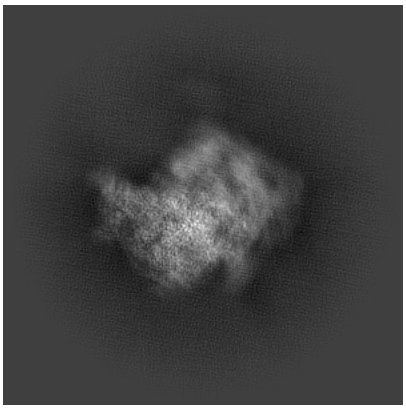
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16895. These allow visual inspection of the internal detail of the map and identification of artifacts.

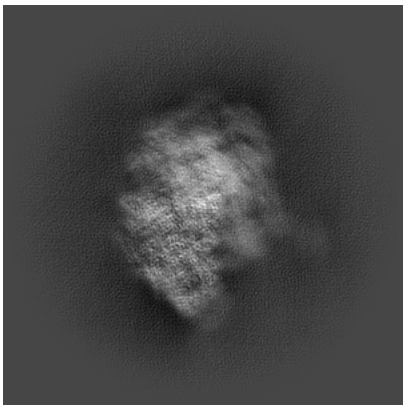
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

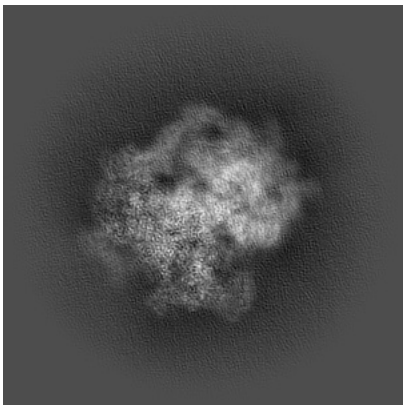
6.1.1 Primary map



X

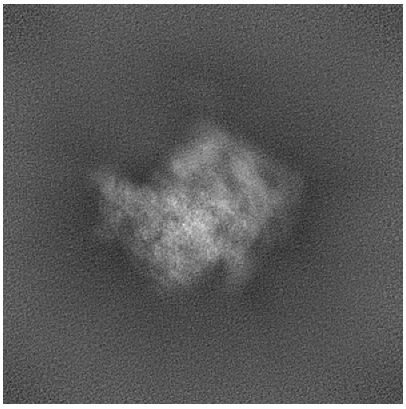


Y

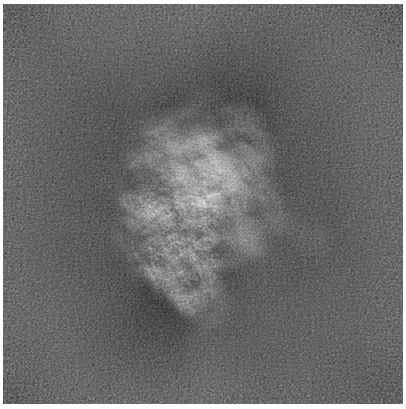


Z

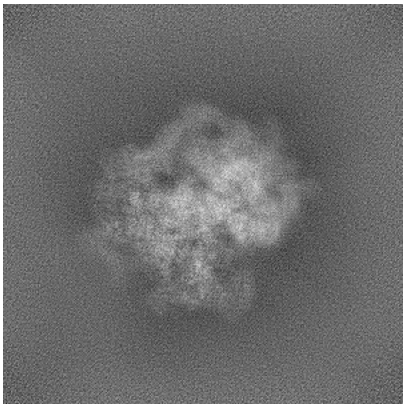
6.1.2 Raw map



X



Y

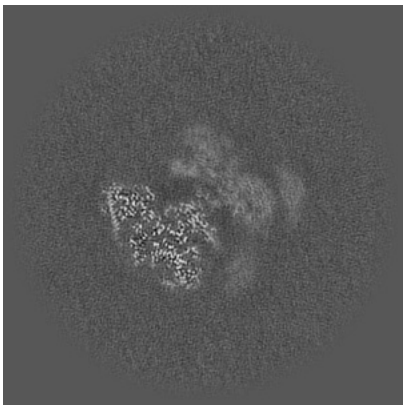


Z

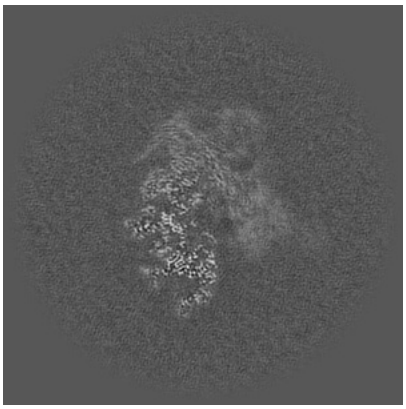
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

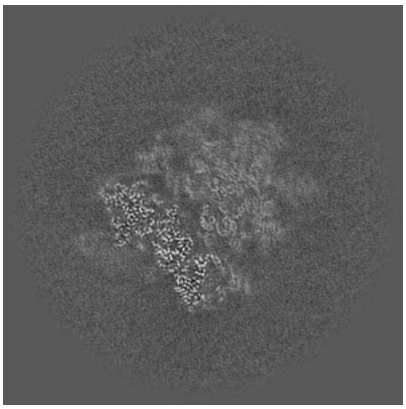
6.2.1 Primary map



X Index: 250

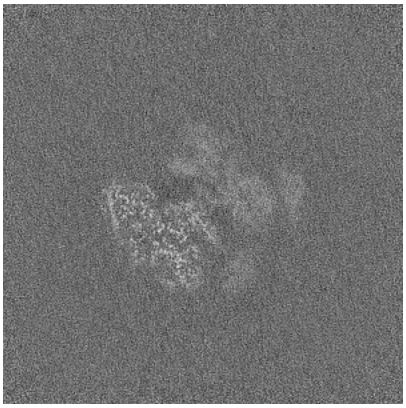


Y Index: 250

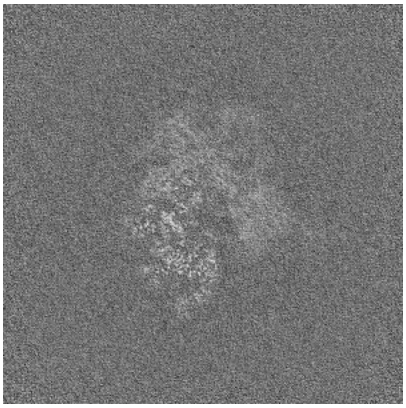


Z Index: 250

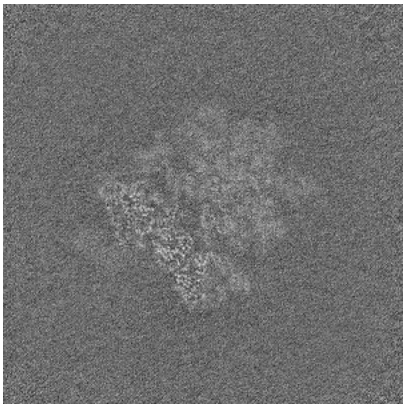
6.2.2 Raw map



X Index: 250



Y Index: 250

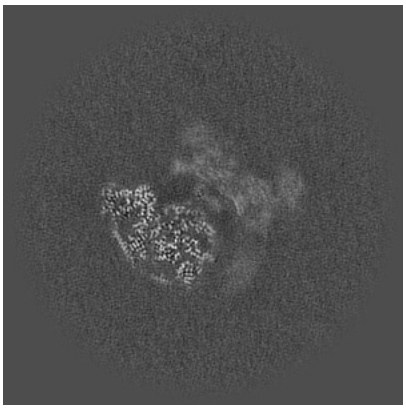


Z Index: 250

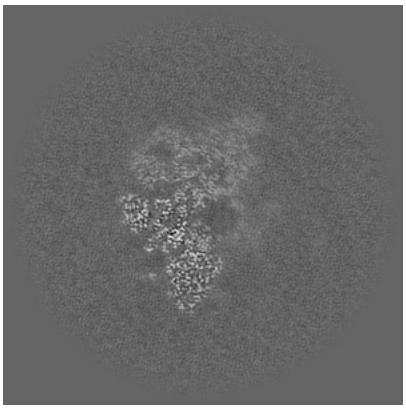
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

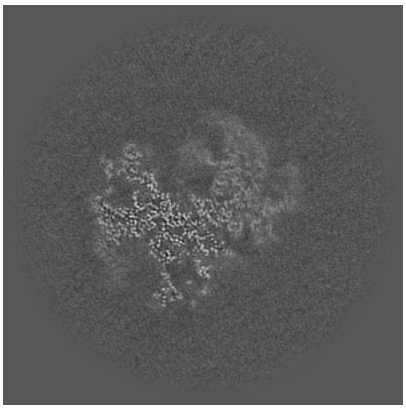
6.3.1 Primary map



X Index: 246

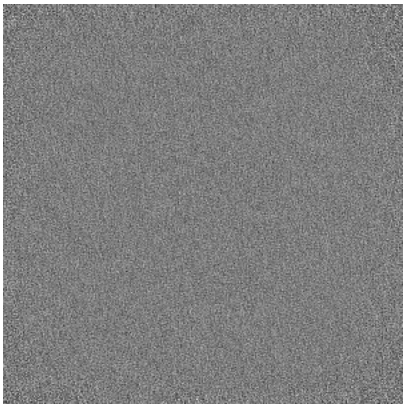


Y Index: 228

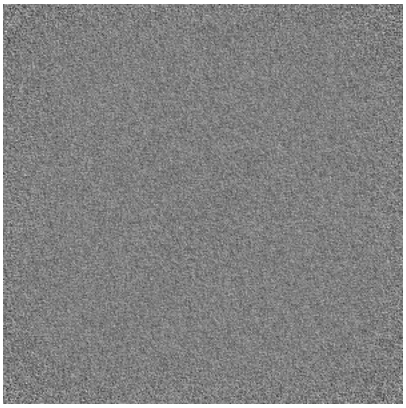


Z Index: 224

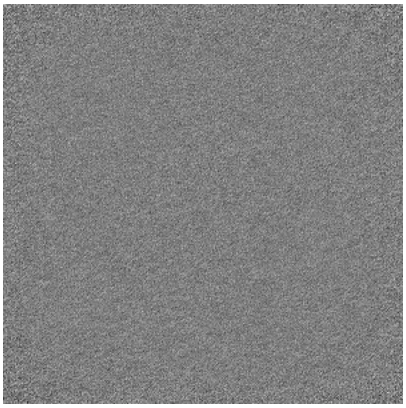
6.3.2 Raw map



X Index: 0



Y Index: 0

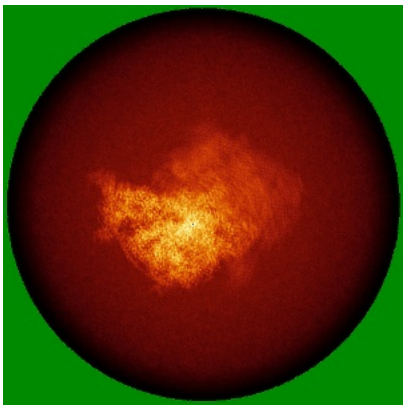


Z Index: 0

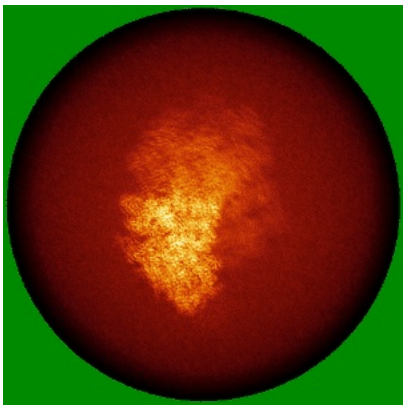
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

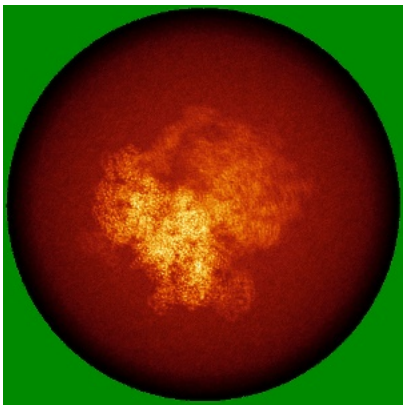
6.4.1 Primary map



X

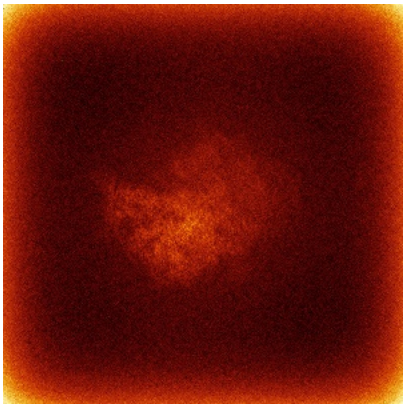


Y

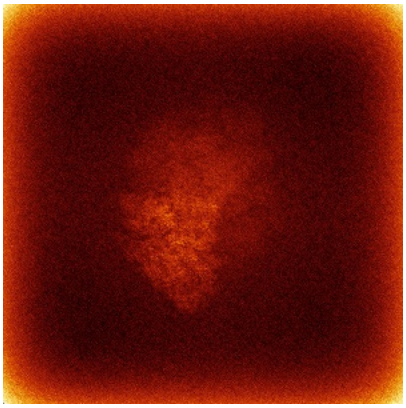


Z

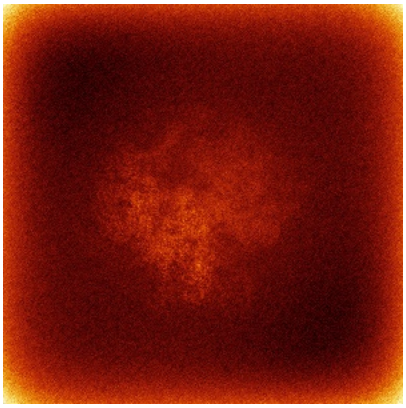
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

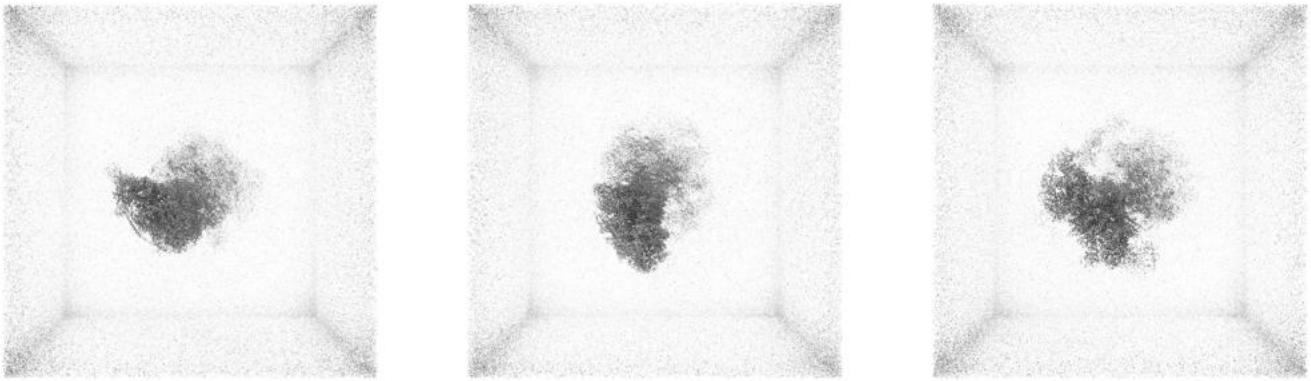
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

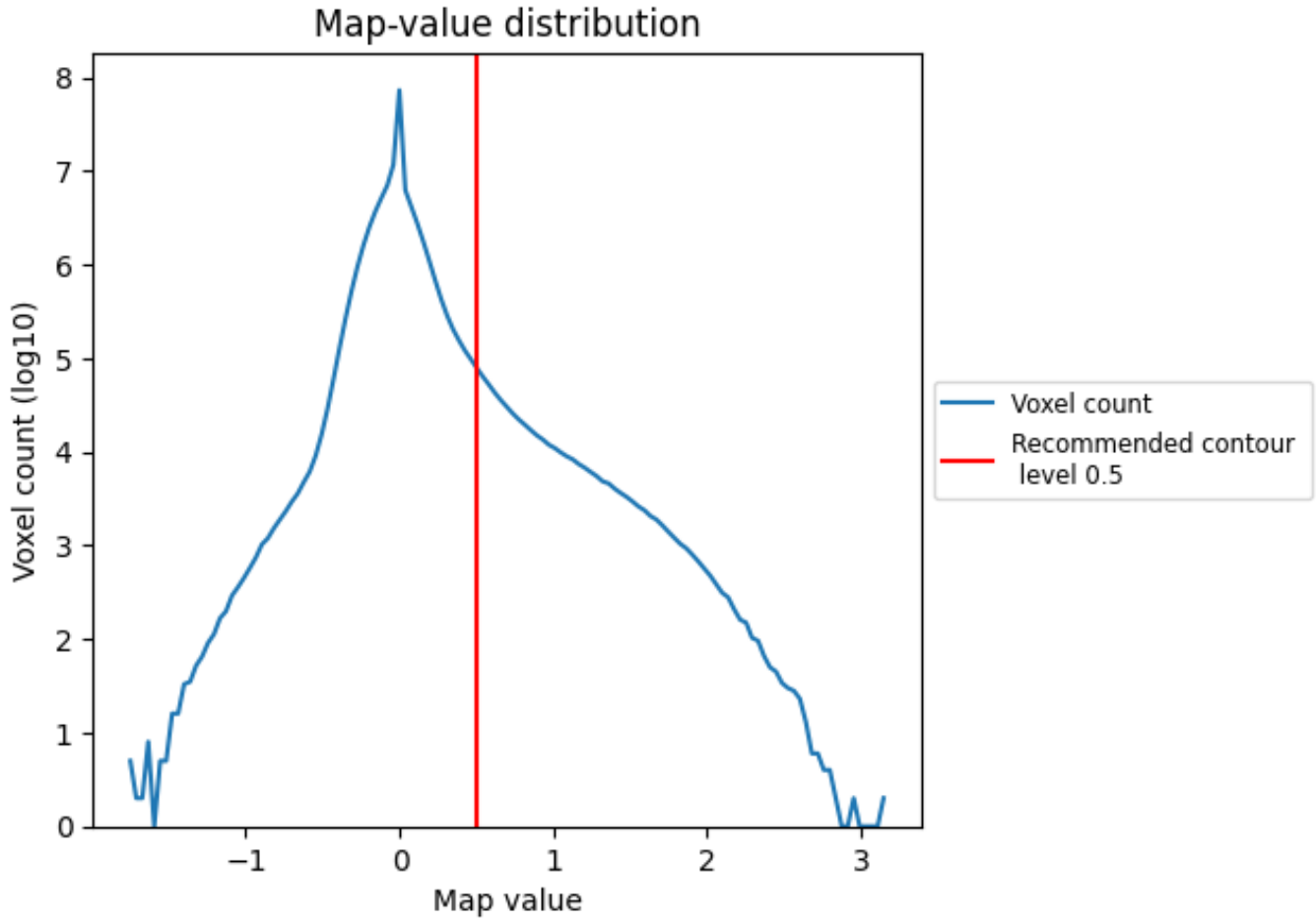
6.6 Mask visualisation (i)

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

7 Map analysis

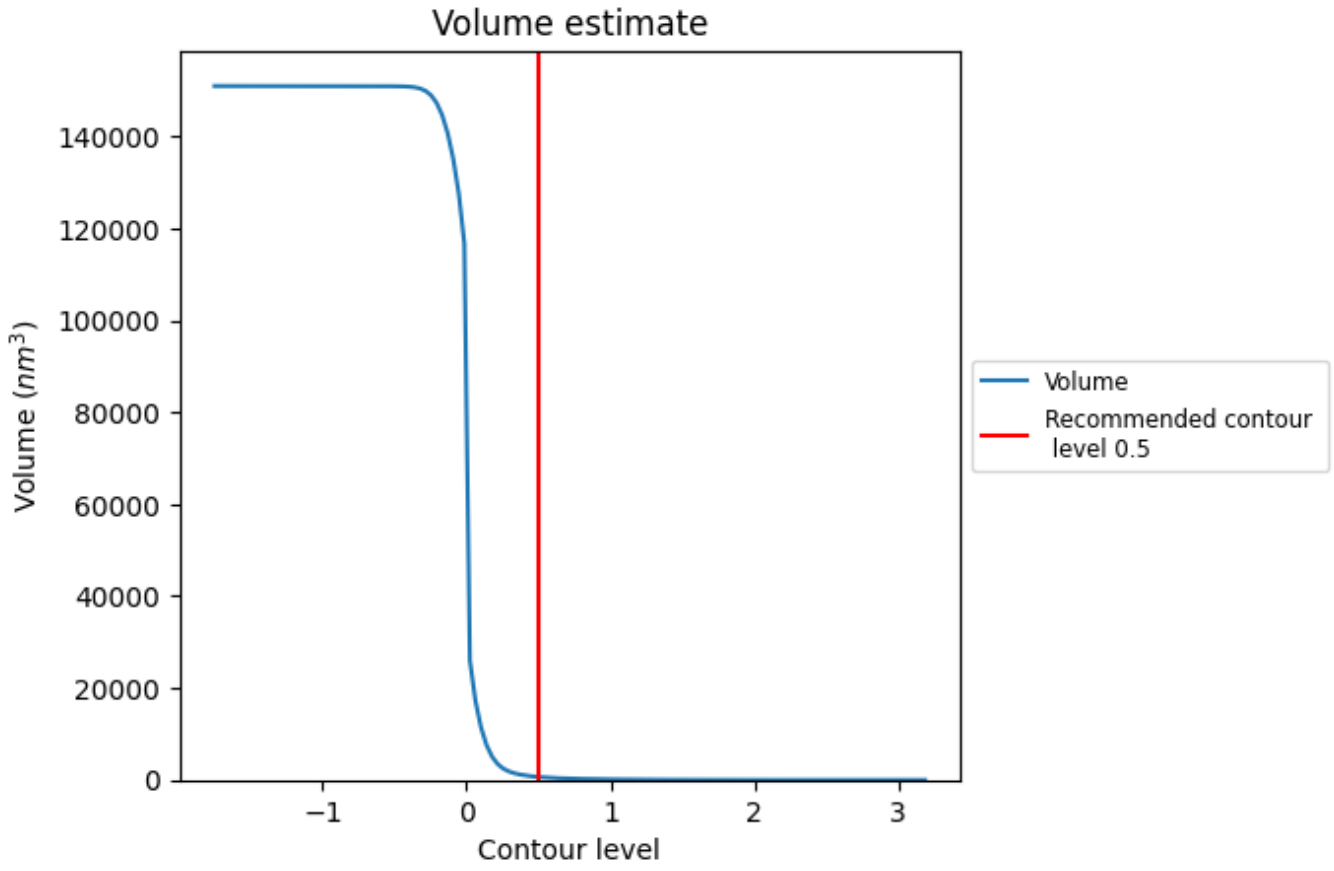
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

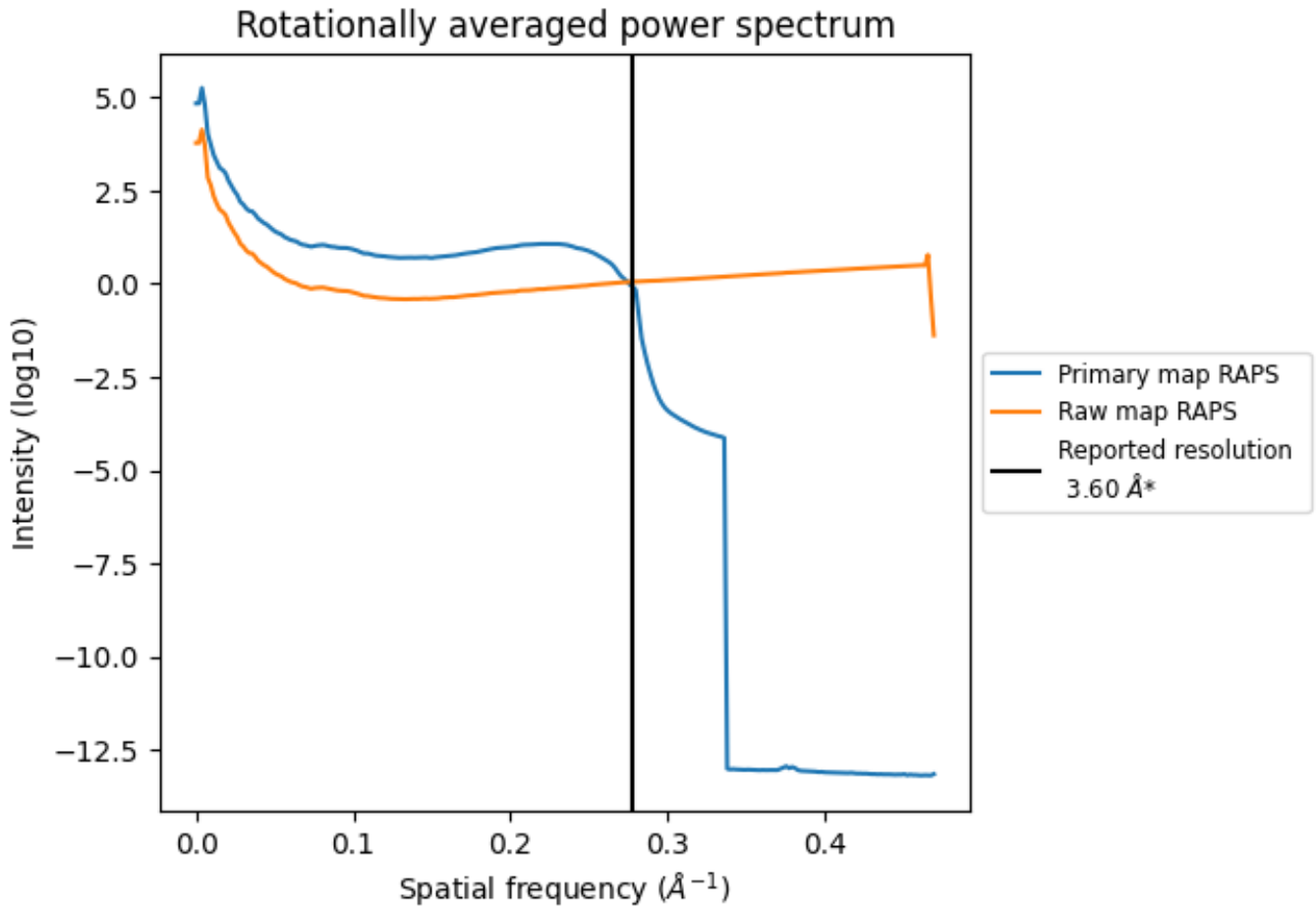
7.2 Volume estimate



The volume at the recommended contour level is 657 nm^3; this corresponds to an approximate mass of 593 kDa.

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

7.3 Rotationally averaged power spectrum (i)

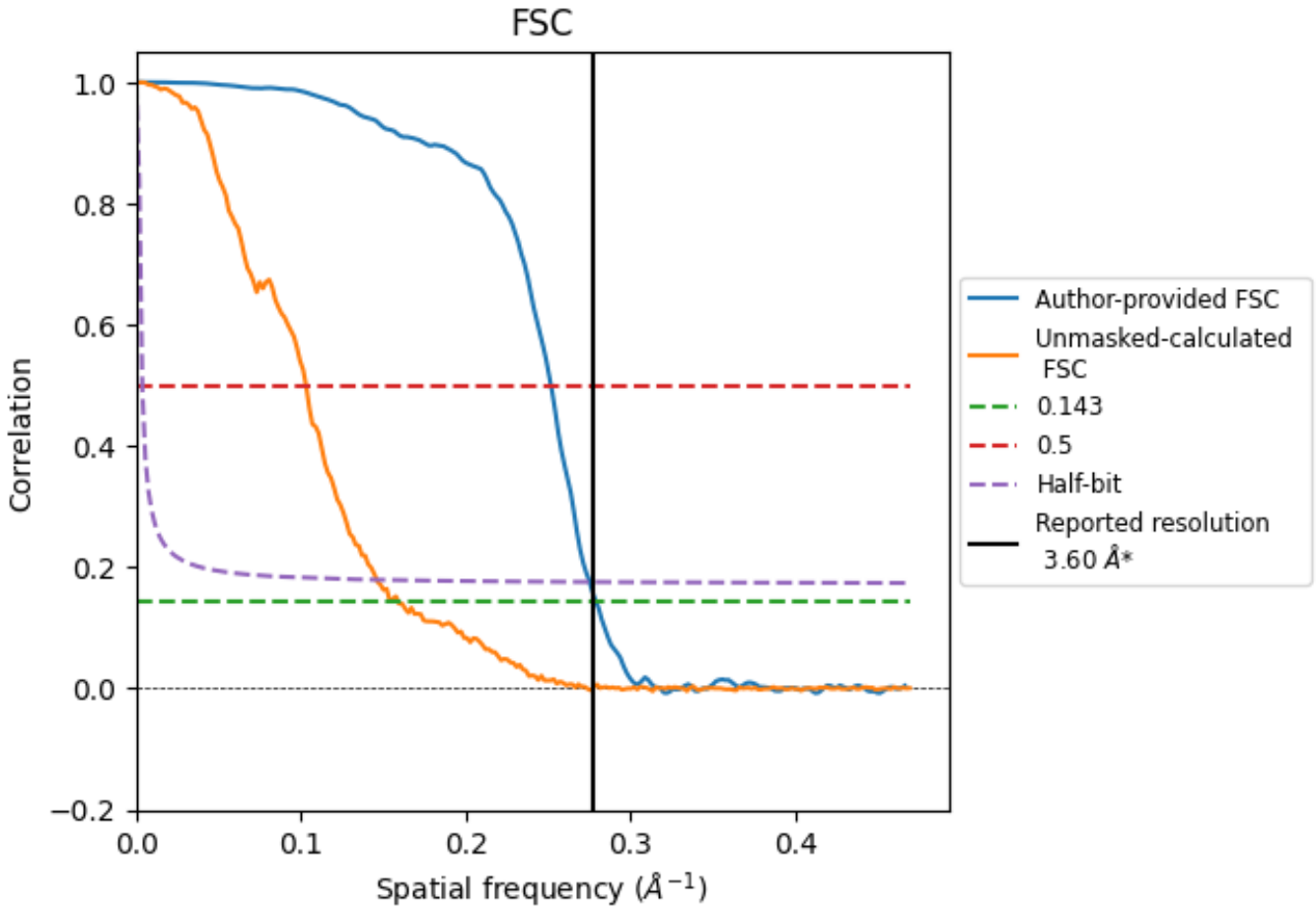


*Reported resolution corresponds to spatial frequency of 0.278 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates (i)

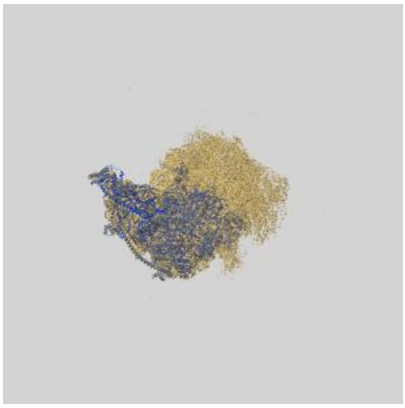
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.58	3.97	3.63
Unmasked-calculated*	6.29	9.70	6.85

*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 6.29 differs from the reported value 3.6 by more than 10 %

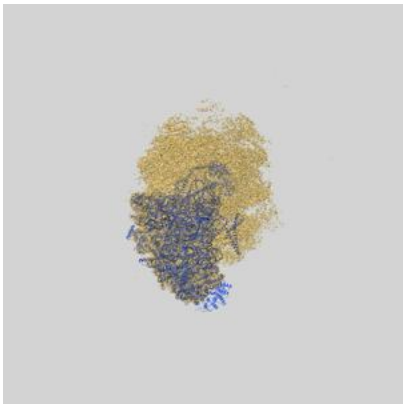
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16895 and PDB model 8OIP. Per-residue inclusion information can be found in section 3 on page 16.

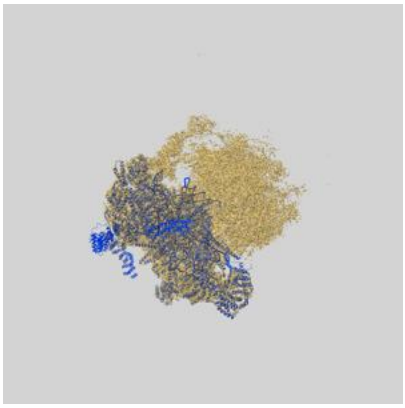
9.1 Map-model overlay



X



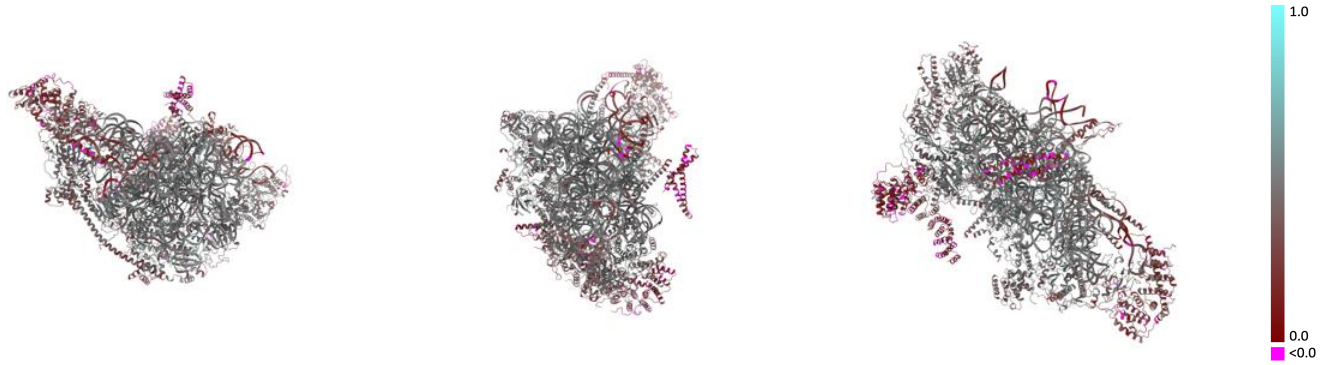
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 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.

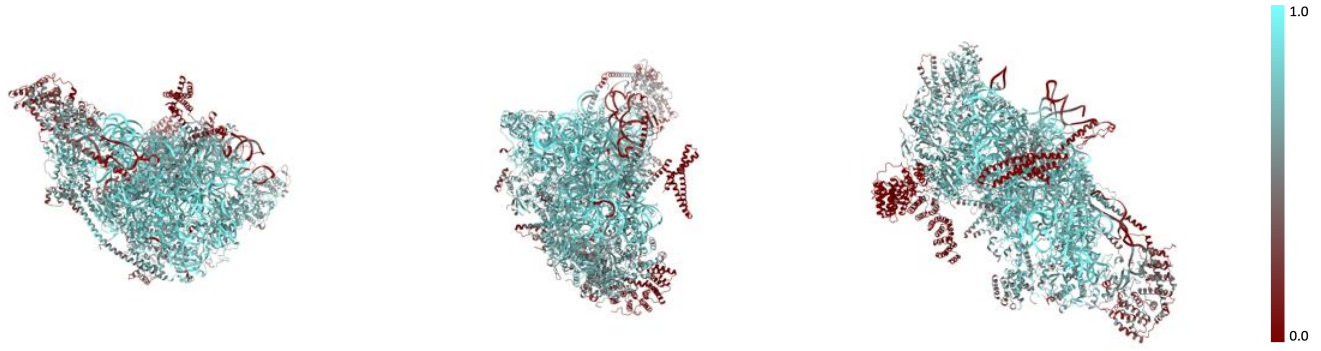
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

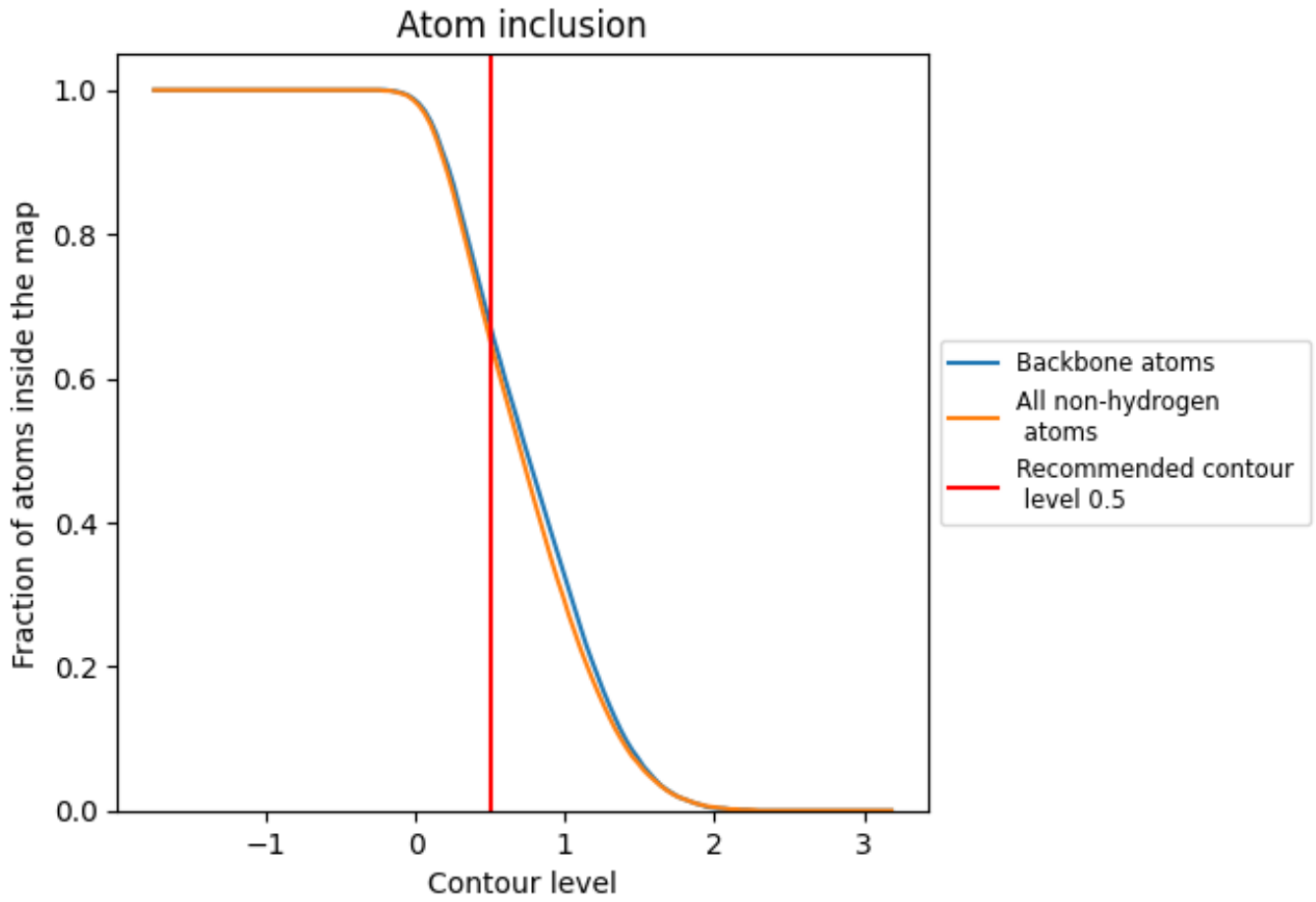
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 67% of all backbone atoms, 65% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6520	0.4180
AA	0.8450	0.4580
AB	0.6500	0.4330
AC	0.7640	0.4920
AD	0.7230	0.4690
AE	0.7220	0.4620
AF	0.7030	0.4340
AG	0.4860	0.3220
AH	0.6680	0.4500
AI	0.7630	0.4740
AJ	0.7200	0.4980
AK	0.7860	0.4910
AL	0.6510	0.4470
AM	0.7590	0.4740
AN	0.7450	0.4690
AO	0.7150	0.4560
AP	0.7380	0.4770
AQ	0.7920	0.4810
AR	0.6260	0.4280
AS	0.6120	0.4160
AT	0.7660	0.4770
AU	0.6680	0.4120
AV	0.3250	0.2600
AW	0.6990	0.4640
AX	0.6530	0.4120
AY	0.4790	0.3500
AZ	0.7150	0.4670
Aa	0.2980	0.3230
Ab	0.7590	0.4620
Ac	0.6560	0.4550
Ad	0.6800	0.4790
Ae	0.1270	0.2150
Ag	0.6790	0.4220
Ai	0.7500	0.4680
Aj	0.5540	0.4000



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
BX	0.1720	0.2790
Bd	0.3460	0.3870