Full wwPDB EM Validation Report ⓘ

Aug 26, 2026 – 12:49 pm BST

PDB ID	:	8CAH / pdb_00008cah
EMDB ID	:	EMD-16525
Title	:	Cryo-EM structure of native Otu2-bound ubiquitinated 43S pre-initiation complex
Authors	:	Ikeuchi, K.; Buschauer, R.; Cheng, J.; Berninghausen, O.; Becker, T.; Beckmann, R.
Deposited on	:	2023-01-24
Resolution	:	3.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

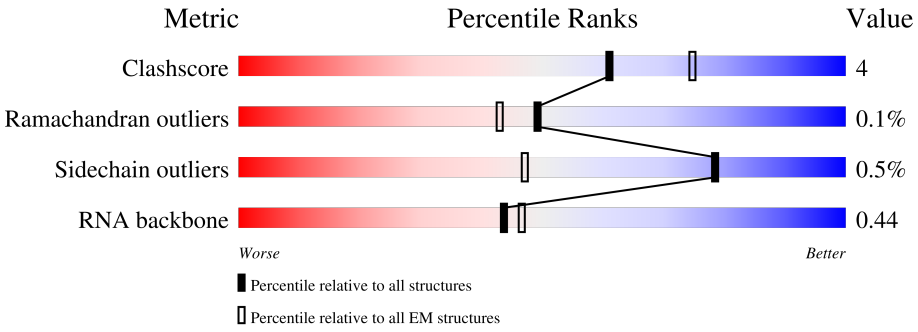
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

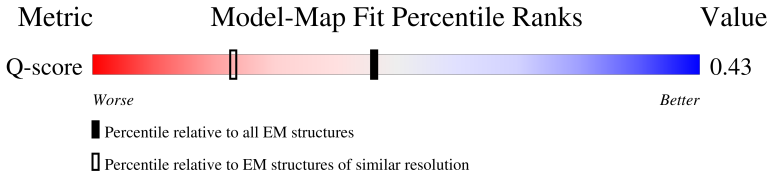
1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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	l	347	95% 93% • 5%
2	r	274	19% 19% 81%
3	o	964	5% 55% 45%

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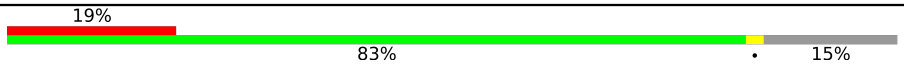
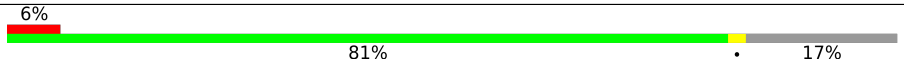
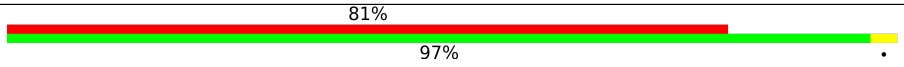
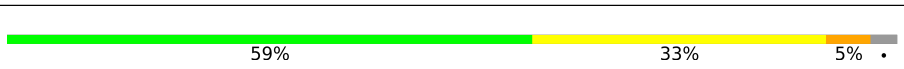
Mol	Chain	Length	Quality of chain
4	p	763	
5	q	812	
6	i	153	
7	m	108	
8	j	77	
9	2	1800	
10	P	252	
11	Q	255	
12	R	254	
13	S	261	
14	T	236	
15	V	200	
16	W	197	
17	X	156	
18	Y	151	
19	Z	137	
20	a	87	
21	b	130	
22	c	145	
23	d	135	
24	e	119	
25	f	82	
26	g	63	
27	E	142	
28	A	240	

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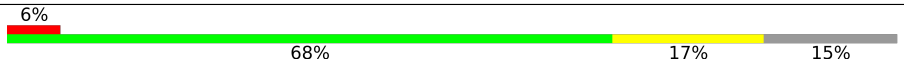
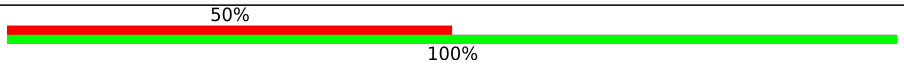
Mol	Chain	Length	Quality of chain
29	B	225	
30	C	105	
31	D	143	
32	F	143	
33	H	136	
34	I	146	
35	J	144	
36	K	121	
37	L	108	
38	M	56	
39	N	76	
40	O	319	
41	h	67	
42	y	265	
42	z	265	
43	x	608	
44	k	76	
45	n	25	
46	G	307	
47	U	190	

2 Entry composition (i)

There are 51 unique types of molecules in this entry. The entry contains 95563 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 Eukaryotic translation initiation factor 3 subunit I.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	l	330	1624	964	330	330	0	0

- Molecule 2 is a protein called Eukaryotic translation initiation factor 3 subunit G.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	r	53	261	155	53	53	0	0

- Molecule 3 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	o	529	2631	1573	529	529	0	0

- Molecule 4 is a protein called Eukaryotic translation initiation factor 3 subunit B.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	p	646	3201	1909	646	646	0	0

- Molecule 5 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	q	636	3169	1897	636	636	0	0

- Molecule 6 is a protein called Eukaryotic translation initiation factor 4C.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	i	97	476	282	97	97	0	0

- Molecule 7 is a protein called SUI1 isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	m	90	Total	C	N	O	0	0
			443	263	90	90		

- Molecule 8 is a protein called RNA recognition motif (unknown).

Mol	Chain	Residues	Atoms				AltConf	Trace
8	j	77	Total	C	N	O	0	0
			385	231	77	77		

- Molecule 9 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	2	1745	Total	C	N	O	P	0	0
			37189	16626	6587	12231	1745		

- Molecule 10 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	206	Total	C	N	O	S	0	0
			1603	1030	284	287	2		

- Molecule 11 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	226	Total	C	N	O	S	0	0
			1798	1139	330	325	4		

- Molecule 12 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	R	216	Total	C	N	O	S	0	0
			1626	1042	287	295	2		

- Molecule 13 is a protein called 40S ribosomal protein S4-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S	258	Total	C	N	O	S	0	0
			2056	1308	387	358	3		

- Molecule 14 is a protein called 40S ribosomal protein S6-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	228	Total	C	N	O	S	0	0
			1815	1138	351	323	3		

- Molecule 15 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	V	187	Total	C	N	O	S	0	0
			1476	916	295	263	2		

- Molecule 16 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	W	184	Total	C	N	O	S	0	0
			1479	935	285	258	1		

- Molecule 17 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	142	Total	C	N	O	S	0	0
			1142	733	217	189	3		

- Molecule 18 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 19 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	127	Total	C	N	O	S	0	0
			923	568	185	167	3		

- Molecule 20 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	a	87	Total	C	N	O	S	0	0
			673	415	125	131	2		

- Molecule 21 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	b	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 22 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	c	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 23 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	d	134	Total	C	N	O	0	0
			1073	676	208	189		

- Molecule 24 is a protein called 40S ribosomal protein S26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	e	97	Total	C	N	O	S	0	0
			765	473	160	127	5		

- Molecule 25 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	f	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 26 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	g	60	Total	C	N	O	S	0	0
			472	298	97	76	1		

- Molecule 27 is a protein called RPS15 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	E	117	Total	C	N	O	S	0	0
			916	583	171	155	7		

- Molecule 28 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	A	222	Total	C	N	O	S	0	0
			1729	1098	312	313	6		

- Molecule 29 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	B	206	Total	C	N	O	S	0	0
			1605	1005	299	298	3		

- Molecule 30 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	C	92	Total	C	N	O	S	0	0
			754	489	122	141	2		

- Molecule 31 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	D	121	Total	C	N	O	S	0	0
			875	551	153	169	2		

- Molecule 32 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	F	141	Total	C	N	O	0	0
			1105	708	203	194		

- Molecule 33 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	H	121	Total	C	N	O	S	0	0
			948	596	179	171	2		

- Molecule 34 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	I	145	Total	C	N	O	S	0	0
			1188	741	237	208	2		

- Molecule 35 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	J	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 36 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	K	100	Total	C	N	O	S	0	0
			797	506	144	146	1		

- Molecule 37 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	L	82	Total	C	N	O	0	0
			651	416	123	112		

- Molecule 38 is a protein called RPS29A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	M	53	Total	C	N	O	S	0	0
			442	274	92	72	4		

- Molecule 39 is a protein called 40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	N	73	Total	C	N	O	S	0	0
			560	355	106	95	4		

- Molecule 40 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	O	312	Total	C	N	O	S	0	0
			2383	1514	409	452	8		

- Molecule 41 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	h	63	Total	C	N	O	S	0	0
			491	303	96	91	1		

- Molecule 42 is a protein called Eukaryotic translation initiation factor 3 subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	z	120	Total 896	C 556	N 172	O 166	S 2	0	0
42	y	79	Total 624	C 389	N 113	O 120	S 2	0	0

- Molecule 43 is a protein called RLI1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	x	582	Total 4607	C 2951	N 795	O 838	S 23	0	0

- Molecule 44 is a protein called 60S ribosomal protein L40-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	k	76	Total 374	C 222	N 76	O 76	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	19	PRO	SER	conflict	UNP P0CH08
k	24	GLU	ASP	conflict	UNP P0CH08
k	28	ALA	SER	conflict	UNP P0CH08

- Molecule 45 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	n	18	Total 175	C 107	N 48	O 19	S 1	0	0

- Molecule 46 is a protein called OTU domain-containing protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	G	259	Total 1509	C 917	N 298	O 292	S 2	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	178	SER	CYS	conflict	UNP P38747

- Molecule 47 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	U	184	Total 1473	C 946	N 263	O 264	0	0

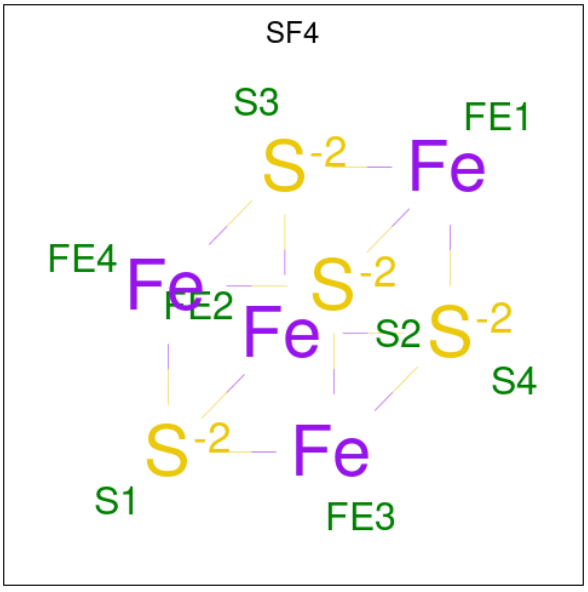
- Molecule 48 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
48	2	77	Total 77	Mg 77	0
48	S	1	Total 1	Mg 1	0
48	B	1	Total 1	Mg 1	0
48	x	1	Total 1	Mg 1	0

- Molecule 49 is ZINC ION (CCD ID: ZN) (formula: Zn).

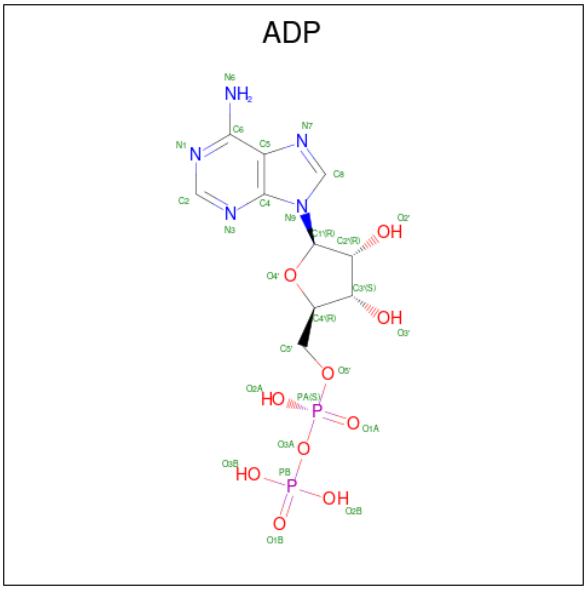
Mol	Chain	Residues	Atoms		AltConf
49	M	1	Total 1	Zn 1	0
49	N	1	Total 1	Zn 1	0

- Molecule 50 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
50	x	1	Total	Fe	S	0
			8	4	4	
50	x	1	Total	Fe	S	0
			8	4	4	

- Molecule 51 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



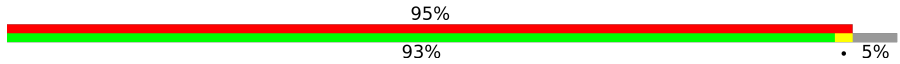
Mol	Chain	Residues	Atoms					AltConf
51	x	1	Total	C	N	O	P	0
			27	10	5	10	2	

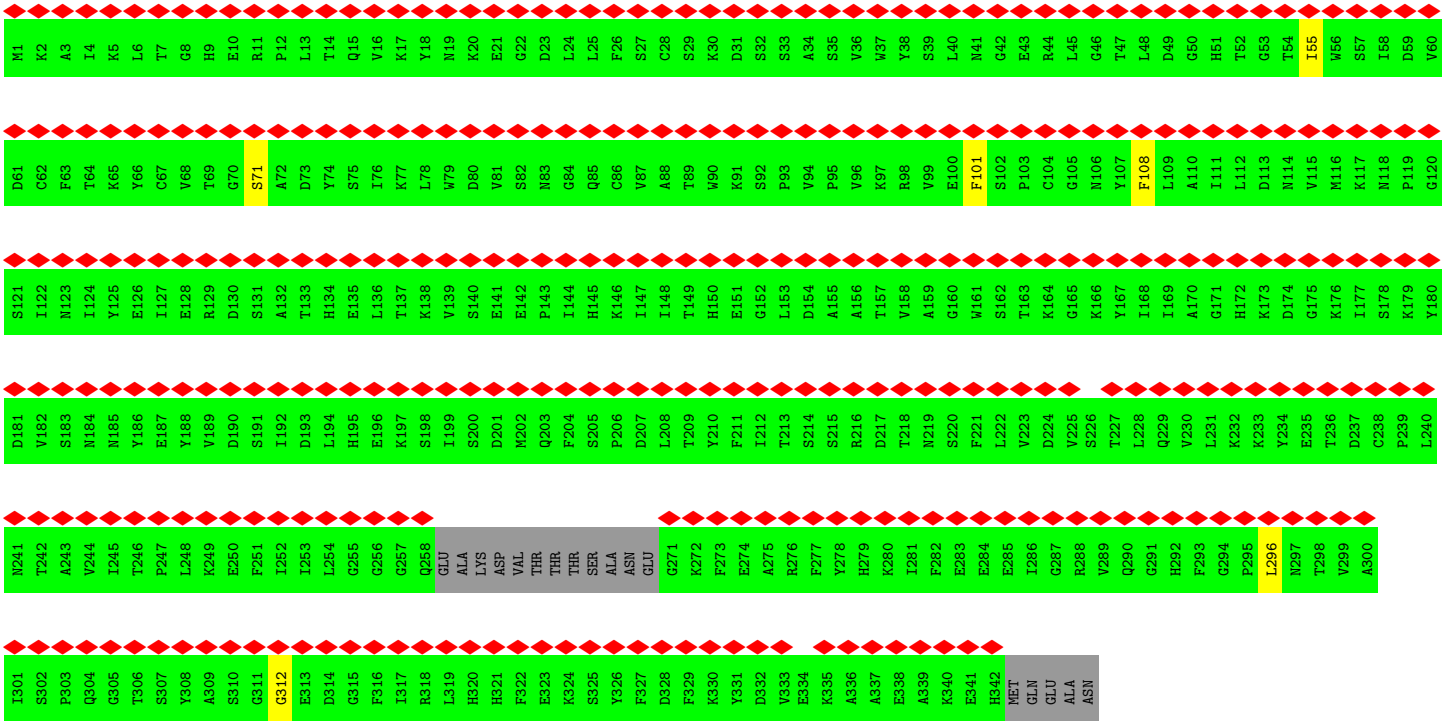
3 Residue-property plots (i)

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: Eukaryotic translation initiation factor 3 subunit I

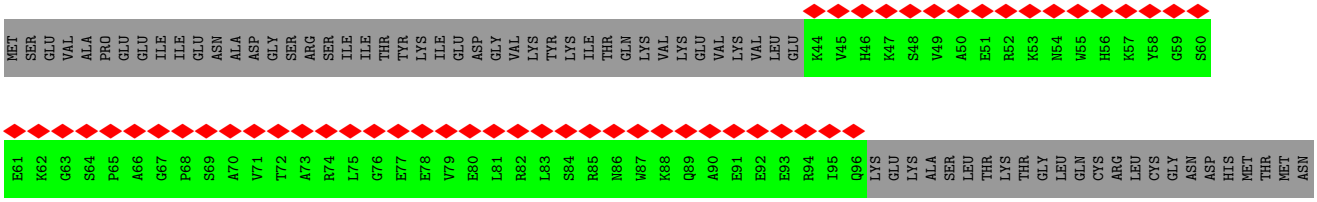
Chain l:

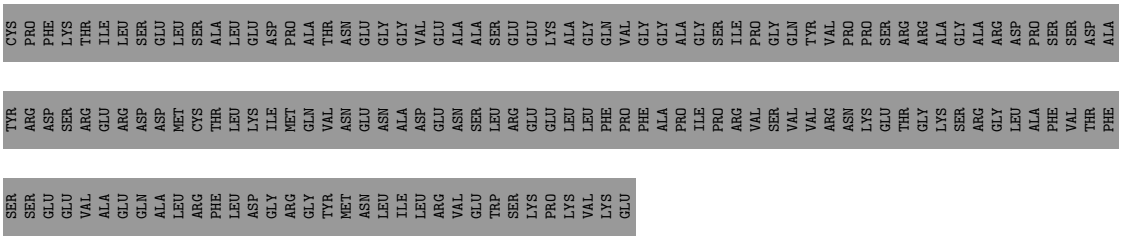




• Molecule 2: Eukaryotic translation initiation factor 3 subunit G

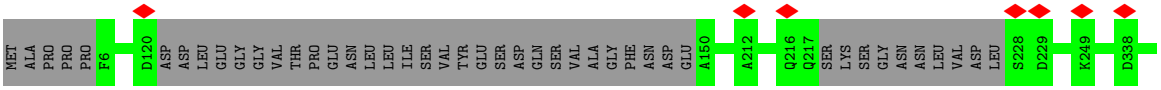
Chain r:

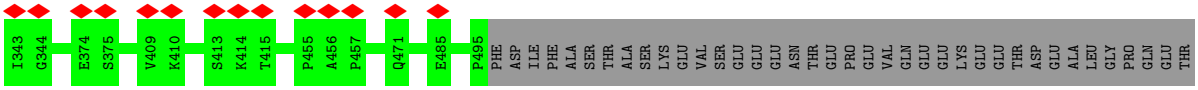


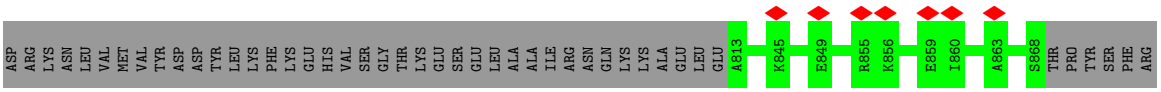


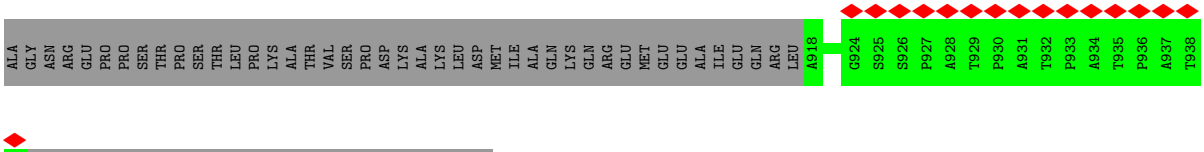
• Molecule 3: Eukaryotic translation initiation factor 3 subunit A

Chain o:



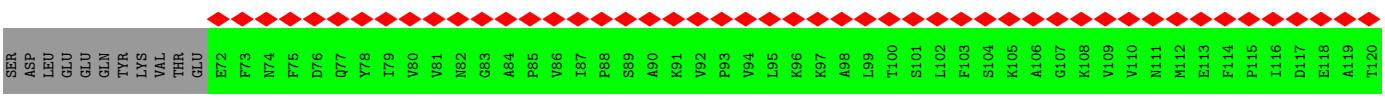


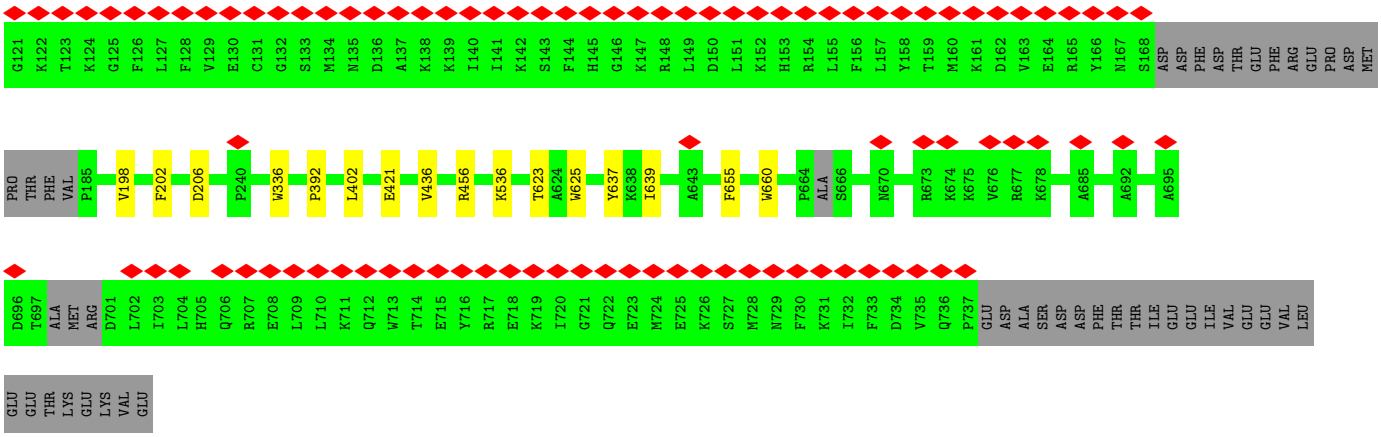




• Molecule 4: Eukaryotic translation initiation factor 3 subunit B

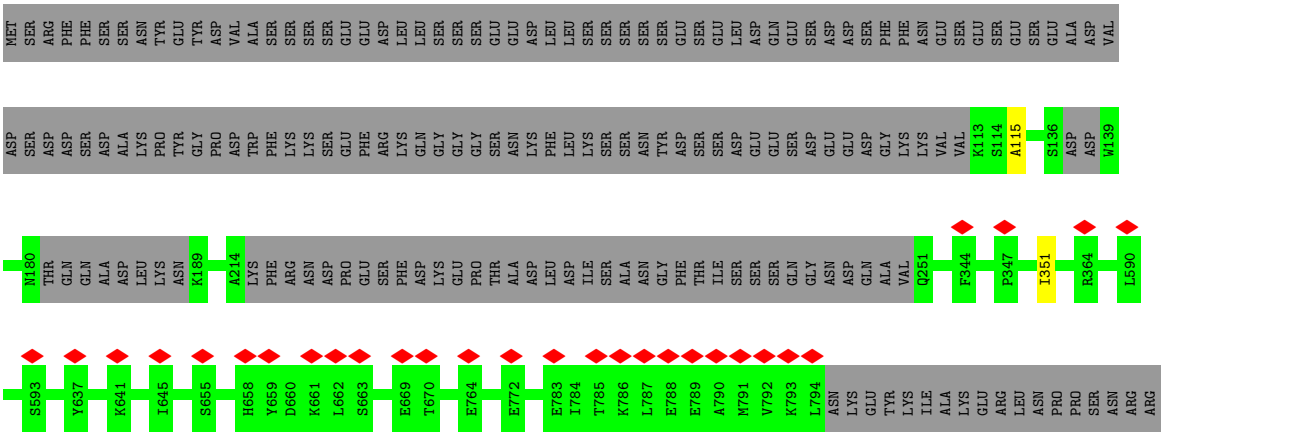
Chain p:





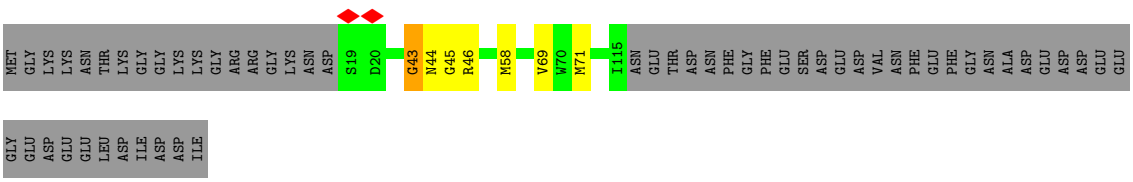
• Molecule 5: Eukaryotic translation initiation factor 3 subunit C

Chain q:



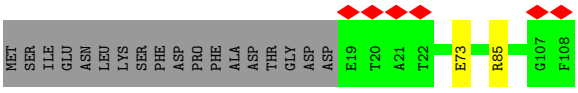
• Molecule 6: Eukaryotic translation initiation factor 4C

Chain i:



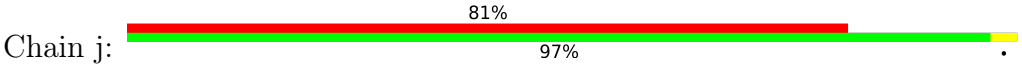
• Molecule 7: SUI1 isoform 1

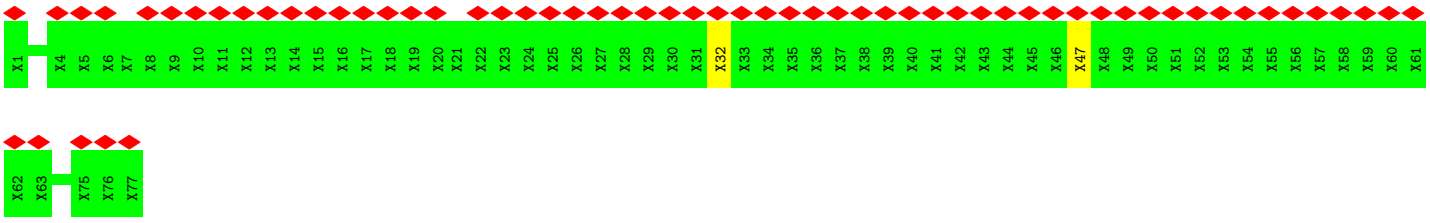
Chain m:



• Molecule 8: RNA recognition motif (unknown)

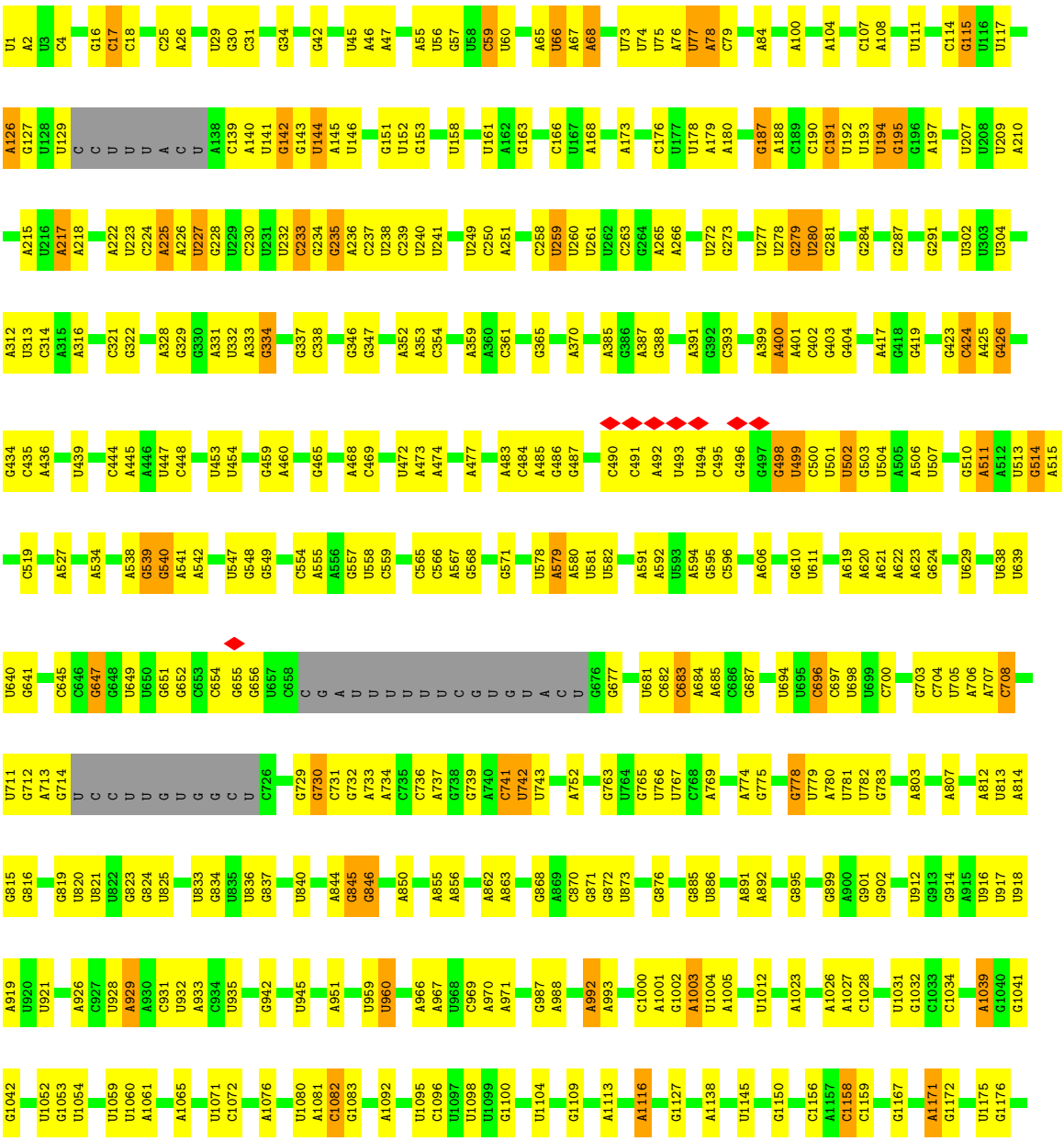
Chain j:

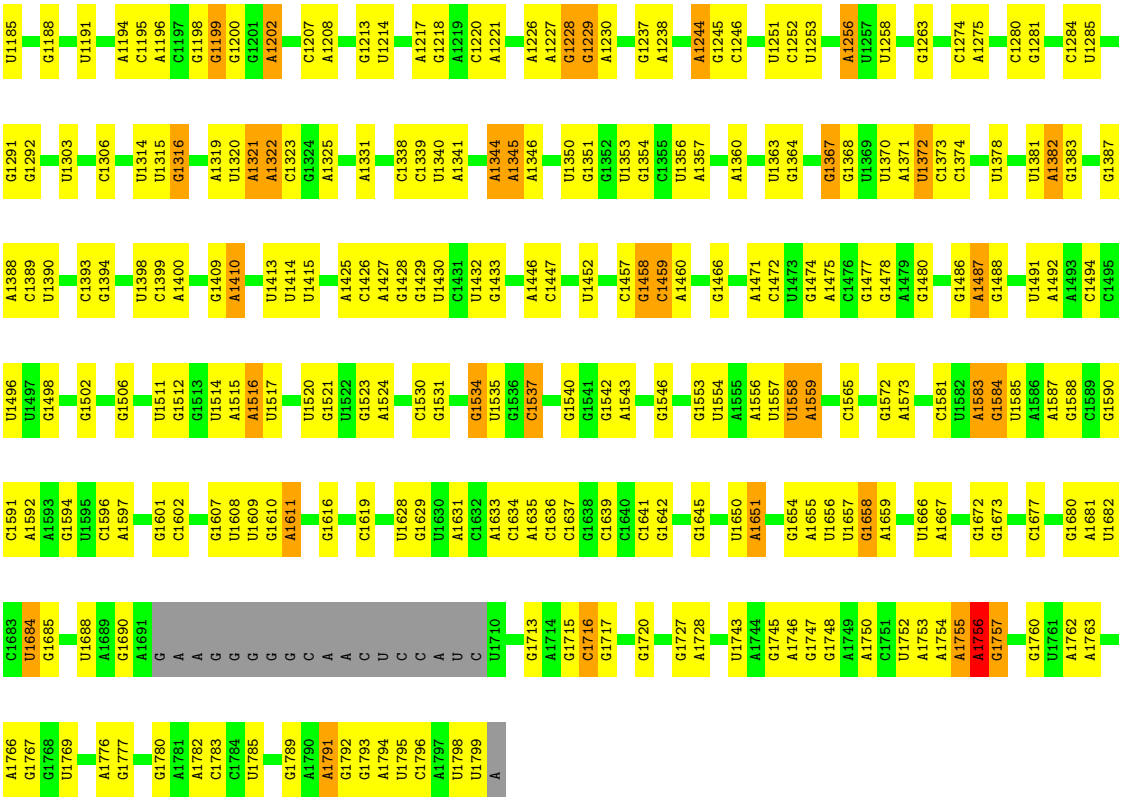




• Molecule 9: 18S ribosomal RNA

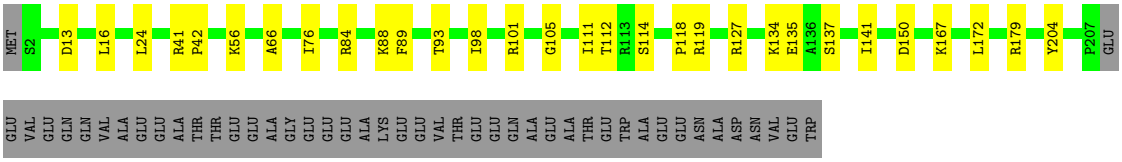
Chain 2:





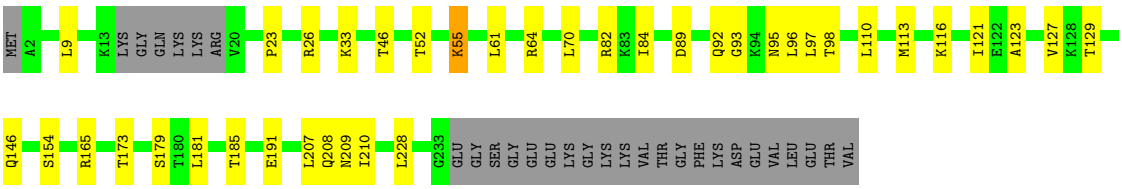
• Molecule 10: 40S ribosomal protein S0-A

Chain P:



• Molecule 11: 40S ribosomal protein S1-A

Chain Q:

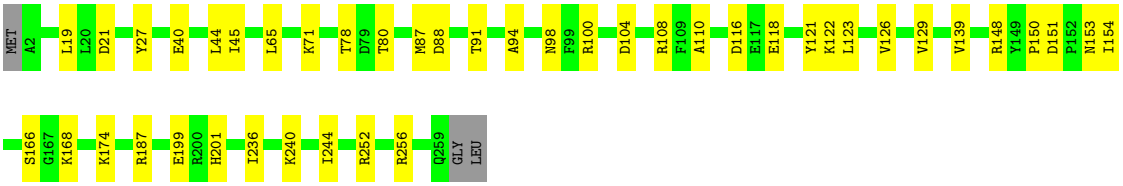


• Molecule 12: 40S ribosomal protein S2

Chain R:

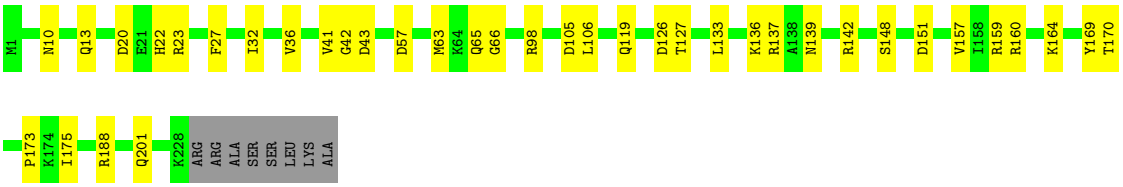
• Molecule 13: 40S ribosomal protein S4-B

Chain S:



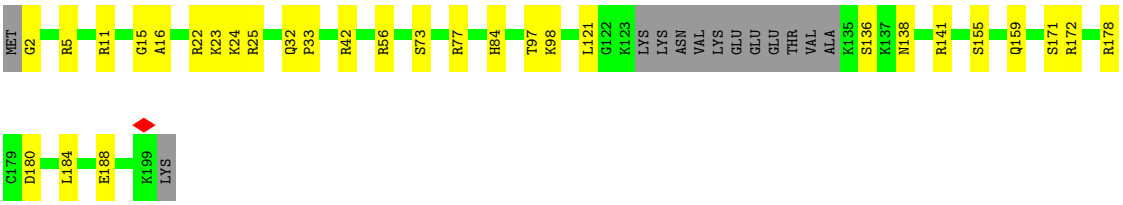
• Molecule 14: 40S ribosomal protein S6-B

Chain T:



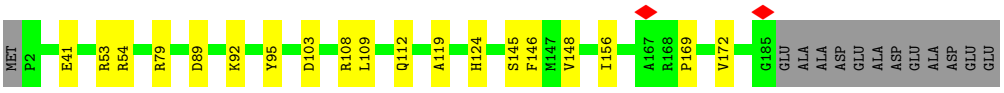
• Molecule 15: 40S ribosomal protein S8-A

Chain V:



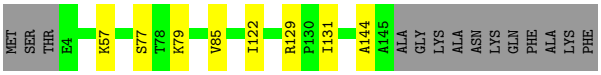
• Molecule 16: 40S ribosomal protein S9-A

Chain W:



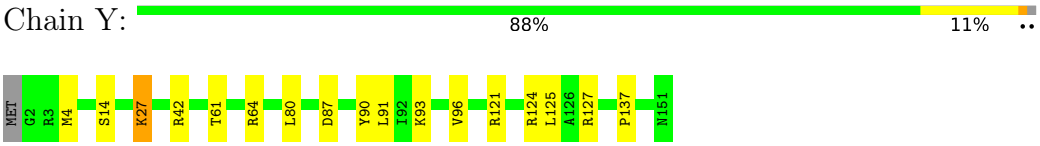
• Molecule 17: 40S ribosomal protein S11-A

Chain X:



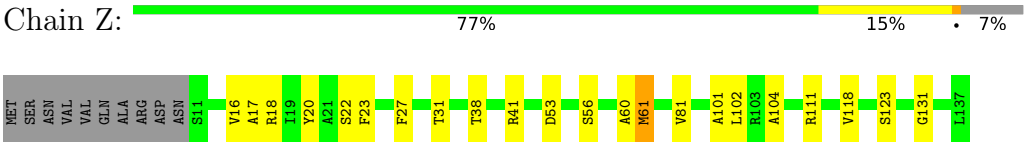
• Molecule 18: 40S ribosomal protein S13

Chain Y:



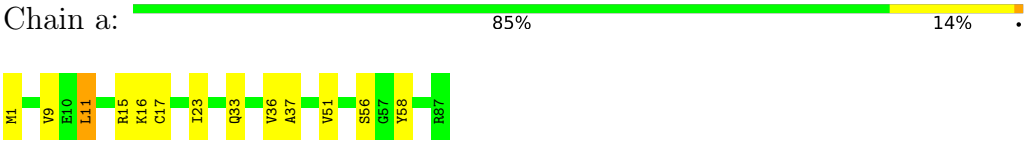
• Molecule 19: 40S ribosomal protein S14-A

Chain Z:



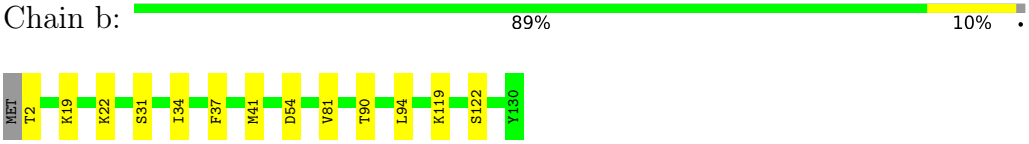
• Molecule 20: 40S ribosomal protein S21-A

Chain a:



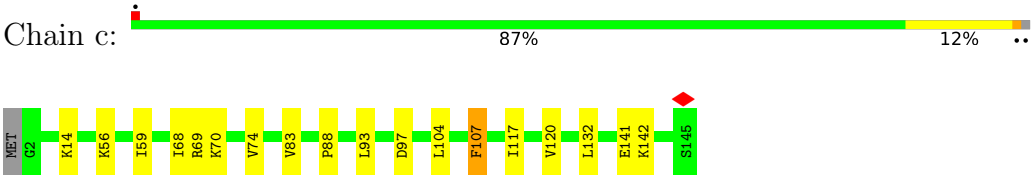
• Molecule 21: 40S ribosomal protein S22-A

Chain b:



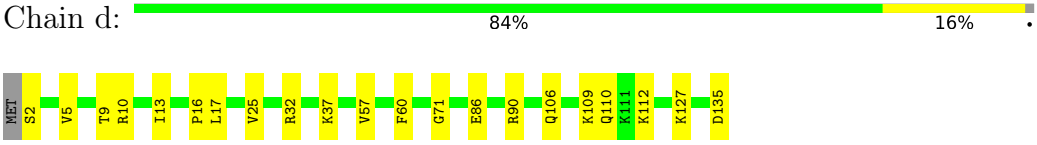
• Molecule 22: 40S ribosomal protein S23-A

Chain c:



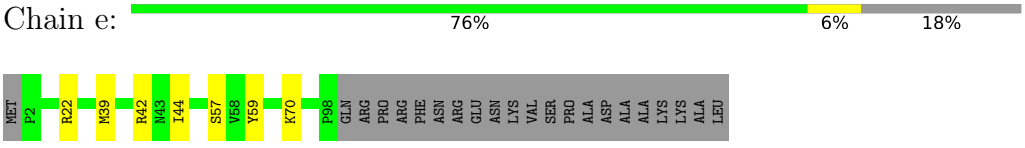
• Molecule 23: 40S ribosomal protein S24-A

Chain d:



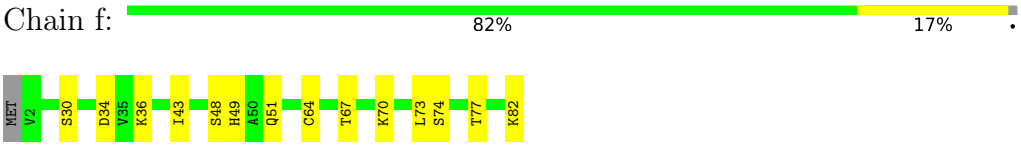
• Molecule 24: 40S ribosomal protein S26-A

Chain e:



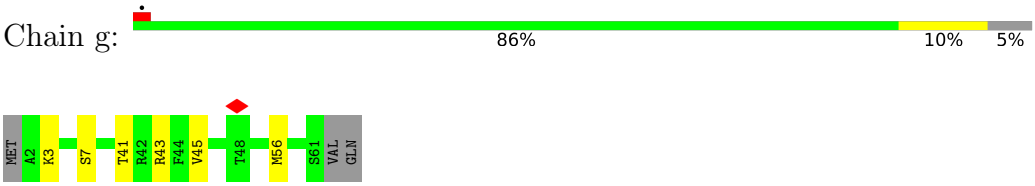
• Molecule 25: 40S ribosomal protein S27-A

Chain f:



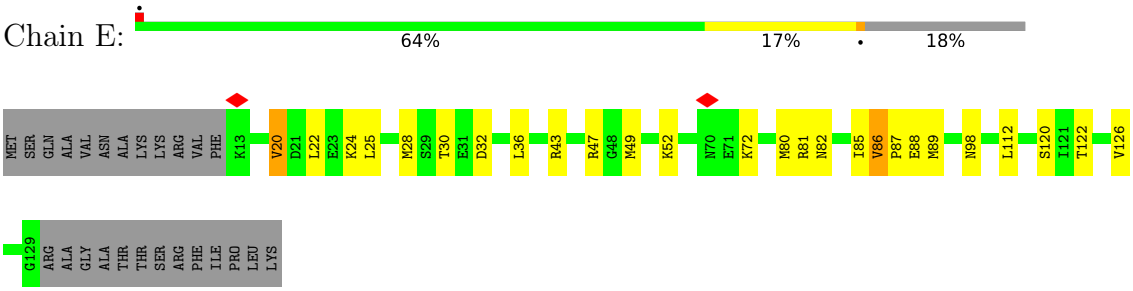
• Molecule 26: 40S ribosomal protein S30-A

Chain g:



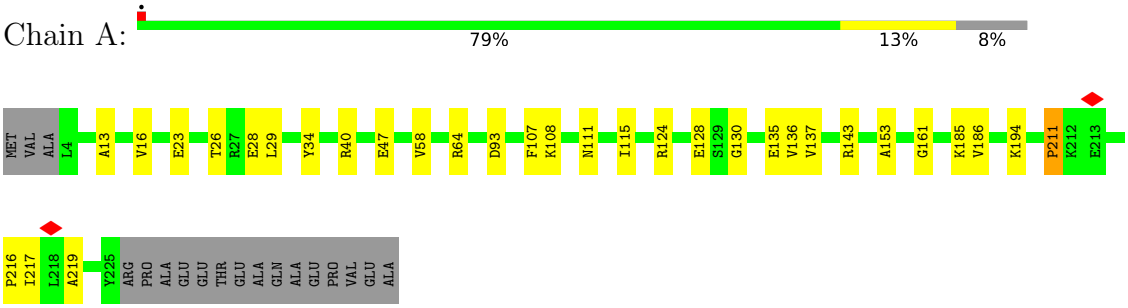
• Molecule 27: RPS15 isoform 1

Chain E:



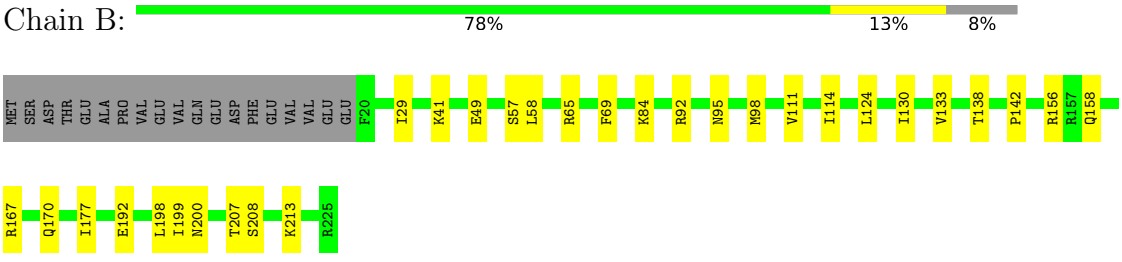
• Molecule 28: 40S ribosomal protein S3

Chain A:



• Molecule 29: 40S ribosomal protein S5

Chain B:

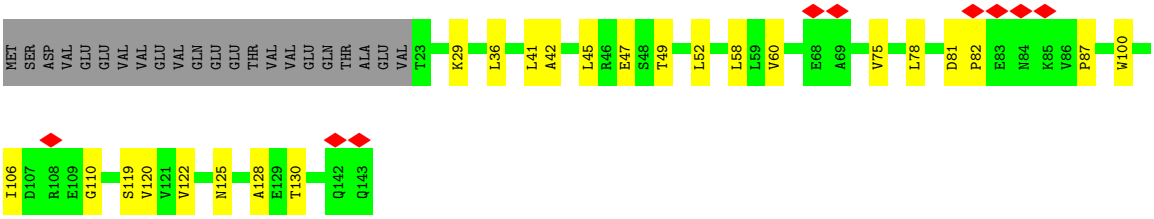


• Molecule 30: 40S ribosomal protein S10-A

Chain C:

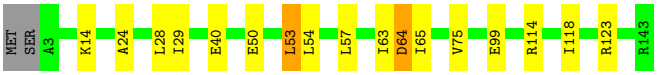
• Molecule 31: 40S ribosomal protein S12

Chain D:



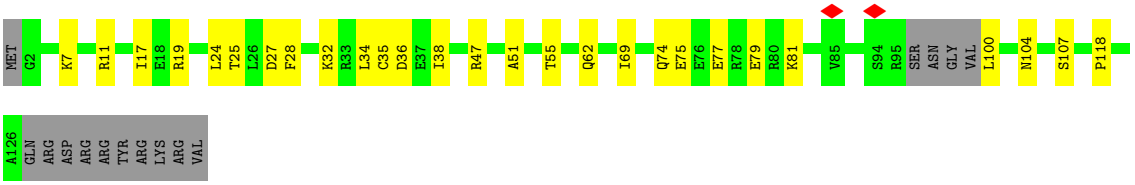
• Molecule 32: 40S ribosomal protein S16-A

Chain F:



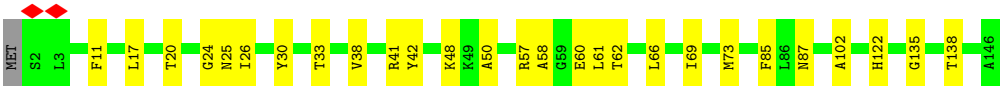
• Molecule 33: 40S ribosomal protein S17-A

Chain H:



• Molecule 34: 40S ribosomal protein S18-A

Chain I:

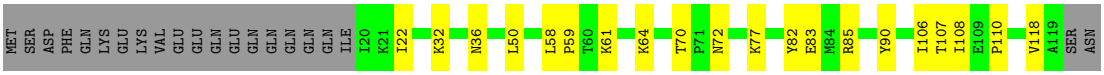


• Molecule 35: 40S ribosomal protein S19-A

Chain J:

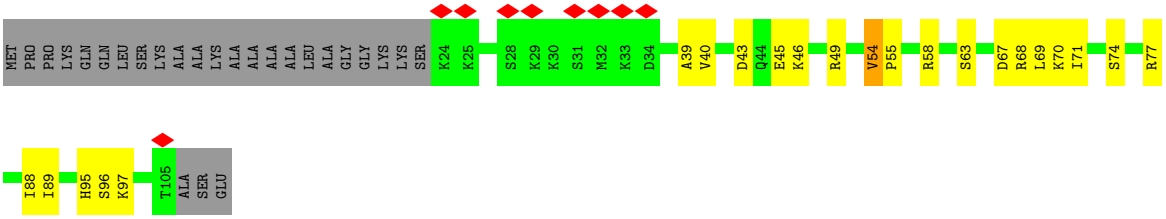
• Molecule 36: 40S ribosomal protein S20

Chain K:



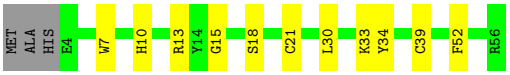
• Molecule 37: 40S ribosomal protein S25-A

Chain L:



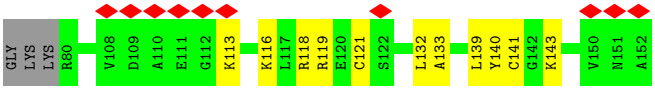
• Molecule 38: RPS29A isoform 1

Chain M:



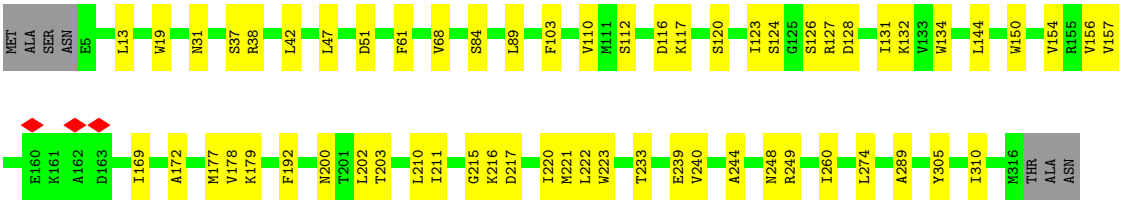
• Molecule 39: 40S ribosomal protein S31

Chain N:



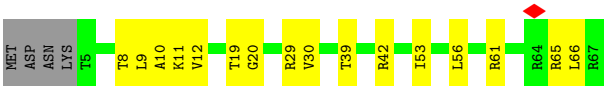
• Molecule 40: Guanine nucleotide-binding protein subunit beta-like protein

Chain O:



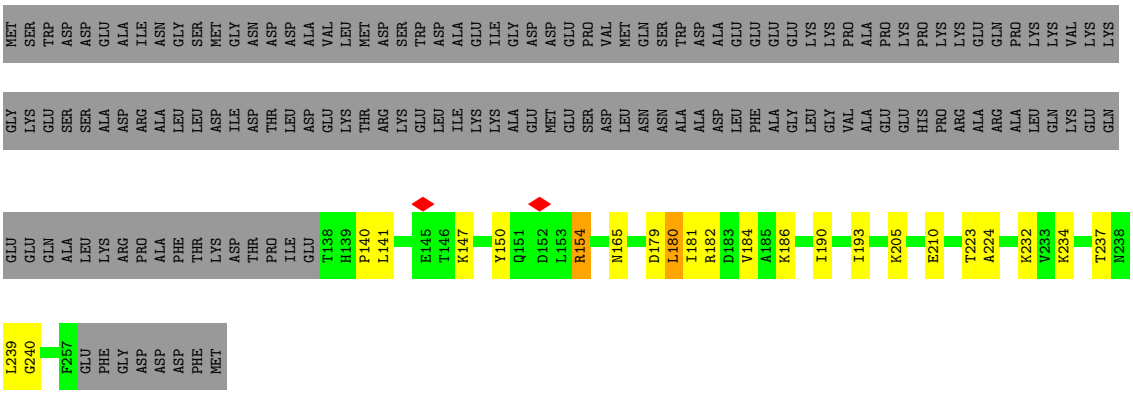
• Molecule 41: 40S ribosomal protein S28-A

Chain h:



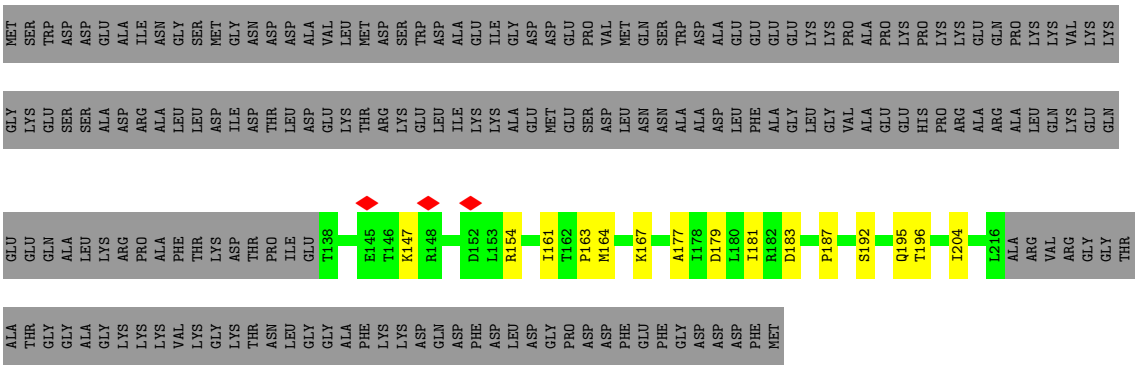
• Molecule 42: Eukaryotic translation initiation factor 3 subunit J

Chain z:



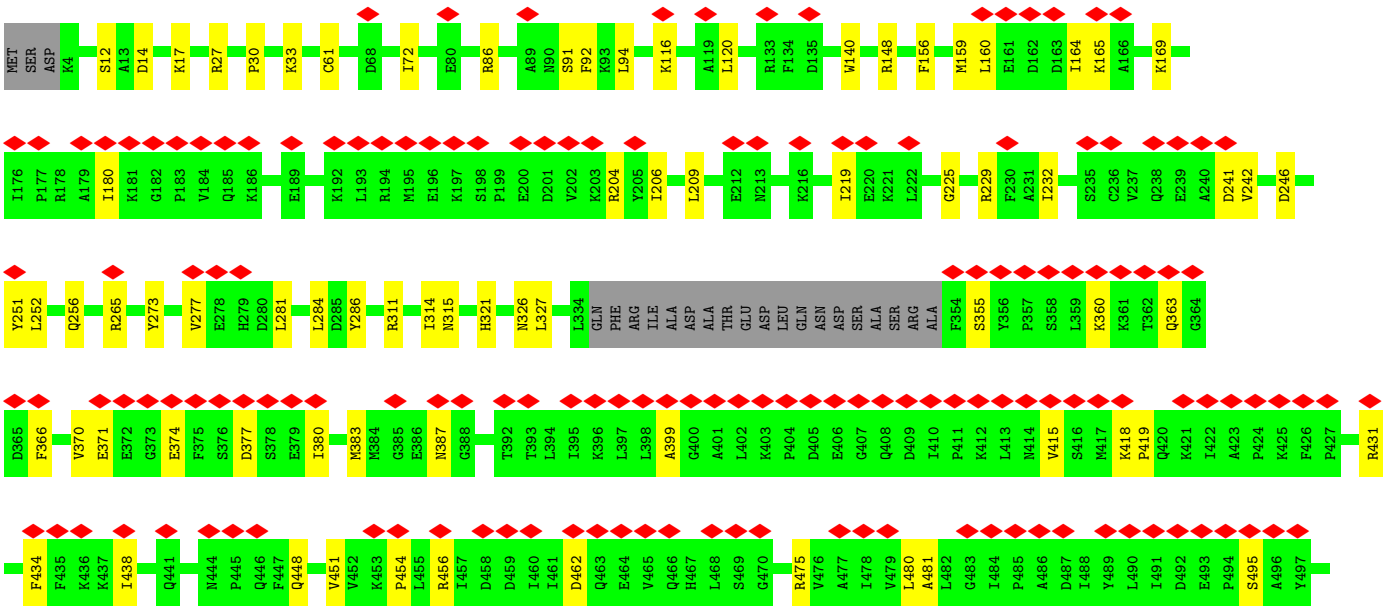
• Molecule 42: Eukaryotic translation initiation factor 3 subunit J

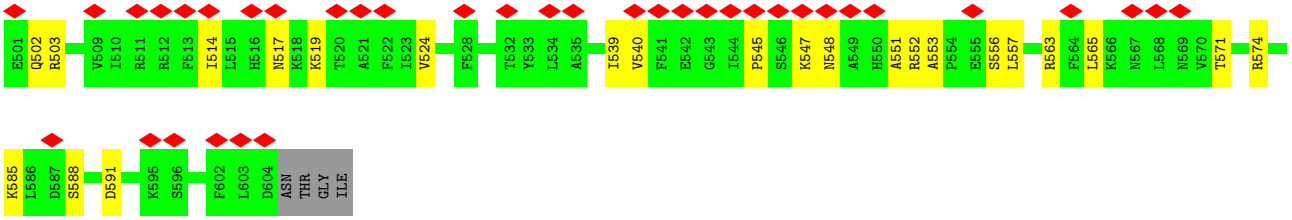
Chain y:



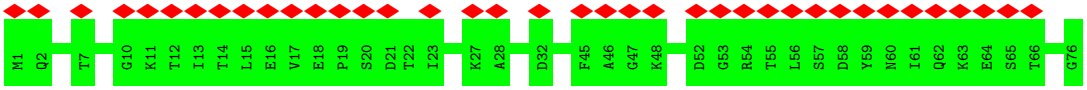
• Molecule 43: RLI1 isoform 1

Chain x:

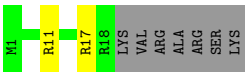




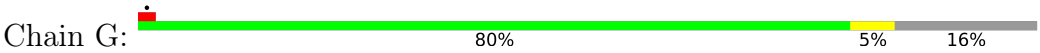
• Molecule 44: 60S ribosomal protein L40-A

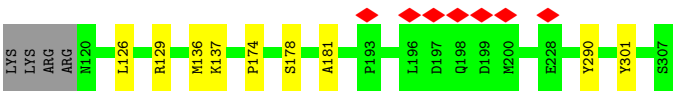


• Molecule 45: 60S ribosomal protein L41-A

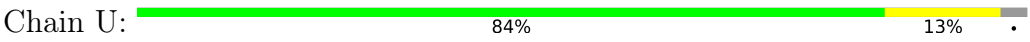


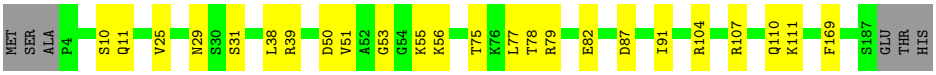
• Molecule 46: OTU domain-containing protein 2





• Molecule 47: 40S ribosomal protein S7-A





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18826	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 ($e^-/Å^2$)	46.4	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.970	Depositor
Minimum map value	-1.905	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.110	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	438.9, 438.9, 438.9	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, ADP, SF4

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	l	0.14	0/1622	0.46	0/2252
2	r	0.10	0/260	0.37	0/360
3	o	0.13	0/2626	0.42	0/3660
4	p	0.18	0/3197	0.50	0/4452
5	q	0.15	0/3165	0.48	1/4418 (0.0%)
6	i	0.38	0/475	0.78	3/658 (0.5%)
7	m	0.19	0/442	0.51	0/613
9	2	0.40	0/41595	0.45	8/64809 (0.0%)
10	P	0.38	0/1644	0.62	0/2249
11	Q	0.34	0/1823	0.67	1/2447 (0.0%)
12	R	0.42	0/1656	0.70	4/2251 (0.2%)
13	S	0.42	0/2097	0.67	0/2823
14	T	0.35	0/1839	0.64	0/2460
15	V	0.42	0/1501	0.58	0/2006
16	W	0.40	0/1504	0.65	0/2016
17	X	0.41	0/1168	0.57	0/1575
18	Y	0.40	0/1215	0.71	3/1638 (0.2%)
19	Z	0.36	0/934	0.72	2/1257 (0.2%)
20	a	0.40	0/682	0.72	0/921
21	b	0.44	0/1038	0.60	0/1395
22	c	0.45	0/1139	0.60	0/1518
23	d	0.41	0/1087	0.61	0/1449
24	e	0.40	0/778	0.65	0/1042
25	f	0.42	0/620	0.66	0/838
26	g	0.34	0/480	0.69	0/639
27	E	0.27	0/936	0.86	4/1259 (0.3%)
28	A	0.40	1/1754 (0.1%)	0.76	5/2361 (0.2%)
29	B	0.23	0/1625	0.61	0/2197
30	C	0.31	0/772	0.85	4/1044 (0.4%)
31	D	0.28	0/883	0.84	0/1199
32	F	0.27	0/1125	0.59	0/1510
33	H	0.33	0/957	0.78	0/1283

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
34	I	0.22	0/1207	0.62	2/1623 (0.1%)
35	J	0.23	0/1130	0.64	1/1517 (0.1%)
36	K	0.30	0/807	0.65	0/1091
37	L	0.23	0/661	0.69	0/888
38	M	0.25	0/452	0.55	0/600
39	N	0.28	0/571	0.77	0/768
40	O	0.21	0/2436	0.56	0/3318
41	h	0.24	0/493	0.71	1/663 (0.2%)
42	y	0.43	0/631	1.11	4/851 (0.5%)
42	z	0.41	0/905	0.94	4/1213 (0.3%)
43	x	0.22	0/4694	0.59	1/6334 (0.0%)
44	k	0.16	0/373	0.52	0/517
45	n	0.30	0/176	0.47	0/225
46	G	0.18	0/1514	0.45	0/2075
47	U	0.35	0/1498	0.69	0/2019
All	All	0.35	1/100187 (0.0%)	0.56	48/144301 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	p	0	1
21	b	0	1
42	z	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	211	PRO	CG-CD	-9.96	1.16	1.50

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	A	211	PRO	N-CD-CG	-12.04	85.13	103.20
28	A	211	PRO	CA-N-CD	-11.39	96.05	112.00
42	y	163	PRO	CA-N-CD	-9.47	98.74	112.00
28	A	216	PRO	CA-N-CD	-7.36	101.69	112.00
28	A	211	PRO	CA-CB-CG	-7.08	91.06	104.50
34	I	73	MET	CA-CB-CG	7.01	128.12	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	i	45	GLY	N-CA-C	6.85	129.41	113.18
30	C	10	LYS	CA-CB-CG	6.78	127.65	114.10
5	q	115	ALA	CB-CA-C	-6.67	108.90	116.63
42	z	180	LEU	CA-CB-CG	6.56	139.27	116.30
35	J	36	ILE	N-CA-C	-6.56	106.44	111.62
18	Y	27	LYS	CB-CG-CD	6.55	126.36	111.30
42	y	147	LYS	CA-CB-CG	6.26	126.63	114.10
9	2	1756	A	O5'-P-OP1	6.11	126.32	108.00
42	z	186	LYS	CB-CG-CD	6.11	125.34	111.30
6	i	43	GLY	CA-C-N	6.07	133.14	121.54
6	i	43	GLY	C-N-CA	6.07	133.14	121.54
42	z	210	GLU	CA-CB-CG	6.00	126.09	114.10
19	Z	118	VAL	CA-CB-CG1	5.99	120.58	110.40
34	I	73	MET	CB-CG-SD	5.98	130.64	112.70
18	Y	137	PRO	CA-C-N	5.97	136.71	126.32
18	Y	137	PRO	C-N-CA	5.97	136.71	126.32
9	2	1756	A	O5'-P-OP2	-5.76	90.72	108.00
27	E	72	LYS	CA-CB-CG	5.76	125.61	114.10
12	R	38	VAL	CA-C-N	5.68	132.39	121.54
12	R	38	VAL	C-N-CA	5.68	132.39	121.54
9	2	1791	A	C2'-C3'-O3'	5.61	117.92	109.50
27	E	36	LEU	CA-C-N	5.52	129.86	121.03
27	E	36	LEU	C-N-CA	5.52	129.86	121.03
12	R	38	VAL	CG1-CB-CG2	-5.51	98.67	110.80
43	x	565	LEU	CA-CB-CG	5.49	135.52	116.30
12	R	147	ASN	N-CA-C	5.46	118.92	111.39
9	2	1791	A	P-O3'-C3'	5.45	128.37	120.20
9	2	1755	A	P-O3'-C3'	5.44	128.36	120.20
30	C	33	GLU	CA-C-N	5.42	131.07	122.61
30	C	33	GLU	C-N-CA	5.42	131.07	122.61
11	Q	55	LYS	CA-CB-CG	5.30	124.71	114.10
19	Z	118	VAL	CB-CA-C	5.30	119.99	111.29
9	2	77	U	P-O3'-C3'	5.23	128.05	120.20
42	z	210	GLU	N-CA-CB	5.20	118.87	110.40
42	y	147	LYS	CB-CG-CD	5.20	123.25	111.30
27	E	49	MET	CA-CB-CG	5.14	124.39	114.10
9	2	59	C	P-O3'-C3'	5.13	127.90	120.20
42	y	195	GLN	CA-CB-CG	5.11	124.32	114.10
41	h	11	LYS	CA-CB-CG	5.07	124.23	114.10
30	C	31	LYS	CA-CB-CG	5.03	124.16	114.10
28	A	211	PRO	N-CA-CB	-5.02	98.98	103.35
9	2	453	U	C2-N1-C1'	5.01	132.74	117.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	b	54	ASP	Peptide
4	p	336	TRP	Peptide
42	z	154	ARG	Sidechain

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	l	1624	0	727	3	0
2	r	261	0	122	0	0
3	o	2631	0	1207	0	0
4	p	3201	0	1398	6	0
5	q	3169	0	1372	0	0
6	i	476	0	215	7	0
7	m	443	0	193	0	0
8	j	385	0	84	1	0
9	2	37189	0	18708	241	0
10	P	1603	0	1610	18	0
11	Q	1798	0	1890	23	0
12	R	1626	0	1715	13	0
13	S	2056	0	2140	28	0
14	T	1815	0	1894	32	0
15	V	1476	0	1501	26	0
16	W	1479	0	1556	13	0
17	X	1142	0	1209	6	0
18	Y	1192	0	1255	13	0
19	Z	923	0	948	13	0
20	a	673	0	662	8	0
21	b	1021	0	1060	8	0
22	c	1121	0	1196	12	0
23	d	1073	0	1132	15	0
24	e	765	0	814	5	0
25	f	610	0	633	12	0
26	g	472	0	521	4	0
27	E	916	0	941	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	A	1729	0	1812	22	0
29	B	1605	0	1669	20	0
30	C	754	0	725	13	0
31	D	875	0	878	14	0
32	F	1105	0	1166	12	0
33	H	948	0	990	16	0
34	I	1188	0	1218	18	0
35	J	1112	0	1124	12	0
36	K	797	0	863	14	0
37	L	651	0	682	16	0
38	M	442	0	428	9	0
39	N	560	0	558	8	0
40	O	2383	0	2332	36	0
41	h	491	0	524	10	0
42	y	624	0	645	13	0
42	z	896	0	926	20	0
43	x	4607	0	4756	64	0
44	k	374	0	163	0	0
45	n	175	0	213	2	0
46	G	1509	0	997	10	0
47	U	1473	0	1555	17	0
48	2	77	0	0	0	0
48	B	1	0	0	0	0
48	S	1	0	0	0	0
48	x	1	0	0	0	0
49	M	1	0	0	0	0
49	N	1	0	0	0	0
50	x	16	0	0	1	0
51	x	27	0	12	0	0
All	All	95563	0	70939	714	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 4.

All (714) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:2:1588:G:H1	9:2:1608:U:H3	1.12	0.92
9:2:1658:G:H1	9:2:1743:U:H3	1.17	0.84
9:2:1688:U:H3	9:2:1713:G:H1	1.34	0.73
9:2:539:G:N3	9:2:540:G:N2	2.37	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:2:647:G:H1	9:2:687:G:H22	1.37	0.72
9:2:1645:G:H1	9:2:1755:A:H2	1.37	0.71
32:F:50:GLU:O	32:F:54:LEU:HB2	1.93	0.69
43:x:61:CYS:HB3	50:x:702:SF4:S2	2.32	0.69
34:I:48:LYS:HD3	35:J:35:ASP:HB3	1.74	0.69
9:2:868:G:H1	9:2:960:U:H3	1.42	0.68
43:x:156:PHE:HA	43:x:159:MET:HG2	1.75	0.67
43:x:399:ALA:HA	43:x:415:VAL:HG11	1.75	0.67
43:x:431:ARG:HH21	43:x:462:ASP:HA	1.60	0.67
43:x:383:MET:HB3	43:x:539:ILE:HB	1.75	0.67
11:Q:23:PRO:HB3	11:Q:26:ARG:HH21	1.59	0.66
9:2:486:G:N1	9:2:502:U:C4	2.64	0.65
9:2:1351:G:H1	9:2:1374:C:H42	1.44	0.65
16:W:119:ALA:O	16:W:124:HIS:ND1	2.30	0.65
9:2:1502:G:N7	35:J:102:ARG:NH2	2.45	0.64
11:Q:93:GLY:O	11:Q:95:ASN:ND2	2.31	0.64
40:O:89:LEU:HB2	40:O:103:PHE:HB2	1.80	0.63
9:2:1410:A:H5'	32:F:118:ILE:HD12	1.81	0.63
9:2:778:G:H22	23:d:10:ARG:HH21	1.47	0.63
37:L:88:ILE:HG23	37:L:89:ILE:HG12	1.81	0.63
42:z:190:ILE:HG23	42:y:204:ILE:HD11	1.80	0.63
9:2:498:G:H21	9:2:499:U:H3	1.45	0.62
13:S:148:ARG:NH2	14:T:201:GLN:OE1	2.32	0.62
31:D:82:PRO:HD3	39:N:113:LYS:HD2	1.82	0.62
9:2:1356:U:H3	9:2:1367:G:H1	1.48	0.61
42:z:181:ILE:HD12	42:y:181:ILE:HG23	1.81	0.61
6:i:46:ARG:N	9:2:1755:A:O3'	2.32	0.61
40:O:13:LEU:HB2	40:O:310:ILE:HB	1.81	0.61
17:X:122:ILE:H	17:X:144:ALA:HB3	1.66	0.61
13:S:100:ARG:NH2	13:S:121:TYR:O	2.34	0.61
9:2:1034:C:HO2'	21:b:2:THR:N	1.98	0.61
13:S:87:MET:HE1	13:S:236:ILE:HG21	1.83	0.61
31:D:52:LEU:HD11	31:D:78:LEU:HB3	1.82	0.61
22:c:74:VAL:HG21	22:c:104:LEU:HD11	1.83	0.60
29:B:200:ASN:HB3	29:B:208:SER:HB2	1.83	0.60
9:2:459:G:OP1	23:d:109:LYS:NZ	2.35	0.60
33:H:7:LYS:O	33:H:11:ARG:HB3	2.02	0.60
19:Z:18:ARG:NH1	19:Z:31:THR:OG1	2.34	0.60
14:T:10:ASN:ND2	14:T:127:THR:O	2.35	0.60
11:Q:23:PRO:HA	11:Q:26:ARG:HE	1.66	0.60
28:A:40:ARG:HG3	36:K:110:PRO:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:2:967:A:OP2	18:Y:124:ARG:NH2	2.34	0.59
33:H:28:PHE:HA	33:H:55:THR:HG21	1.84	0.59
12:R:80:VAL:HG12	12:R:102:VAL:HG22	1.84	0.59
40:O:221:MET:HG2	40:O:233:THR:HG23	1.84	0.59
9:2:151:G:N3	14:T:13:GLN:NE2	2.50	0.59
36:K:106:ILE:HG23	36:K:107:THR:HG23	1.84	0.59
9:2:1685:G:N3	46:G:37:GLN:NE2	2.50	0.59
29:B:58:LEU:HG	29:B:138:THR:HG22	1.85	0.59
39:N:116:LYS:HE3	39:N:119:ARG:HA	1.85	0.59
42:z:140:PRO:HD2	42:z:141:LEU:HD22	1.85	0.59
47:U:55:LYS:HE2	47:U:87:ASP:HA	1.85	0.59
11:Q:82:ARG:NH2	11:Q:191:GLU:OE2	2.36	0.58
11:Q:110:LEU:HA	11:Q:113:MET:HE2	1.84	0.58
42:z:193:ILE:HD11	42:y:204:ILE:HD13	1.85	0.58
11:Q:46:THR:OG1	11:Q:64:ARG:NH2	2.37	0.58
20:a:15:ARG:NH1	20:a:33:GLN:OE1	2.36	0.58
27:E:20:VAL:HG23	27:E:24:LYS:HE2	1.85	0.58
9:2:1065:A:N3	11:Q:146:GLN:NE2	2.51	0.58
43:x:383:MET:HE1	43:x:524:VAL:HG13	1.85	0.58
31:D:60:VAL:HG23	31:D:87:PRO:HG2	1.85	0.58
9:2:115:G:H5'	17:X:129:ARG:HD3	1.85	0.58
9:2:870:C:O2	25:f:51:GLN:NE2	2.36	0.58
13:S:19:LEU:HD11	13:S:108:ARG:HD2	1.84	0.58
15:V:77:ARG:NH2	46:G:52:ASP:OD1	2.36	0.58
27:E:98:ASN:HB2	27:E:122:THR:HA	1.86	0.58
9:2:1554:U:OP1	38:M:13:ARG:NH1	2.37	0.57
9:2:331:A:N7	15:V:172:ARG:NH2	2.49	0.57
9:2:742:U:H1'	47:U:107:ARG:HH12	1.68	0.57
33:H:69:ILE:O	33:H:74:GLN:NE2	2.35	0.57
43:x:371:GLU:OE1	43:x:552:ARG:NH1	2.36	0.57
42:z:180:LEU:HD13	42:y:154:ARG:HG2	1.86	0.57
28:A:40:ARG:NH2	28:A:47:GLU:OE1	2.37	0.57
28:A:211:PRO:HG3	33:H:19:ARG:HB2	1.86	0.57
43:x:229:ARG:HA	43:x:232:ILE:HD12	1.86	0.57
9:2:579:A:N6	42:z:237:THR:OG1	2.36	0.57
6:i:69:VAL:O	9:2:1756:A:N6	2.38	0.57
9:2:567:A:OP1	22:c:70:LYS:NZ	2.36	0.57
13:S:88:ASP:OD1	13:S:122:LYS:NZ	2.37	0.57
47:U:25:VAL:O	47:U:29:ASN:ND2	2.38	0.57
14:T:27:PHE:HE2	14:T:36:VAL:HG21	1.70	0.56
23:d:86:GLU:OE2	23:d:90:ARG:NH1	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:O:200:ASN:ND2	40:O:239:GLU:OE2	2.38	0.56
9:2:354:C:H5"	15:V:16:ALA:HB2	1.86	0.56
9:2:1681:A:H1'	14:T:66:GLY:HA2	1.87	0.56
11:Q:52:THR:OG1	11:Q:55:LYS:NZ	2.34	0.56
22:c:97:ASP:OD1	22:c:97:ASP:N	2.38	0.56
36:K:32:LYS:O	36:K:36:ASN:ND2	2.39	0.56
9:2:126:A:H2	9:2:291:G:H21	1.52	0.56
38:M:30:LEU:HA	38:M:39:CYS:HA	1.86	0.56
43:x:545:PRO:O	43:x:547:LYS:NZ	2.36	0.56
9:2:217:A:N1	9:2:844:A:O2'	2.35	0.56
27:E:43:ARG:HE	27:E:47:ARG:HD3	1.70	0.56
43:x:585:LYS:HB3	43:x:588:SER:HB3	1.85	0.56
9:2:1339:C:O2'	9:2:1341:A:N7	2.35	0.56
13:S:98:ASN:ND2	13:S:116:ASP:OD1	2.38	0.56
15:V:11:ARG:NH1	15:V:15:GLY:O	2.38	0.56
43:x:434:PHE:HA	43:x:438:ILE:HG22	1.88	0.56
9:2:1591:C:H2'	9:2:1592:A:H8	1.71	0.55
9:2:1594:G:OP2	9:2:1596:C:N4	2.39	0.55
9:2:1565:C:OP1	34:I:41:ARG:NH1	2.39	0.55
9:2:629:U:OP1	18:Y:127:ARG:NH2	2.40	0.55
4:p:623:THR:HA	4:p:639:ILE:HA	1.88	0.55
9:2:152:U:OP2	23:d:127:LYS:NZ	2.40	0.55
9:2:1516:A:OP2	36:K:61:LYS:NZ	2.34	0.55
9:2:1387:G:OP1	33:H:32:LYS:NZ	2.38	0.55
9:2:1127:G:OP1	45:n:11:ARG:NH2	2.39	0.55
43:x:14:ASP:OD2	43:x:14:ASP:N	2.39	0.55
13:S:104:ASP:HB3	13:S:110:ALA:HB2	1.88	0.55
16:W:41:GLU:OE1	16:W:108:ARG:NH2	2.40	0.55
17:X:57:LYS:HD3	17:X:131:ILE:HG23	1.87	0.55
9:2:1116:A:OP1	45:n:17:ARG:NH1	2.40	0.55
11:Q:129:THR:OG1	11:Q:179:SER:O	2.24	0.55
32:F:50:GLU:HA	32:F:53:LEU:HB2	1.89	0.55
42:z:147:LYS:HA	42:z:150:TYR:HB2	1.89	0.55
29:B:156:ARG:NH2	29:B:158:GLN:OE1	2.40	0.55
9:2:511:A:H5"	16:W:172:VAL:HG23	1.88	0.54
19:Z:17:ALA:HB3	19:Z:81:VAL:HA	1.89	0.54
31:D:42:ALA:HB1	31:D:47:GLU:HG2	1.89	0.54
37:L:46:LYS:HE2	37:L:49:ARG:HD2	1.89	0.54
43:x:377:ASP:OD1	43:x:377:ASP:N	2.40	0.54
9:2:916:U:O4	19:Z:41:ARG:NH2	2.40	0.54
35:J:73:VAL:O	35:J:77:ASN:ND2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:x:27:ARG:O	43:x:33:LYS:NZ	2.40	0.54
9:2:65:A:H2	9:2:84:A:H62	1.56	0.54
9:2:1303:U:O2'	9:2:1322:A:OP2	2.25	0.54
9:2:329:G:H5"	15:V:98:LYS:HB3	1.90	0.54
9:2:862:A:OP2	18:Y:64:ARG:NH1	2.38	0.54
10:P:13:ASP:OD1	10:P:179:ARG:NH2	2.41	0.54
13:S:100:ARG:NH1	13:S:118:GLU:OE2	2.41	0.54
43:x:72:ILE:O	43:x:326:ASN:ND2	2.40	0.54
12:R:139:ILE:HD12	12:R:218:ILE:HB	1.89	0.54
9:2:1537:C:OP2	9:2:1572:G:N2	2.41	0.54
12:R:180:ALA:HB1	12:R:184:VAL:HG13	1.90	0.54
9:2:708:C:O2'	9:2:730:G:N7	2.41	0.53
28:A:23:GLU:OE1	30:C:61:TRP:NE1	2.35	0.53
34:I:25:ASN:HB3	37:L:40:VAL:HG11	1.90	0.53
36:K:82:TYR:HB3	38:M:52:PHE:HB3	1.90	0.53
9:2:959:U:H6	18:Y:61:THR:HG23	1.73	0.53
9:2:1356:U:H2'	9:2:1357:A:H8	1.73	0.53
9:2:1584:G:N2	9:2:1611:A:OP2	2.31	0.53
37:L:43:ASP:N	37:L:43:ASP:OD1	2.38	0.53
9:2:652:G:O2'	9:2:683:C:N4	2.41	0.53
30:C:7:ASP:OD1	30:C:7:ASP:N	2.40	0.53
39:N:121:CYS:HB3	39:N:132:LEU:HD21	1.90	0.53
9:2:741:C:O2	47:U:107:ARG:NH2	2.42	0.53
9:2:992:A:O2'	9:2:1785:U:O2	2.25	0.53
36:K:22:ILE:HG22	36:K:118:VAL:HG22	1.90	0.53
47:U:10:SER:OG	47:U:11:GLN:N	2.41	0.53
16:W:109:LEU:HB2	16:W:146:PHE:HB3	1.90	0.53
33:H:100:LEU:N	33:H:118:PRO:O	2.40	0.53
40:O:210:LEU:HD11	40:O:222:LEU:HD12	1.89	0.53
9:2:1039:A:OP1	21:b:22:LYS:NZ	2.39	0.53
9:2:1320:U:O2'	9:2:1322:A:OP1	2.26	0.53
9:2:1459:C:OP2	34:I:138:THR:OG1	2.25	0.53
30:C:1:MET:HB3	30:C:3:MET:HG3	1.91	0.53
14:T:98:ARG:NE	14:T:105:ASP:OD2	2.38	0.53
43:x:495:SER:O	43:x:503:ARG:NH1	2.41	0.53
40:O:123:ILE:HG21	40:O:169:ILE:HG21	1.91	0.53
12:R:170:ILE:HB	12:R:197:TYR:HB2	1.90	0.53
42:z:165:ASN:ND2	42:y:187:PRO:O	2.43	0.52
10:P:105:GLY:N	10:P:135:GLU:OE2	2.41	0.52
34:I:17:LEU:HD21	34:I:66:LEU:HD12	1.91	0.52
41:h:9:LEU:HD12	41:h:53:ILE:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:x:30:PRO:HA	43:x:33:LYS:HD2	1.90	0.52
9:2:1:U:O2	16:W:54:ARG:NH2	2.42	0.52
43:x:556:SER:OG	43:x:557:LEU:N	2.42	0.52
9:2:31:C:O2'	9:2:547:U:OP1	2.27	0.52
40:O:156:VAL:HG12	40:O:169:ILE:HG22	1.91	0.52
9:2:68:A:OP1	14:T:160:ARG:NH2	2.37	0.52
12:R:222:TYR:OH	20:a:11:LEU:O	2.28	0.52
28:A:28:GLU:HA	30:C:58:GLN:HE22	1.75	0.52
40:O:289:ALA:HA	40:O:305:TYR:HA	1.92	0.52
9:2:1340:U:H5"	9:2:1341:A:H5"	1.93	0.52
21:b:90:THR:HG23	21:b:94:LEU:HD12	1.92	0.52
43:x:204:ARG:HE	43:x:206:ILE:H	1.58	0.52
15:V:136:SER:OG	15:V:138:ASN:OD1	2.28	0.51
22:c:69:ARG:HG3	22:c:117:ILE:HG12	1.92	0.51
6:i:43:GLY:HA3	9:2:1757:G:H8	1.74	0.51
9:2:558:U:H1'	42:z:240:GLY:HA2	1.92	0.51
9:2:1429:G:O2'	36:K:72:ASN:ND2	2.43	0.51
10:P:112:THR:HG22	10:P:114:SER:H	1.75	0.51
33:H:77:GLU:O	33:H:81:LYS:NZ	2.39	0.51
34:I:38:VAL:HG23	34:I:42:TYR:HB3	1.91	0.51
13:S:153:ASN:O	13:S:174:LYS:NZ	2.37	0.51
31:D:58:LEU:HD12	31:D:125:ASN:H	1.75	0.51
37:L:67:ASP:O	37:L:70:LYS:NZ	2.43	0.51
46:G:174:PRO:HD3	47:U:79:ARG:HH21	1.75	0.51
9:2:1655:A:N6	9:2:1745:G:O2'	2.39	0.51
11:Q:181:LEU:O	11:Q:185:THR:OG1	2.26	0.51
14:T:164:LYS:NZ	14:T:169:TYR:OH	2.44	0.51
41:h:42:ARG:NH1	41:h:61:ARG:O	2.42	0.51
43:x:169:LYS:NZ	43:x:246:ASP:O	2.42	0.51
9:2:992:A:H2	9:2:1012:U:H3	1.59	0.51
22:c:68:ILE:HD13	26:g:7:SER:H	1.76	0.51
28:A:107:PHE:O	28:A:111:ASN:ND2	2.43	0.51
9:2:845:G:H3'	9:2:846:G:H21	1.76	0.51
15:V:84:HIS:NE2	15:V:97:THR:OG1	2.44	0.51
17:X:77:SER:HB3	17:X:85:VAL:HB	1.92	0.51
14:T:57:ASP:HA	14:T:106:LEU:HA	1.91	0.51
41:h:12:VAL:HG12	41:h:30:VAL:HG12	1.91	0.51
12:R:120:GLU:HG2	12:R:123:GLY:H	1.74	0.51
9:2:65:A:O2'	9:2:67:A:OP2	2.28	0.51
9:2:513:U:H2'	9:2:514:G:C8	2.46	0.51
28:A:130:GLY:O	28:A:194:LYS:NZ	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:2:1558:U:OP1	34:I:122:HIS:ND1	2.44	0.51
18:Y:42:ARG:HG2	18:Y:80:LEU:HD21	1.92	0.51
31:D:60:VAL:HG22	31:D:122:VAL:HG23	1.92	0.51
42:z:154:ARG:NH2	42:y:183:ASP:OD2	2.39	0.51
43:x:86:ARG:HH21	43:x:91:SER:H	1.59	0.51
9:2:65:A:OP1	14:T:136:LYS:NZ	2.40	0.50
33:H:35:CYS:HA	33:H:38:ILE:HG22	1.94	0.50
37:L:96:SER:OG	37:L:97:LYS:NZ	2.41	0.50
40:O:126:SER:OG	40:O:128:ASP:OD1	2.28	0.50
9:2:729:G:OP2	9:2:729:G:N2	2.44	0.50
9:2:1474:G:H2'	9:2:1475:A:H8	1.77	0.50
9:2:1480:G:O2'	32:F:40:GLU:OE2	2.24	0.50
28:A:137:VAL:HB	28:A:185:LYS:HB2	1.93	0.50
9:2:194:U:H2'	9:2:195:G:H4'	1.94	0.50
9:2:1321:A:OP2	10:P:101:ARG:NH2	2.41	0.50
9:2:1292:G:H21	10:P:111:ILE:HD11	1.75	0.50
19:Z:131:GLY:O	24:e:22:ARG:NH2	2.44	0.50
40:O:248:ASN:HD21	40:O:249:ARG:HE	1.57	0.50
43:x:571:THR:OG1	43:x:591:ASP:OD1	2.22	0.50
4:p:202:PHE:HA	4:p:660:TRP:HA	1.94	0.50
9:2:687:G:OP1	21:b:119:LYS:NZ	2.45	0.50
15:V:2:GLY:O	15:V:24:LYS:NZ	2.38	0.50
27:E:30:THR:HG23	27:E:86:VAL:HG21	1.93	0.50
27:E:32:ASP:OD1	27:E:32:ASP:N	2.38	0.50
43:x:418:LYS:HB2	43:x:481:ALA:HB2	1.94	0.50
43:x:418:LYS:HD3	43:x:419:PRO:HD2	1.93	0.50
9:2:142:G:H22	9:2:173:A:H2	1.60	0.50
42:z:184:VAL:HG22	42:y:161:ILE:HG21	1.94	0.50
11:Q:89:ASP:HB3	11:Q:228:LEU:HD21	1.94	0.50
18:Y:91:LEU:HD12	18:Y:125:LEU:HD12	1.94	0.50
34:I:26:ILE:HA	34:I:57:ARG:HH11	1.76	0.50
37:L:54:VAL:HG23	37:L:55:PRO:HD3	1.94	0.50
43:x:311:ARG:O	43:x:315:ASN:ND2	2.44	0.50
9:2:1252:C:OP1	39:N:118:ARG:NH1	2.44	0.50
42:z:179:ASP:HA	42:z:182:ARG:HG2	1.94	0.50
19:Z:22:SER:OG	19:Z:23:PHE:O	2.30	0.49
43:x:265:ARG:NH1	43:x:286:TYR:O	2.42	0.49
9:2:959:U:O2	25:f:30:SER:OG	2.30	0.49
13:S:129:VAL:HG22	13:S:139:VAL:HG12	1.94	0.49
28:A:124:ARG:O	28:A:128:GLU:HB2	2.12	0.49
31:D:81:ASP:N	31:D:81:ASP:OD1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:i:44:ASN:H	9:2:1756:A:H4'	1.78	0.49
15:V:138:ASN:OD1	15:V:138:ASN:N	2.45	0.49
43:x:91:SER:OG	43:x:92:PHE:N	2.46	0.49
9:2:55:A:H5'	23:d:109:LYS:HZ3	1.78	0.49
29:B:29:ILE:HD12	32:F:57:LEU:HD21	1.94	0.49
39:N:132:LEU:HD22	39:N:141:CYS:HA	1.94	0.49
40:O:110:VAL:HA	40:O:126:SER:HA	1.94	0.49
9:2:931:C:H5"	11:Q:116:LYS:HB3	1.95	0.49
9:2:959:U:H5"	18:Y:14:SER:HB3	1.95	0.49
28:A:136:VAL:HG22	28:A:186:VAL:HG22	1.95	0.49
43:x:517:ASN:HB3	43:x:519:LYS:HG2	1.94	0.49
9:2:1095:U:O2'	21:b:19:LYS:NZ	2.44	0.49
9:2:1553:G:N1	9:2:1556:A:OP2	2.46	0.49
43:x:281:LEU:HD12	43:x:314:ILE:HG12	1.94	0.49
9:2:895:G:H1	9:2:917:U:H3	1.59	0.49
9:2:1452:U:OP1	38:M:10:HIS:ND1	2.46	0.49
14:T:43:ASP:OD2	14:T:43:ASP:N	2.44	0.49
16:W:92:LYS:HE2	16:W:95:TYR:HE2	1.76	0.49
30:C:20:VAL:HG12	30:C:67:THR:HG22	1.95	0.49
8:j:32:UNK:O	8:j:47:UNK:N	2.46	0.49
31:D:36:LEU:HD13	31:D:41:LEU:HB2	1.95	0.49
41:h:10:ALA:HB1	41:h:30:VAL:HB	1.93	0.49
42:y:192:SER:O	42:y:196:THR:OG1	2.24	0.49
1:l:296:LEU:HA	1:l:312:GLY:HA2	1.94	0.49
9:2:334:G:O6	15:V:5:ARG:NH2	2.45	0.48
9:2:1027:A:OP1	9:2:1789:G:O2'	2.27	0.48
9:2:1477:G:H2'	9:2:1478:G:C8	2.49	0.48
9:2:554:C:H1'	9:2:555:A:H2	1.78	0.48
28:A:135:GLU:HG2	28:A:153:ALA:HB2	1.95	0.48
32:F:14:LYS:O	32:F:123:ARG:NH2	2.46	0.48
9:2:1258:U:OP1	30:C:1:MET:N	2.37	0.48
9:2:1641:C:H2'	9:2:1642:G:C8	2.48	0.48
13:S:71:LYS:HG3	13:S:91:THR:HB	1.94	0.48
20:a:1:MET:HG2	20:a:9:VAL:HG23	1.95	0.48
29:B:84:LYS:HD3	29:B:92:ARG:HH12	1.78	0.48
40:O:116:ASP:OD2	40:O:120:SER:OG	2.31	0.48
23:d:57:VAL:HB	23:d:60:PHE:HE2	1.78	0.48
9:2:1639:C:H5	9:2:1763:A:H61	1.60	0.48
22:c:56:LYS:HE2	22:c:93:LEU:HG	1.96	0.48
35:J:60:SER:OG	35:J:80:TYR:OH	2.29	0.48
43:x:116:LYS:HD2	43:x:277:VAL:HG21	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:x:370:VAL:HA	43:x:551:ALA:HB3	1.96	0.48
46:G:178:SER:HA	46:G:181:ALA:HB3	1.95	0.48
13:S:94:ALA:HB1	23:d:16:PRO:HB2	1.96	0.48
43:x:540:VAL:HG21	43:x:563:ARG:HD3	1.95	0.48
9:2:1672:G:H2'	9:2:1673:G:C8	2.48	0.48
13:S:78:THR:O	13:S:78:THR:OG1	2.26	0.48
25:f:34:ASP:HB3	25:f:82:LYS:HE3	1.96	0.48
47:U:31:SER:O	47:U:31:SER:OG	2.26	0.48
9:2:190:C:N4	9:2:191:C:O2	2.46	0.48
9:2:1413:U:H3	9:2:1583:A:H5'	1.78	0.48
10:P:127:ARG:NH2	10:P:150:ASP:O	2.47	0.48
18:Y:87:ASP:OD1	18:Y:87:ASP:N	2.45	0.48
19:Z:61:MET:HG2	19:Z:104:ALA:HB2	1.95	0.48
37:L:68:ARG:HG3	37:L:69:LEU:HD22	1.96	0.48
9:2:144:U:O4	14:T:137:ARG:NH2	2.46	0.48
9:2:1486:G:OP1	36:K:64:LYS:NZ	2.46	0.48
24:e:39:MET:HG2	24:e:70:LYS:HG3	1.95	0.48
25:f:67:THR:OG1	25:f:70:LYS:O	2.32	0.48
40:O:217:ASP:OD1	40:O:217:ASP:N	2.47	0.48
20:a:36:VAL:HB	20:a:51:VAL:HG22	1.96	0.47
9:2:1511:U:H2'	9:2:1512:G:H8	1.79	0.47
11:Q:33:LYS:O	11:Q:98:THR:OG1	2.32	0.47
43:x:475:ARG:NH1	43:x:502:GLN:OE1	2.46	0.47
35:J:12:GLN:O	35:J:16:ASN:ND2	2.47	0.47
9:2:78:A:O2'	14:T:173:PRO:O	2.27	0.47
11:Q:127:VAL:HG21	11:Q:173:THR:HG23	1.96	0.47
29:B:49:GLU:OE1	29:B:65:ARG:NH2	2.47	0.47
40:O:172:ALA:HA	40:O:178:VAL:HG12	1.96	0.47
40:O:203:THR:HG21	40:O:244:ALA:HA	1.95	0.47
9:2:486:G:C6	9:2:502:U:O4	2.68	0.47
9:2:1477:G:H2'	9:2:1478:G:H8	1.79	0.47
13:S:174:LYS:HD3	13:S:174:LYS:HA	1.73	0.47
29:B:124:LEU:HD22	29:B:199:ILE:HD13	1.96	0.47
9:2:1534:G:OP2	37:L:74:SER:OG	2.32	0.47
35:J:25:GLN:HG2	35:J:27:LYS:HE2	1.96	0.47
4:p:436:VAL:HA	4:p:456:ARG:HA	1.96	0.47
9:2:1220:C:H2'	9:2:1221:A:H8	1.79	0.47
9:2:1498:G:H5"	35:J:72:GLY:HA3	1.95	0.47
10:P:76:ILE:HD13	10:P:98:ILE:HB	1.97	0.47
33:H:24:LEU:HB3	33:H:34:LEU:HD21	1.96	0.47
35:J:117:SER:HB2	35:J:123:ARG:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:M:15:GLY:O	38:M:18:SER:OG	2.31	0.47
40:O:124:SER:OG	40:O:132:LYS:O	2.33	0.47
9:2:1280:C:H2'	9:2:1281:G:H8	1.79	0.47
23:d:106:GLN:O	23:d:110:GLN:HG2	2.15	0.47
25:f:48:SER:HG	25:f:49:HIS:HD1	1.63	0.47
27:E:85:ILE:HG22	27:E:112:LEU:HD23	1.97	0.47
9:2:836:U:H2'	9:2:837:G:C8	2.50	0.47
9:2:1082:C:H4'	20:a:58:TYR:HE1	1.80	0.47
9:2:1104:U:OP1	22:c:14:LYS:NZ	2.43	0.47
25:f:64:CYS:HB3	25:f:73:LEU:HD23	1.96	0.47
35:J:22:LEU:HB3	35:J:55:TYR:HD1	1.80	0.47
40:O:131:ILE:HB	40:O:144:LEU:HB2	1.96	0.47
47:U:51:VAL:HG23	47:U:53:GLY:H	1.79	0.47
14:T:23:ARG:NE	14:T:41:VAL:O	2.41	0.46
15:V:138:ASN:HA	15:V:141:ARG:HD3	1.97	0.46
27:E:52:LYS:HB3	27:E:80:MET:HE1	1.96	0.46
43:x:180:ILE:HD11	43:x:219:ILE:HD13	1.97	0.46
4:p:625:TRP:HA	4:p:637:TYR:HA	1.97	0.46
9:2:209:U:H2'	9:2:210:A:C8	2.51	0.46
9:2:1195:C:OP1	36:K:77:LYS:NZ	2.44	0.46
9:2:1658:G:O6	9:2:1743:U:O4	2.33	0.46
46:G:126:LEU:HD22	46:G:129:ARG:HH11	1.79	0.46
9:2:696:C:H4'	9:2:697:C:H5'	1.97	0.46
9:2:1331:A:H61	28:A:161:GLY:HA3	1.81	0.46
10:P:89:PHE:O	10:P:93:THR:OG1	2.31	0.46
14:T:20:ASP:OD1	14:T:22:HIS:ND1	2.44	0.46
14:T:159:ARG:HB3	14:T:170:THR:HB	1.96	0.46
30:C:15:LEU:HG	30:C:68:LEU:HD23	1.97	0.46
37:L:95:HIS:ND1	37:L:96:SER:O	2.48	0.46
43:x:17:LYS:HE2	43:x:17:LYS:HB2	1.81	0.46
43:x:225:GLY:HA2	43:x:251:TYR:HB3	1.97	0.46
9:2:207:U:O2	15:V:178:ARG:NH1	2.47	0.46
9:2:1316:G:OP1	33:H:7:LYS:N	2.47	0.46
9:2:1393:C:H2'	9:2:1394:G:H8	1.80	0.46
29:B:41:LYS:HZ3	29:B:69:PHE:HE2	1.63	0.46
9:2:142:G:H5"	14:T:139:ASN:HD21	1.80	0.46
10:P:134:LYS:O	10:P:137:SER:OG	2.33	0.46
25:f:74:SER:O	25:f:77:THR:OG1	2.33	0.46
29:B:200:ASN:HD21	29:B:207:THR:HB	1.80	0.46
43:x:116:LYS:NZ	43:x:246:ASP:OD1	2.48	0.46
6:i:58:MET:O	26:g:3:LYS:NZ	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:2:55:A:OP1	23:d:112:LYS:NZ	2.45	0.46
9:2:514:G:H2'	9:2:515:A:H8	1.80	0.46
9:2:1727:G:N2	15:V:32:GLN:OE1	2.39	0.46
10:P:24:LEU:HA	10:P:24:LEU:HD23	1.84	0.46
12:R:245:ASP:OD1	12:R:245:ASP:N	2.45	0.46
13:S:44:LEU:HD23	13:S:65:LEU:HD21	1.97	0.46
23:d:2:SER:HA	23:d:32:ARG:HH21	1.79	0.46
31:D:128:ALA:HB1	31:D:130:THR:HG23	1.98	0.46
9:2:474:A:OP1	16:W:145:SER:OG	2.30	0.46
9:2:1658:G:N2	9:2:1743:U:O2	2.35	0.46
12:R:120:GLU:OE2	12:R:120:GLU:N	2.47	0.46
13:S:166:SER:HB2	13:S:168:LYS:HG2	1.97	0.46
19:Z:31:THR:HG22	19:Z:38:THR:HA	1.97	0.46
27:E:22:LEU:HA	27:E:25:LEU:HG	1.98	0.46
27:E:81:ARG:NH2	27:E:120:SER:O	2.48	0.46
28:A:29:LEU:HD23	28:A:34:TYR:HB2	1.98	0.46
32:F:64:ASP:OD1	32:F:64:ASP:N	2.38	0.46
37:L:45:GLU:O	37:L:49:ARG:NE	2.42	0.46
40:O:37:SER:OG	40:O:38:ARG:N	2.48	0.46
43:x:209:LEU:O	43:x:229:ARG:NH1	2.47	0.46
47:U:50:ASP:HB2	47:U:56:LYS:HD2	1.97	0.46
9:2:126:A:N6	9:2:263:C:O2'	2.48	0.46
9:2:486:G:O6	9:2:502:U:O4	2.34	0.46
20:a:17:CYS:HB2	20:a:56:SER:HB3	1.97	0.46
43:x:164:ILE:HG23	43:x:241:ASP:HB3	1.98	0.46
9:2:346:G:H5'	17:X:79:LYS:HD2	1.97	0.46
9:2:1716:C:H2'	9:2:1717:G:H8	1.80	0.46
23:d:135:ASP:N	23:d:135:ASP:OD1	2.49	0.46
27:E:86:VAL:H	27:E:89:MET:HE1	1.81	0.46
1:l:55:ILE:HA	1:l:71:SER:HA	1.97	0.46
14:T:23:ARG:HH21	14:T:42:GLY:HA2	1.81	0.46
15:V:184:LEU:HD22	15:V:188:GLU:HG2	1.98	0.46
16:W:103:ASP:OD1	16:W:103:ASP:N	2.49	0.46
25:f:36:LYS:HE2	25:f:43:ILE:HD11	1.97	0.46
43:x:548:ASN:N	43:x:548:ASN:OD1	2.48	0.46
9:2:465:G:O2'	43:x:148:ARG:NH1	2.49	0.45
9:2:1041:G:H2'	9:2:1042:G:C8	2.50	0.45
41:h:8:THR:HG23	41:h:56:LEU:HB3	1.98	0.45
9:2:391:A:OP2	15:V:23:LYS:NZ	2.49	0.45
9:2:1409:G:N7	32:F:114:ARG:NH2	2.63	0.45
31:D:106:ILE:O	31:D:110:GLY:N	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:O:51:ASP:OD1	40:O:51:ASP:N	2.49	0.45
42:z:150:TYR:OH	42:y:164:MET:SD	2.61	0.45
43:x:252:LEU:HD22	43:x:256:GLN:HB3	1.97	0.45
43:x:454:PRO:O	43:x:456:ARG:NH1	2.48	0.45
9:2:279:G:H2'	9:2:280:U:H4'	1.97	0.45
9:2:472:U:O2'	9:2:769:A:N3	2.42	0.45
9:2:554:C:H1'	9:2:555:A:C2	2.50	0.45
9:2:912:U:H5	11:Q:9:LEU:HD12	1.80	0.45
9:2:1488:G:H3'	9:2:1515:A:H61	1.82	0.45
9:2:1591:C:H2'	9:2:1592:A:C8	2.52	0.45
11:Q:61:LEU:HD13	11:Q:96:LEU:HD13	1.98	0.45
11:Q:154:SER:O	11:Q:154:SER:OG	2.30	0.45
19:Z:20:TYR:HB3	19:Z:27:PHE:HB2	1.98	0.45
19:Z:60:ALA:HB1	19:Z:101:ALA:HB2	1.99	0.45
20:a:16:LYS:HG2	20:a:23:ILE:HD13	1.98	0.45
39:N:132:LEU:HD12	39:N:139:LEU:HD23	1.98	0.45
40:O:42:LEU:HB2	40:O:61:PHE:HB2	1.98	0.45
14:T:98:ARG:HH21	14:T:105:ASP:HB3	1.81	0.45
47:U:75:THR:O	47:U:79:ARG:HG2	2.17	0.45
9:2:1466:G:O2'	9:2:1602:C:OP1	2.33	0.45
13:S:252:ARG:HD2	13:S:256:ARG:HH22	1.82	0.45
43:x:380:ILE:HB	43:x:514:ILE:HD13	1.99	0.45
36:K:83:GLU:OE2	36:K:85:ARG:NH2	2.49	0.45
43:x:448:GLN:HA	43:x:451:VAL:HG22	1.98	0.45
9:2:424:C:O2'	9:2:426:G:OP1	2.28	0.45
9:2:1681:A:H8	14:T:65:GLN:HG3	1.81	0.45
13:S:87:MET:HE3	13:S:87:MET:HB3	1.78	0.45
19:Z:111:ARG:NH2	24:e:57:SER:O	2.50	0.45
43:x:242:VAL:HG22	43:x:273:TYR:HB2	1.98	0.45
46:G:137:LYS:HA	47:U:39:ARG:HH12	1.80	0.45
47:U:78:THR:O	47:U:82:GLU:HG3	2.17	0.45
9:2:1003:A:O2'	9:2:1005:A:N7	2.44	0.45
27:E:89:MET:SD	27:E:89:MET:N	2.90	0.45
9:2:591:A:H2'	9:2:592:A:C8	2.52	0.45
9:2:1237:G:H2'	9:2:1238:A:H8	1.82	0.45
43:x:140:TRP:HB3	43:x:160:LEU:HD11	1.99	0.45
9:2:1546:G:N2	34:I:87:ASN:O	2.50	0.45
33:H:75:GLU:O	33:H:79:GLU:HB2	2.17	0.45
40:O:68:VAL:HA	40:O:84:SER:HA	1.99	0.45
42:z:232:LYS:O	42:z:234:LYS:NZ	2.48	0.45
43:x:438:ILE:HD12	43:x:480:LEU:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:U:91:ILE:HG12	47:U:169:PHE:HE1	1.81	0.45
9:2:447:U:O2'	13:S:27:TYR:O	2.31	0.44
9:2:1353:U:H3	9:2:1372:U:H3	1.64	0.44
12:R:45:VAL:HG21	12:R:68:ILE:HG23	1.98	0.44
40:O:177:MET:HG3	40:O:179:LYS:HZ1	1.82	0.44
10:P:16:LEU:HB3	10:P:172:LEU:HD21	1.98	0.44
14:T:157:VAL:HG21	14:T:175:ILE:HD11	1.99	0.44
9:2:332:U:P	15:V:56:ARG:HH22	2.40	0.44
9:2:385:A:H5"	15:V:22:ARG:HG3	1.99	0.44
9:2:1171:A:H2'	9:2:1172:G:C8	2.52	0.44
30:C:35:ILE:HG22	30:C:37:THR:H	1.82	0.44
9:2:78:A:H1'	14:T:175:ILE:HG12	2.00	0.44
9:2:258:C:O2	15:V:178:ARG:NH1	2.50	0.44
9:2:331:A:H5'	15:V:33:PRO:HA	1.99	0.44
9:2:846:G:OP2	9:2:846:G:N2	2.47	0.44
9:2:1188:G:O2'	9:2:1430:U:OP1	2.30	0.44
9:2:1727:G:H2'	9:2:1728:A:C8	2.53	0.44
27:E:82:ASN:OD1	27:E:82:ASN:N	2.50	0.44
29:B:57:SER:HB2	29:B:167:ARG:HH22	1.82	0.44
34:I:61:LEU:HD23	34:I:61:LEU:HA	1.88	0.44
36:K:70:THR:OG1	36:K:72:ASN:O	2.24	0.44
9:2:581:U:OP2	28:A:143:ARG:NH2	2.51	0.44
9:2:885:G:N2	19:Z:123:SER:O	2.50	0.44
9:2:1585:U:H3	9:2:1611:A:H2	1.65	0.44
9:2:1611:A:O2'	29:B:95:ASN:O	2.35	0.44
13:S:199:GLU:OE1	13:S:201:HIS:NE2	2.50	0.44
33:H:36:ASP:OD1	33:H:47:ARG:NE	2.41	0.44
35:J:109:GLU:HG3	35:J:114:VAL:HG13	1.99	0.44
9:2:1202:A:N6	9:2:1457:C:OP1	2.50	0.44
9:2:1213:G:O2'	9:2:1244:A:N7	2.46	0.44
9:2:1628:U:H2'	9:2:1629:G:C8	2.53	0.44
31:D:29:LYS:HG3	31:D:100:TRP:HB3	1.99	0.44
33:H:25:THR:OG1	33:H:27:ASP:OD1	2.32	0.44
37:L:54:VAL:HB	37:L:89:ILE:HD11	1.99	0.44
42:z:165:ASN:HD22	42:y:187:PRO:HB2	1.83	0.44
42:z:223:THR:OG1	42:z:224:ALA:N	2.49	0.44
9:2:400:A:H5"	15:V:25:ARG:HA	2.00	0.44
25:f:43:ILE:HD13	25:f:43:ILE:HA	1.85	0.44
28:A:108:LYS:HA	28:A:111:ASN:HD21	1.82	0.44
46:G:290:TYR:HA	46:G:301:TYR:HA	2.00	0.44
9:2:1559:A:H5"	34:I:135:GLY:HA3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:D:75:VAL:HG21	31:D:120:VAL:HG21	2.00	0.44
40:O:211:ILE:HG13	40:O:223:TRP:HB2	1.99	0.44
43:x:418:LYS:HD3	43:x:418:LYS:HA	1.82	0.44
9:2:237:C:O2'	9:2:238:U:O2	2.32	0.44
9:2:1776:A:H2'	9:2:1777:G:C8	2.52	0.44
11:Q:208:GLN:HG3	11:Q:209:ASN:HB2	2.00	0.44
13:S:87:MET:HE2	13:S:123:LEU:HB2	2.00	0.44
34:I:24:GLY:HA2	34:I:58:ALA:HB3	1.99	0.44
40:O:260:ILE:HD12	40:O:274:LEU:HD11	1.99	0.44
9:2:187:G:H3'	15:V:138:ASN:HD21	1.82	0.43
9:2:1677:C:OP1	15:V:42:ARG:NH1	2.46	0.43
13:S:139:VAL:HG13	13:S:150:PRO:HG3	2.00	0.43
14:T:148:SER:N	14:T:151:ASP:OD1	2.42	0.43
33:H:104:ASN:O	33:H:107:SER:OG	2.32	0.43
40:O:110:VAL:HG12	40:O:126:SER:HB3	2.00	0.43
4:p:402:LEU:HA	4:p:421:GLU:HA	2.00	0.43
9:2:929:A:OP1	9:2:931:C:N4	2.46	0.43
9:2:1081:A:H2	9:2:1082:C:H42	1.66	0.43
19:Z:53:ASP:O	19:Z:56:SER:OG	2.34	0.43
21:b:81:VAL:O	21:b:122:SER:OG	2.29	0.43
18:Y:93:LYS:HA	18:Y:96:VAL:HG22	1.99	0.43
29:B:124:LEU:O	37:L:58:ARG:NH1	2.51	0.43
42:z:205:LYS:HE3	42:z:205:LYS:HB3	1.90	0.43
9:2:1253:U:H4'	39:N:143:LYS:HB2	1.99	0.43
12:R:54:GLU:H	12:R:54:GLU:HG2	1.68	0.43
29:B:111:VAL:HA	29:B:114:ILE:HG22	2.00	0.43
9:2:1175:U:H2'	9:2:1176:G:C8	2.52	0.43
9:2:1344:A:H2'	9:2:1345:A:C8	2.53	0.43
10:P:66:ALA:HB2	20:a:37:ALA:HB2	2.01	0.43
13:S:151:ASP:HB3	13:S:154:ILE:HG13	2.00	0.43
34:I:17:LEU:O	34:I:20:THR:OG1	2.34	0.43
42:z:154:ARG:HH22	42:y:179:ASP:CG	2.26	0.43
9:2:16:G:H2'	9:2:17:C:C6	2.53	0.43
9:2:1458:G:H21	27:E:126:VAL:HG11	1.84	0.43
18:Y:90:TYR:HA	18:Y:93:LYS:HG2	2.01	0.43
32:F:29:ILE:HG23	32:F:65:ILE:HB	2.00	0.43
35:J:93:HIS:NE2	35:J:95:ASP:OD1	2.51	0.43
40:O:200:ASN:H	40:O:215:GLY:HA2	1.83	0.43
9:2:1587:A:H2'	9:2:1588:G:H8	1.83	0.43
11:Q:123:ALA:HB2	11:Q:165:ARG:HG3	2.00	0.43
15:V:171:SER:HB3	15:V:180:ASP:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:c:59:ILE:HD12	22:c:59:ILE:H	1.83	0.43
34:I:30:TYR:O	34:I:33:THR:OG1	2.35	0.43
9:2:502:U:H2'	9:2:503:G:C8	2.54	0.43
9:2:1381:U:H2'	9:2:1382:A:C8	2.54	0.43
38:M:21:CYS:HB2	38:M:39:CYS:HB3	2.01	0.43
40:O:117:LYS:NZ	40:O:157:VAL:O	2.42	0.43
40:O:216:LYS:HA	40:O:239:GLU:HG2	2.00	0.43
41:h:29:ARG:HD2	41:h:29:ARG:HA	1.76	0.43
9:2:17:C:H2'	9:2:18:C:C6	2.53	0.43
9:2:803:A:O2'	47:U:104:ARG:NH2	2.51	0.43
9:2:1158:C:O2'	9:2:1581:C:OP2	2.33	0.43
22:c:107:PHE:HE2	22:c:120:VAL:HG23	1.84	0.43
27:E:86:VAL:HG13	27:E:88:GLU:H	1.83	0.43
29:B:177:ILE:HD13	29:B:177:ILE:HA	1.89	0.43
43:x:363:GLN:HG2	43:x:366:PHE:H	1.83	0.43
9:2:235:G:H2'	9:2:236:A:H8	1.83	0.43
9:2:259:U:OP2	46:G:44:LYS:NZ	2.52	0.43
12:R:87:GLN:OE1	12:R:96:THR:OG1	2.31	0.43
28:A:143:ARG:HG2	42:z:239:LEU:HD22	2.00	0.43
40:O:172:ALA:HB2	40:O:202:LEU:HD13	2.01	0.43
6:i:44:ASN:N	9:2:1756:A:H4'	2.34	0.42
9:2:163:G:OP2	9:2:163:G:N2	2.44	0.42
9:2:347:G:OP1	17:X:77:SER:OG	2.31	0.42
22:c:141:GLU:OE2	22:c:142:LYS:N	2.50	0.42
40:O:220:ILE:HD11	40:O:240:VAL:HG11	2.00	0.42
9:2:871:G:H2'	9:2:872:G:C8	2.54	0.42
18:Y:93:LYS:HB2	18:Y:93:LYS:HE2	1.85	0.42
21:b:31:SER:H	21:b:34:ILE:HD12	1.84	0.42
21:b:37:PHE:O	21:b:41:MET:HG3	2.19	0.42
22:c:132:LEU:HD23	22:c:132:LEU:HA	1.91	0.42
41:h:29:ARG:NE	41:h:39:THR:OG1	2.51	0.42
9:2:1229:G:H21	9:2:1256:A:H62	1.66	0.42
10:P:167:LYS:NZ	10:P:204:TYR:O	2.52	0.42
14:T:126:ASP:OD2	14:T:126:ASP:N	2.52	0.42
16:W:112:GLN:HG3	16:W:148:VAL:HG21	2.01	0.42
4:p:206:ASP:HA	4:p:655:PHE:HA	2.00	0.42
9:2:1000:C:O2'	9:2:1002:G:N7	2.44	0.42
9:2:1752:U:H2'	9:2:1753:A:C8	2.54	0.42
29:B:198:LEU:HD23	29:B:198:LEU:HA	1.91	0.42
9:2:1368:G:OP1	35:J:69:LYS:NZ	2.45	0.42
9:2:1474:G:H2'	9:2:1475:A:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:32:ILE:HD11	14:T:63:MET:HE3	2.02	0.42
41:h:19:THR:HG1	41:h:20:GLY:H	1.67	0.42
43:x:552:ARG:HE	43:x:553:ALA:H	1.68	0.42
43:x:574:ARG:HA	43:x:574:ARG:HD3	1.85	0.42
9:2:763:G:OP2	16:W:79:ARG:NH1	2.52	0.42
9:2:1487:A:OP1	38:M:34:TYR:OH	2.34	0.42
9:2:1666:U:O4	9:2:1667:A:N6	2.53	0.42
11:Q:70:LEU:HD13	11:Q:84:ILE:HG13	2.01	0.42
14:T:139:ASN:HA	14:T:142:ARG:HB2	2.00	0.42
26:g:41:THR:HA	26:g:45:VAL:HG22	2.01	0.42
9:2:79:C:OP1	14:T:159:ARG:NH2	2.43	0.42
28:A:13:ALA:HA	28:A:16:VAL:HG12	2.02	0.42
34:I:69:ILE:HD12	34:I:69:ILE:HA	1.89	0.42
43:x:360:LYS:HA	43:x:360:LYS:HD2	1.92	0.42
9:2:227:U:O4	9:2:233:C:O2'	2.26	0.42
9:2:284:G:O6	14:T:188:ARG:NH1	2.53	0.42
9:2:959:U:OP1	25:f:30:SER:OG	2.37	0.42
9:2:1515:A:O2'	9:2:1517:U:OP2	2.34	0.42
13:S:240:LYS:HE2	13:S:240:LYS:HB2	1.83	0.42
15:V:32:GLN:HE21	15:V:32:GLN:HB3	1.57	0.42
25:f:36:LYS:HE2	25:f:36:LYS:HB3	1.89	0.42
27:E:86:VAL:HG22	27:E:87:PRO:HD2	2.02	0.42
32:F:24:ALA:HA	32:F:63:ILE:HG22	2.02	0.42
33:H:51:ALA:O	33:H:55:THR:HG23	2.20	0.42
43:x:380:ILE:HB	43:x:514:ILE:HG21	2.02	0.42
9:2:1071:U:H2'	9:2:1072:C:C6	2.55	0.42
28:A:29:LEU:HD11	28:A:58:VAL:HG22	2.00	0.42
34:I:42:TYR:HA	34:I:85:PHE:HE2	1.85	0.42
40:O:127:ARG:HA	40:O:150:TRP:HB2	2.02	0.42
9:2:891:A:H2'	9:2:892:A:C8	2.55	0.42
11:Q:181:LEU:HA	11:Q:181:LEU:HD23	1.82	0.42
12:R:142:GLY:N	12:R:153:SER:O	2.42	0.42
13:S:21:ASP:OD1	13:S:21:ASP:N	2.52	0.42
36:K:58:LEU:HD21	36:K:90:TYR:HE2	1.85	0.42
43:x:229:ARG:HE	43:x:387:ASN:HD22	1.67	0.42
9:2:1280:C:H2'	9:2:1281:G:C8	2.54	0.41
9:2:1658:G:H2'	9:2:1659:A:C8	2.55	0.41
23:d:9:THR:HG22	23:d:25:VAL:HG12	2.02	0.41
28:A:23:GLU:HA	28:A:26:THR:HG22	2.02	0.41
9:2:166:C:O2'	14:T:133:LEU:O	2.35	0.41
9:2:1175:U:H2'	9:2:1176:G:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:2:1228:G:OP2	31:D:119:SER:OG	2.29	0.41
9:2:1530:C:H2'	9:2:1531:G:H8	1.85	0.41
29:B:192:GLU:OE1	37:L:63:SER:OG	2.31	0.41
41:h:19:THR:OG1	41:h:20:GLY:N	2.53	0.41
46:G:136:MET:O	47:U:39:ARG:NH1	2.53	0.41
6:i:71:MET:N	9:2:1756:A:H62	2.19	0.41
9:2:29:U:H2'	9:2:30:G:H8	1.86	0.41
9:2:66:U:H5'	14:T:173:PRO:HA	2.02	0.41
9:2:250:C:H2'	9:2:251:A:H8	1.85	0.41
10:P:118:PRO:HG2	10:P:141:ILE:HD13	2.02	0.41
23:d:37:LYS:HB2	23:d:37:LYS:HE2	1.92	0.41
24:e:57:SER:OG	24:e:59:TYR:O	2.30	0.41
39:N:133:ALA:HB3	39:N:140:TYR:HB3	2.02	0.41
9:2:1534:G:N7	37:L:77:ARG:NH2	2.68	0.41
9:2:1594:G:H5'	38:M:33:LYS:HE2	2.02	0.41
9:2:1610:G:H4'	29:B:98:MET:HE1	2.02	0.41
15:V:155:SER:O	15:V:159:GLN:HG3	2.20	0.41
16:W:148:VAL:HG11	16:W:156:ILE:HD11	2.02	0.41
28:A:93:ASP:OD1	28:A:93:ASP:N	2.53	0.41
29:B:130:ILE:HA	29:B:133:VAL:HG12	2.02	0.41
41:h:65:ARG:NH1	41:h:66:LEU:O	2.44	0.41
42:z:154:ARG:HH12	42:y:179:ASP:HB3	1.86	0.41
43:x:284:LEU:HB3	43:x:314:ILE:HD11	2.03	0.41
1:l:101:PHE:HA	1:l:108:PHE:HA	2.03	0.41
9:2:225:A:H2'	9:2:226:A:C8	2.55	0.41
9:2:1588:G:N2	9:2:1608:U:O2	2.43	0.41
9:2:1684:U:H3	9:2:1717:G:H1	1.68	0.41
10:P:84:ARG:O	10:P:88:LYS:HG2	2.20	0.41
11:Q:92:GLN:HE21	11:Q:97:LEU:HD11	1.86	0.41
14:T:119:GLN:N	14:T:119:GLN:OE1	2.53	0.41
22:c:69:ARG:HA	22:c:69:ARG:HD3	1.86	0.41
23:d:60:PHE:H	23:d:71:GLY:HA2	1.85	0.41
30:C:28:ASN:OD1	38:M:7:TRP:NE1	2.47	0.41
30:C:29:GLN:O	30:C:31:LYS:NZ	2.40	0.41
43:x:180:ILE:HD13	43:x:180:ILE:HA	1.94	0.41
43:x:552:ARG:NE	43:x:553:ALA:H	2.18	0.41
9:2:142:G:H5"	14:T:139:ASN:ND2	2.36	0.41
10:P:41:ARG:HG3	10:P:42:PRO:HD2	2.02	0.41
10:P:119:ARG:NH2	12:R:241:ASP:OD1	2.54	0.41
16:W:89:ASP:OD1	16:W:89:ASP:N	2.47	0.41
18:Y:27:LYS:HE3	18:Y:27:LYS:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:I:11:PHE:HD2	34:I:60:GLU:HB3	1.86	0.41
34:I:50:ALA:HB2	34:I:69:ILE:HD13	2.02	0.41
40:O:31:ASN:HA	40:O:47:LEU:HB2	2.02	0.41
43:x:321:HIS:ND1	43:x:327:LEU:O	2.51	0.41
46:G:57:LEU:HA	46:G:60:LYS:HE3	2.02	0.41
18:Y:4:MET:HE2	18:Y:121:ARG:HG2	2.03	0.41
19:Z:81:VAL:HG11	19:Z:102:LEU:HD13	2.01	0.41
30:C:10:LYS:HZ3	30:C:35:ILE:HG12	1.86	0.41
40:O:112:SER:HB3	40:O:154:VAL:H	1.85	0.41
9:2:891:A:H2'	9:2:892:A:H8	1.86	0.41
13:S:45:ILE:HB	13:S:80:THR:HG22	2.03	0.41
29:B:213:LYS:HA	29:B:213:LYS:HD3	1.84	0.41
30:C:80:LEU:HB2	30:C:82:LEU:HD22	2.03	0.41
47:U:110:GLN:HB3	47:U:111:LYS:H	1.69	0.41
9:2:107:C:H2'	9:2:108:A:H8	1.86	0.41
9:2:1145:U:H5	9:2:1633:A:N1	2.19	0.41
9:2:1198:G:OP1	9:2:1199:G:O2'	2.29	0.41
9:2:1681:A:N6	9:2:1720:G:O2'	2.54	0.41
13:S:94:ALA:HB3	23:d:17:LEU:HD23	2.03	0.41
31:D:45:LEU:O	31:D:49:THR:OG1	2.30	0.41
32:F:28:LEU:H	32:F:64:ASP:HB3	1.86	0.41
33:H:17:ILE:HA	33:H:17:ILE:HD13	1.79	0.41
37:L:39:ALA:HB3	37:L:71:ILE:HG22	2.03	0.41
40:O:19:TRP:HB2	40:O:38:ARG:HD2	2.03	0.41
40:O:124:SER:OG	40:O:134:TRP:NE1	2.40	0.41
42:y:177:ALA:O	42:y:181:ILE:HG12	2.20	0.41
9:2:498:G:O2'	9:2:499:U:O2	2.35	0.40
10:P:56:LYS:HA	10:P:56:LYS:HD2	1.95	0.40
29:B:142:PRO:HG2	29:B:170:GLN:HG2	2.01	0.40
43:x:12:SER:OG	43:x:14:ASP:O	2.36	0.40
9:2:107:C:H2'	9:2:108:A:C8	2.57	0.40
9:2:592:A:O2'	9:2:596:C:OP1	2.36	0.40
9:2:684:A:H2'	9:2:685:A:C8	2.56	0.40
9:2:918:U:H2'	9:2:919:A:C8	2.56	0.40
9:2:1381:U:H4'	36:K:59:PRO:HG3	2.04	0.40
9:2:1650:U:H2'	9:2:1651:A:C8	2.57	0.40
15:V:121:LEU:HD23	15:V:121:LEU:HA	1.88	0.40
24:e:42:ARG:HE	24:e:42:ARG:HB2	1.54	0.40
25:f:82:LYS:HE3	25:f:82:LYS:HB2	1.87	0.40
26:g:43:ARG:HD3	26:g:56:MET:HE2	2.03	0.40
28:A:64:ARG:NH2	30:C:70:GLU:OE2	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:K:108:ILE:HD13	36:K:108:ILE:HA	1.89	0.40
40:O:178:VAL:HG23	40:O:192:PHE:HB2	2.03	0.40
43:x:94:LEU:HD12	43:x:94:LEU:HA	1.93	0.40
43:x:355:SER:OG	43:x:374:GLU:OE1	2.33	0.40
43:x:462:ASP:OD1	43:x:462:ASP:N	2.53	0.40
47:U:38:LEU:HD21	47:U:77:LEU:HD21	2.04	0.40
9:2:238:U:H6	9:2:238:U:H2'	1.72	0.40
9:2:752:A:H3'	13:S:187:ARG:HH12	1.87	0.40
43:x:165:LYS:HZ2	43:x:165:LYS:HG3	1.79	0.40
9:2:1:U:O4	16:W:53:ARG:NH1	2.55	0.40
9:2:1609:U:H5"	32:F:75:VAL:HG12	2.02	0.40
11:Q:121:ILE:HD12	11:Q:207:LEU:HD11	2.03	0.40
28:A:217:ILE:HG22	28:A:219:ALA:H	1.86	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	l	326/347 (94%)	321 (98%)	5 (2%)	0	100	100
2	r	51/274 (19%)	49 (96%)	2 (4%)	0	100	100
3	o	519/964 (54%)	509 (98%)	10 (2%)	0	100	100
4	p	638/763 (84%)	604 (95%)	31 (5%)	3 (0%)	24	60
5	q	628/812 (77%)	601 (96%)	26 (4%)	1 (0%)	43	76
6	i	95/153 (62%)	87 (92%)	8 (8%)	0	100	100
7	m	88/108 (82%)	81 (92%)	5 (6%)	2 (2%)	5	25
10	P	204/252 (81%)	190 (93%)	14 (7%)	0	100	100
11	Q	222/255 (87%)	201 (90%)	21 (10%)	0	100	100
12	R	214/254 (84%)	202 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	S	256/261 (98%)	238 (93%)	18 (7%)	0	100	100
14	T	226/236 (96%)	217 (96%)	9 (4%)	0	100	100
15	V	183/200 (92%)	176 (96%)	7 (4%)	0	100	100
16	W	182/197 (92%)	172 (94%)	9 (5%)	1 (0%)	24	60
17	X	140/156 (90%)	134 (96%)	6 (4%)	0	100	100
18	Y	148/151 (98%)	143 (97%)	5 (3%)	0	100	100
19	Z	125/137 (91%)	111 (89%)	14 (11%)	0	100	100
20	a	85/87 (98%)	75 (88%)	10 (12%)	0	100	100
21	b	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
22	c	142/145 (98%)	135 (95%)	6 (4%)	1 (1%)	18	53
23	d	132/135 (98%)	126 (96%)	6 (4%)	0	100	100
24	e	95/119 (80%)	88 (93%)	7 (7%)	0	100	100
25	f	79/82 (96%)	71 (90%)	8 (10%)	0	100	100
26	g	58/63 (92%)	55 (95%)	3 (5%)	0	100	100
27	E	115/142 (81%)	110 (96%)	5 (4%)	0	100	100
28	A	220/240 (92%)	208 (94%)	12 (6%)	0	100	100
29	B	204/225 (91%)	194 (95%)	10 (5%)	0	100	100
30	C	90/105 (86%)	81 (90%)	9 (10%)	0	100	100
31	D	119/143 (83%)	103 (87%)	16 (13%)	0	100	100
32	F	139/143 (97%)	133 (96%)	6 (4%)	0	100	100
33	H	117/136 (86%)	111 (95%)	6 (5%)	0	100	100
34	I	143/146 (98%)	137 (96%)	5 (4%)	1 (1%)	18	53
35	J	141/144 (98%)	136 (96%)	5 (4%)	0	100	100
36	K	98/121 (81%)	93 (95%)	5 (5%)	0	100	100
37	L	80/108 (74%)	76 (95%)	4 (5%)	0	100	100
38	M	51/56 (91%)	51 (100%)	0	0	100	100
39	N	71/76 (93%)	60 (84%)	11 (16%)	0	100	100
40	O	310/319 (97%)	293 (94%)	17 (6%)	0	100	100
41	h	61/67 (91%)	57 (93%)	4 (7%)	0	100	100
42	y	77/265 (29%)	71 (92%)	6 (8%)	0	100	100
42	z	118/265 (44%)	109 (92%)	9 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	x	578/608 (95%)	549 (95%)	29 (5%)	0	100	100
44	k	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
45	n	16/25 (64%)	16 (100%)	0	0	100	100
46	G	253/307 (82%)	251 (99%)	2 (1%)	0	100	100
47	U	182/190 (96%)	171 (94%)	11 (6%)	0	100	100
All	All	8220/10188 (81%)	7788 (95%)	423 (5%)	9 (0%)	49	80

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	p	392	PRO
7	m	85	ARG
34	I	102	ALA
4	p	536	LYS
22	c	88	PRO
7	m	73	GLU
16	W	169	PRO
4	p	198	VAL
5	q	351	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	
10	P	170/210 (81%)	170 (100%)	0	100	100
11	Q	200/224 (89%)	199 (100%)	1 (0%)	81	89
12	R	175/205 (85%)	175 (100%)	0	100	100
13	S	220/222 (99%)	217 (99%)	3 (1%)	59	80
14	T	189/201 (94%)	189 (100%)	0	100	100
15	V	148/161 (92%)	147 (99%)	1 (1%)	76	86
16	W	156/166 (94%)	156 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	X	126/137 (92%)	126 (100%)	0	100	100
18	Y	127/128 (99%)	127 (100%)	0	100	100
19	Z	90/105 (86%)	88 (98%)	2 (2%)	45	74
20	a	71/74 (96%)	70 (99%)	1 (1%)	59	80
21	b	110/111 (99%)	110 (100%)	0	100	100
22	c	119/120 (99%)	117 (98%)	2 (2%)	53	78
23	d	112/113 (99%)	110 (98%)	2 (2%)	51	77
24	e	82/101 (81%)	81 (99%)	1 (1%)	63	82
25	f	70/71 (99%)	70 (100%)	0	100	100
26	g	50/54 (93%)	50 (100%)	0	100	100
27	E	95/118 (80%)	92 (97%)	3 (3%)	34	67
28	A	182/195 (93%)	181 (100%)	1 (0%)	81	89
29	B	172/191 (90%)	172 (100%)	0	100	100
30	C	78/98 (80%)	78 (100%)	0	100	100
31	D	88/119 (74%)	88 (100%)	0	100	100
32	F	117/119 (98%)	114 (97%)	3 (3%)	40	72
33	H	101/124 (82%)	100 (99%)	1 (1%)	68	84
34	I	127/129 (98%)	126 (99%)	1 (1%)	73	86
35	J	115/116 (99%)	115 (100%)	0	100	100
36	K	93/114 (82%)	92 (99%)	1 (1%)	65	83
37	L	67/89 (75%)	66 (98%)	1 (2%)	57	80
38	M	47/49 (96%)	47 (100%)	0	100	100
39	N	57/66 (86%)	57 (100%)	0	100	100
40	O	250/262 (95%)	250 (100%)	0	100	100
41	h	55/60 (92%)	55 (100%)	0	100	100
42	y	69/221 (31%)	68 (99%)	1 (1%)	59	80
42	z	90/221 (41%)	90 (100%)	0	100	100
43	x	516/537 (96%)	515 (100%)	1 (0%)	87	92
45	n	17/23 (74%)	17 (100%)	0	100	100
46	G	62/282 (22%)	62 (100%)	0	100	100
47	U	163/170 (96%)	163 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4776/5706 (84%)	4750 (100%)	26 (0%)	78 89

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	Q	210	ILE
13	S	40	GLU
13	S	126	VAL
13	S	244	ILE
15	V	73	SER
19	Z	16	VAL
19	Z	61	MET
20	a	11	LEU
22	c	83	VAL
22	c	107	PHE
23	d	5	VAL
23	d	13	ILE
24	e	44	ILE
27	E	20	VAL
27	E	28	MET
27	E	86	VAL
28	A	115	ILE
32	F	53	LEU
32	F	64	ASP
32	F	99	GLU
33	H	62	GLN
34	I	62	THR
36	K	50	LEU
37	L	54	VAL
42	y	167	LYS
43	x	120	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
10	P	28	ASN
10	P	33	GLN
11	Q	92	GLN
11	Q	95	ASN
12	R	59	HIS
12	R	110	HIS

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Mol	Chain	Res	Type
13	S	96	ASN
13	S	98	ASN
13	S	197	HIS
14	T	182	GLN
15	V	88	ASN
15	V	111	GLN
18	Y	58	HIS
18	Y	105	ASN
21	b	12	ASN
21	b	56	HIS
23	d	31	ASN
23	d	34	ASN
25	f	9	HIS
28	A	111	ASN
30	C	58	GLN
31	D	80	ASN
31	D	96	GLN
32	F	32	ASN
32	F	77	GLN
32	F	100	GLN
34	I	13	HIS
34	I	19	ASN
34	I	90	ASN
35	J	101	ASN
36	K	36	ASN
38	M	53	ASN
40	O	101	GLN
40	O	182	ASN
40	O	237	GLN
42	z	165	ASN
43	x	82	HIS
43	x	85	HIS
43	x	127	GLN
43	x	154	ASN
43	x	185	GLN
43	x	228	GLN
43	x	463	GLN

5.3.3 RNA (i)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
9	2	1740/1800 (96%)	459 (26%)	16 (0%)

All (459) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	2	2	A
9	2	4	C
9	2	17	C
9	2	25	C
9	2	26	A
9	2	34	G
9	2	42	G
9	2	45	U
9	2	46	A
9	2	47	A
9	2	56	U
9	2	57	G
9	2	59	C
9	2	60	U
9	2	66	U
9	2	68	A
9	2	73	U
9	2	74	U
9	2	75	U
9	2	76	A
9	2	77	U
9	2	78	A
9	2	100	A
9	2	104	A
9	2	111	U
9	2	114	C
9	2	115	G
9	2	117	U
9	2	126	A
9	2	127	G
9	2	129	U
9	2	140	A
9	2	141	U
9	2	142	G
9	2	143	G
9	2	144	U

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Mol	Chain	Res	Type
9	2	145	A
9	2	146	U
9	2	153	G
9	2	158	U
9	2	161	U
9	2	168	A
9	2	176	C
9	2	178	U
9	2	179	A
9	2	180	A
9	2	187	G
9	2	188	A
9	2	191	C
9	2	192	U
9	2	193	U
9	2	194	U
9	2	195	G
9	2	197	A
9	2	215	A
9	2	217	A
9	2	218	A
9	2	222	A
9	2	223	U
9	2	224	C
9	2	225	A
9	2	227	U
9	2	228	G
9	2	230	C
9	2	232	U
9	2	233	C
9	2	234	G
9	2	235	G
9	2	239	C
9	2	240	U
9	2	241	U
9	2	249	U
9	2	259	U
9	2	260	U
9	2	261	U
9	2	265	A
9	2	266	A
9	2	272	U

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Mol	Chain	Res	Type
9	2	273	G
9	2	277	U
9	2	278	U
9	2	279	G
9	2	280	U
9	2	281	G
9	2	287	G
9	2	302	U
9	2	304	U
9	2	312	A
9	2	313	U
9	2	314	C
9	2	316	A
9	2	321	C
9	2	322	G
9	2	328	A
9	2	333	A
9	2	334	G
9	2	337	G
9	2	338	C
9	2	352	A
9	2	353	A
9	2	359	A
9	2	361	C
9	2	365	G
9	2	370	A
9	2	387	A
9	2	388	G
9	2	393	C
9	2	399	A
9	2	400	A
9	2	401	A
9	2	402	C
9	2	403	G
9	2	404	G
9	2	417	A
9	2	419	G
9	2	423	G
9	2	424	C
9	2	425	A
9	2	426	G
9	2	434	G

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Mol	Chain	Res	Type
9	2	435	C
9	2	436	A
9	2	439	U
9	2	444	C
9	2	445	A
9	2	448	C
9	2	454	U
9	2	460	A
9	2	468	A
9	2	469	C
9	2	473	A
9	2	477	A
9	2	483	A
9	2	484	C
9	2	485	A
9	2	487	G
9	2	490	C
9	2	491	C
9	2	492	A
9	2	493	U
9	2	494	U
9	2	495	C
9	2	496	G
9	2	498	G
9	2	499	U
9	2	500	C
9	2	501	U
9	2	502	U
9	2	504	U
9	2	506	A
9	2	507	U
9	2	510	G
9	2	511	A
9	2	514	G
9	2	519	C
9	2	527	A
9	2	534	A
9	2	538	A
9	2	539	G
9	2	540	G
9	2	541	A
9	2	542	A

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Mol	Chain	Res	Type
9	2	548	G
9	2	549	G
9	2	557	G
9	2	559	C
9	2	565	C
9	2	566	C
9	2	568	G
9	2	571	G
9	2	578	U
9	2	579	A
9	2	580	A
9	2	582	U
9	2	594	A
9	2	595	G
9	2	606	A
9	2	610	G
9	2	611	U
9	2	619	A
9	2	620	A
9	2	621	A
9	2	622	A
9	2	623	A
9	2	624	G
9	2	638	U
9	2	639	U
9	2	640	U
9	2	641	G
9	2	645	C
9	2	647	G
9	2	649	U
9	2	651	G
9	2	654	C
9	2	655	G
9	2	656	G
9	2	677	G
9	2	681	U
9	2	682	C
9	2	683	C
9	2	694	U
9	2	696	C
9	2	698	U
9	2	700	C

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Mol	Chain	Res	Type
9	2	703	G
9	2	704	C
9	2	705	U
9	2	706	A
9	2	707	A
9	2	708	C
9	2	711	U
9	2	712	G
9	2	713	A
9	2	714	G
9	2	730	G
9	2	731	C
9	2	732	G
9	2	733	A
9	2	734	A
9	2	736	C
9	2	737	A
9	2	739	G
9	2	741	C
9	2	742	U
9	2	743	U
9	2	765	G
9	2	766	U
9	2	767	U
9	2	774	A
9	2	775	G
9	2	778	G
9	2	779	U
9	2	780	A
9	2	781	U
9	2	782	U
9	2	783	G
9	2	807	A
9	2	812	A
9	2	813	U
9	2	814	A
9	2	815	G
9	2	816	G
9	2	819	G
9	2	820	U
9	2	821	U
9	2	823	G

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Mol	Chain	Res	Type
9	2	824	G
9	2	825	U
9	2	833	U
9	2	834	G
9	2	840	U
9	2	845	G
9	2	846	G
9	2	850	A
9	2	855	A
9	2	856	A
9	2	863	A
9	2	873	U
9	2	876	G
9	2	886	U
9	2	899	G
9	2	901	G
9	2	902	G
9	2	914	G
9	2	921	U
9	2	926	A
9	2	928	U
9	2	929	A
9	2	932	U
9	2	933	A
9	2	935	U
9	2	942	G
9	2	945	U
9	2	951	A
9	2	960	U
9	2	966	A
9	2	969	C
9	2	970	A
9	2	971	A
9	2	987	G
9	2	988	A
9	2	992	A
9	2	993	A
9	2	1001	A
9	2	1003	A
9	2	1004	U
9	2	1023	A
9	2	1026	A

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Mol	Chain	Res	Type
9	2	1028	C
9	2	1031	U
9	2	1032	G
9	2	1039	A
9	2	1052	U
9	2	1053	G
9	2	1054	U
9	2	1059	U
9	2	1060	U
9	2	1061	A
9	2	1076	A
9	2	1080	U
9	2	1082	C
9	2	1083	G
9	2	1092	A
9	2	1096	C
9	2	1098	U
9	2	1100	G
9	2	1109	G
9	2	1113	A
9	2	1116	A
9	2	1138	A
9	2	1150	G
9	2	1156	C
9	2	1158	C
9	2	1159	C
9	2	1167	G
9	2	1171	A
9	2	1185	U
9	2	1191	U
9	2	1194	A
9	2	1196	A
9	2	1199	G
9	2	1200	G
9	2	1202	A
9	2	1207	C
9	2	1208	A
9	2	1214	U
9	2	1217	A
9	2	1218	G
9	2	1227	A
9	2	1228	G

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Mol	Chain	Res	Type
9	2	1229	G
9	2	1230	A
9	2	1244	A
9	2	1245	G
9	2	1246	C
9	2	1251	U
9	2	1256	A
9	2	1263	G
9	2	1274	C
9	2	1275	A
9	2	1284	C
9	2	1285	U
9	2	1291	G
9	2	1306	C
9	2	1314	U
9	2	1315	U
9	2	1316	G
9	2	1319	A
9	2	1321	A
9	2	1322	A
9	2	1323	C
9	2	1325	A
9	2	1338	C
9	2	1344	A
9	2	1345	A
9	2	1346	A
9	2	1350	U
9	2	1354	G
9	2	1360	A
9	2	1363	U
9	2	1364	G
9	2	1367	G
9	2	1370	U
9	2	1371	A
9	2	1372	U
9	2	1373	C
9	2	1378	U
9	2	1383	G
9	2	1388	A
9	2	1389	C
9	2	1390	U
9	2	1398	U

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Mol	Chain	Res	Type
9	2	1399	C
9	2	1400	A
9	2	1410	A
9	2	1414	U
9	2	1415	U
9	2	1425	A
9	2	1426	C
9	2	1427	A
9	2	1428	G
9	2	1432	U
9	2	1433	G
9	2	1446	A
9	2	1447	C
9	2	1458	G
9	2	1459	C
9	2	1460	A
9	2	1471	A
9	2	1472	C
9	2	1487	A
9	2	1491	U
9	2	1492	A
9	2	1494	C
9	2	1496	U
9	2	1506	G
9	2	1514	U
9	2	1516	A
9	2	1520	U
9	2	1521	G
9	2	1523	G
9	2	1524	A
9	2	1534	G
9	2	1535	U
9	2	1537	C
9	2	1540	G
9	2	1542	G
9	2	1543	A
9	2	1557	U
9	2	1558	U
9	2	1559	A
9	2	1573	A
9	2	1583	A
9	2	1584	G

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Mol	Chain	Res	Type
9	2	1590	G
9	2	1597	A
9	2	1601	G
9	2	1607	G
9	2	1611	A
9	2	1616	G
9	2	1619	C
9	2	1631	A
9	2	1634	C
9	2	1635	A
9	2	1637	C
9	2	1651	A
9	2	1654	G
9	2	1656	U
9	2	1657	U
9	2	1658	G
9	2	1680	G
9	2	1682	U
9	2	1684	U
9	2	1690	G
9	2	1715	G
9	2	1716	C
9	2	1746	A
9	2	1747	G
9	2	1748	G
9	2	1750	A
9	2	1754	A
9	2	1756	A
9	2	1757	G
9	2	1760	G
9	2	1762	A
9	2	1766	A
9	2	1767	G
9	2	1769	U
9	2	1780	G
9	2	1782	A
9	2	1783	C
9	2	1791	A
9	2	1792	G
9	2	1793	G
9	2	1794	A
9	2	1795	U

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Mol	Chain	Res	Type
9	2	1796	C
9	2	1798	U
9	2	1799	U

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	2	59	C
9	2	77	U
9	2	139	C
9	2	280	U
9	2	387	A
9	2	400	A
9	2	639	U
9	2	640	U
9	2	711	U
9	2	928	U
9	2	1226	A
9	2	1274	C
9	2	1344	A
9	2	1382	A
9	2	1636	C
9	2	1791	A

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 85 ligands modelled in this entry, 82 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
51	ADP	x	703	48,43	27,29,29	1.35	4 (14%)	42,45,45	1.91	11 (26%)
50	SF4	x	701	43	0,12,12	-	-	-		
50	SF4	x	702	43	0,12,12	-	-	-		

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
51	ADP	x	703	48,43	-	2/16/32/32	0/3/3/3
50	SF4	x	701	43	-	-	0/6/5/5
50	SF4	x	702	43	-	-	0/6/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	x	703	ADP	C5-C4	4.48	1.47	1.39
51	x	703	ADP	C5-C6	2.66	1.48	1.41
51	x	703	ADP	C8-N7	2.33	1.36	1.31
51	x	703	ADP	C5-N7	-2.21	1.34	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	x	703	ADP	C5-C4-N3	-6.06	118.85	126.75
51	x	703	ADP	N3-C4-N9	4.82	135.03	127.08
51	x	703	ADP	C2-N3-C4	3.77	120.66	111.75
51	x	703	ADP	C4-C5-N7	-3.18	106.75	110.62
51	x	703	ADP	N3-C2-N1	-3.07	123.80	128.60
51	x	703	ADP	C4-N9-C8	2.76	108.71	105.73
51	x	703	ADP	C5-N7-C8	2.72	107.37	103.51
51	x	703	ADP	C3'-C2'-C1'	2.43	106.04	101.43
51	x	703	ADP	C6-C5-N7	2.10	135.94	132.02
51	x	703	ADP	N9-C8-N7	-2.09	111.05	113.91
51	x	703	ADP	PA-O3A-PB	-2.09	125.67	132.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

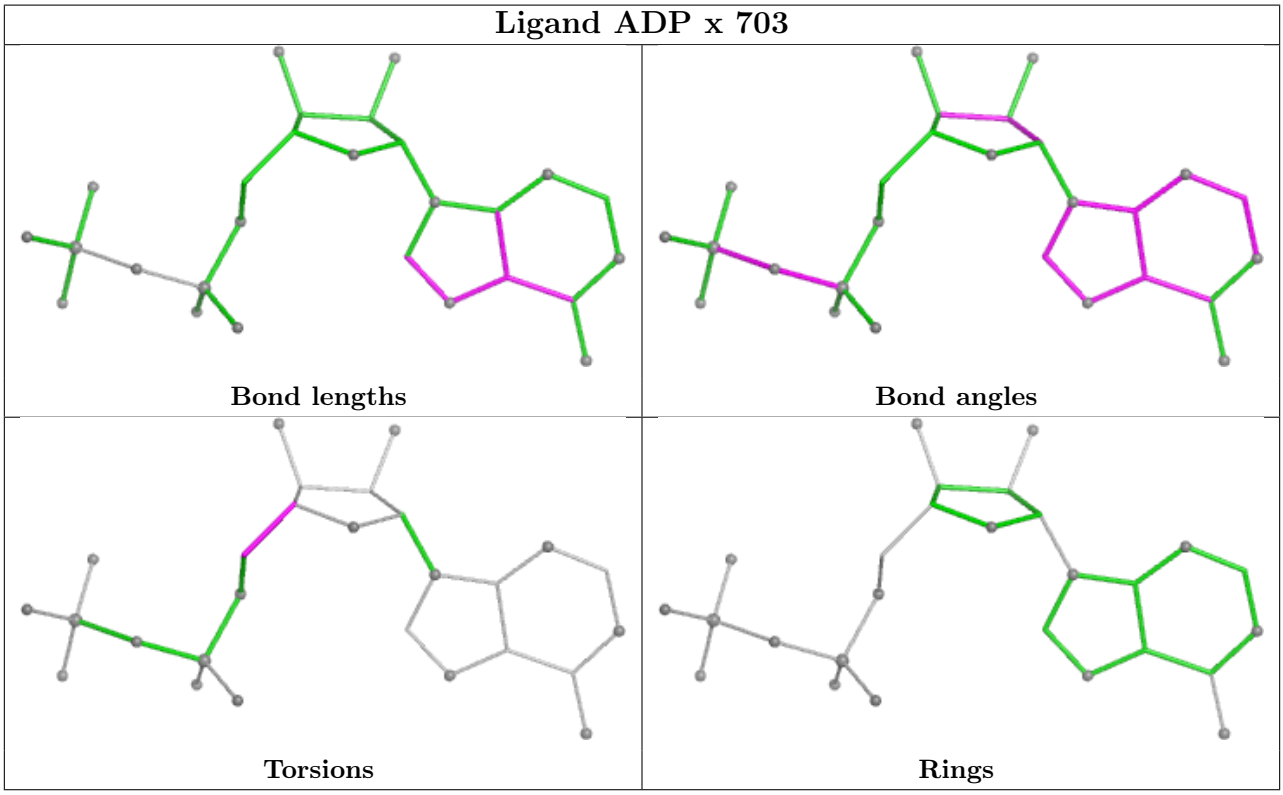
Mol	Chain	Res	Type	Atoms
51	x	703	ADP	O4'-C4'-C5'-O5'
51	x	703	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	x	702	SF4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

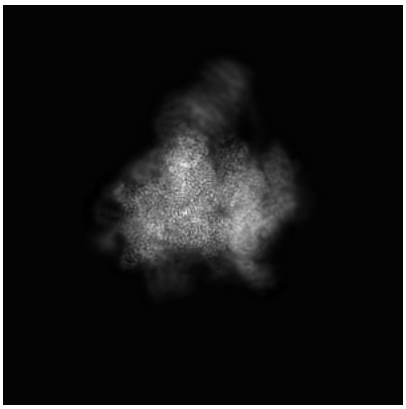
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16525. These allow visual inspection of the internal detail of the map and identification of artifacts.

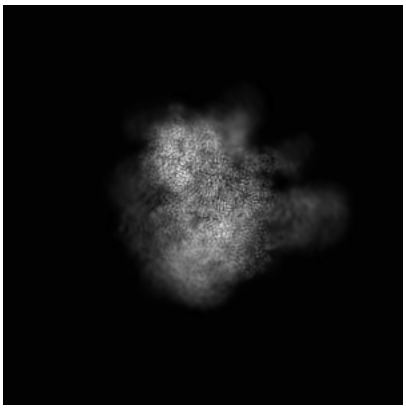
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

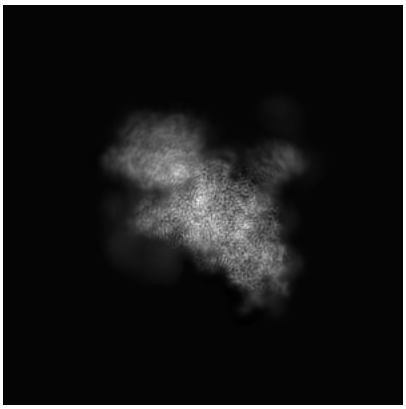
6.1.1 Primary map



X

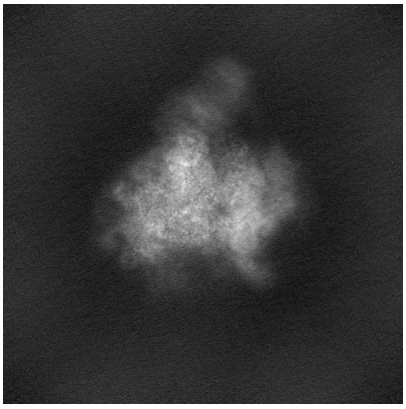


Y

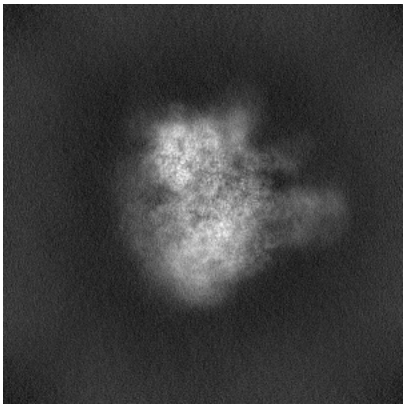


Z

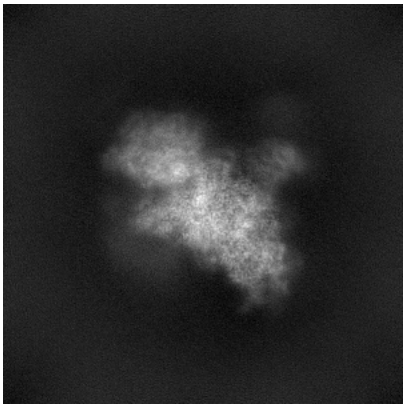
6.1.2 Raw map



X



Y



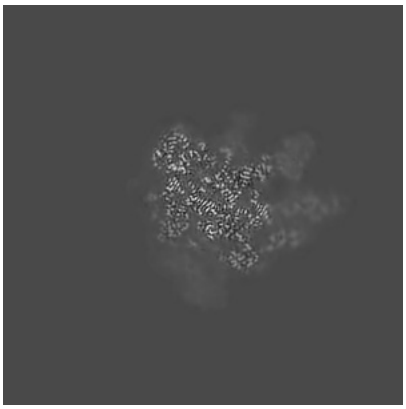
Z

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

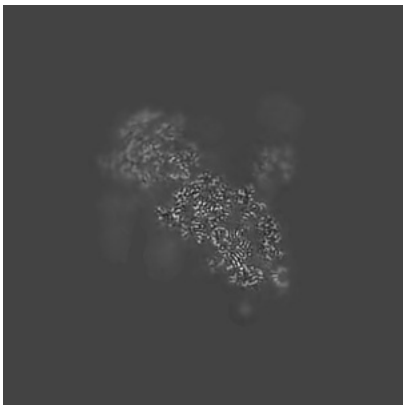
6.2 Central slices (i)

6.2.1 Primary map

X Index: 210

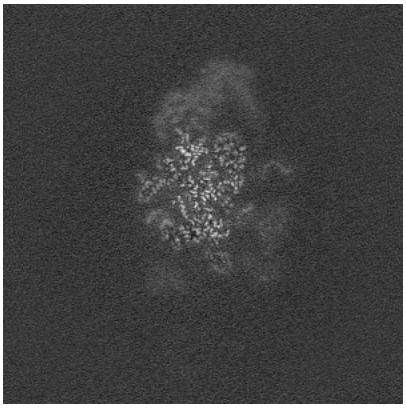


Y Index: 210

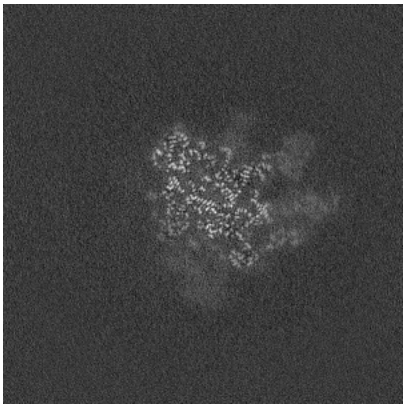


Z Index: 210

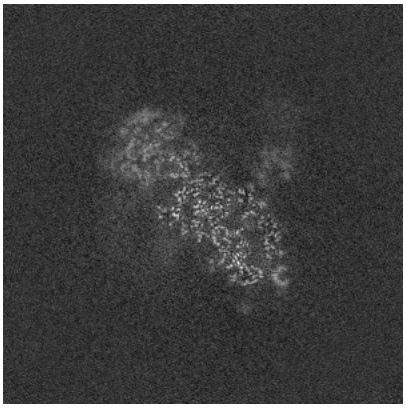
6.2.2 Raw map



X Index: 210



Y Index: 210

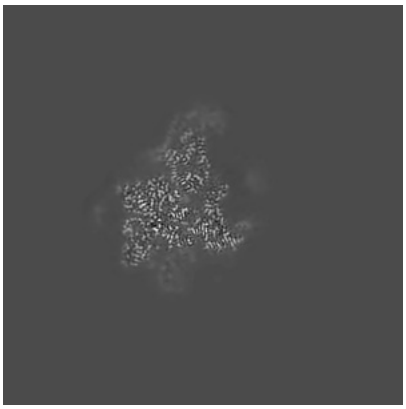


Z Index: 210

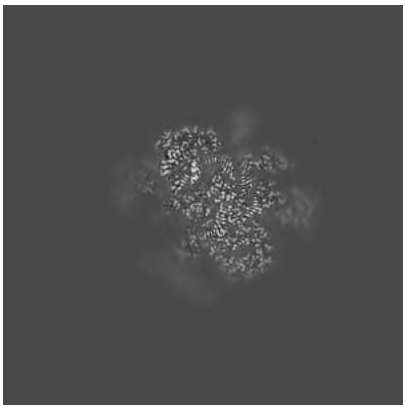
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

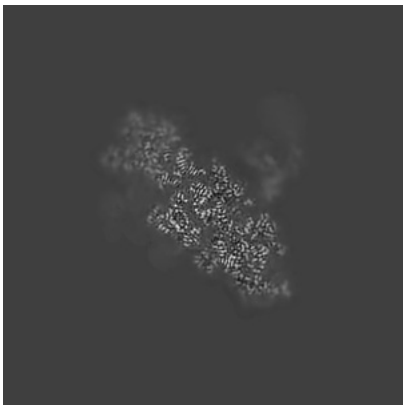
6.3.1 Primary map



X Index: 247

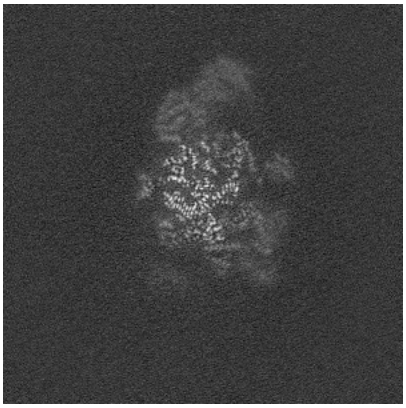


Y Index: 189

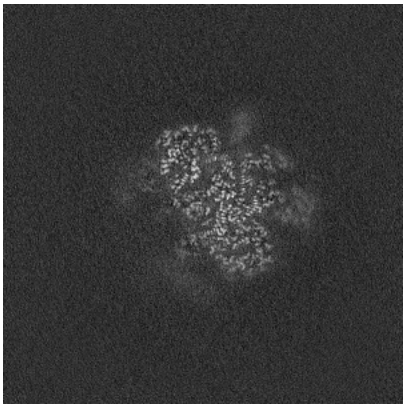


Z Index: 222

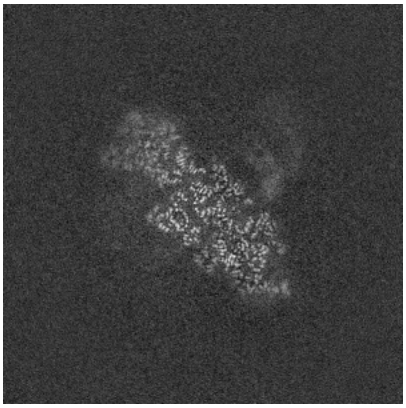
6.3.2 Raw map



X Index: 205



Y Index: 189

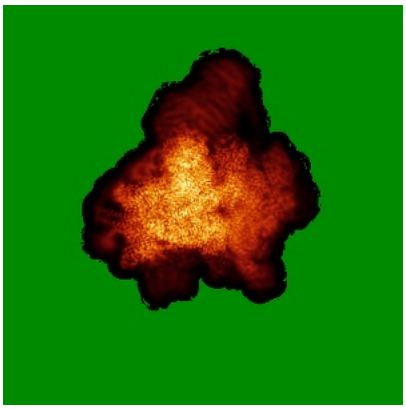


Z Index: 222

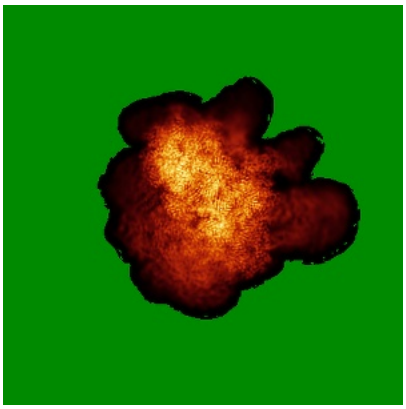
The images above show the largest variance slices of the map in three orthogonal directions.

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

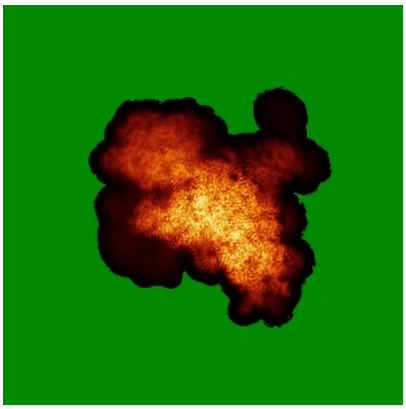
6.4.1 Primary map



X

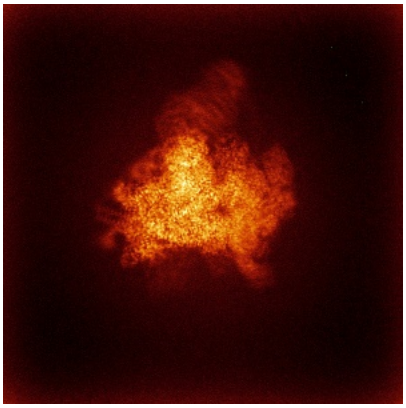


Y

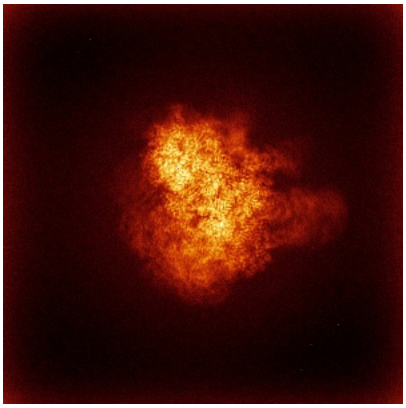


Z

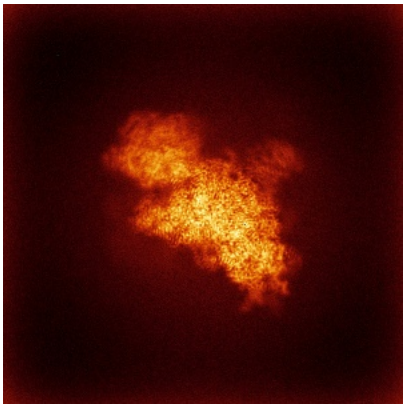
6.4.2 Raw map



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.

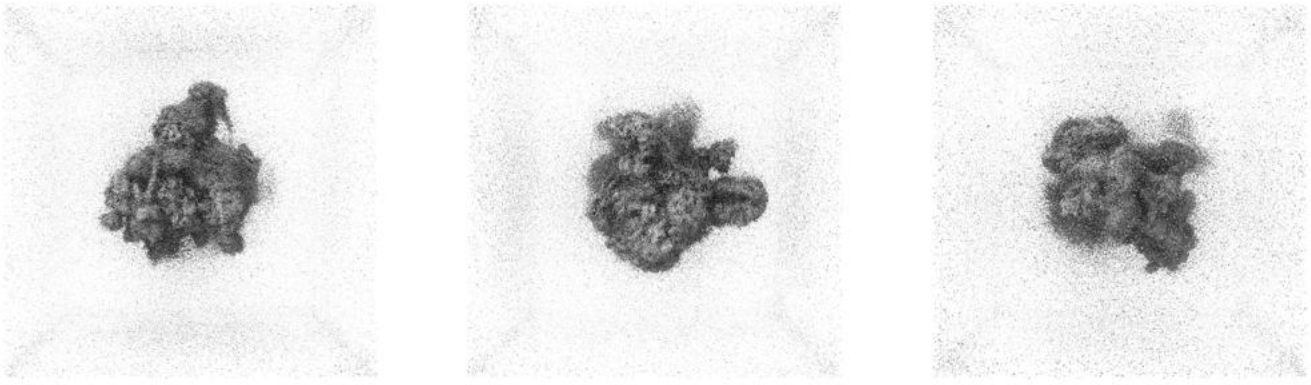
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. 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.

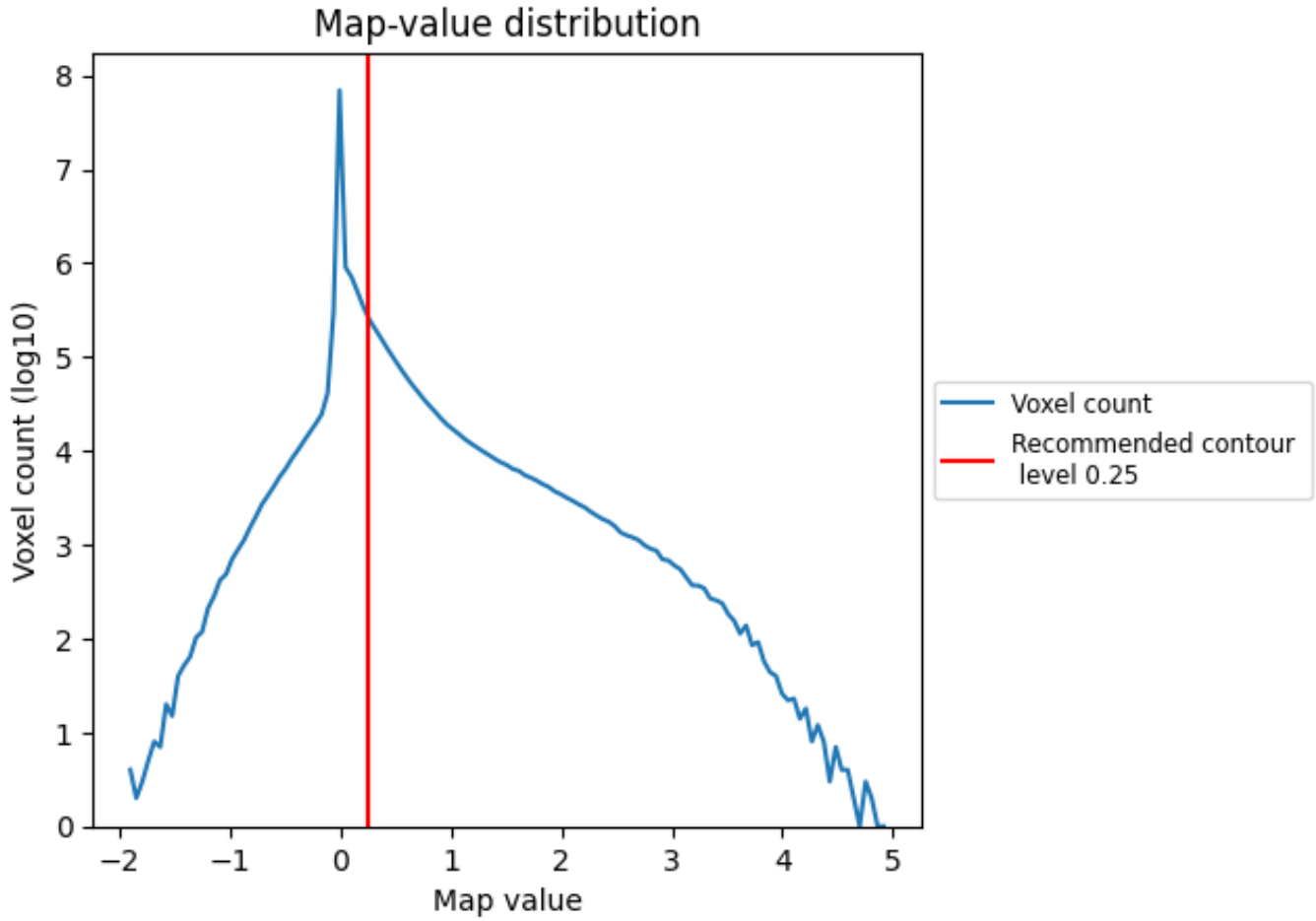
6.6 Mask visualisation (i)

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

7 Map analysis

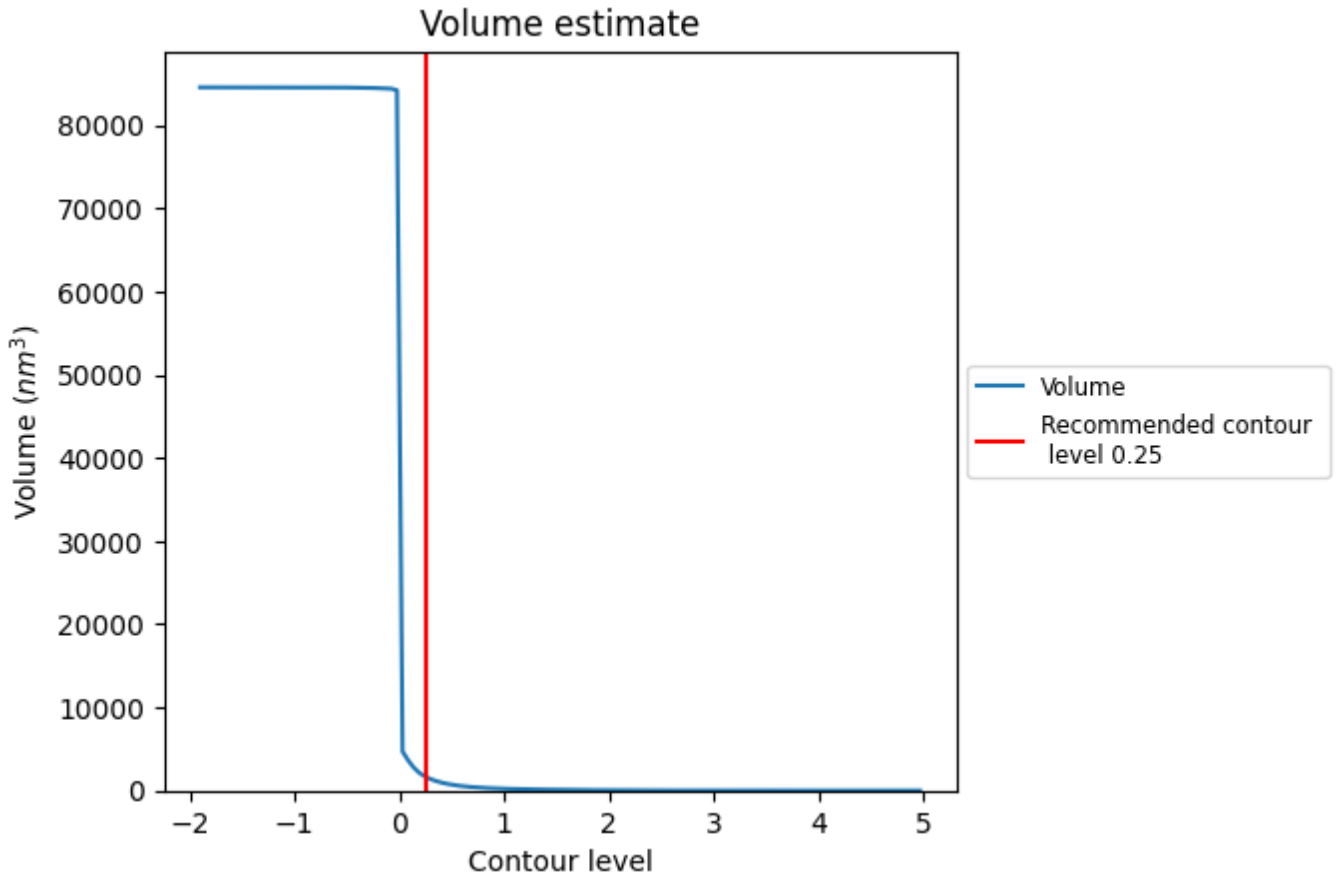
This section contains the results of statistical analysis of the map.

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.

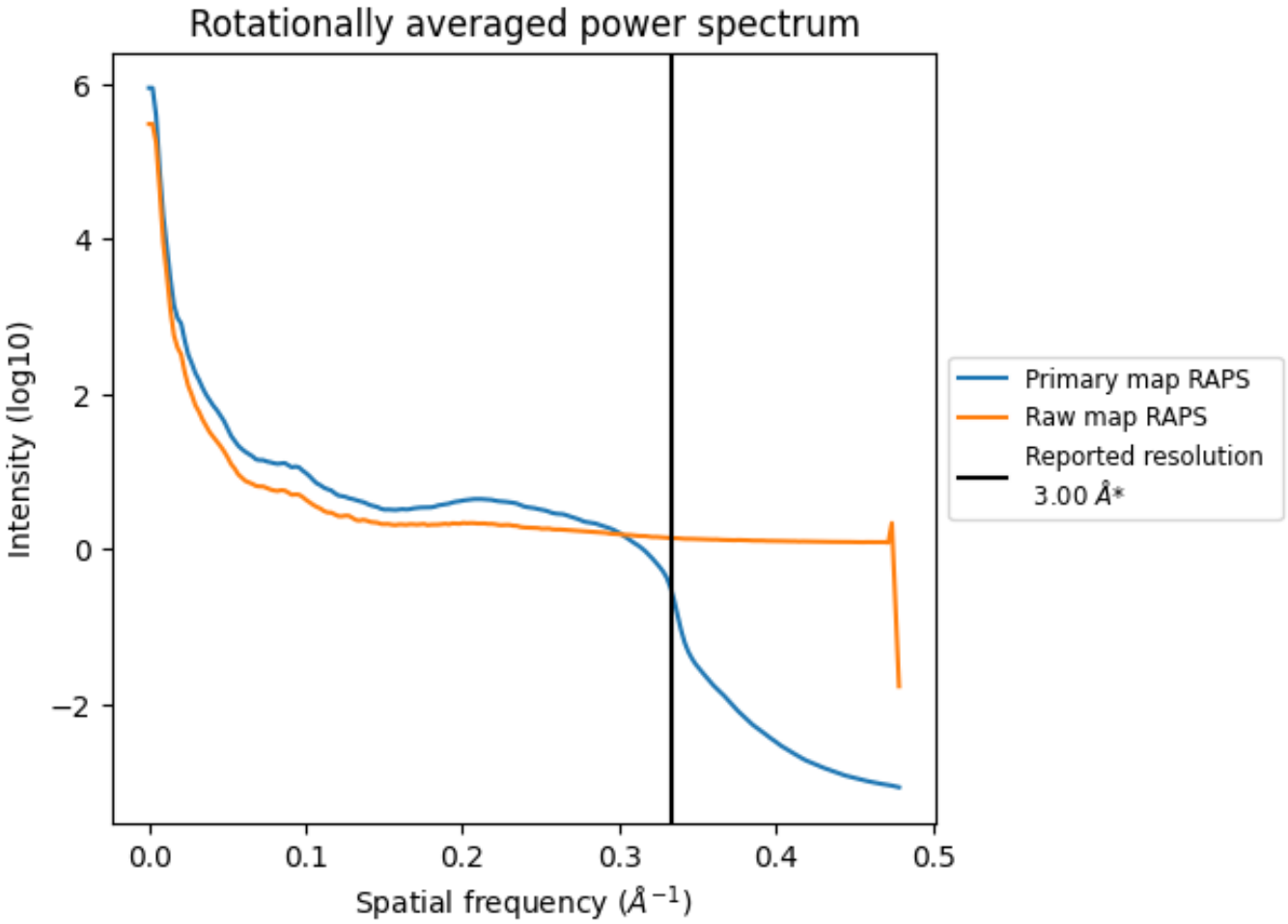
7.2 Volume estimate (i)



The volume at the recommended contour level is 1650 nm^3; this corresponds to an approximate mass of 1491 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)

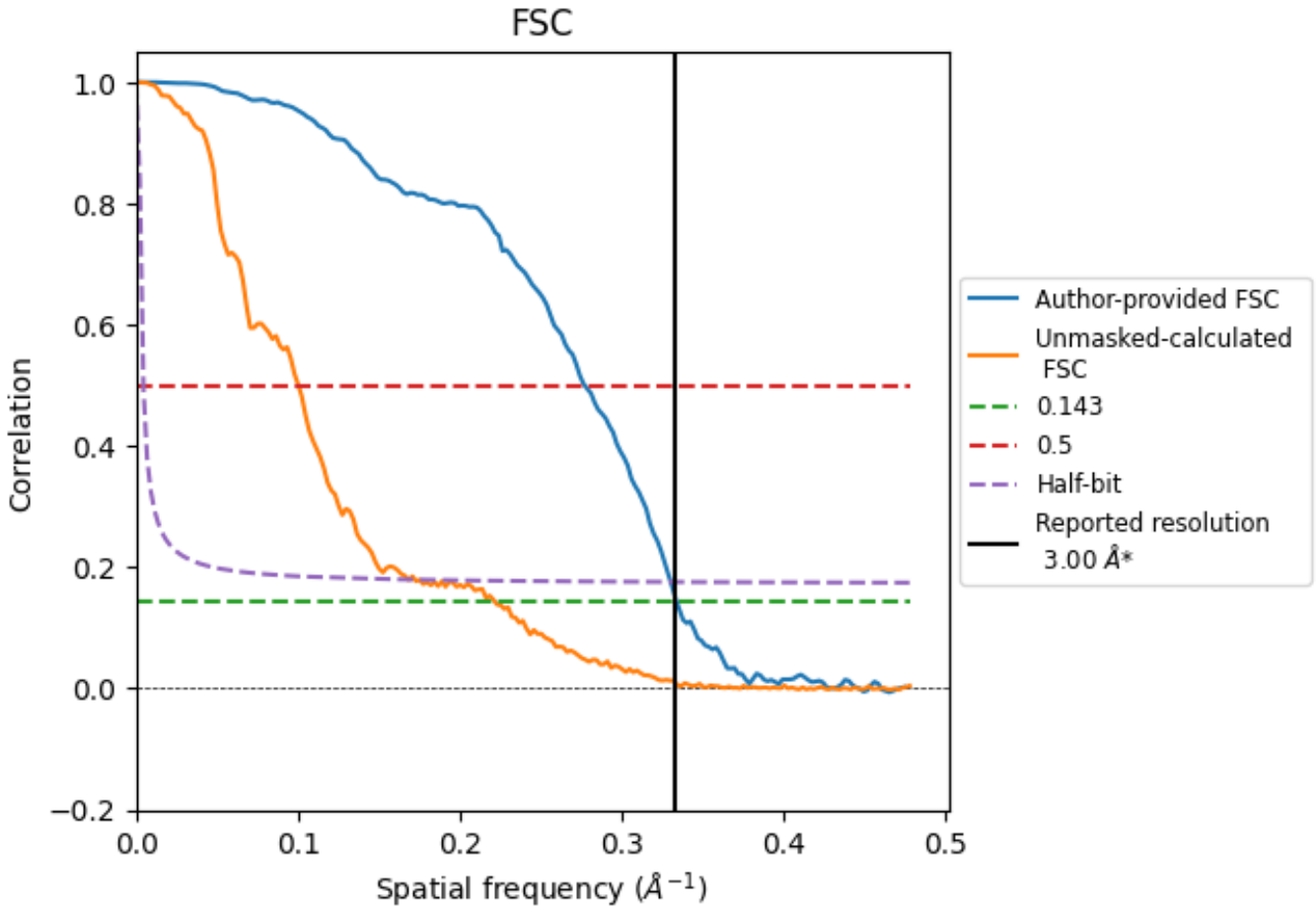


*Reported resolution corresponds to spatial frequency of 0.333 $Å^{-1}$

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 0.333 $Å^{-1}$

8.2 Resolution estimates (i)

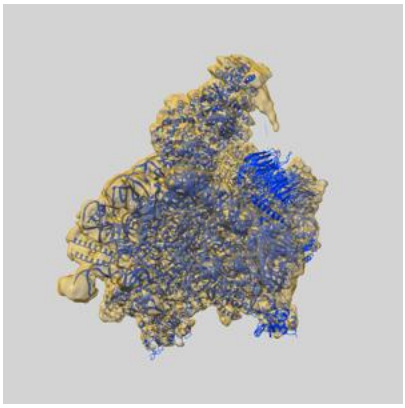
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.99	3.60	3.02
Unmasked-calculated*	4.50	9.97	5.94

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.50 differs from the reported value 3.0 by more than 10 %

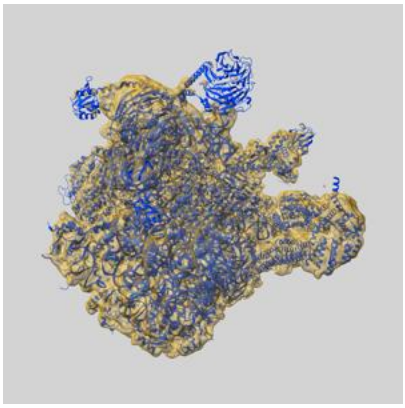
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16525 and PDB model 8CAH. Per-residue inclusion information can be found in section 3 on page 14.

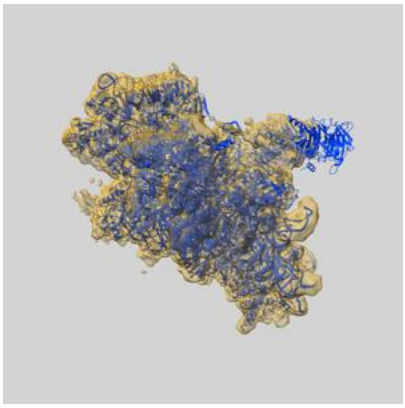
9.1 Map-model overlay



X



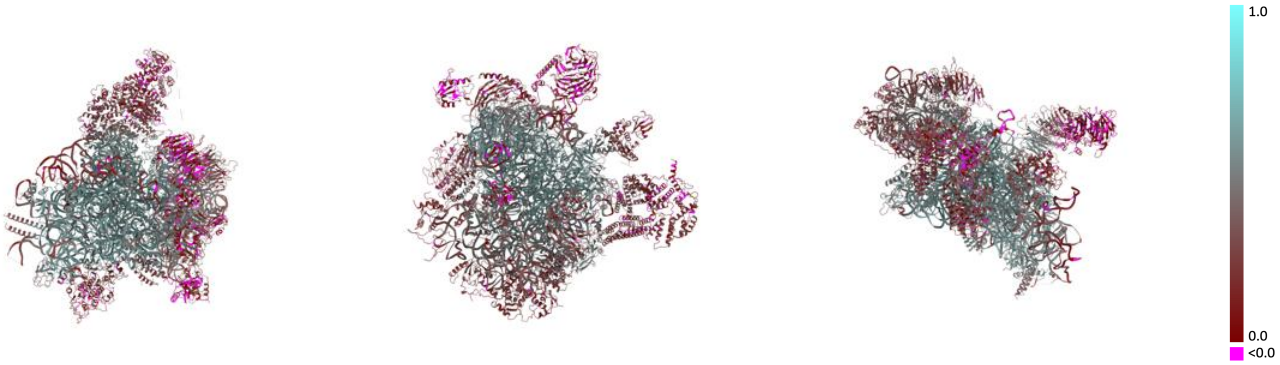
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25 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.

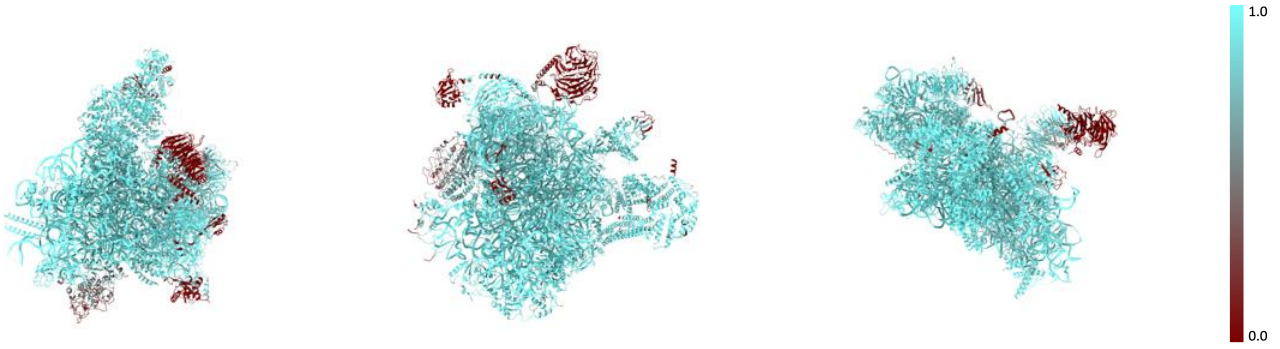
9.2 Q-score mapped to coordinate model (i)



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.

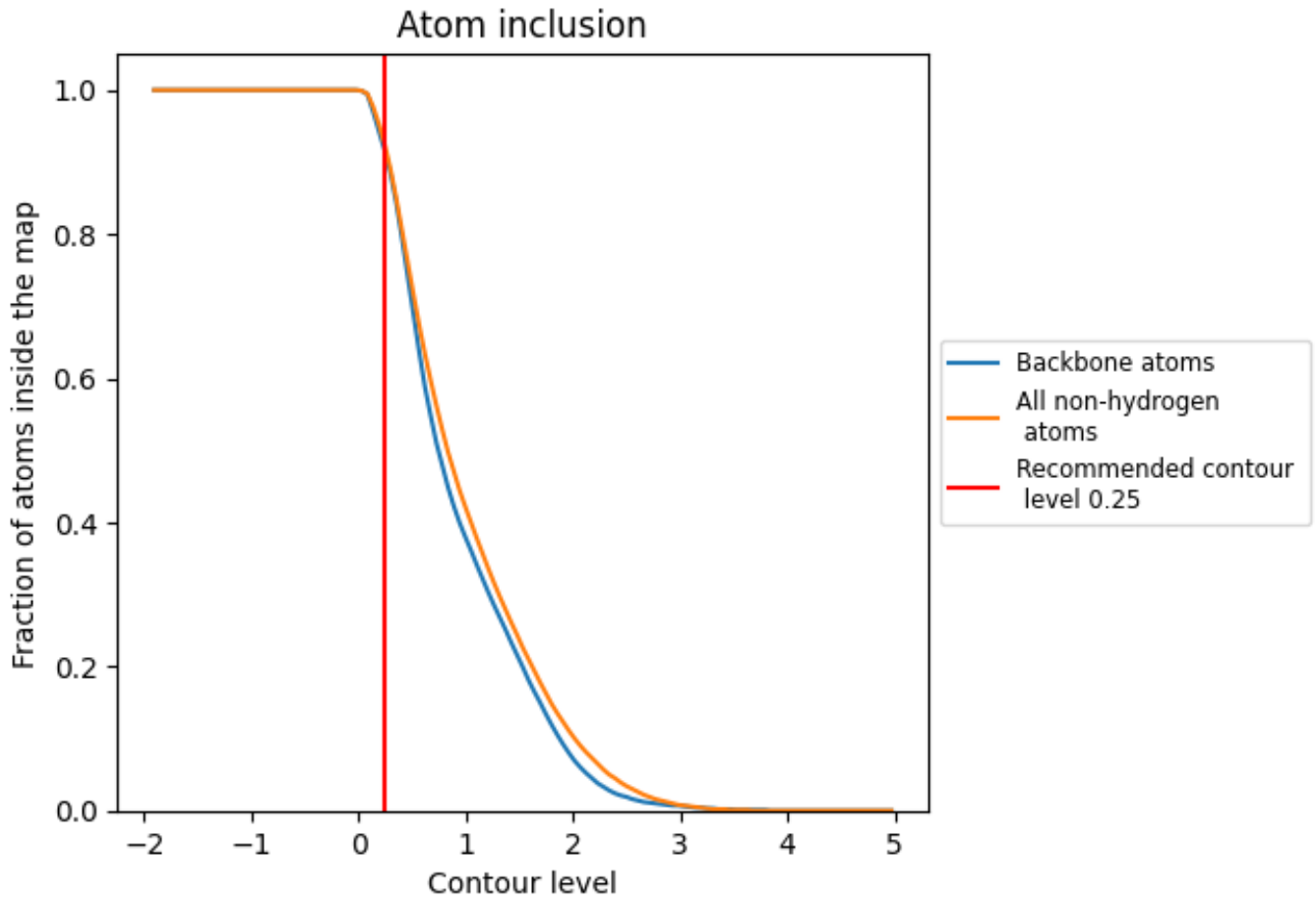
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.25).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 92% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9210	0.4300
2	0.9910	0.5070
A	0.9450	0.4170
B	0.9610	0.3310
C	0.9780	0.3710
D	0.8090	0.1960
E	0.9480	0.2660
F	0.9930	0.3680
G	0.9480	0.3100
H	0.9640	0.4310
I	0.9520	0.2390
J	0.9790	0.2800
K	0.9460	0.3820
L	0.8700	0.1940
M	1.0000	0.4810
N	0.8070	0.1840
O	0.9360	0.2810
P	0.9930	0.5580
Q	0.9810	0.5110
R	0.9940	0.5820
S	0.9960	0.5850
T	0.9830	0.5030
U	0.9770	0.4820
V	0.9940	0.5700
W	0.9820	0.5760
X	0.9870	0.5920
Y	0.9890	0.5620
Z	0.9870	0.5350
a	0.9890	0.5720
b	0.9990	0.6120
c	0.9930	0.5910
d	0.9880	0.5540
e	0.9910	0.5710
f	0.9780	0.5400
g	0.9360	0.4980

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Chain	Atom inclusion	Q-score
h	0.9370	0.3410
i	0.9500	0.4380
j	0.1950	0.0630
k	0.4920	0.1840
l	0.0110	0.0720
m	0.9320	0.3930
n	1.0000	0.5870
o	0.8920	0.1950
p	0.7640	0.2750
q	0.9420	0.2330
r	0.0000	0.1080
x	0.5460	0.2130
y	0.8360	0.3210
z	0.8890	0.3550