



## Full wwPDB EM Validation Report ⓘ

Jun 18, 2026 – 11:39 am BST

PDB ID : 28ZY / pdb\_000028zy  
EMDB ID : EMD-57010  
Title : human 48S PIC with mRNA (Kozak\_2)  
Authors : von Loeffelholz, O.; Barchet, C.; Klaholz, B.  
Deposited on : 2026-03-03  
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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

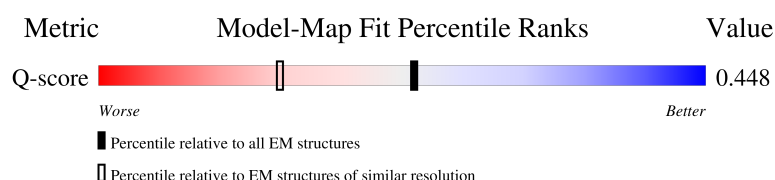
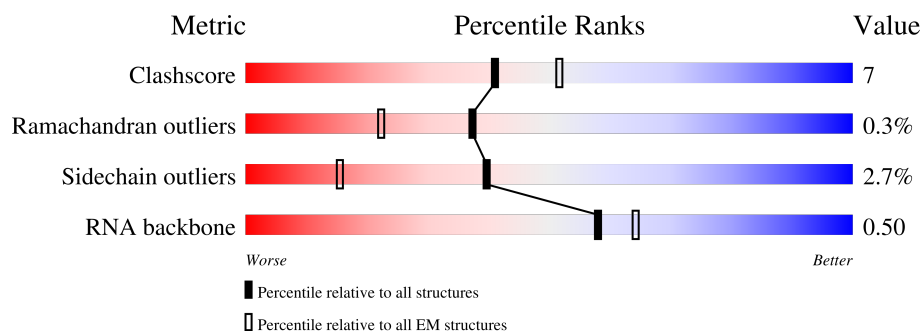
# 1 Overall quality at a glance

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.









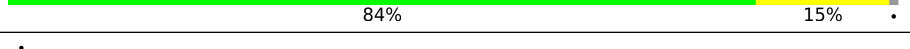
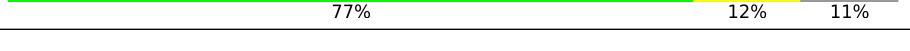
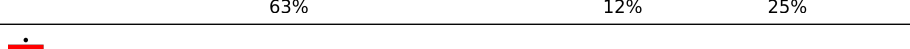
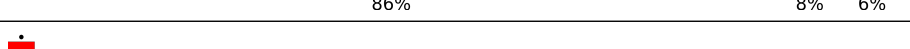
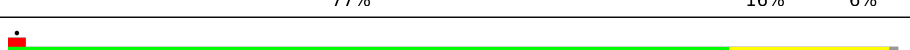

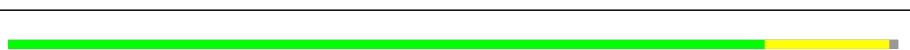

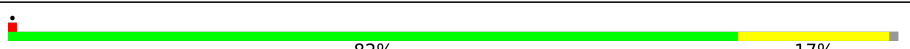





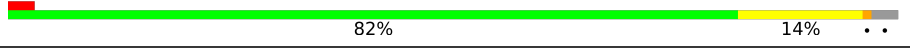
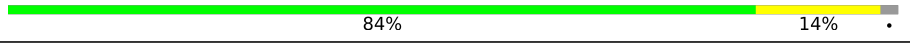



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14081 ( 2.50 - 3.50 )

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	S2	1869	
2	Ln	25	
3	SE	263	

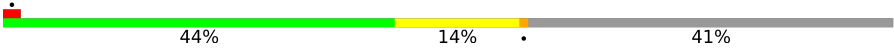





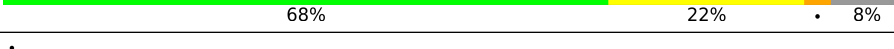
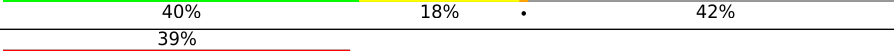
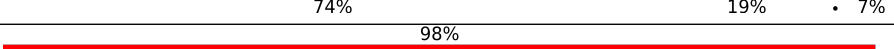
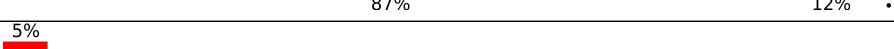
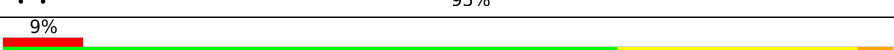

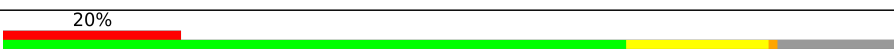

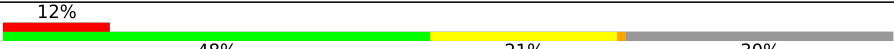




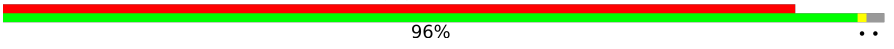
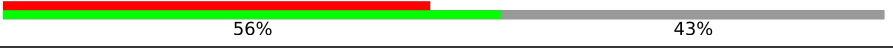

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Mol	Chain	Length	Quality of chain
4	SA	295	
5	SB	264	
6	SH	194	
7	SI	208	
8	SL	158	
9	SV	83	
10	SX	143	
11	Sa	115	
12	SC	293	
13	SG	249	
14	SJ	194	
15	SN	151	
16	SO	151	
17	SW	130	
18	SY	133	
19	Sb	84	
20	Se	133	
21	B	50	
22	SD	243	
23	SF	204	
24	Sf	156	
25	SR	135	
26	Sd	56	
27	Sg	317	
28	Sc	69	

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Mol	Chain	Length	Quality of chain
29	SK	165	
30	SM	132	
31	SU	119	
32	SQ	146	
33	SS	152	
34	ST	145	
35	SP	145	
36	SZ	125	
37	D	315	
38	E	472	
39	F	333	
40	G	75	
41	H	144	
42	e	445	
43	d	548	
44	c	913	
45	a	1382	
46	3f	357	
47	m	374	
48	h	352	
49	k	218	
50	l	564	

## 2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 108768 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	S2	1740	Total	C	N	O	P	0	0
			36955	16511	6600	12105	1739		

- Molecule 2 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ln	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 3 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	SE	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SA	219	Total	C	N	O	S	0	0
			1727	1096	302	320	9		

- Molecule 5 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SB	223	Total	C	N	O	S	0	0
			1806	1145	325	322	14		

- Molecule 6 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SH	189	Total	C	N	O	S	0	0
			1523	972	280	270	1		

- Molecule 7 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SI	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

- Molecule 8 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SL	154	Total	C	N	O	S	0	0
			1258	802	235	215	6		

- Molecule 9 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SV	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 10 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SX	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 11 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Sa	102	Total	C	N	O	S	0	0
			821	512	171	133	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SC	220	Total	C	N	O	S	0	0
			1709	1106	294	299	10		

- Molecule 13 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SG	234	Total	C	N	O	S	0	0
			1903	1188	384	324	7		

- Molecule 14 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	SJ	182	Total	C	N	O	S	0	0
			1512	962	303	245	2		

- Molecule 15 is a protein called 40S ribosomal protein S13.

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

- Molecule 16 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	SO	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 17 is a protein called 40S ribosomal protein S15a.

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

- Molecule 18 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SY	124	Total	C	N	O	S	0	0
			1014	641	198	170	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Sb	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 20 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Se	59	Total	C	N	O	S	0	0
			468	290	102	75	1		

- Molecule 21 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	B	28	Total	C	N	O	P	0	0
			594	267	109	190	28		

- Molecule 22 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	SD	227	Total	C	N	O	S	0	0
			1765	1125	317	315	8		

- Molecule 23 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	SF	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 24 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Sf	63	Total	C	N	O	S	0	0
			515	324	98	86	7		

- Molecule 25 is a protein called 40S ribosomal protein S17.

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

- Molecule 26 is a protein called 40S ribosomal protein S29.

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

- Molecule 27 is a protein called Receptor of activated protein C kinase 1.



Mol	Chain	Residues	Atoms					AltConf	Trace
27	Sg	314	Total	C	N	O	S	0	0
			2440	1537	425	466	12		

- Molecule 28 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Sc	65	Total	C	N	O	S	0	0
			517	314	106	95	2		

- Molecule 29 is a protein called 40S ribosomal protein S10.

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

- Molecule 30 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	SM	118	Total	C	N	O	S	0	0
			906	568	158	172	8		

- Molecule 31 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	SU	102	Total	C	N	O	S	0	0
			811	508	154	145	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	SQ	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 33 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	SS	145	Total	C	N	O	S	0	0
			1198	751	242	203	2		

- Molecule 34 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	ST	143	Total	C	N	O	S	0	0
			1113	698	214	198	3		

- Molecule 35 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	SP	134	Total	C	N	O	S	0	0
			1103	703	208	185	7		

- Molecule 36 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	SZ	73	Total	C	N	O	S	0	0
			585	374	108	102	1		

- Molecule 37 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	D	294	Total	C	N	O	S	0	0
			2367	1487	413	453	14		

- Molecule 38 is a protein called Eukaryotic translation initiation factor 2 subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	E	472	Total	C	N	O	S	0	0
			3585	2272	628	667	18		

- Molecule 39 is a protein called Eukaryotic translation initiation factor 2 subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	F	16	Total	C	N	O	S	0	0
			143	91	25	26	1		

- Molecule 40 is a RNA chain called initiator tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	G	75	Total	C	N	O	P	1	0
			1623	728	299	521	75		

- Molecule 41 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	H	111	Total	C	N	O	S	0	0
			895	556	170	164	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	e	384	Total	C	N	O	S	0	0
			2635	1657	477	489	12		

- Molecule 43 is a protein called Eukaryotic translation initiation factor 3 subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	d	414	Total	C	N	O	S	0	0
			2778	1714	511	544	9		

- Molecule 44 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	c	642	Total	C	N	O	S	0	0
			5197	3274	925	963	35		

- Molecule 45 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	a	589	Total	C	N	O	S	1	0
			4799	3029	865	882	23		

- Molecule 46 is a protein called Eukaryotic translation initiation factor 3 subunit F.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	3f	257	Total	C	N	O	0	0
			1272	757	257	258		

- Molecule 47 is a protein called Eukaryotic translation initiation factor 3 subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	m	350	Total	C	N	O	S	0	0
			1917	1159	376	380	2		

- Molecule 48 is a protein called Eukaryotic translation initiation factor 3 subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	h	317	Total	C	N	O	0	0
			1571	936	317	318		

- Molecule 49 is a protein called Eukaryotic translation initiation factor 3 subunit K.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	k	213	Total	C	N	O	0	0
			1057	631	213	213		

- Molecule 50 is a protein called Eukaryotic translation initiation factor 3 subunit L.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	l	319	Total	C	N	O	0	0
			1581	943	319	319		

- Molecule 51 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
51	S2	17	Total	K	0
			17	17	
51	SX	1	Total	K	0
			1	1	
51	Sd	1	Total	K	0
			1	1	

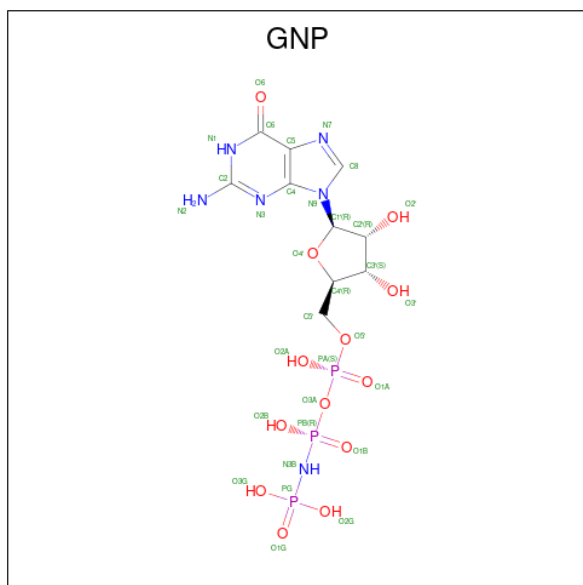
- Molecule 52 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
52	S2	76	Total	Mg	0
			76	76	
52	SE	1	Total	Mg	0
			1	1	
52	SN	1	Total	Mg	0
			1	1	
52	SO	1	Total	Mg	0
			1	1	
52	B	7	Total	Mg	0
			7	7	
52	H	1	Total	Mg	0
			1	1	

- Molecule 53 is ZINC ION (CCD ID: ZN) (formula: Zn).

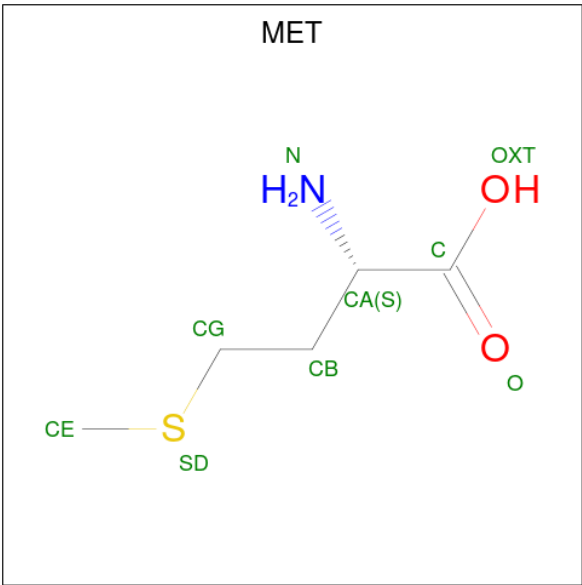
Mol	Chain	Residues	Atoms		AltConf
53	Sa	1	Total	Zn	0
			1	1	
53	Sf	1	Total	Zn	0
			1	1	
53	Sd	1	Total	Zn	0
			1	1	

- Molecule 54 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula:  $C_{10}H_{17}N_6O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					AltConf
54	E	1	Total	C	N	O	P	0
			32	10	6	13	3	

- Molecule 55 is METHIONINE (CCD ID: MET) (formula:  $C_5H_{11}NO_2S$ ).



Mol	Chain	Residues	Atoms					AltConf
55	E	1	Total	C	N	O	S	0
			8	5	1	1	1	

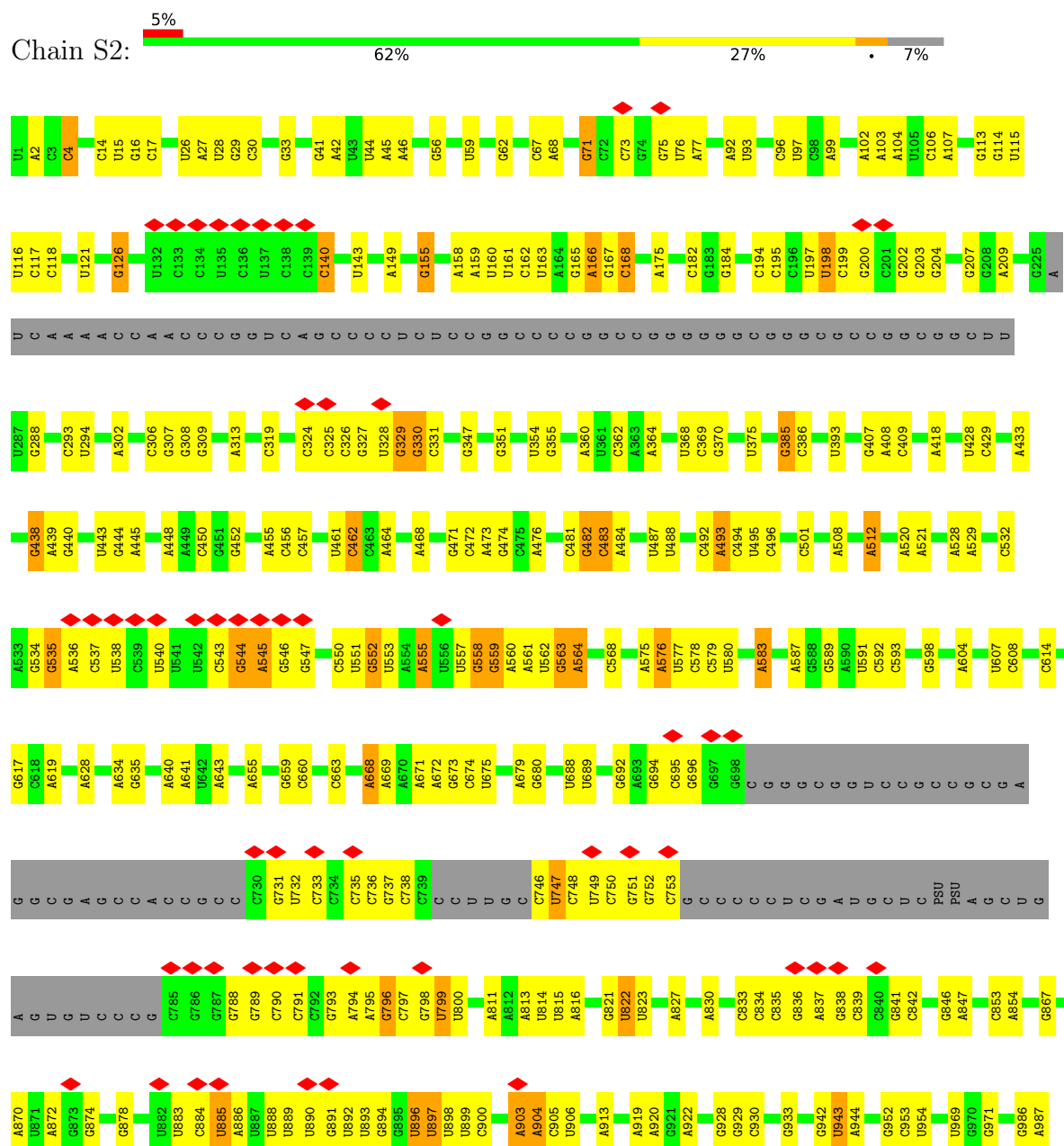
- Molecule 56 is water.

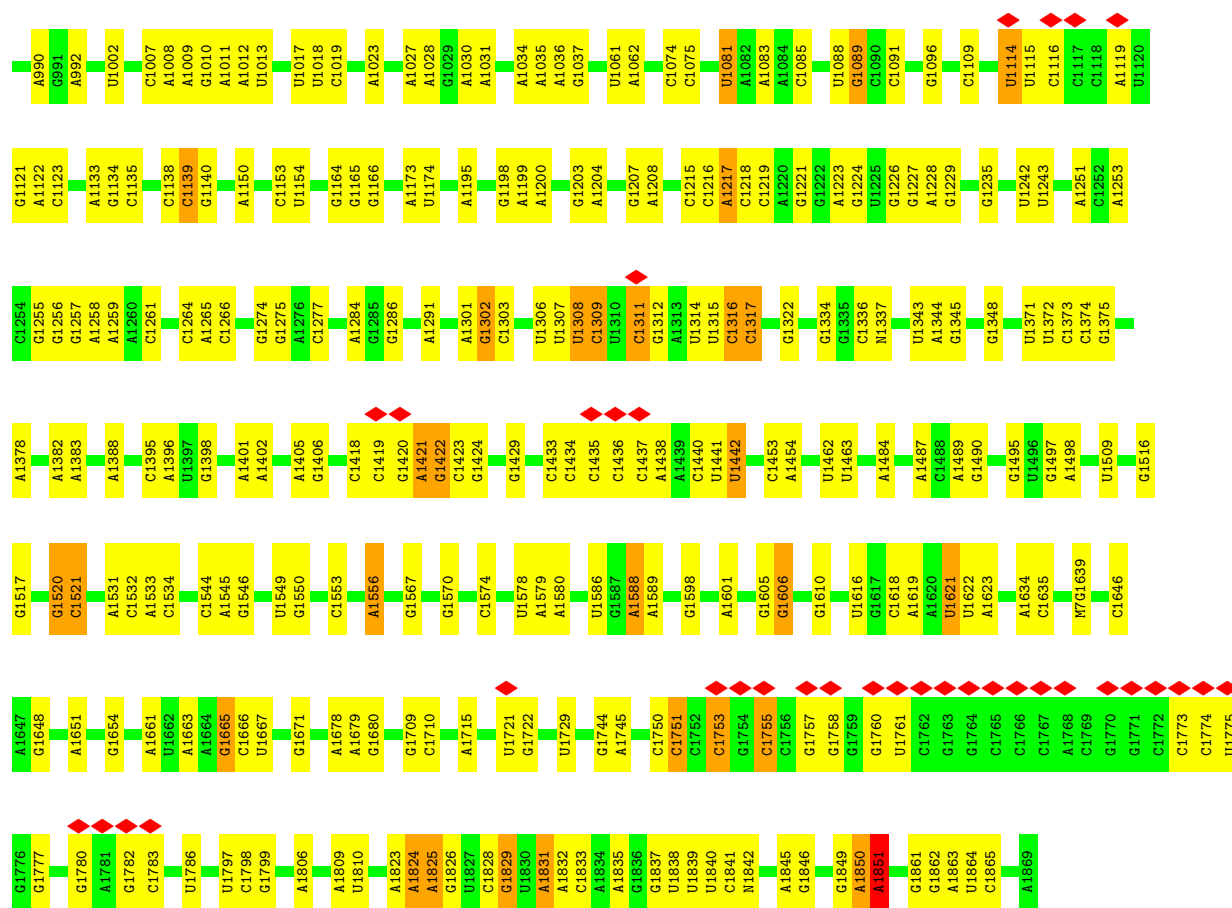
Mol	Chain	Residues	Atoms		AltConf
56	S2	349	Total	O	0
			349	349	
56	SE	1	Total	O	0
			1	1	
56	SB	1	Total	O	0
			1	1	
56	SL	2	Total	O	0
			2	2	
56	Sa	1	Total	O	0
			1	1	
56	SC	1	Total	O	0
			1	1	
56	SN	3	Total	O	0
			3	3	
56	SO	2	Total	O	0
			2	2	
56	SQ	1	Total	O	0
			1	1	
56	SS	1	Total	O	0
			1	1	
56	ST	1	Total	O	0
			1	1	

### 3 Residue-property plots

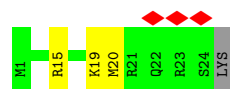
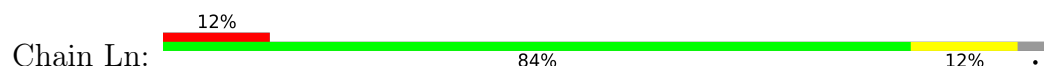
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: 18S ribosomal RNA

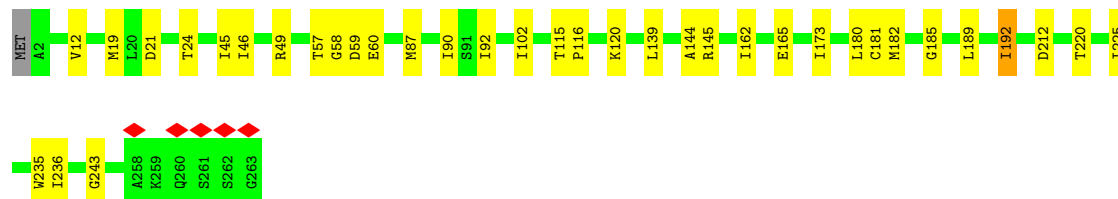
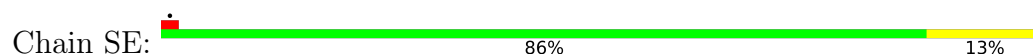




• Molecule 2: 60S ribosomal protein L41



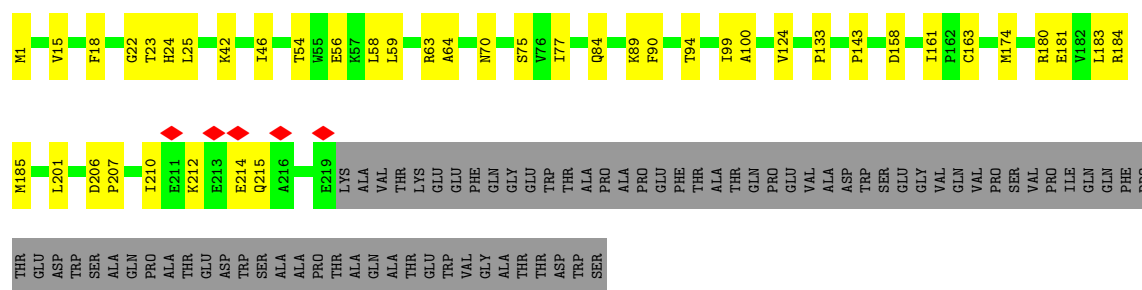
• Molecule 3: Small ribosomal subunit protein eS4, X isoform



• Molecule 4: 40S ribosomal protein SA

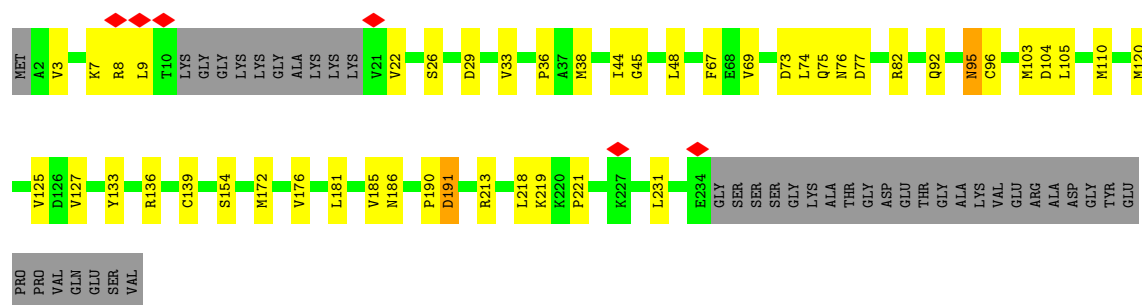






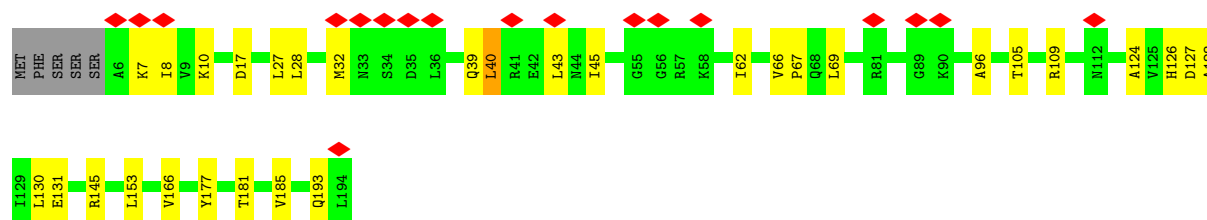
- Molecule 5: 40S ribosomal protein S3a

Chain SB: 67% 17% 16%



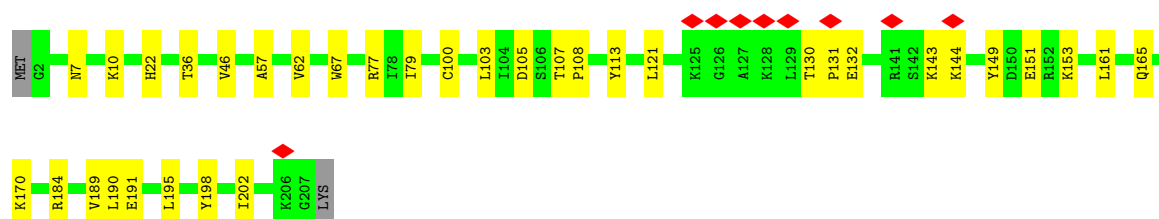
- Molecule 6: 40S ribosomal protein S7

Chain SH: 9% 81% 15%



- Molecule 7: 40S ribosomal protein S8

Chain SI: 82% 17%

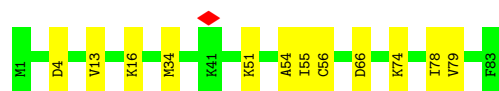
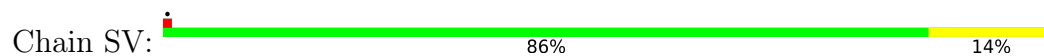


- Molecule 8: Small ribosomal subunit protein uS17

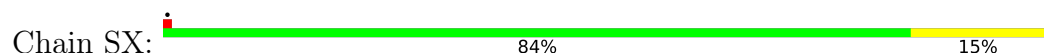
Chain SL: 9% 84% 13%



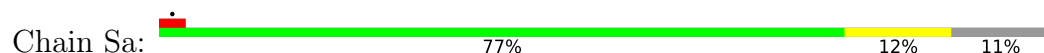
- Molecule 9: 40S ribosomal protein S21



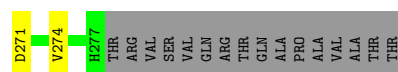
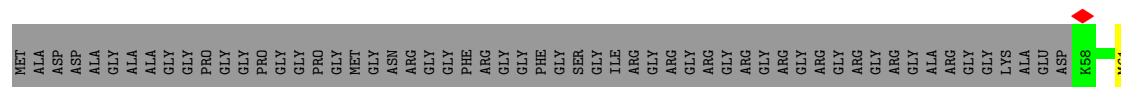
- Molecule 10: 40S ribosomal protein S23



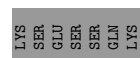
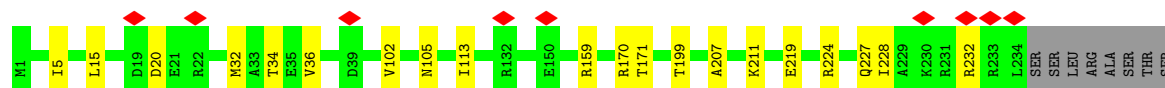
- Molecule 11: 40S ribosomal protein S26



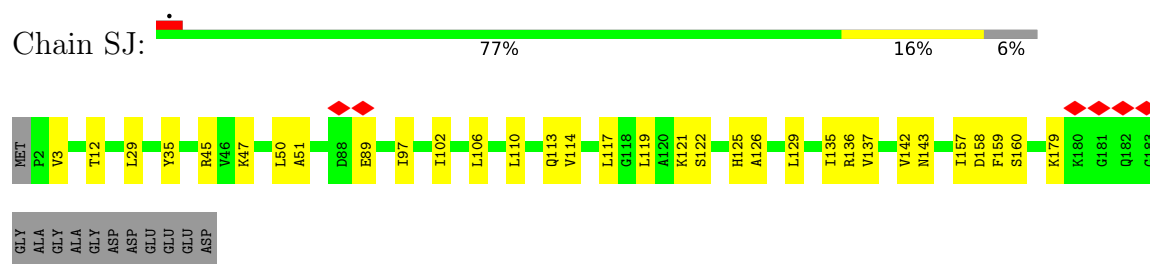
- Molecule 12: 40S ribosomal protein S2



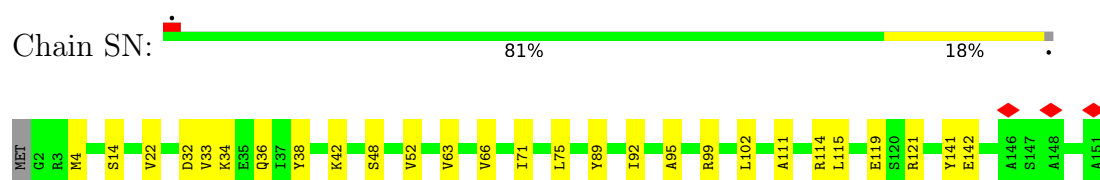
- Molecule 13: 40S ribosomal protein S6



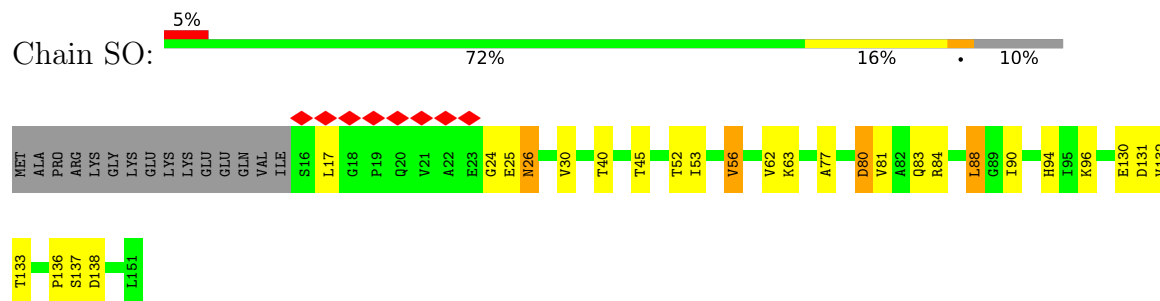
- Molecule 14: 40S ribosomal protein S9



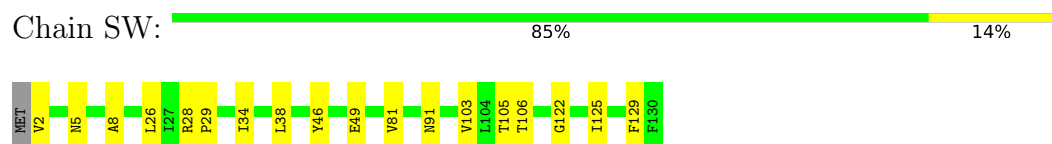
- Molecule 15: 40S ribosomal protein S13



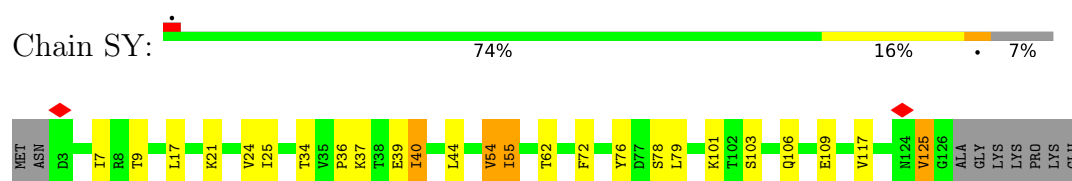
- Molecule 16: 40S ribosomal protein S14



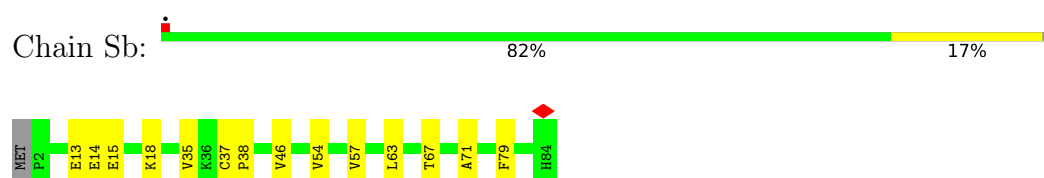
- Molecule 17: 40S ribosomal protein S15a



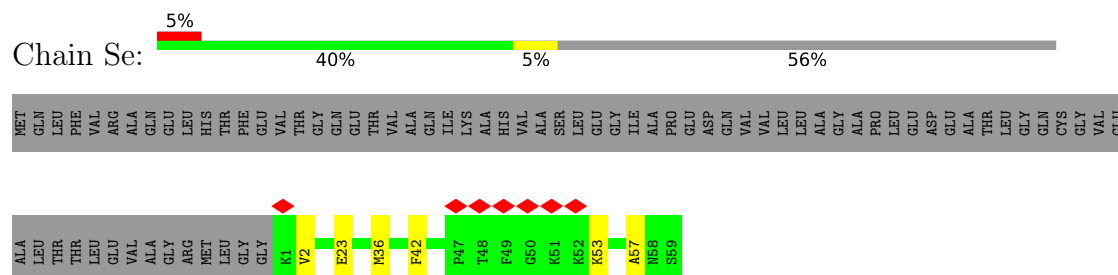
- Molecule 18: 40S ribosomal protein S24



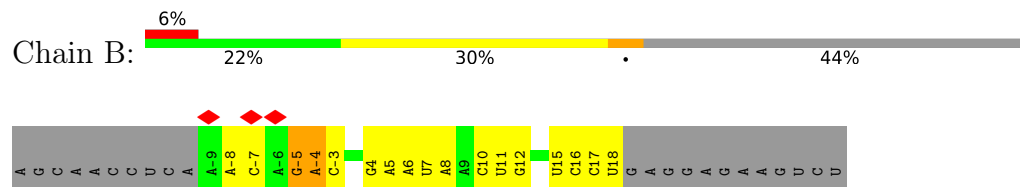
- Molecule 19: 40S ribosomal protein S27



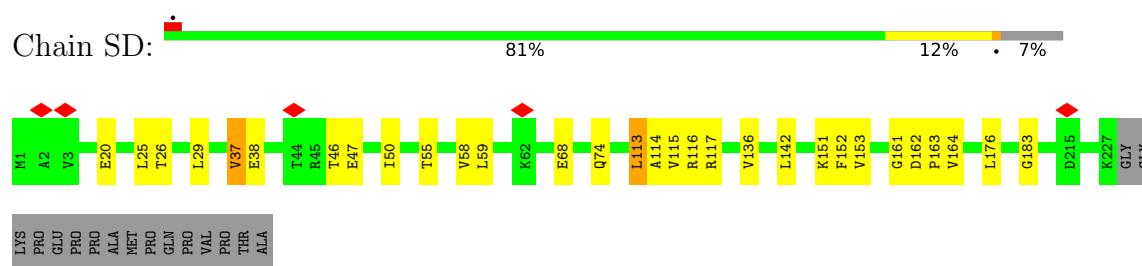
- Molecule 20: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein



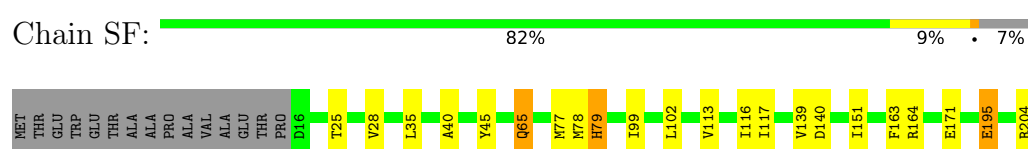
- Molecule 21: mRNA



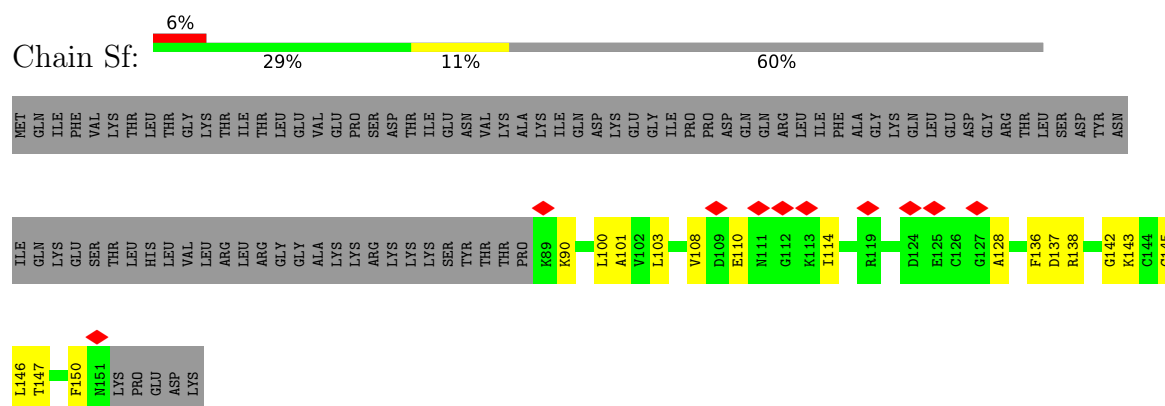
- Molecule 22: 40S ribosomal protein S3




- Molecule 23: 40S ribosomal protein S5

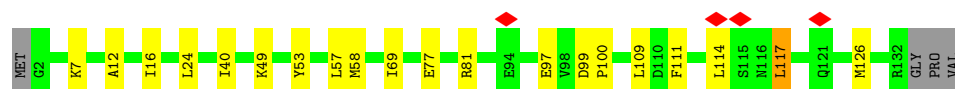


- Molecule 24: Ubiquitin




- Molecule 25: 40S ribosomal protein S17

Chain SR:  82% 14%




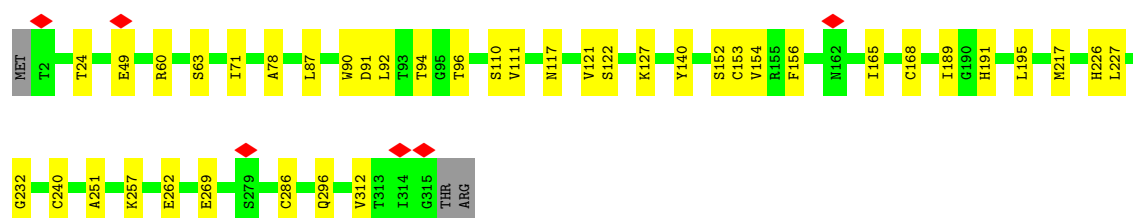
- Molecule 26: 40S ribosomal protein S29

Chain Sd:  84% 14%




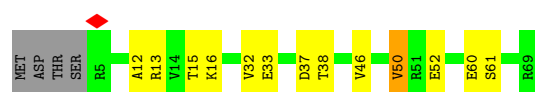
- Molecule 27: Receptor of activated protein C kinase 1

Chain Sg:  86% 13%



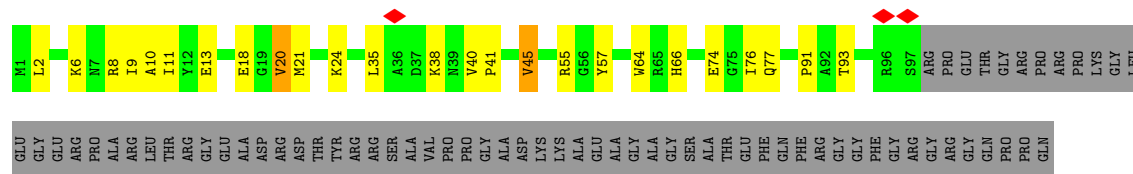
- Molecule 28: 40S ribosomal protein S28

Chain Sc:  75% 17% 6%



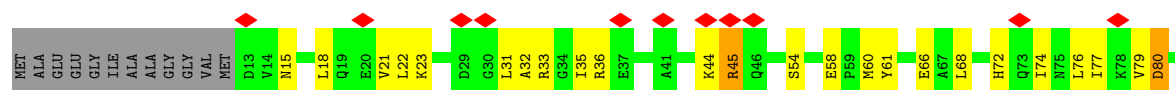
- Molecule 29: 40S ribosomal protein S10

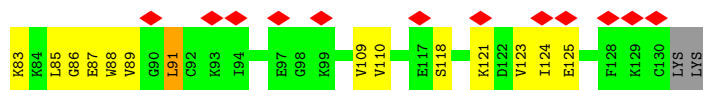
Chain SK:  44% 14% 41%



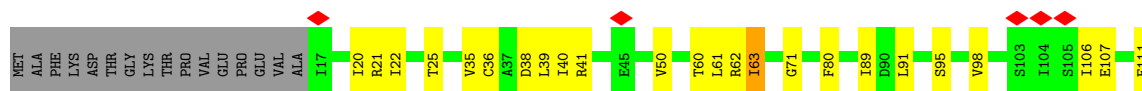
- Molecule 30: 40S ribosomal protein S12

Chain SM:  17% 61% 27% 11%

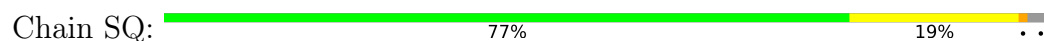




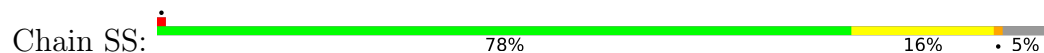
- Molecule 31: 40S ribosomal protein S20



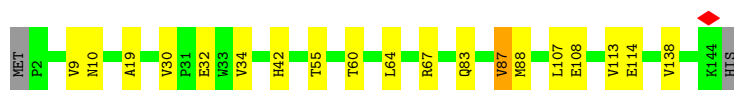
- Molecule 32: 40S ribosomal protein S16



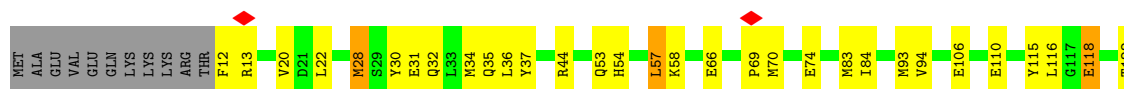
- Molecule 33: 40S ribosomal protein S18



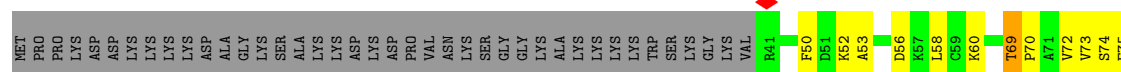
- Molecule 34: Small ribosomal subunit protein eS19



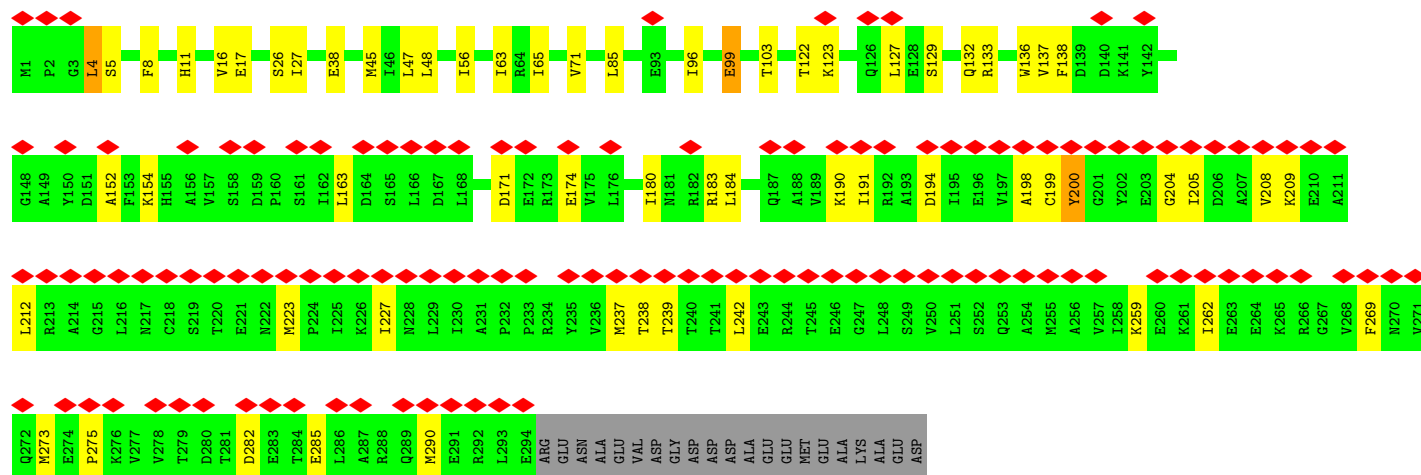
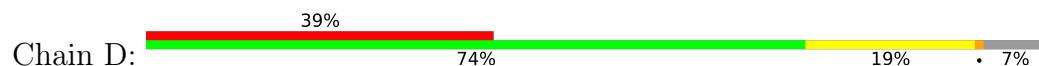
- Molecule 35: 40S ribosomal protein S15



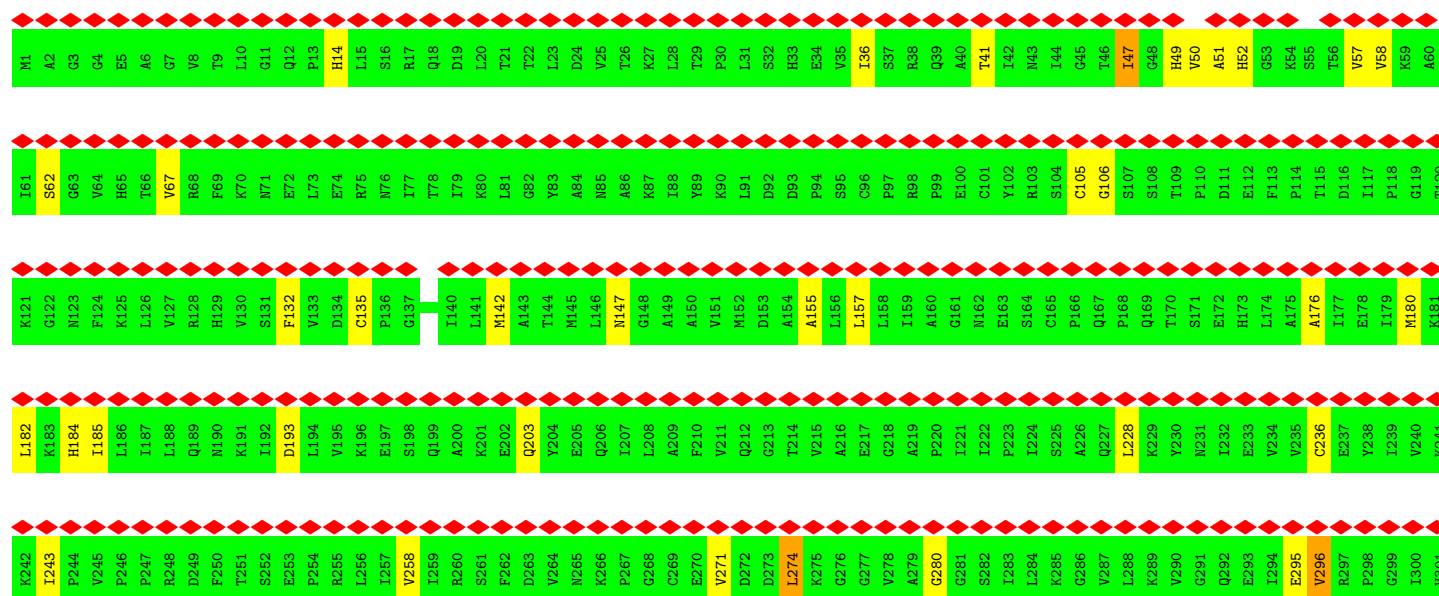
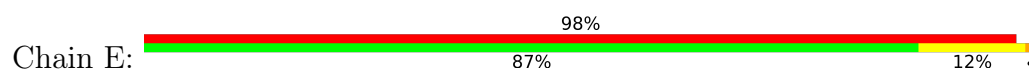
- Molecule 36: Small ribosomal subunit protein eS25

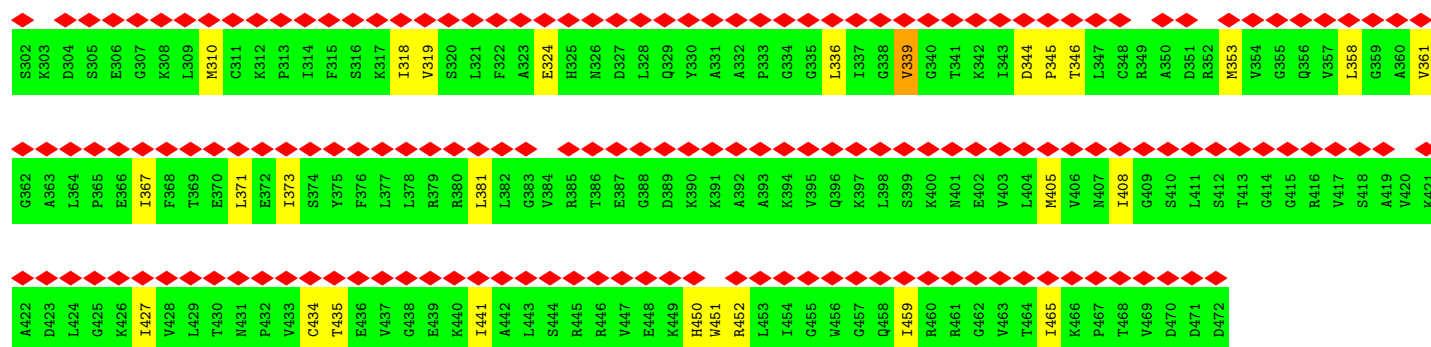


• Molecule 37: Eukaryotic translation initiation factor 2 subunit 1



• Molecule 38: Eukaryotic translation initiation factor 2 subunit 3

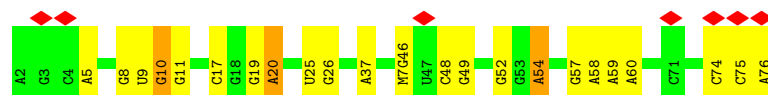




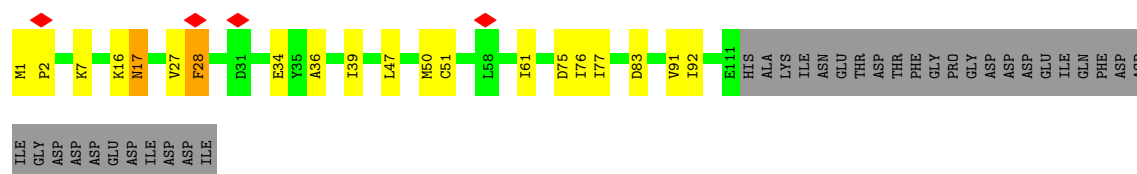
• Molecule 39: Eukaryotic translation initiation factor 2 subunit 2



• Molecule 40: initiator tRNA

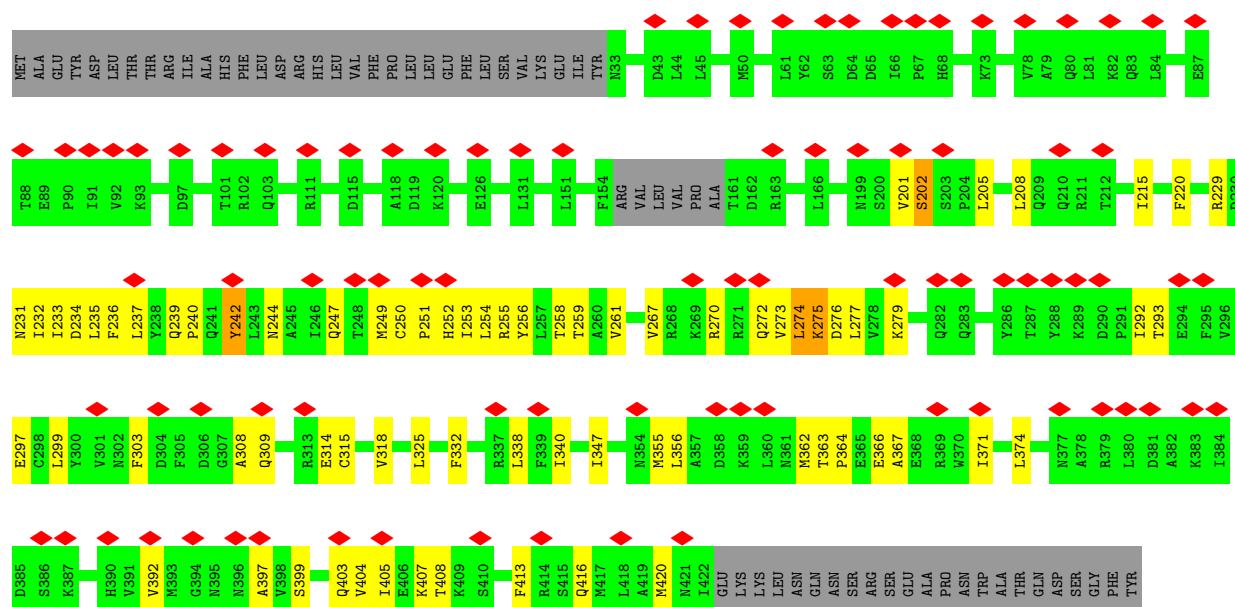


• Molecule 41: Eukaryotic translation initiation factor 1A, X-chromosomal

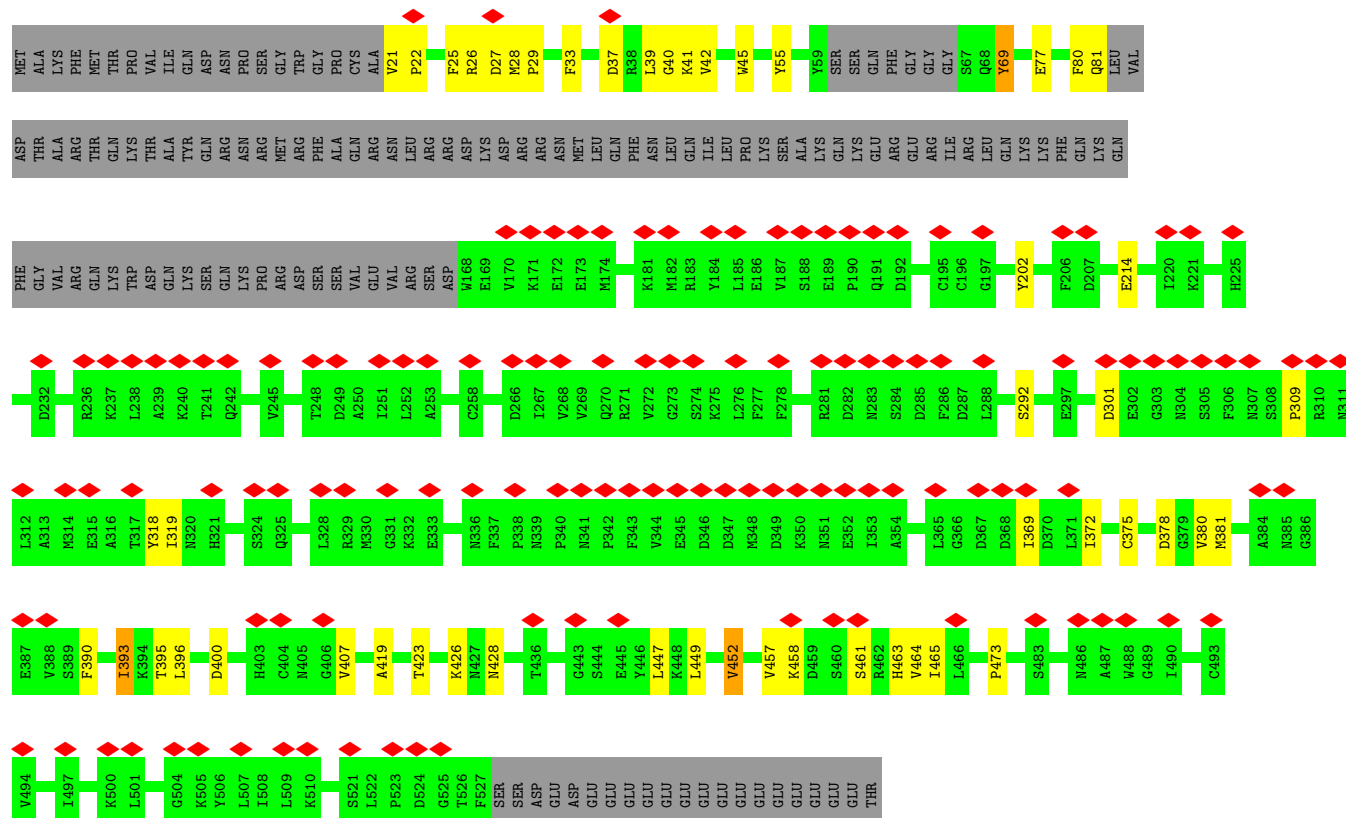


• Molecule 42: Eukaryotic translation initiation factor 3 subunit E





• Molecule 43: Eukaryotic translation initiation factor 3 subunit D



• Molecule 44: Eukaryotic translation initiation factor 3 subunit C

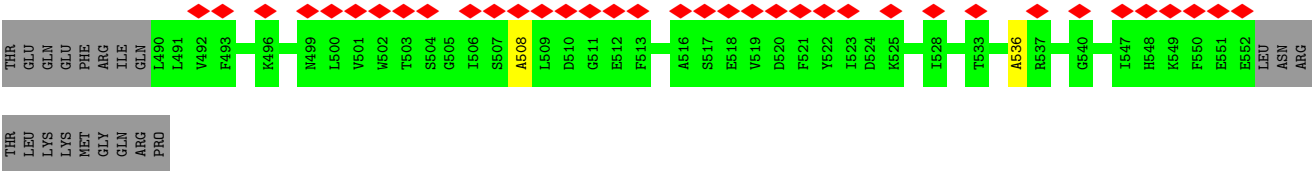




Response	Percentage
Good	15%
Not good	70%
Don't know	28%







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36575	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	42.118	Depositor
Minimum map value	-17.754	Depositor
Average map value	0.052	Depositor
Map value standard deviation	1.246	Depositor
Recommended contour level	3.88	Depositor
Map size (Å)	374.40002, 374.40002, 374.40002	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.72, 0.72, 0.72	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: B8N, 1MA, 5MC, T6A, NMM, 4AC, OMU, PSU, OMC, M7G, K, A2M, 6MZ, GNP, 1MG, IAS, UY1, MG, OMG, 2MG, H2U, MA6, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	S2	0.21	0/39125	0.26	0/60957
2	Ln	0.19	0/231	0.39	0/294
3	SE	0.18	0/2118	0.34	0/2849
4	SA	0.17	0/1764	0.36	0/2396
5	SB	0.17	0/1832	0.36	0/2449
6	SH	0.15	0/1546	0.35	0/2071
7	SI	0.16	0/1715	0.34	0/2287
8	SL	0.17	0/1280	0.32	0/1712
9	SV	0.18	0/643	0.30	0/860
10	SX	0.17	0/1116	0.35	0/1490
11	Sa	0.17	0/836	0.29	0/1121
12	SC	0.18	0/1746	0.33	0/2358
13	SG	0.16	0/1926	0.33	0/2563
14	SJ	0.15	0/1537	0.31	0/2052
15	SN	0.17	0/1232	0.33	0/1656
16	SO	0.46	1/1020 (0.1%)	0.38	0/1366
17	SW	0.19	0/1051	0.35	0/1406
18	SY	0.16	0/1031	0.37	0/1370
19	Sb	0.18	0/665	0.34	0/891
20	Se	0.16	0/474	0.33	0/623
21	B	0.13	0/664	0.27	0/1031
22	SD	0.16	0/1793	0.32	0/2414
23	SF	0.16	0/1516	0.29	0/2037
24	Sf	0.19	0/525	0.49	0/695
25	SR	0.19	0/1078	0.42	0/1447
26	Sd	0.19	0/470	0.35	0/623
27	Sg	0.16	0/2497	0.35	0/3399
28	Sc	0.17	0/519	0.33	0/694
29	SK	0.20	0/840	0.44	0/1133
30	SM	0.18	0/916	0.52	0/1233
31	SU	0.17	0/821	0.37	0/1103



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	SQ	0.18	0/1142	0.36	0/1528
33	SS	0.17	0/1216	0.34	0/1628
34	ST	0.16	0/1119	0.32	0/1498
35	SP	0.18	0/1126	0.46	0/1505
36	SZ	0.17	0/591	0.42	0/794
37	D	0.15	0/2400	0.37	0/3235
38	E	0.12	0/3643	0.31	0/4929
39	F	0.14	0/144	0.45	0/191
40	G	0.17	0/1600	0.22	0/2492
41	H	0.16	0/905	0.41	0/1202
42	e	0.16	0/2672	0.45	0/3647
43	d	0.14	0/2821	0.37	0/3852
44	c	0.19	0/5284	0.41	0/7123
45	a	0.19	0/4891	0.44	0/6615
46	3f	0.12	0/1269	0.30	0/1762
47	m	0.14	0/1926	0.39	0/2669
48	h	0.14	0/1569	0.39	0/2183
49	k	0.09	0/1055	0.25	0/1469
50	l	0.10	0/1575	0.27	0/2187
All	All	0.19	1/111475 (0.0%)	0.33	0/159089

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	SO	136	PRO	C-N	-13.20	1.14	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	S2	36955	0	18671	232	0
2	Ln	230	0	276	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	SE	2076	0	2177	26	0
4	SA	1727	0	1729	40	0
5	SB	1806	0	1888	34	0
6	SH	1523	0	1622	22	0
7	SI	1686	0	1771	17	0
8	SL	1258	0	1332	16	0
9	SV	636	0	637	11	0
10	SX	1098	0	1167	14	0
11	Sa	821	0	870	7	0
12	SC	1709	0	1797	22	0
13	SG	1903	0	2068	12	0
14	SJ	1512	0	1629	27	0
15	SN	1208	0	1293	19	0
16	SO	1016	0	1037	20	0
17	SW	1034	0	1080	13	0
18	SY	1014	0	1082	18	0
19	Sb	651	0	672	9	0
20	Se	468	0	519	5	0
21	B	594	0	304	1	0
22	SD	1765	0	1865	20	0
23	SF	1495	0	1549	15	0
24	Sf	515	0	523	15	0
25	SR	1064	0	1118	18	0
26	Sd	459	0	448	6	0
27	Sg	2440	0	2396	26	0
28	Sc	517	0	549	11	0
29	SK	816	0	841	17	0
30	SM	906	0	921	33	0
31	SU	811	0	877	17	0
32	SQ	1124	0	1193	20	0
33	SS	1198	0	1261	18	0
34	ST	1113	0	1145	14	0
35	SP	1103	0	1156	33	0
36	SZ	585	0	640	16	0
37	D	2367	0	2411	45	0
38	E	3585	0	3736	41	0
39	F	143	0	144	5	0
40	G	1623	0	828	5	0
41	H	895	0	924	17	0
42	e	2635	0	2207	65	0
43	d	2778	0	2143	48	0
44	c	5197	0	5201	186	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	a	4799	0	4830	158	0
46	3f	1272	0	564	4	0
47	m	1917	0	1096	25	0
48	h	1571	0	683	4	0
49	k	1057	0	475	1	0
50	l	1581	0	689	3	0
51	S2	17	0	0	0	0
51	SX	1	0	0	0	0
51	Sd	1	0	0	0	0
52	B	7	0	0	0	0
52	H	1	0	0	0	0
52	S2	76	0	0	0	0
52	SE	1	0	0	0	0
52	SN	1	0	0	0	0
52	SO	1	0	0	0	0
53	Sa	1	0	0	0	0
53	Sd	1	0	0	0	0
53	Sf	1	0	0	0	0
54	E	32	0	13	0	0
55	E	8	0	8	1	0
56	S2	349	0	0	1	0
56	SB	1	0	0	0	0
56	SC	1	0	0	0	0
56	SE	1	0	0	0	0
56	SL	2	0	0	0	0
56	SN	3	0	0	0	0
56	SO	2	0	0	0	0
56	SQ	1	0	0	0	0
56	SS	1	0	0	0	0
56	ST	1	0	0	0	0
56	Sa	1	0	0	0	0
All	All	108768	0	86055	1346	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 7.

All (1346) 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)
45:a:11:ALA:HB2	45:a:34:VAL:HG21	1.48	0.96
44:c:371:ILE:HD11	44:c:411:ILE:HD13	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:e:215:ILE:HD12	42:e:232:ILE:HD12	1.56	0.88
43:d:28:MET:HE2	44:c:591:MET:HE1	1.61	0.82
7:SI:198:TYR:O	7:SI:202:ILE:HD12	1.81	0.81
47:m:46:ILE:O	47:m:50:ASP:CB	2.28	0.81
30:SM:31:LEU:HD13	30:SM:31:LEU:O	1.82	0.79
1:S2:165:G:H2'	1:S2:166:A2M:H5''	1.64	0.79
47:m:320:MET:HA	47:m:320:MET:HE2	1.64	0.79
45:a:390:LEU:HD13	45:a:410:VAL:HG21	1.65	0.77
1:S2:952:G:H21	16:SO:52:THR:HG21	1.49	0.76
18:SY:7:ILE:HD11	18:SY:40:ILE:HD11	1.69	0.75
12:SC:61:MET:HE3	12:SC:61:MET:HA	1.69	0.75
44:c:684:CYS:SG	44:c:765:VAL:HG21	2.26	0.75
43:d:419:ALA:O	43:d:423:THR:HG23	1.86	0.74
25:SR:12:ALA:O	25:SR:16:ILE:HD12	1.88	0.73
45:a:179:GLN:HG2	45:a:235:VAL:HG11	1.71	0.72
7:SI:113:TYR:CD2	7:SI:121:LEU:HD22	2.25	0.71
1:S2:512:A2M:H4'	1:S2:576:A2M:H2	1.71	0.71
44:c:459:MET:HE3	44:c:473:LEU:HG	1.70	0.71
44:c:512:TYR:CE2	44:c:675:LEU:HD21	2.26	0.71
44:c:455:PHE:CD2	44:c:479:VAL:HG21	2.26	0.71
44:c:75:ASP:OD1	44:c:75:ASP:O	2.09	0.70
44:c:409:MET:HE3	44:c:409:MET:HA	1.72	0.70
16:SO:56:VAL:HG22	16:SO:81:VAL:HG23	1.74	0.70
5:SB:125:VAL:HG22	5:SB:172:MET:HE3	1.73	0.69
1:S2:575:A:H3'	1:S2:576:A2M:H5''	1.75	0.69
1:S2:1850:MA6:H103	1:S2:1851:MA6:H102	1.75	0.69
4:SA:58:LEU:HD21	4:SA:174:MET:SD	2.33	0.69
44:c:743:ALA:HB1	44:c:751:THR:HG23	1.73	0.69
44:c:393:MET:HE2	44:c:454:GLU:OE1	1.93	0.68
44:c:473:LEU:HD13	45:a:129:LEU:HD21	1.75	0.68
45:a:157:TYR:O	45:a:161:LEU:HD22	1.94	0.68
3:SE:180:LEU:HD21	3:SE:192:ILE:HG23	1.75	0.68
1:S2:165:G:C2'	1:S2:166:A2M:H5''	2.23	0.67
44:c:451:MET:HE2	44:c:479:VAL:HG22	1.74	0.67
18:SY:7:ILE:HD11	18:SY:40:ILE:CD1	2.24	0.67
47:m:338:THR:HG21	47:m:347:TRP:CZ3	2.30	0.67
1:S2:99:A2M:O5'	1:S2:99:A2M:H8	1.95	0.67
27:Sg:121:VAL:HG21	27:Sg:165:ILE:HD11	1.77	0.67
37:D:56:ILE:HD12	37:D:56:ILE:O	1.94	0.67
37:D:208:VAL:HG23	37:D:209:LYS:CE	2.25	0.66
40:G:46:M7G:H3'	40:G:46:M7G:O2A	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:D:16:VAL:HG12	37:D:17:GLU:HG2	1.75	0.66
45:a:519:ILE:HD12	45:a:519:ILE:H	1.61	0.66
14:SJ:137:VAL:HG23	14:SJ:142:VAL:HG21	1.76	0.65
45:a:28:LEU:HD11	45:a:66:LEU:CD2	2.26	0.65
35:SP:144:LEU:HD12	35:SP:145:LYS:N	2.10	0.65
38:E:367:ILE:HD12	38:E:367:ILE:O	1.96	0.65
44:c:512:TYR:CD2	44:c:675:LEU:HD11	2.31	0.65
35:SP:83:MET:HE2	35:SP:83:MET:HA	1.79	0.65
45:a:55:LEU:HD11	45:a:71:LEU:HD21	1.77	0.65
5:SB:136:ARG:HB2	5:SB:218:LEU:HD11	1.78	0.64
1:S2:166:A2M:H5'	1:S2:166:A2M:H8	1.79	0.64
1:S2:903:A:C6	1:S2:904:A:N6	2.65	0.64
17:SW:34:ILE:O	17:SW:38:LEU:HD13	1.98	0.64
42:e:355:MET:HE3	42:e:356:LEU:N	2.13	0.64
1:S2:428:OMU:H6	1:S2:428:OMU:HM23	1.79	0.64
24:Sf:103:LEU:HD12	24:Sf:103:LEU:O	1.97	0.64
1:S2:483:C:O2'	1:S2:484:A2M:H5'	1.97	0.64
6:SH:28:LEU:HD13	6:SH:28:LEU:O	1.98	0.64
45:a:437:LEU:HD12	45:a:437:LEU:O	1.97	0.64
1:S2:1622:U:H3	35:SP:122:THR:HG22	1.62	0.63
17:SW:105:THR:HG23	17:SW:105:THR:O	1.98	0.63
44:c:106:TYR:HA	44:c:109:ILE:HD12	1.81	0.63
1:S2:166:A2M:H8	1:S2:166:A2M:C5'	2.29	0.63
37:D:209:LYS:HZ2	38:E:274:LEU:HD23	1.63	0.63
45:a:83:ILE:HD12	45:a:84:LYS:N	2.14	0.63
14:SJ:137:VAL:HG22	14:SJ:157:ILE:HD13	1.80	0.63
44:c:455:PHE:HE1	44:c:459:MET:HE2	1.63	0.63
45:a:15:ALA:HB2	45:a:31:LEU:HD21	1.80	0.63
30:SM:31:LEU:HD12	30:SM:33:ARG:CD	2.29	0.63
33:SS:30:ILE:HD11	33:SS:41:ALA:HB1	1.82	0.62
37:D:184:LEU:HD13	37:D:184:LEU:O	1.99	0.62
33:SS:65:GLU:O	33:SS:69:THR:HG23	2.00	0.62
44:c:691:MET:HE1	44:c:756:ILE:HD12	1.82	0.62
5:SB:3:VAL:HG13	16:SO:62:VAL:O	2.00	0.61
45:a:15:ALA:CB	45:a:31:LEU:HD21	2.29	0.61
32:SQ:32:ILE:HD13	32:SQ:68:ILE:HB	1.81	0.61
41:H:16:LYS:O	41:H:17:ASN:HB2	2.01	0.61
42:e:256:TYR:CD1	42:e:325:LEU:HD21	2.35	0.61
45:a:167:ASN:OD1	45:a:170:VAL:HG22	2.00	0.61
47:m:324:LYS:C	47:m:325:ILE:HD12	2.26	0.61
44:c:679:LEU:HD13	44:c:679:LEU:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:d:452:VAL:HG12	43:d:465:ILE:HG22	1.82	0.61
44:c:409:MET:CE	44:c:412:LEU:HD22	2.31	0.61
1:S2:1832:6MZ:H9C2	1:S2:1833:C:H41	1.64	0.61
1:S2:1832:6MZ:H9C2	1:S2:1833:C:N4	2.15	0.61
3:SE:236:ILE:C	3:SE:236:ILE:HD12	2.25	0.61
44:c:483:ILE:HD11	44:c:505:LEU:HD11	1.83	0.61
45:a:283:PHE:CZ	45:a:355:LEU:HD21	2.36	0.61
45:a:401:LEU:H	45:a:401:LEU:HD23	1.66	0.61
43:d:319:ILE:HG22	43:d:395:THR:HG21	1.81	0.61
37:D:27:ILE:HD11	37:D:63:ILE:HG21	1.82	0.60
44:c:445:LEU:HD12	44:c:498:GLU:HB2	1.83	0.60
45:a:285:LYS:O	45:a:285:LYS:HD3	2.00	0.60
1:S2:116:OMU:H6	1:S2:116:OMU:O5'	2.02	0.60
37:D:208:VAL:HG23	37:D:209:LYS:HE2	1.82	0.60
38:E:408:ILE:HG22	38:E:441:ILE:HD12	1.83	0.60
5:SB:95:ASN:C	5:SB:95:ASN:HD22	2.10	0.60
5:SB:33:VAL:HG11	5:SB:67:PHE:CZ	2.37	0.59
44:c:451:MET:HE1	44:c:479:VAL:HG13	1.83	0.59
28:Sc:37:ASP:O	28:Sc:38:THR:HG22	2.02	0.59
42:e:399:SER:O	42:e:404:VAL:HG22	2.03	0.59
3:SE:180:LEU:HD23	3:SE:181:CYS:N	2.17	0.59
45:a:331:ILE:C	45:a:333:PRO:HD3	2.27	0.59
35:SP:28:MET:HE3	35:SP:32:GLN:OE1	2.03	0.59
44:c:804:MET:HE2	44:c:822:ILE:HD13	1.84	0.59
45:a:283:PHE:CE2	45:a:355:LEU:HD21	2.37	0.59
1:S2:1091:C:HO2'	17:SW:2:VAL:N	1.99	0.59
47:m:338:THR:HG21	47:m:347:TRP:HZ3	1.66	0.59
43:d:28:MET:CE	44:c:591:MET:HE1	2.30	0.59
1:S2:1388:A:H61	22:SD:161:GLY:HA3	1.67	0.58
28:Sc:13:ARG:CZ	43:d:423:THR:HG22	2.33	0.58
1:S2:793:G:N2	1:S2:795:A:H61	2.00	0.58
42:e:399:SER:HB3	42:e:404:VAL:HG13	1.84	0.58
30:SM:60:MET:HE3	30:SM:60:MET:H	1.67	0.58
42:e:256:TYR:HD1	42:e:325:LEU:HD21	1.67	0.58
6:SH:69:LEU:HD22	6:SH:96:ALA:HB2	1.86	0.58
42:e:229:ARG:O	42:e:232:ILE:HG22	2.04	0.58
45:a:411:LEU:HD12	45:a:428:VAL:HG23	1.84	0.58
1:S2:27:A2M:OP1	1:S2:484:A2M:HM'1	2.03	0.58
1:S2:529:A:H61	1:S2:555:A:H61	1.50	0.58
4:SA:89:LYS:HD2	4:SA:201:LEU:HD11	1.84	0.58
32:SQ:44:PRO:HD2	32:SQ:81:ILE:HD11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:d:42:VAL:HG23	44:c:610:ASN:OD1	2.04	0.58
45:a:19:LEU:HD21	45:a:57:LEU:HD11	1.84	0.58
1:S2:4:C:H4'	12:SC:207:ALA:HB2	1.84	0.58
43:d:40:GLY:HA2	44:c:613:MET:HE1	1.85	0.58
43:d:407:VAL:HG22	43:d:423:THR:HG21	1.85	0.58
44:c:412:LEU:C	44:c:412:LEU:HD23	2.29	0.58
18:SY:34:THR:HG22	18:SY:62:THR:HG21	1.85	0.57
45:a:26:PRO:O	45:a:30:VAL:HG13	2.04	0.57
47:m:333:VAL:HG13	47:m:334:VAL:N	2.18	0.57
44:c:510:THR:O	44:c:510:THR:HG22	2.03	0.57
8:SL:128:VAL:HG12	8:SL:142:VAL:HA	1.86	0.57
30:SM:22:LEU:HD12	30:SM:23:LYS:N	2.19	0.57
44:c:555:ILE:HG21	44:c:568:ALA:HB3	1.85	0.57
37:D:204:GLY:O	37:D:208:VAL:HG22	2.04	0.57
44:c:455:PHE:CE2	44:c:479:VAL:HG21	2.39	0.57
1:S2:512:A2M:H5'	1:S2:576:A2M:N1	2.20	0.57
45:a:111:MET:HA	45:a:111:MET:HE2	1.87	0.57
44:c:625:LEU:H	44:c:625:LEU:HD12	1.70	0.57
1:S2:1841:C:H2'	1:S2:1842:4AC:H6	1.86	0.57
44:c:691:MET:HE1	44:c:756:ILE:CD1	2.35	0.57
1:S2:846:G:C4	3:SE:19:MET:HE3	2.40	0.56
44:c:709:MET:HE1	44:c:712:LYS:HD3	1.86	0.56
45:a:232:THR:O	45:a:235:VAL:HG12	2.05	0.56
45:a:446:ILE:HD11	47:m:316:VAL:HG11	1.85	0.56
4:SA:15:VAL:HG21	25:SR:111:PHE:CD2	2.41	0.56
42:e:205:LEU:HD21	43:d:26:ARG:HG3	1.87	0.56
1:S2:1229:G:H21	34:ST:87:VAL:CG2	2.18	0.56
3:SE:181:CYS:SG	3:SE:225:ILE:HG23	2.45	0.56
4:SA:201:LEU:HD13	4:SA:201:LEU:O	2.05	0.56
30:SM:44:LYS:O	30:SM:45:ARG:HB2	2.05	0.56
47:m:127:LEU:O	47:m:131:ALA:HB3	2.04	0.56
1:S2:126:G:H8	13:SG:199:THR:HG21	1.70	0.56
5:SB:33:VAL:HG23	5:SB:44:ILE:HB	1.88	0.56
31:SU:35:VAL:O	31:SU:39:LEU:HD22	2.05	0.56
37:D:212:LEU:HD12	37:D:227:ILE:HG21	1.87	0.56
37:D:259:LYS:HA	37:D:262:ILE:HG22	1.88	0.56
38:E:228:LEU:HD23	38:E:228:LEU:H	1.70	0.56
45:a:447:TYR:CE2	45:a:450:ILE:HD12	2.40	0.56
3:SE:173:ILE:HD11	3:SE:235:TRP:CE3	2.39	0.56
37:D:191:ILE:HG23	37:D:275:PRO:HB3	1.87	0.56
1:S2:1484:A:N7	56:S2:2011:HOH:O	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:SA:18:PHE:CD1	4:SA:23:THR:HG21	2.40	0.56
44:c:756:ILE:HG22	44:c:756:ILE:O	2.06	0.56
5:SB:219:LYS:HD2	5:SB:219:LYS:C	2.30	0.56
44:c:500:CYS:SG	44:c:564:ILE:HG21	2.45	0.56
15:SN:4:MET:HE3	15:SN:121:ARG:HG2	1.88	0.56
15:SN:38:TYR:O	15:SN:42:LYS:HG2	2.06	0.56
23:SF:65:GLN:HE21	23:SF:65:GLN:C	2.14	0.56
37:D:26:SER:C	37:D:27:ILE:HD12	2.31	0.56
44:c:822:ILE:O	44:c:826:ILE:HG12	2.05	0.56
44:c:448:VAL:HG21	44:c:486:VAL:HG21	1.88	0.56
45:a:229:HIS:HB3	45:a:259:LEU:HD11	1.88	0.55
30:SM:124:ILE:HD12	30:SM:125:GLU:N	2.21	0.55
37:D:262:ILE:HD13	37:D:269:PHE:HB2	1.87	0.55
44:c:64:ILE:HG13	44:c:109:ILE:HD11	1.88	0.55
44:c:358:VAL:HA	44:c:374:ILE:HD11	1.88	0.55
44:c:548:MET:HE1	44:c:572:HIS:HA	1.86	0.55
47:m:324:LYS:O	47:m:325:ILE:HD12	2.06	0.55
1:S2:1517:G:OP1	35:SP:122:THR:HG21	2.06	0.55
45:a:467:LEU:C	45:a:467:LEU:HD13	2.31	0.55
45:a:549:GLN:O	45:a:553:ALA:HB3	2.06	0.55
10:SX:58:GLU:OE1	10:SX:58:GLU:HA	2.07	0.55
25:SR:97:GLU:N	25:SR:97:GLU:OE1	2.39	0.55
38:E:344:ASP:OD2	38:E:346:THR:HG23	2.06	0.55
42:e:273:VAL:HG23	42:e:274:LEU:N	2.22	0.55
43:d:447:LEU:HD11	43:d:473:PRO:HA	1.89	0.55
14:SJ:114:VAL:HG23	14:SJ:119:LEU:HB3	1.88	0.55
27:Sg:121:VAL:HG21	27:Sg:165:ILE:CD1	2.36	0.55
1:S2:550:C:H2'	1:S2:551:U:C6	2.42	0.55
44:c:368:GLU:OE1	44:c:411:ILE:HD11	2.07	0.55
16:SO:83:GLN:C	16:SO:83:GLN:OE1	2.50	0.55
16:SO:130:GLU:N	16:SO:130:GLU:OE1	2.40	0.55
34:ST:9:VAL:HG21	34:ST:138:VAL:HG13	1.87	0.55
44:c:555:ILE:HG21	44:c:568:ALA:CB	2.37	0.55
45:a:447:TYR:HE2	45:a:450:ILE:HD12	1.72	0.55
1:S2:1750:C:H2'	1:S2:1751:C:C1'	2.38	0.54
1:S2:1850:MA6:H103	1:S2:1851:MA6:C10	2.37	0.54
29:SK:74:GLU:C	29:SK:74:GLU:OE1	2.49	0.54
22:SD:25:LEU:CD1	22:SD:37:VAL:HG11	2.38	0.54
22:SD:162:ASP:C	22:SD:162:ASP:OD1	2.50	0.54
43:d:319:ILE:HD12	43:d:452:VAL:HG21	1.89	0.54
44:c:409:MET:HE1	44:c:412:LEU:HD22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:c:611:ARG:NH2	44:c:675:LEU:HD12	2.23	0.54
45:a:374:MET:HA	45:a:374:MET:HE3	1.89	0.54
3:SE:102:ILE:HG22	3:SE:182:MET:HE1	1.89	0.54
43:d:40:GLY:O	43:d:41:LYS:HD2	2.07	0.54
45:a:230:LEU:HD13	45:a:230:LEU:O	2.07	0.54
14:SJ:114:VAL:CG1	14:SJ:126:ALA:HB1	2.37	0.54
38:E:258:VAL:HG11	38:E:353:MET:HE3	1.88	0.54
5:SB:92:GLN:OE1	5:SB:92:GLN:HA	2.07	0.54
30:SM:85:LEU:HD12	30:SM:89:VAL:HG13	1.90	0.54
45:a:11:ALA:CB	45:a:34:VAL:HG21	2.30	0.54
6:SH:40:LEU:HD23	6:SH:40:LEU:O	2.08	0.54
37:D:198:ALA:HA	38:E:346:THR:HG21	1.90	0.54
44:c:548:MET:HE1	44:c:571:CYS:C	2.33	0.54
44:c:832:MET:CE	44:c:843:VAL:HG22	2.38	0.54
1:S2:619:A:N6	10:SX:115:ILE:HD11	2.23	0.54
8:SL:126:VAL:HG13	8:SL:142:VAL:HG13	1.89	0.54
19:Sb:67:THR:HG22	19:Sb:71:ALA:HA	1.90	0.54
44:c:832:MET:HE3	44:c:843:VAL:HG22	1.88	0.54
45:a:530:LEU:HD23	45:a:531:ALA:N	2.22	0.53
5:SB:33:VAL:HG22	5:SB:45:GLY:O	2.08	0.53
12:SC:166:ARG:O	12:SC:247:THR:HG21	2.09	0.53
42:e:215:ILE:CD1	42:e:232:ILE:HD12	2.34	0.53
44:c:105:PHE:O	44:c:109:ILE:HD12	2.07	0.53
45:a:432:GLN:HA	45:a:435:THR:HG22	1.90	0.53
1:S2:1442:OMU:O5'	1:S2:1442:OMU:H6	2.07	0.53
25:SR:114:LEU:HB2	25:SR:117:LEU:HD11	1.88	0.53
43:d:27:ASP:O	44:c:557:ALA:HB2	2.08	0.53
43:d:80:PHE:O	43:d:81:GLN:HG3	2.08	0.53
5:SB:190:PRO:O	5:SB:191:ASP:OD1	2.27	0.53
24:Sf:100:LEU:HD23	24:Sf:101:ALA:O	2.09	0.53
31:SU:21:ARG:C	31:SU:22:ILE:HD13	2.34	0.53
35:SP:53:GLN:O	35:SP:57:LEU:HD22	2.08	0.53
44:c:64:ILE:HG23	44:c:109:ILE:HG12	1.89	0.53
44:c:684:CYS:HA	44:c:733:MET:CE	2.39	0.53
44:c:700:ALA:HB2	44:c:793:PHE:CG	2.43	0.53
3:SE:212:ASP:C	3:SE:212:ASP:OD1	2.52	0.53
5:SB:38:MET:HE3	5:SB:185:VAL:HG21	1.90	0.53
29:SK:41:PRO:O	29:SK:45:VAL:HG13	2.09	0.53
43:d:21:VAL:N	43:d:22:PRO:CD	2.72	0.53
45:a:290:LEU:HA	45:a:329:ILE:HD12	1.91	0.53
11:Sa:67:LEU:HD11	16:SO:131:ASP:OD2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:SD:113:LEU:HD23	22:SD:114:ALA:N	2.24	0.53
35:SP:36:LEU:HD23	35:SP:36:LEU:H	1.73	0.53
42:e:303:PHE:HD2	42:e:347:ILE:HD11	1.74	0.53
43:d:372:ILE:N	43:d:372:ILE:HD12	2.24	0.53
5:SB:133:TYR:CE2	5:SB:181:LEU:HD22	2.44	0.53
44:c:153:GLU:OE1	44:c:153:GLU:O	2.27	0.53
44:c:681:LEU:HD12	44:c:768:LEU:HD12	1.91	0.53
30:SM:31:LEU:HD12	30:SM:33:ARG:HD3	1.91	0.52
36:SZ:60:LYS:N	36:SZ:60:LYS:HE2	2.24	0.52
1:S2:194:C:H2'	1:S2:195:C:C1'	2.39	0.52
30:SM:35:ILE:HD12	30:SM:36:ARG:N	2.23	0.52
35:SP:93:MET:HE2	35:SP:93:MET:HA	1.91	0.52
35:SP:44:ARG:HG2	35:SP:84:ILE:HD11	1.92	0.52
1:S2:1226:G:C2	1:S2:1639:M7G:HM71	2.44	0.52
35:SP:30:TYR:O	35:SP:34:MET:HG3	2.10	0.52
30:SM:89:VAL:HG11	30:SM:109:VAL:HG21	1.90	0.52
45:a:101:THR:HG21	45:a:153:LEU:HD13	1.92	0.52
25:SR:109:LEU:HD12	25:SR:109:LEU:O	2.10	0.52
32:SQ:97:GLN:HB2	32:SQ:105:LYS:HG3	1.90	0.52
1:S2:1235:G:H21	35:SP:135:ALA:HA	1.74	0.52
1:S2:1315:U:H4'	29:SK:2:LEU:HD22	1.90	0.52
5:SB:8:ARG:HA	5:SB:8:ARG:NE	2.25	0.52
15:SN:22:VAL:HG12	15:SN:66:VAL:HG22	1.90	0.52
22:SD:151:LYS:HG2	22:SD:153:VAL:HG13	1.91	0.52
37:D:133:ARG:O	37:D:137:VAL:HG13	2.08	0.52
42:e:233:ILE:HG23	42:e:234:ASP:N	2.25	0.52
8:SL:40:ILE:HD11	8:SL:61:PRO:O	2.10	0.52
44:c:548:MET:HE1	44:c:571:CYS:O	2.10	0.52
4:SA:24:HIS:C	4:SA:25:LEU:HD12	2.34	0.52
8:SL:40:ILE:HD13	8:SL:62:PHE:CD1	2.45	0.52
26:Sd:38:MET:HE1	26:Sd:50:ILE:HD11	1.92	0.52
33:SS:108:ARG:O	33:SS:112:GLU:HG2	2.09	0.52
33:SS:110:ASP:OD1	33:SS:110:ASP:C	2.53	0.52
44:c:65:ARG:NE	44:c:65:ARG:HA	2.24	0.52
44:c:733:MET:SD	44:c:733:MET:C	2.93	0.52
1:S2:27:A2M:HM'2	1:S2:28:U:O4'	2.10	0.51
33:SS:61:GLU:OE2	33:SS:61:GLU:HA	2.09	0.51
18:SY:37:LYS:O	18:SY:40:ILE:HG22	2.10	0.51
19:Sb:35:VAL:HG21	19:Sb:63:LEU:HD21	1.91	0.51
44:c:512:TYR:CZ	44:c:675:LEU:HD21	2.44	0.51
44:c:573:ILE:HD13	44:c:589:MET:HE2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:c:627:LYS:HA	44:c:693:LEU:HD11	1.92	0.51
44:c:735:GLU:HA	44:c:738:VAL:HG12	1.91	0.51
45:a:452:PHE:CE1	45:a:467:LEU:HD12	2.45	0.51
37:D:27:ILE:HD13	37:D:65:ILE:HD11	1.93	0.51
43:d:25:PHE:O	43:d:25:PHE:CD1	2.63	0.51
1:S2:501:C:H2'	1:S2:501:C:O2	2.11	0.51
1:S2:1824:A:O5'	10:SX:61:GLN:HG3	2.11	0.51
3:SE:165:GLU:OE2	3:SE:165:GLU:N	2.43	0.51
4:SA:54:THR:O	4:SA:58:LEU:HD23	2.10	0.51
30:SM:79:VAL:HG13	30:SM:80:ASP:N	2.25	0.51
33:SS:16:LEU:O	33:SS:16:LEU:HD23	2.09	0.51
42:e:235:LEU:HD23	42:e:239:GLN:HG3	1.93	0.51
42:e:255:ARG:O	42:e:259:THR:HG22	2.10	0.51
45:a:358:LEU:HD23	45:a:358:LEU:C	2.35	0.51
22:SD:68:GLU:CD	22:SD:68:GLU:C	2.77	0.51
22:SD:113:LEU:HD23	22:SD:114:ALA:H	1.75	0.51
24:Sf:108:VAL:HG12	24:Sf:114:ILE:HG22	1.92	0.51
29:SK:21:MET:HE1	29:SK:45:VAL:HB	1.93	0.51
45:a:543:LEU:HD12	45:a:544:GLN:N	2.26	0.51
24:Sf:103:LEU:HD21	30:SM:36:ARG:HD3	1.92	0.51
32:SQ:76:GLY:O	32:SQ:80:GLN:HG2	2.10	0.51
37:D:290:MET:O	37:D:290:MET:HE3	2.10	0.51
44:c:358:VAL:HG22	44:c:374:ILE:HD11	1.91	0.51
45:a:92:ALA:O	45:a:96:MET:SD	2.69	0.51
45:a:105:LYS:HG3	45:a:149:TRP:CD1	2.46	0.51
2:Ln:20:MET:SD	2:Ln:20:MET:C	2.94	0.51
45:a:400:PRO:HD2	47:m:313:ILE:HD13	1.93	0.51
1:S2:140:C:H42	1:S2:313:A:H61	1.59	0.51
1:S2:1831:A:O2'	1:S2:1832:6MZ:H5'1	2.10	0.51
3:SE:192:ILE:HD12	3:SE:243:GLY:HA3	1.92	0.51
8:SL:15:THR:O	8:SL:16:ILE:HD12	2.11	0.51
15:SN:142:GLU:OE1	15:SN:142:GLU:HA	2.09	0.51
32:SQ:47:LEU:HB2	32:SQ:81:ILE:HD13	1.93	0.51
42:e:255:ARG:HG2	42:e:292:ILE:CG2	2.41	0.51
22:SD:55:THR:HA	22:SD:58:VAL:HG12	1.91	0.51
23:SF:65:GLN:O	23:SF:65:GLN:NE2	2.39	0.51
36:SZ:58:LEU:C	36:SZ:58:LEU:HD23	2.35	0.51
37:D:208:VAL:HG23	37:D:209:LYS:HE3	1.93	0.51
42:e:259:THR:HG21	42:e:325:LEU:HD11	1.93	0.51
44:c:681:LEU:HD11	44:c:769:PHE:CE1	2.46	0.51
45:a:279:VAL:HG12	45:a:295:THR:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:SA:70:ASN:ND2	12:SC:274:VAL:HG12	2.27	0.50
30:SM:86:GLY:O	30:SM:89:VAL:HG22	2.11	0.50
32:SQ:31:LEU:HB3	32:SQ:67:ASP:OD1	2.12	0.50
35:SP:137:HIS:O	35:SP:138:SER:CB	2.58	0.50
37:D:199:CYS:O	37:D:200:TYR:C	2.54	0.50
3:SE:45:ILE:HG23	3:SE:46:ILE:HD12	1.92	0.50
41:H:47:LEU:C	41:H:47:LEU:HD12	2.36	0.50
1:S2:551:U:H2'	1:S2:552:G:N9	2.25	0.50
3:SE:139:LEU:HD12	3:SE:139:LEU:C	2.37	0.50
13:SG:227:GLN:C	13:SG:227:GLN:OE1	2.54	0.50
6:SH:66:VAL:HG23	6:SH:67:PRO:HD3	1.94	0.50
14:SJ:143:ASN:OD1	14:SJ:143:ASN:O	2.29	0.50
30:SM:31:LEU:HD11	30:SM:89:VAL:HB	1.94	0.50
37:D:209:LYS:NZ	38:E:274:LEU:HD23	2.27	0.50
44:c:370:VAL:O	44:c:374:ILE:HG23	2.10	0.50
1:S2:928:G:H2'	1:S2:929:G:C8	2.46	0.50
15:SN:89:TYR:O	15:SN:92:ILE:HG22	2.11	0.50
1:S2:484:A2M:O5'	1:S2:484:A2M:H8	2.10	0.50
4:SA:1:MET:HE1	9:SV:78:ILE:C	2.36	0.50
4:SA:214:GLU:HA	4:SA:214:GLU:OE2	2.12	0.50
6:SH:105:THR:HG22	6:SH:105:THR:O	2.12	0.50
19:Sb:15:GLU:OE2	19:Sb:15:GLU:O	2.30	0.50
27:Sg:226:HIS:CE1	27:Sg:227:LEU:O	2.64	0.50
39:F:184:PHE:O	39:F:188:ARG:HG2	2.12	0.50
42:e:292:ILE:HD11	42:e:332:PHE:CZ	2.46	0.50
44:c:86:LEU:HD11	44:c:106:TYR:CE1	2.47	0.50
1:S2:815:PSU:C4	1:S2:816:A:C8	3.00	0.50
25:SR:99:ASP:OD1	25:SR:100:PRO:N	2.45	0.50
28:Sc:12:ALA:HB1	28:Sc:32:VAL:HG22	1.93	0.50
44:c:826:ILE:HD12	44:c:832:MET:HB2	1.94	0.50
45:a:519:ILE:O	45:a:522:GLN:HG3	2.12	0.50
5:SB:82:ARG:CD	5:SB:103:MET:HE2	2.42	0.50
20:Se:23:GLU:OE2	20:Se:23:GLU:C	2.55	0.50
27:Sg:87:LEU:HD21	27:Sg:122:SER:HB3	1.94	0.50
44:c:499:VAL:HA	44:c:502:ILE:HG22	1.93	0.50
44:c:552:CYS:O	44:c:556:TYR:CD2	2.65	0.50
1:S2:158:A:H2'	1:S2:159:A2M:O4'	2.12	0.50
9:SV:4:ASP:OD2	12:SC:172:ASN:ND2	2.43	0.50
30:SM:66:GLU:C	30:SM:66:GLU:OE1	2.55	0.50
47:m:312:VAL:O	47:m:316:VAL:HG13	2.12	0.50
15:SN:102:LEU:HD21	15:SN:111:ALA:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:SK:77:GLN:OE1	29:SK:77:GLN:N	2.45	0.49
43:d:202:TYR:CB	43:d:381:MET:HE3	2.42	0.49
44:c:857:LEU:C	44:c:857:LEU:HD23	2.37	0.49
1:S2:155:G:H4'	13:SG:15:LEU:HD13	1.93	0.49
15:SN:95:ALA:O	15:SN:99:ARG:HG3	2.12	0.49
16:SO:84:ARG:O	16:SO:88:LEU:HD12	2.11	0.49
43:d:465:ILE:O	43:d:465:ILE:CD1	2.60	0.49
45:a:128:LEU:O	45:a:132:VAL:HG23	2.11	0.49
1:S2:14:C:O2	1:S2:668:A2M:H2	2.12	0.49
1:S2:118:C:H1'	1:S2:445:A:C5	2.47	0.49
38:E:271:VAL:HA	38:E:274:LEU:HD13	1.93	0.49
41:H:61:ILE:HA	41:H:91:VAL:HG22	1.95	0.49
45:a:128:LEU:HD12	45:a:128:LEU:H	1.78	0.49
3:SE:59:ASP:OD1	3:SE:60:GLU:N	2.46	0.49
4:SA:1:MET:HB3	4:SA:59:LEU:CB	2.43	0.49
7:SI:191:GLU:HA	7:SI:195:LEU:HD23	1.94	0.49
16:SO:17:LEU:O	16:SO:17:LEU:HG	2.12	0.49
18:SY:9:THR:HG22	18:SY:25:ILE:HG22	1.95	0.49
23:SF:116:ILE:HD11	23:SF:151:ILE:HD11	1.94	0.49
42:e:299:LEU:HD13	42:e:299:LEU:O	2.12	0.49
43:d:400:ASP:HB2	43:d:457:VAL:HG13	1.94	0.49
1:S2:1831:A:H2'	1:S2:1832:6MZ:H8	1.94	0.49
23:SF:35:LEU:HD12	23:SF:117:ILE:HD13	1.93	0.49
27:Sg:296:GLN:HB2	27:Sg:312:VAL:HG22	1.94	0.49
33:SS:10:GLN:OE1	33:SS:10:GLN:HA	2.12	0.49
35:SP:144:LEU:HD12	35:SP:145:LYS:H	1.75	0.49
38:E:367:ILE:HD11	38:E:465:ILE:O	2.12	0.49
39:F:184:PHE:HA	39:F:187:MET:SD	2.52	0.49
44:c:804:MET:SD	44:c:804:MET:N	2.85	0.49
44:c:819:HIS:HD1	44:c:819:HIS:C	2.20	0.49
1:S2:953:C:H2'	1:S2:954:U:O4'	2.12	0.49
1:S2:1373:C:OP1	25:SR:7:LYS:HG3	2.13	0.49
4:SA:15:VAL:HG21	25:SR:111:PHE:HD2	1.77	0.49
5:SB:33:VAL:HG12	5:SB:96:CYS:SG	2.52	0.49
30:SM:31:LEU:HD12	30:SM:33:ARG:HD2	1.94	0.49
37:D:129:SER:O	37:D:132:GLN:HG2	2.13	0.49
49:k:154:ASP:CB	50:l:508:ALA:HB2	2.43	0.49
1:S2:659:G:H21	10:SX:17:ARG:NH2	2.11	0.49
1:S2:1227:G:C2	1:S2:1228:A:C8	3.00	0.49
12:SC:63:VAL:HG22	12:SC:90:GLU:OE2	2.13	0.49
14:SJ:136:ARG:HD2	14:SJ:160:SER:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Sd:5:GLN:OE1	26:Sd:5:GLN:C	2.55	0.49
28:Sc:33:GLU:OE1	28:Sc:33:GLU:C	2.55	0.49
45:a:338:ILE:O	45:a:342:LEU:HD22	2.12	0.49
47:m:333:VAL:HG13	47:m:334:VAL:H	1.77	0.49
6:SH:126:HIS:NE2	6:SH:181:THR:HG23	2.28	0.49
9:SV:13:VAL:HG23	9:SV:13:VAL:O	2.12	0.49
12:SC:266:TYR:O	12:SC:270:THR:HG23	2.13	0.49
30:SM:15:ASN:OD1	30:SM:15:ASN:C	2.56	0.49
36:SZ:75:GLU:OE2	36:SZ:75:GLU:O	2.31	0.49
37:D:242:LEU:HD13	37:D:242:LEU:O	2.13	0.49
38:E:36:ILE:HD12	38:E:41:THR:HG21	1.94	0.49
42:e:374:LEU:HD13	42:e:374:LEU:C	2.37	0.49
44:c:762:ASN:O	44:c:767:ASP:HB2	2.13	0.49
42:e:363:THR:HG23	42:e:364:PRO:HD2	1.95	0.49
45:a:109:GLN:HA	45:a:112:VAL:HG22	1.95	0.49
1:S2:1824:A:O2'	1:S2:1825:A:H5'	2.12	0.48
13:SG:5:ILE:HG22	13:SG:113:ILE:HD11	1.94	0.48
29:SK:35:LEU:HD12	29:SK:40:VAL:HG11	1.94	0.48
38:E:367:ILE:HD12	38:E:367:ILE:C	2.38	0.48
44:c:757:ILE:HG22	44:c:757:ILE:O	2.13	0.48
5:SB:104:ASP:OD1	5:SB:105:LEU:O	2.31	0.48
12:SC:98:LEU:HB2	12:SC:102:LEU:HD21	1.94	0.48
24:Sf:90:LYS:HE2	24:Sf:90:LYS:N	2.28	0.48
28:Sc:15:THR:HG22	28:Sc:16:LYS:H	1.78	0.48
33:SS:51:ASP:OD1	33:SS:51:ASP:C	2.56	0.48
43:d:39:LEU:O	44:c:613:MET:HE1	2.13	0.48
44:c:329:VAL:HG11	44:c:366:LEU:HD13	1.95	0.48
44:c:854:ASN:O	44:c:858:GLN:HG2	2.12	0.48
4:SA:58:LEU:HD22	4:SA:161:ILE:HG21	1.95	0.48
15:SN:63:VAL:HG11	15:SN:71:ILE:HD13	1.95	0.48
22:SD:161:GLY:O	22:SD:164:VAL:HG12	2.12	0.48
10:SX:85:VAL:O	10:SX:85:VAL:HG23	2.13	0.48
30:SM:68:LEU:HD22	30:SM:68:LEU:H	1.79	0.48
31:SU:60:THR:HG22	31:SU:62:ARG:HG2	1.94	0.48
44:c:417:ASN:OD1	44:c:418:ILE:HD12	2.13	0.48
6:SH:177:TYR:CD2	6:SH:185:VAL:HG21	2.48	0.48
30:SM:85:LEU:HD12	30:SM:85:LEU:O	2.13	0.48
35:SP:66:GLU:C	35:SP:66:GLU:OE2	2.56	0.48
42:e:399:SER:HA	42:e:403:GLN:H	1.78	0.48
43:d:33:PHE:HB3	44:c:591:MET:HA	1.95	0.48
44:c:504:LEU:HD13	44:c:508:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:a:450:ILE:HD13	45:a:455:LEU:HD13	1.95	0.48
47:m:343:GLY:O	47:m:347:TRP:CD2	2.66	0.48
44:c:570:LEU:HD21	44:c:594:LEU:HD13	1.96	0.48
44:c:718:LEU:HB2	44:c:738:VAL:HG23	1.95	0.48
6:SH:153:LEU:C	6:SH:153:LEU:HD23	2.38	0.48
38:E:184:HIS:ND1	38:E:243:ILE:HG23	2.29	0.48
1:S2:1709:G:C2	1:S2:1710:C:C5	3.01	0.48
4:SA:63:ARG:NH1	9:SV:78:ILE:HD11	2.28	0.48
7:SI:151:GLU:C	7:SI:151:GLU:OE2	2.56	0.48
37:D:45:MET:O	37:D:85:LEU:HD12	2.14	0.48
42:e:251:PRO:O	42:e:255:ARG:HG3	2.13	0.48
45:a:437:LEU:HD11	45:a:507:ILE:HD12	1.96	0.48
1:S2:833:C:H2'	1:S2:834:C:C6	2.49	0.48
1:S2:943:U:C2	1:S2:944:A:C8	3.02	0.48
4:SA:1:MET:HB3	4:SA:59:LEU:HB3	1.96	0.48
31:SU:106:ILE:C	31:SU:106:ILE:HD12	2.39	0.48
44:c:338:GLN:HA	44:c:338:GLN:NE2	2.28	0.48
44:c:465:HIS:N	44:c:465:HIS:ND1	2.62	0.48
44:c:668:ARG:CZ	44:c:668:ARG:O	2.62	0.48
45:a:372:ASN:HA	45:a:375:VAL:HG12	1.96	0.48
46:3f:261:ARG:O	46:3f:262:VAL:CB	2.61	0.48
19:Sb:46:VAL:HG12	19:Sb:54:VAL:HG21	1.96	0.48
27:Sg:24:THR:HB	27:Sg:71:ILE:HG21	1.96	0.48
44:c:379:ILE:HG22	44:c:383:TYR:CE2	2.49	0.48
45:a:55:LEU:HD13	45:a:93:TYR:HB2	1.96	0.48
45:a:241:ILE:HD11	45:a:282:VAL:CG2	2.43	0.48
1:S2:1164:G:O2'	1:S2:1165:G:H5'	2.14	0.47
1:S2:1203:G:H2'	1:S2:1204:A:C8	2.49	0.47
1:S2:1336:C:O2'	1:S2:1337:4AC:H5'	2.14	0.47
7:SI:67:TRP:HA	7:SI:189:VAL:HG22	1.96	0.47
34:ST:42:HIS:HB2	34:ST:83:GLN:HA	1.96	0.47
38:E:176:ALA:O	38:E:180:MET:HG3	2.14	0.47
38:E:182:LEU:HB3	38:E:185:ILE:HD11	1.96	0.47
44:c:549:GLU:OE2	44:c:549:GLU:HA	2.14	0.47
22:SD:29:LEU:HD12	22:SD:50:ILE:HD11	1.96	0.47
30:SM:79:VAL:HG13	30:SM:80:ASP:H	1.78	0.47
44:c:394:LYS:HA	44:c:394:LYS:HE2	1.95	0.47
13:SG:20:ASP:OD1	13:SG:20:ASP:C	2.57	0.47
20:Se:2:VAL:HG22	41:H:92:ILE:HD12	1.95	0.47
37:D:154:LYS:HD3	37:D:184:LEU:HD11	1.96	0.47
43:d:378:ASP:HB2	43:d:393:ILE:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:a:467:LEU:O	45:a:471:ILE:HG12	2.14	0.47
47:m:322:TYR:HA	47:m:333:VAL:HG12	1.97	0.47
10:SX:59:ALA:HB1	10:SX:114:ASP:OD2	2.14	0.47
14:SJ:143:ASN:OD1	14:SJ:143:ASN:C	2.57	0.47
31:SU:38:ASP:OD1	31:SU:38:ASP:C	2.57	0.47
35:SP:69:PRO:C	35:SP:70:MET:HE3	2.39	0.47
43:d:40:GLY:HA2	44:c:613:MET:CE	2.43	0.47
44:c:786:GLU:OE1	44:c:786:GLU:HA	2.15	0.47
1:S2:1395:C:O2'	1:S2:1396:A:H5'	2.15	0.47
36:SZ:58:LEU:HD21	36:SZ:91:LEU:HD11	1.97	0.47
38:E:258:VAL:HG13	38:E:280:GLY:O	2.15	0.47
38:E:336:LEU:HD22	55:E:502:MET:HE3	1.96	0.47
42:e:252:HIS:O	42:e:256:TYR:CD2	2.67	0.47
44:c:695:ILE:HG21	44:c:744:MET:HG2	1.97	0.47
1:S2:551:U:H2'	1:S2:552:G:C1'	2.44	0.47
1:S2:813:A:C5	1:S2:814:PSU:C6	3.03	0.47
1:S2:1030:A:H2'	1:S2:1031:A2M:H8	1.95	0.47
1:S2:1217:A:H2'	1:S2:1218:C:H6	1.79	0.47
15:SN:115:LEU:O	15:SN:119:GLU:HG2	2.14	0.47
42:e:273:VAL:CG2	42:e:274:LEU:N	2.77	0.47
42:e:355:MET:SD	42:e:355:MET:C	2.98	0.47
45:a:186:LEU:HD11	45:a:239:SER:HA	1.94	0.47
1:S2:1018:U:C2	1:S2:1019:C:C5	3.03	0.47
1:S2:1173:A:H2'	1:S2:1174:PSU:O4'	2.15	0.47
1:S2:1556:A:H2'	1:S2:1556:A:N3	2.30	0.47
7:SI:190:LEU:O	7:SI:195:LEU:HD21	2.14	0.47
14:SJ:137:VAL:HG23	14:SJ:142:VAL:CG2	2.44	0.47
23:SF:40:ALA:HB1	23:SF:45:TYR:CD2	2.50	0.47
29:SK:57:TYR:CD1	29:SK:74:GLU:OE1	2.68	0.47
42:e:364:PRO:HA	42:e:367:ALA:HB3	1.97	0.47
44:c:60:LEU:O	44:c:64:ILE:HG12	2.14	0.47
44:c:455:PHE:CE1	44:c:459:MET:HE2	2.48	0.47
44:c:464:PRO:HA	44:c:469:TYR:CD2	2.50	0.47
44:c:586:ARG:O	44:c:590:LEU:HD23	2.14	0.47
1:S2:1824:A:H4'	1:S2:1825:A:OP1	2.15	0.47
1:S2:1850:MA6:O5'	1:S2:1850:MA6:H8	2.15	0.47
3:SE:21:ASP:CG	3:SE:24:THR:HG1	2.23	0.47
4:SA:64:ALA:CB	9:SV:34:MET:HE3	2.45	0.47
6:SH:124:ALA:O	6:SH:127:ASP:OD1	2.33	0.47
8:SL:40:ILE:HD11	8:SL:61:PRO:C	2.40	0.47
27:Sg:60:ARG:CB	27:Sg:60:ARG:NH1	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:c:465:HIS:HB2	45:a:143:ARG:HD2	1.97	0.47
1:S2:159:A2M:H2	1:S2:468:A2M:O4'	2.15	0.47
1:S2:1798:C:H2'	1:S2:1799:G:O4'	2.15	0.47
14:SJ:35:TYR:CD2	14:SJ:106:LEU:HD13	2.49	0.47
31:SU:50:VAL:HG22	31:SU:91:LEU:HG	1.96	0.47
31:SU:106:ILE:HD12	31:SU:106:ILE:O	2.15	0.47
37:D:96:ILE:O	37:D:99:GLU:HG3	2.14	0.47
42:e:233:ILE:HG23	42:e:234:ASP:H	1.80	0.47
42:e:404:VAL:HG23	42:e:405:ILE:N	2.30	0.47
43:d:465:ILE:O	43:d:465:ILE:HD12	2.14	0.47
1:S2:1034:A:N7	1:S2:1081:U:O4	2.48	0.47
1:S2:1229:G:H21	34:ST:87:VAL:HG22	1.79	0.47
34:ST:60:THR:O	34:ST:64:LEU:HD23	2.14	0.47
44:c:371:ILE:CD1	44:c:411:ILE:HD13	2.37	0.47
45:a:348:ILE:N	45:a:348:ILE:HD12	2.29	0.47
36:SZ:52:LYS:HD3	36:SZ:52:LYS:O	2.15	0.46
42:e:299:LEU:HD13	42:e:299:LEU:C	2.40	0.46
45:a:25:GLN:HB3	45:a:26:PRO:HD3	1.97	0.46
1:S2:354:OMU:HM22	1:S2:355:G:O4'	2.15	0.46
1:S2:814:PSU:C4	1:S2:815:PSU:C6	3.03	0.46
1:S2:1226:G:N2	1:S2:1639:M7G:H81	2.30	0.46
44:c:153:GLU:O	44:c:156:ILE:HG22	2.14	0.46
15:SN:34:LYS:O	15:SN:38:TYR:CD2	2.68	0.46
15:SN:102:LEU:HD21	15:SN:111:ALA:CB	2.46	0.46
37:D:47:LEU:HD22	37:D:47:LEU:H	1.81	0.46
44:c:153:GLU:OE1	44:c:153:GLU:C	2.58	0.46
45:a:205:LEU:HD22	45:a:233:ARG:NH2	2.29	0.46
45:a:306:MET:SD	45:a:306:MET:C	2.99	0.46
47:m:197:ALA:HB1	47:m:200:ALA:HB3	1.97	0.46
16:SO:80:ASP:OD1	16:SO:80:ASP:C	2.58	0.46
22:SD:176:LEU:HD13	22:SD:176:LEU:O	2.15	0.46
33:SS:21:ASP:OD1	33:SS:21:ASP:O	2.33	0.46
35:SP:69:PRO:O	35:SP:70:MET:SD	2.74	0.46
43:d:21:VAL:HG12	43:d:22:PRO:HD3	1.98	0.46
44:c:459:MET:HE1	44:c:472:HIS:HB3	1.97	0.46
1:S2:952:G:H2'	1:S2:953:C:C6	2.51	0.46
1:S2:1373:C:OP1	25:SR:7:LYS:HE2	2.15	0.46
1:S2:1578:U:H2'	1:S2:1578:U:O2	2.16	0.46
4:SA:163:CYS:SG	4:SA:174:MET:HE3	2.55	0.46
8:SL:14:PRO:C	8:SL:15:THR:HG23	2.40	0.46
45:a:56:GLU:OE2	45:a:60:ASP:OD2	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1850:MA6:H2'	1:S2:1851:MA6:O4'	2.16	0.46
16:SO:131:ASP:OD1	16:SO:133:THR:HG22	2.15	0.46
24:Sf:136:PHE:CD1	24:Sf:136:PHE:C	2.93	0.46
30:SM:32:ALA:HB3	30:SM:110:VAL:O	2.16	0.46
34:ST:19:ALA:HB2	34:ST:55:THR:HA	1.98	0.46
38:E:381:LEU:HD11	38:E:452:ARG:HB3	1.98	0.46
44:c:445:LEU:HD21	44:c:490:LEU:HD22	1.97	0.46
45:a:291:PHE:O	45:a:295:THR:HG23	2.15	0.46
1:S2:198:U:H2'	1:S2:199:C:H2'	1.98	0.46
5:SB:69:VAL:HG22	5:SB:73:ASP:HB2	1.98	0.46
25:SR:57:LEU:HD13	25:SR:69:ILE:HD11	1.98	0.46
34:ST:30:VAL:HG13	34:ST:34:VAL:HG11	1.97	0.46
42:e:249:MET:O	42:e:250:CYS:C	2.58	0.46
45:a:248:GLU:OE1	45:a:248:GLU:HA	2.16	0.46
45:a:314:GLU:OE2	45:a:314:GLU:HA	2.16	0.46
45:a:534:LEU:O	45:a:537:ILE:HG22	2.16	0.46
1:S2:1316:C:O2'	1:S2:1317:C:P	2.73	0.46
3:SE:45:ILE:HD11	3:SE:49:ARG:HH21	1.79	0.46
5:SB:110:MET:HE2	5:SB:213:ARG:HD2	1.98	0.46
16:SO:30:VAL:HG22	16:SO:96:LYS:HG3	1.97	0.46
34:ST:9:VAL:HG22	34:ST:10:ASN:N	2.31	0.46
40:G:46:M7G:H2'	40:G:46:M7G:N3	2.31	0.46
41:H:83:ASP:OD1	41:H:83:ASP:N	2.47	0.46
42:e:308:ALA:HB2	42:e:340:ILE:HD12	1.98	0.46
42:e:338:LEU:HG	42:e:374:LEU:HD23	1.98	0.46
1:S2:796:G:H2'	1:S2:796:G:N3	2.31	0.46
1:S2:1453:C:H4'	25:SR:49:LYS:HA	1.98	0.46
14:SJ:114:VAL:HG13	14:SJ:126:ALA:HB1	1.97	0.46
30:SM:83:LYS:O	30:SM:87:GLU:OE2	2.34	0.46
44:c:86:LEU:C	44:c:86:LEU:HD13	2.40	0.46
1:S2:579:C:C4	1:S2:580:U:C5	3.04	0.46
3:SE:185:GLY:N	3:SE:189:LEU:HD23	2.31	0.46
30:SM:79:VAL:O	30:SM:80:ASP:HB2	2.16	0.46
1:S2:668:A2M:HM'3	1:S2:668:A2M:H1'	1.48	0.45
14:SJ:89:GLU:OE2	14:SJ:89:GLU:HA	2.15	0.45
19:Sb:79:PHE:CD1	19:Sb:79:PHE:C	2.94	0.45
42:e:208:LEU:HD11	42:e:242:TYR:HA	1.98	0.45
42:e:254:LEU:O	42:e:258:THR:HG22	2.16	0.45
45:a:47:HIS:CE1	45:a:77:ILE:HD12	2.51	0.45
45:a:161:LEU:HD12	45:a:174:TYR:CD1	2.51	0.45
45:a:548:GLU:O	45:a:549:GLN:C	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:SH:130:LEU:HD13	6:SH:130:LEU:O	2.17	0.45
8:SL:68:ILE:HG12	8:SL:143:LEU:HD21	1.99	0.45
14:SJ:158:ASP:OD1	14:SJ:159:PHE:N	2.48	0.45
31:SU:41:ARG:HG2	31:SU:41:ARG:HH11	1.82	0.45
36:SZ:72:VAL:O	36:SZ:76:ARG:HG2	2.16	0.45
44:c:682:LEU:HD23	44:c:682:LEU:O	2.17	0.45
45:a:469:ARG:O	45:a:473:ASP:OD1	2.33	0.45
45:a:530:LEU:HD23	45:a:530:LEU:C	2.40	0.45
47:m:327:GLN:O	47:m:328:THR:C	2.60	0.45
1:S2:27:A2M:H2'	1:S2:28:U:C6	2.51	0.45
1:S2:461:U:O2'	1:S2:462:OMC:P	2.74	0.45
5:SB:127:VAL:HG13	5:SB:176:VAL:HG11	1.99	0.45
16:SO:26:ASN:N	16:SO:26:ASN:ND2	2.63	0.45
17:SW:26:LEU:C	17:SW:26:LEU:HD13	2.40	0.45
36:SZ:69:THR:O	36:SZ:73:VAL:HG12	2.17	0.45
38:E:142:MET:SD	38:E:142:MET:C	3.00	0.45
41:H:36:ALA:HB2	41:H:51:CYS:SG	2.56	0.45
42:e:276:ASP:OD1	42:e:277:LEU:HD12	2.17	0.45
45:a:237:LEU:HD11	45:a:253:VAL:HG23	1.97	0.45
45:a:523:LEU:HD22	45:a:527:SER:CB	2.46	0.45
47:m:60:VAL:O	47:m:61:GLU:C	2.59	0.45
48:h:222:SER:HA	48:h:229:GLU:CB	2.46	0.45
1:S2:578:C:C4	1:S2:579:C:C5	3.05	0.45
3:SE:57:THR:HG22	3:SE:58:GLY:N	2.31	0.45
3:SE:139:LEU:HD12	3:SE:139:LEU:O	2.17	0.45
8:SL:66:VAL:HG11	8:SL:141:ASN:ND2	2.31	0.45
14:SJ:47:LYS:HG3	14:SJ:102:ILE:HD12	1.98	0.45
16:SO:132:VAL:O	16:SO:132:VAL:HG12	2.17	0.45
42:e:399:SER:HA	42:e:403:GLN:HB2	1.97	0.45
45:a:331:ILE:O	45:a:331:ILE:HG22	2.17	0.45
1:S2:942:G:H2'	1:S2:943:U:C6	2.51	0.45
1:S2:987:A:C6	5:SB:120:MET:HE1	2.52	0.45
1:S2:1421:A:H2'	1:S2:1422:G:O4'	2.16	0.45
13:SG:32:MET:O	13:SG:34:THR:HG23	2.16	0.45
15:SN:141:TYR:CD1	15:SN:141:TYR:C	2.94	0.45
19:Sb:13:GLU:HG2	19:Sb:14:GLU:N	2.32	0.45
34:ST:113:VAL:HG22	34:ST:114:GLU:N	2.32	0.45
37:D:71:VAL:HG21	37:D:85:LEU:HD22	1.98	0.45
38:E:296:VAL:HG22	38:E:358:LEU:HD12	1.98	0.45
44:c:336:ILE:HG13	44:c:353:LEU:HD22	1.97	0.45
45:a:230:LEU:HD13	45:a:230:LEU:C	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:a:519:ILE:HD12	45:a:519:ILE:N	2.30	0.45
45:a:533:ALA:O	45:a:536:VAL:HG12	2.16	0.45
1:S2:1809:A:H2'	1:S2:1810:U:C6	2.51	0.45
4:SA:84:GLN:HG2	4:SA:100:ALA:HB1	1.98	0.45
36:SZ:52:LYS:HE2	36:SZ:52:LYS:HA	1.98	0.45
37:D:282:ASP:HA	37:D:285:GLU:OE1	2.17	0.45
41:H:27:VAL:O	41:H:28:PHE:HB2	2.16	0.45
42:e:234:ASP:OD1	42:e:234:ASP:O	2.35	0.45
43:d:395:THR:O	43:d:396:LEU:HD12	2.16	0.45
45:a:317:ARG:HA	45:a:317:ARG:NE	2.32	0.45
1:S2:896:U:H2'	1:S2:897:U:H5	1.82	0.45
1:S2:1374:C:H2'	1:S2:1375:G:O4'	2.17	0.45
7:SI:79:ILE:HD11	7:SI:105:ASP:OD1	2.15	0.45
9:SV:54:ALA:O	9:SV:55:ILE:HD13	2.17	0.45
10:SX:46:HIS:CD2	10:SX:103:ALA:HB2	2.52	0.45
17:SW:28:ARG:HB3	17:SW:29:PRO:HD3	1.98	0.45
44:c:505:LEU:HD12	44:c:505:LEU:O	2.17	0.45
45:a:15:ALA:O	45:a:19:LEU:HG	2.17	0.45
45:a:122:GLN:O	45:a:122:GLN:CG	2.64	0.45
45:a:482:VAL:O	45:a:482:VAL:HG13	2.17	0.45
1:S2:121:OMU:HM23	3:SE:144:ALA:HB3	1.99	0.45
1:S2:679:A:C5	1:S2:680:G:C8	3.05	0.45
24:Sf:138:ARG:HB2	24:Sf:147:THR:HG23	1.99	0.45
27:Sg:269:GLU:OE2	27:Sg:269:GLU:HA	2.16	0.45
28:Sc:37:ASP:O	28:Sc:38:THR:CG2	2.65	0.45
43:d:69:TYR:N	43:d:69:TYR:CD1	2.82	0.45
45:a:283:PHE:O	45:a:287:GLY:O	2.34	0.45
1:S2:27:A2M:HM'3	1:S2:27:A2M:H1'	1.79	0.45
1:S2:96:C:H2'	1:S2:97:U:C6	2.51	0.45
1:S2:1520:G:H2'	1:S2:1520:G:N3	2.31	0.45
7:SI:131:PRO:O	7:SI:132:GLU:HB3	2.17	0.45
27:Sg:168:CYS:HB2	27:Sg:195:LEU:HD13	1.99	0.45
32:SQ:31:LEU:HD13	32:SQ:31:LEU:C	2.41	0.45
35:SP:74:GLU:OE2	35:SP:74:GLU:N	2.50	0.45
37:D:205:ILE:HD13	38:E:345:PRO:HD3	1.98	0.45
43:d:214:GLU:O	43:d:465:ILE:HD12	2.16	0.45
1:S2:1277:C:H5''	29:SK:55:ARG:HD3	1.98	0.45
1:S2:1405:A:H2'	1:S2:1406:G:O4'	2.16	0.45
5:SB:36:PRO:HB3	5:SB:231:LEU:HD11	1.99	0.45
12:SC:102:LEU:HD12	12:SC:130:ILE:HG12	1.99	0.45
12:SC:191:VAL:HG11	12:SC:236:PHE:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:SW:105:THR:O	17:SW:105:THR:CG2	2.65	0.45
36:SZ:53:ALA:O	36:SZ:56:ASP:OD1	2.34	0.45
42:e:261:VAL:HG11	42:e:274:LEU:HG	1.99	0.45
42:e:392:VAL:HG13	42:e:392:VAL:O	2.17	0.45
44:c:781:ARG:O	44:c:785:GLU:OE1	2.35	0.45
45:a:43:TRP:CD1	45:a:43:TRP:C	2.95	0.45
45:a:538:LYS:HB2	45:a:539:PRO:HD3	1.99	0.45
1:S2:563:G:HO2'	1:S2:564:A:P	2.39	0.44
1:S2:575:A:C3'	1:S2:576:A2M:H5''	2.45	0.44
1:S2:1223:A:O2'	1:S2:1651:A:H4'	2.18	0.44
4:SA:77:ILE:HD11	4:SA:124:VAL:HG22	1.99	0.44
19:Sb:14:GLU:O	19:Sb:18:LYS:HG2	2.18	0.44
37:D:194:ASP:OD1	37:D:273:MET:HB2	2.17	0.44
42:e:416:GLN:C	42:e:416:GLN:OE1	2.60	0.44
44:c:739:ALA:HB1	44:c:755:PHE:CE2	2.51	0.44
44:c:819:HIS:C	44:c:819:HIS:ND1	2.76	0.44
44:c:831:LEU:HD12	44:c:831:LEU:N	2.32	0.44
45:a:521:ASN:HA	45:a:524:THR:HG23	1.99	0.44
15:SN:33:VAL:O	15:SN:36:GLN:OE1	2.35	0.44
44:c:412:LEU:HD21	44:c:489:TYR:CE1	2.53	0.44
45:a:265:LYS:C	45:a:265:LYS:HD2	2.42	0.44
47:m:322:TYR:HB3	47:m:332:VAL:HA	2.00	0.44
1:S2:885:U:H2'	1:S2:886:A:C4	2.52	0.44
1:S2:1218:C:N3	1:S2:1219:C:C5	2.85	0.44
1:S2:1545:A:H2'	1:S2:1546:G:C8	2.52	0.44
3:SE:102:ILE:CG2	3:SE:182:MET:HE1	2.47	0.44
6:SH:32:MET:SD	6:SH:32:MET:N	2.90	0.44
15:SN:33:VAL:HA	15:SN:36:GLN:OE1	2.18	0.44
24:Sf:110:GLU:OE1	24:Sf:110:GLU:N	2.50	0.44
24:Sf:136:PHE:CD1	24:Sf:137:ASP:OD1	2.71	0.44
43:d:28:MET:HE2	44:c:591:MET:CE	2.40	0.44
44:c:418:ILE:HG13	44:c:425:LEU:HD11	1.99	0.44
44:c:424:ILE:HD11	44:c:437:PRO:HB2	1.99	0.44
44:c:743:ALA:HB1	44:c:751:THR:CG2	2.45	0.44
45:a:27:ALA:O	45:a:30:VAL:HG22	2.17	0.44
45:a:379:VAL:HG12	45:a:383:VAL:HG13	2.00	0.44
45:a:481:GLN:CD	45:a:518:GLN:NE2	2.76	0.44
1:S2:1035:A:C4	1:S2:1036:A:C8	3.05	0.44
17:SW:106:THR:HG22	17:SW:122:GLY:O	2.17	0.44
18:SY:40:ILE:HD12	18:SY:40:ILE:HA	1.87	0.44
25:SR:126:MET:O	25:SR:126:MET:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:SK:76:ILE:HD12	29:SK:91:PRO:HG2	1.99	0.44
31:SU:25:THR:HG22	31:SU:111:GLU:CG	2.47	0.44
34:ST:108:GLU:OE1	34:ST:108:GLU:HA	2.17	0.44
43:d:214:GLU:O	43:d:464:VAL:HG13	2.17	0.44
44:c:357:LEU:HD23	44:c:357:LEU:O	2.18	0.44
44:c:398:TRP:CD1	44:c:398:TRP:C	2.95	0.44
44:c:573:ILE:CD1	44:c:589:MET:HE2	2.48	0.44
45:a:327:LEU:HD23	45:a:370:LEU:HD11	2.00	0.44
1:S2:493:A:C2	1:S2:494:C:C6	3.06	0.44
4:SA:90:PHE:CE1	4:SA:94:THR:HG21	2.52	0.44
5:SB:191:ASP:O	5:SB:191:ASP:CG	2.60	0.44
10:SX:122:VAL:HG23	10:SX:130:LEU:HD22	2.00	0.44
12:SC:70:VAL:HG21	12:SC:93:ILE:HG23	2.00	0.44
24:Sf:150:PHE:C	24:Sf:150:PHE:CD1	2.93	0.44
33:SS:33:ILE:HD13	33:SS:71:MET:HE1	1.99	0.44
38:E:310:MET:SD	38:E:310:MET:C	3.00	0.44
43:d:45:TRP:CZ3	44:c:607:ILE:HG23	2.52	0.44
44:c:398:TRP:CE3	44:c:458:ILE:HD12	2.52	0.44
44:c:611:ARG:HD2	44:c:646:LEU:HD21	2.00	0.44
1:S2:1114:U:H3'	1:S2:1115:U:H2'	2.00	0.44
6:SH:27:LEU:HD21	6:SH:40:LEU:HD21	2.00	0.44
8:SL:75:GLY:HA3	8:SL:88:ILE:HD12	1.99	0.44
19:Sb:35:VAL:HG21	19:Sb:63:LEU:CD2	2.48	0.44
32:SQ:96:TYR:HD1	32:SQ:100:VAL:HG11	1.82	0.44
41:H:16:LYS:O	41:H:17:ASN:CB	2.65	0.44
44:c:75:ASP:OD1	44:c:78:LYS:HB3	2.17	0.44
44:c:152:PHE:CD1	44:c:152:PHE:N	2.85	0.44
44:c:756:ILE:O	44:c:756:ILE:CG2	2.66	0.44
45:a:41:ARG:HB2	45:a:41:ARG:NH1	2.33	0.44
45:a:55:LEU:CD1	45:a:71:LEU:HD21	2.47	0.44
45:a:147:THR:N	45:a:148:PRO:CD	2.81	0.44
1:S2:2:A:O4'	1:S2:418:A:C8	2.71	0.44
1:S2:634:A:C2	1:S2:635:G:N7	2.85	0.44
1:S2:1598:G:H2'	36:SZ:80:ARG:HG2	1.99	0.44
10:SX:85:VAL:O	10:SX:85:VAL:CG2	2.66	0.44
13:SG:228:ILE:O	13:SG:232:ARG:HG2	2.17	0.44
16:SO:30:VAL:HG23	16:SO:94:HIS:HB2	2.00	0.44
18:SY:79:LEU:HD13	18:SY:79:LEU:O	2.17	0.44
30:SM:18:LEU:O	30:SM:22:LEU:HG	2.17	0.44
30:SM:22:LEU:HD12	30:SM:23:LYS:H	1.82	0.44
32:SQ:45:ARG:O	32:SQ:45:ARG:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:SP:12:PHE:CD1	35:SP:12:PHE:C	2.96	0.44
37:D:4:LEU:HB3	37:D:127:LEU:HD22	2.00	0.44
38:E:258:VAL:HG11	38:E:353:MET:CE	2.47	0.44
38:E:371:LEU:HD13	38:E:459:ILE:HD11	1.99	0.44
43:d:458:LYS:HG2	43:d:458:LYS:O	2.17	0.44
45:a:234:LEU:HD11	45:a:274:ASN:HB3	1.99	0.44
45:a:417:GLN:N	45:a:418:PRO:HD3	2.33	0.44
45:a:544:GLN:O	45:a:548:GLU:HB2	2.18	0.44
1:S2:1396:A:O2'	1:S2:1398:G:N7	2.50	0.44
1:S2:1442:OMU:HM23	1:S2:1442:OMU:H1'	1.53	0.44
1:S2:1753:C:H2'	1:S2:1755:C:H41	1.83	0.44
2:Ln:15:ARG:O	2:Ln:19:LYS:HG2	2.17	0.44
4:SA:1:MET:N	4:SA:56:GLU:HA	2.33	0.44
4:SA:181:GLU:O	4:SA:185:MET:HG3	2.17	0.44
22:SD:55:THR:O	22:SD:59:LEU:HG	2.17	0.44
23:SF:102:LEU:HD11	36:SZ:110:THR:HG21	1.99	0.44
23:SF:163:PHE:CD2	23:SF:164:ARG:HG3	2.53	0.44
30:SM:22:LEU:HD13	30:SM:88:TRP:O	2.18	0.44
30:SM:121:LYS:O	30:SM:124:ILE:HD12	2.18	0.44
44:c:368:GLU:O	44:c:372:VAL:HG23	2.18	0.44
45:a:516:SER:C	45:a:517:GLU:HG3	2.43	0.44
12:SC:271:ASP:O	12:SC:274:VAL:HG22	2.18	0.44
18:SY:117:VAL:HG11	18:SY:125:VAL:HG21	2.00	0.44
39:F:183:VAL:O	39:F:187:MET:SD	2.76	0.44
41:H:1:MET:N	41:H:2:PRO:CD	2.81	0.44
41:H:1:MET:N	41:H:2:PRO:HD2	2.33	0.44
42:e:413:PHE:HE2	50:l:536:ALA:CB	2.30	0.44
43:d:319:ILE:HD11	43:d:463:HIS:CG	2.52	0.44
45:a:443:VAL:HG22	45:a:447:TYR:HB2	2.00	0.44
1:S2:455:A:H2'	1:S2:456:C:H6	1.81	0.43
1:S2:1009:A:O2'	15:SN:114:ARG:HG2	2.18	0.43
4:SA:1:MET:SD	9:SV:79:VAL:HG22	2.58	0.43
5:SB:75:GLN:O	5:SB:76:ASN:OD1	2.36	0.43
6:SH:166:VAL:HG12	6:SH:166:VAL:O	2.18	0.43
14:SJ:117:LEU:CD2	14:SJ:157:ILE:HG21	2.48	0.43
25:SR:53:TYR:CE2	25:SR:57:LEU:HD11	2.53	0.43
34:ST:108:GLU:OE1	34:ST:113:VAL:HG13	2.18	0.43
36:SZ:96:LEU:HD23	36:SZ:96:LEU:H	1.82	0.43
38:E:50:VAL:O	38:E:51:ALA:HB3	2.18	0.43
45:a:535:GLU:O	45:a:539:PRO:HD3	2.18	0.43
45:a:549:GLN:CD	45:a:550:HIS:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1036:A:C4	1:S2:1037:G:C8	3.07	0.43
3:SE:59:ASP:OD1	3:SE:59:ASP:C	2.61	0.43
14:SJ:113:GLN:OE1	14:SJ:113:GLN:HA	2.18	0.43
25:SR:12:ALA:O	25:SR:16:ILE:CD1	2.63	0.43
38:E:105:CYS:SG	38:E:106:GLY:N	2.91	0.43
42:e:252:HIS:HB3	42:e:256:TYR:OH	2.17	0.43
44:c:566:THR:HG23	44:c:594:LEU:HD21	2.01	0.43
44:c:621:PHE:N	44:c:629:ALA:HB2	2.33	0.43
44:c:785:GLU:O	44:c:789:ARG:HG3	2.18	0.43
45:a:175:HIS:CD2	45:a:232:THR:HG21	2.53	0.43
27:Sg:78:ALA:HB2	27:Sg:92:LEU:HD21	2.00	0.43
29:SK:8:ARG:O	29:SK:11:ILE:HG12	2.18	0.43
30:SM:76:LEU:C	30:SM:77:ILE:HD13	2.43	0.43
38:E:373:ILE:HD12	38:E:427:ILE:HD12	1.99	0.43
42:e:201:VAL:O	42:e:202:SER:OG	2.33	0.43
42:e:366:GLU:OE1	42:e:366:GLU:O	2.35	0.43
44:c:383:TYR:OH	44:c:451:MET:HB2	2.18	0.43
44:c:718:LEU:HD11	45:a:344:MET:SD	2.59	0.43
44:c:780:VAL:HA	44:c:783:ILE:HD11	2.00	0.43
44:c:823:SER:HA	44:c:826:ILE:HG12	1.99	0.43
45:a:268:LYS:HD3	45:a:271:LEU:HD12	2.00	0.43
47:m:48:ALA:C	47:m:50:ASP:H	2.26	0.43
47:m:327:GLN:O	47:m:327:GLN:HG2	2.18	0.43
1:S2:521:A:OP1	14:SJ:45:ARG:HD3	2.18	0.43
1:S2:558:G:H1'	1:S2:559:G:C8	2.53	0.43
4:SA:18:PHE:HD1	4:SA:23:THR:HG21	1.82	0.43
4:SA:206:ASP:OD1	4:SA:207:PRO:HD2	2.18	0.43
12:SC:127:PHE:HD2	12:SC:141:VAL:HG22	1.83	0.43
28:Sc:37:ASP:C	28:Sc:38:THR:HG22	2.43	0.43
35:SP:35:GLN:OE1	35:SP:35:GLN:HA	2.16	0.43
42:e:252:HIS:HB3	42:e:256:TYR:CZ	2.53	0.43
44:c:515:ASP:H	44:c:579:HIS:HE2	1.64	0.43
45:a:153:LEU:O	45:a:157:TYR:HD1	2.01	0.43
1:S2:2:A:C2	12:SC:196:ILE:HD13	2.53	0.43
1:S2:2:A:C8	12:SC:223:TYR:CD2	3.07	0.43
1:S2:1199:A:H2'	1:S2:1200:A:O4'	2.19	0.43
1:S2:1334:G:O3'	22:SD:183:GLY:HA3	2.18	0.43
4:SA:23:THR:HG22	4:SA:23:THR:O	2.19	0.43
6:SH:126:HIS:CE1	6:SH:181:THR:HG23	2.53	0.43
14:SJ:137:VAL:CG2	14:SJ:142:VAL:HG21	2.47	0.43
16:SO:30:VAL:HG12	16:SO:45:THR:HG23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:D:122:THR:HG23	37:D:123:LYS:CD	2.48	0.43
41:H:1:MET:H3	41:H:2:PRO:CD	2.31	0.43
42:e:362:MET:HE2	42:e:363:THR:N	2.34	0.43
44:c:64:ILE:HG13	44:c:109:ILE:CD1	2.48	0.43
44:c:443:CYS:HB3	44:c:446:THR:OG1	2.18	0.43
44:c:700:ALA:HB2	44:c:793:PHE:CD1	2.54	0.43
44:c:815:LEU:N	44:c:816:PRO:HD2	2.33	0.43
45:a:380:LEU:O	45:a:383:VAL:HG22	2.18	0.43
6:SH:45:ILE:HD12	6:SH:62:ILE:HG23	2.01	0.43
8:SL:25:LEU:HD23	8:SL:25:LEU:H	1.84	0.43
10:SX:81:ILE:HD12	10:SX:120:PHE:CD2	2.54	0.43
24:Sf:146:LEU:O	24:Sf:146:LEU:HD12	2.18	0.43
25:SR:99:ASP:OD1	25:SR:99:ASP:C	2.62	0.43
29:SK:9:ILE:O	29:SK:13:GLU:HG3	2.18	0.43
32:SQ:100:VAL:HG13	32:SQ:101:ASP:H	1.83	0.43
42:e:407:LYS:HG3	42:e:408:THR:N	2.34	0.43
45:a:141:THR:HG22	45:a:145:LEU:HD13	1.99	0.43
45:a:534:LEU:O	45:a:534:LEU:HD23	2.18	0.43
1:S2:166:A2M:H5'	1:S2:166:A2M:C8	2.48	0.43
5:SB:186:ASN:O	45:a:17:GLU:OE2	2.36	0.43
24:Sf:137:ASP:O	24:Sf:150:PHE:HB3	2.19	0.43
27:Sg:217:MET:HG2	27:Sg:226:HIS:HE1	1.83	0.43
35:SP:93:MET:HE1	35:SP:106:GLU:HB2	2.00	0.43
44:c:504:LEU:HG	44:c:564:ILE:HG23	2.00	0.43
45:a:175:HIS:CG	45:a:232:THR:HG21	2.52	0.43
48:h:225:ALA:HA	48:h:229:GLU:CB	2.48	0.43
1:S2:428:OMU:H6	1:S2:428:OMU:CM2	2.48	0.43
1:S2:443:U:H2'	1:S2:444:G:O4'	2.19	0.43
1:S2:456:C:C2	1:S2:457:C:C5	3.07	0.43
1:S2:619:A:H61	10:SX:115:ILE:HD11	1.83	0.43
1:S2:1678:A2M:O2'	1:S2:1679:A:H5'	2.19	0.43
4:SA:1:MET:H1	4:SA:56:GLU:HA	1.83	0.43
6:SH:128:ALA:O	6:SH:131:GLU:HG3	2.18	0.43
8:SL:16:ILE:HD13	8:SL:36:TYR:HB2	2.00	0.43
10:SX:94:ILE:HG22	10:SX:125:VAL:HG21	1.99	0.43
20:Se:2:VAL:CG2	41:H:92:ILE:HD12	2.49	0.43
27:Sg:92:LEU:N	27:Sg:92:LEU:HD22	2.33	0.43
29:SK:10:ALA:HB1	29:SK:38:LYS:HD2	2.00	0.43
31:SU:61:LEU:HD12	31:SU:61:LEU:N	2.33	0.43
42:e:247:GLN:NE2	42:e:253:ILE:HG13	2.34	0.43
42:e:356:LEU:HD21	42:e:371:ILE:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:a:518:GLN:HG2	45:a:519:ILE:HD12	2.00	0.43
45:a:532:LYS:NZ	46:3f:280:GLN:CB	2.82	0.43
47:m:345:GLN:CD	47:m:345:GLN:C	2.86	0.43
1:S2:563:G:C2	1:S2:564:A:C8	3.05	0.43
1:S2:929:G:H2'	1:S2:930:C:O4'	2.19	0.43
1:S2:1255:G:O4'	31:SU:71:GLY:HA3	2.19	0.43
1:S2:1284:A:N1	30:SM:91:LEU:HD21	2.34	0.43
23:SF:78:MET:O	23:SF:79:HIS:HB2	2.18	0.43
23:SF:195:GLU:OE1	37:D:45:MET:SD	2.77	0.43
26:Sd:6:LEU:O	26:Sd:6:LEU:HG	2.19	0.43
38:E:405:MET:SD	38:E:451:TRP:CD1	3.12	0.43
43:d:369:ILE:O	43:d:369:ILE:HG13	2.19	0.43
44:c:520:GLN:O	44:c:521:ARG:HB3	2.18	0.43
45:a:25:GLN:O	45:a:29:ASP:OD2	2.37	0.43
45:a:30:VAL:O	45:a:33:ASP:OD1	2.36	0.43
1:S2:29:G:H2'	1:S2:30:C:C6	2.54	0.43
1:S2:102:A:H4'	1:S2:104:A:C8	2.54	0.43
11:Sa:94:ASP:OD1	11:Sa:96:THR:HG22	2.19	0.43
12:SC:78:LEU:HD13	12:SC:97:PHE:CD2	2.54	0.43
15:SN:71:ILE:O	15:SN:75:LEU:HD22	2.18	0.43
16:SO:63:LYS:H	16:SO:63:LYS:HD3	1.84	0.43
17:SW:5:ASN:HB3	17:SW:8:ALA:HB3	2.01	0.43
24:Sf:137:ASP:HB2	24:Sf:138:ARG:HD3	2.01	0.43
32:SQ:100:VAL:HG13	32:SQ:101:ASP:N	2.34	0.43
37:D:56:ILE:O	37:D:56:ILE:CD1	2.65	0.43
38:E:49:HIS:O	38:E:52:HIS:ND1	2.52	0.43
44:c:504:LEU:HD21	44:c:567:CYS:HB3	2.00	0.43
3:SE:116:PRO:O	3:SE:120:LYS:HG2	2.19	0.42
16:SO:56:VAL:HG23	16:SO:77:ALA:HB1	2.00	0.42
21:B:-5:G:H2'	21:B:-4:A:C4'	2.49	0.42
28:Sc:46:VAL:CG1	28:Sc:50:VAL:HG21	2.48	0.42
31:SU:63:ILE:HG23	31:SU:80:PHE:HB2	2.01	0.42
37:D:237:MET:SD	37:D:237:MET:C	3.02	0.42
40:G:54:A:H2'	40:G:54:A:N3	2.34	0.42
41:H:39:ILE:HD11	41:H:50:MET:HB2	2.00	0.42
42:e:413:PHE:HE2	50:l:536:ALA:HB1	1.84	0.42
44:c:520:GLN:O	44:c:520:GLN:HG3	2.19	0.42
44:c:607:ILE:HG13	44:c:608:LEU:N	2.33	0.42
45:a:438:ARG:CZ	45:a:510:HIS:NE2	2.82	0.42
1:S2:1516:G:H4'	35:SP:122:THR:OG1	2.19	0.42
1:S2:1828:C:H2'	1:S2:1829:G:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:SA:77:ILE:HG22	4:SA:99:ILE:HB	2.00	0.42
15:SN:48:SER:O	15:SN:52:VAL:HG13	2.19	0.42
18:SY:54:VAL:O	18:SY:54:VAL:HG13	2.18	0.42
23:SF:139:VAL:HG12	23:SF:140:ASP:O	2.18	0.42
27:Sg:152:SER:O	27:Sg:153:CYS:C	2.61	0.42
34:ST:32:GLU:OE2	34:ST:32:GLU:N	2.51	0.42
37:D:171:ASP:O	37:D:174:GLU:HG3	2.19	0.42
38:E:367:ILE:HG22	38:E:434:CYS:HA	2.01	0.42
44:c:384:ASP:O	44:c:385:TYR:C	2.61	0.42
44:c:403:ASP:O	44:c:407:GLU:HG2	2.18	0.42
1:S2:1610:G:O3'	33:SS:110:ASP:OD2	2.37	0.42
7:SI:143:LYS:HG2	7:SI:144:LYS:N	2.34	0.42
27:Sg:121:VAL:HG12	27:Sg:156:PHE:CE2	2.54	0.42
33:SS:62:ASP:OD1	33:SS:63:GLU:N	2.53	0.42
35:SP:22:LEU:HD13	35:SP:22:LEU:C	2.44	0.42
35:SP:22:LEU:HD13	35:SP:22:LEU:O	2.20	0.42
36:SZ:92:LEU:HD13	36:SZ:92:LEU:O	2.19	0.42
38:E:57:VAL:HG23	38:E:58:VAL:N	2.33	0.42
44:c:349:ALA:HA	44:c:352:GLU:HG2	2.01	0.42
47:m:312:VAL:HA	47:m:322:TYR:OH	2.20	0.42
1:S2:433:A:H5''	7:SI:22:HIS:HB3	2.01	0.42
1:S2:495:U:H2'	1:S2:496:C:O4'	2.19	0.42
1:S2:1139:C:O2	1:S2:1139:C:O4'	2.36	0.42
1:S2:1308:U:H2'	1:S2:1309:C:O5'	2.19	0.42
5:SB:104:ASP:OD1	5:SB:105:LEU:N	2.52	0.42
6:SH:10:LYS:NZ	6:SH:45:ILE:HD11	2.34	0.42
11:Sa:41:ILE:CD1	11:Sa:68:TYR:CD2	3.02	0.42
25:SR:24:LEU:O	25:SR:58:MET:HE1	2.20	0.42
27:Sg:191:HIS:CE1	27:Sg:217:MET:HE3	2.54	0.42
30:SM:31:LEU:O	30:SM:32:ALA:C	2.62	0.42
36:SZ:99:LEU:HD13	36:SZ:109:TYR:CE1	2.55	0.42
38:E:147:ASN:OD1	38:E:147:ASN:C	2.62	0.42
42:e:293:THR:O	42:e:297:GLU:HG2	2.20	0.42
44:c:52:ALA:O	44:c:56:ARG:HG2	2.19	0.42
44:c:328:VAL:O	44:c:328:VAL:HG22	2.18	0.42
44:c:406:ASN:OD1	44:c:482:ILE:HD11	2.20	0.42
45:a:47:HIS:HE1	45:a:77:ILE:HD12	1.84	0.42
45:a:145:LEU:N	45:a:145:LEU:HD12	2.34	0.42
45:a:373:ASP:O	45:a:378:ASN:HA	2.19	0.42
45:a:380:LEU:HA	45:a:383:VAL:HG22	2.02	0.42
45:a:412:ASN:O	45:a:416:GLU:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:578:C:C2	1:S2:579:C:C6	3.07	0.42
1:S2:1531:A:H2'	1:S2:1532:C:C6	2.55	0.42
4:SA:180:ARG:O	4:SA:184:ARG:HG2	2.20	0.42
6:SH:130:LEU:HD13	6:SH:130:LEU:C	2.44	0.42
15:SN:32:ASP:O	15:SN:36:GLN:OE1	2.38	0.42
18:SY:44:LEU:HD12	18:SY:55:ILE:HD11	2.01	0.42
23:SF:113:VAL:O	23:SF:117:ILE:HG12	2.20	0.42
27:Sg:91:ASP:OD1	27:Sg:91:ASP:O	2.37	0.42
28:Sc:33:GLU:OE1	28:Sc:33:GLU:O	2.37	0.42
42:e:356:LEU:HD12	42:e:356:LEU:C	2.45	0.42
44:c:424:ILE:C	44:c:425:LEU:HD12	2.45	0.42
1:S2:562:U:H5'	1:S2:563:G:OP1	2.20	0.42
1:S2:853:C:C2	1:S2:854:A:C8	3.07	0.42
1:S2:903:A:H2'	1:S2:904:A:C8	2.54	0.42
4:SA:64:ALA:HB2	9:SV:34:MET:HE3	2.00	0.42
27:Sg:49:GLU:OE2	27:Sg:49:GLU:N	2.53	0.42
35:SP:69:PRO:HB2	35:SP:70:MET:HE3	2.01	0.42
44:c:626:THR:CB	44:c:693:LEU:HD21	2.50	0.42
44:c:733:MET:SD	44:c:734:ARG:N	2.92	0.42
44:c:848:GLU:OE2	44:c:851:ALA:HB3	2.20	0.42
1:S2:640:A:H2'	1:S2:641:A:C8	2.55	0.42
1:S2:1139:C:H2'	1:S2:1140:G:O4'	2.20	0.42
1:S2:1665:G:C5	34:ST:88:MET:SD	3.13	0.42
5:SB:133:TYR:CE1	5:SB:221:PRO:HD2	2.54	0.42
12:SC:148:ALA:O	12:SC:152:ARG:HG2	2.20	0.42
29:SK:18:GLU:O	29:SK:93:THR:HG23	2.19	0.42
38:E:318:ILE:HD13	38:E:339:VAL:HG23	2.00	0.42
42:e:220:PHE:N	42:e:220:PHE:CD1	2.86	0.42
42:e:275:LYS:O	42:e:279:LYS:HG3	2.18	0.42
43:d:37:ASP:OD1	44:c:590:LEU:CD1	2.68	0.42
44:c:409:MET:HB3	44:c:485:ARG:NH2	2.35	0.42
45:a:113:LEU:HD11	45:a:138:GLN:OE1	2.19	0.42
1:S2:429:C:H4'	3:SE:12:VAL:HG23	2.02	0.42
1:S2:481:C:H2'	1:S2:482:G:O4'	2.19	0.42
1:S2:534:G:H2'	1:S2:535:G:C1'	2.50	0.42
1:S2:1261:C:C6	1:S2:1619:A:N1	2.88	0.42
11:Sa:26:CYS:SG	11:Sa:28:ARG:HB2	2.60	0.42
23:SF:99:ILE:HD13	23:SF:171:GLU:HG3	2.01	0.42
25:SR:77:GLU:CD	25:SR:81:ARG:HE	2.27	0.42
31:SU:95:SER:O	31:SU:98:VAL:HG12	2.20	0.42
35:SP:106:GLU:HA	35:SP:106:GLU:OE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:SP:110:GLU:OE2	35:SP:110:GLU:N	2.52	0.42
43:d:28:MET:O	43:d:29:PRO:C	2.63	0.42
44:c:682:LEU:HD23	44:c:682:LEU:C	2.45	0.42
44:c:733:MET:SD	44:c:734:ARG:HG3	2.60	0.42
45:a:30:VAL:HG23	45:a:31:LEU:HD23	2.02	0.42
45:a:48:GLU:HB3	45:a:49:PRO:HD3	2.02	0.42
45:a:277:ASN:O	45:a:281:THR:HG22	2.20	0.42
47:m:336:HIS:ND1	47:m:338:THR:HG22	2.35	0.42
1:S2:27:A2M:H2'	1:S2:28:U:H6	1.85	0.42
1:S2:106:C:H2'	1:S2:107:A:H8	1.85	0.42
1:S2:116:OMU:H2'	1:S2:117:C:O4'	2.20	0.42
1:S2:468:A2M:HM'3	1:S2:468:A2M:H1'	1.81	0.42
1:S2:1666:C:H2'	1:S2:1667:U:O4'	2.19	0.42
3:SE:180:LEU:HD23	3:SE:181:CYS:H	1.84	0.42
4:SA:94:THR:HG22	4:SA:183:LEU:HD21	2.00	0.42
13:SG:224:ARG:O	13:SG:227:GLN:HG3	2.20	0.42
22:SD:68:GLU:HG2	29:SK:20:VAL:HG12	2.02	0.42
28:Sc:15:THR:O	28:Sc:16:LYS:C	2.62	0.42
32:SQ:112:LEU:HD13	32:SQ:120:LEU:HD11	2.02	0.42
33:SS:21:ASP:OD1	33:SS:24:ARG:HG2	2.19	0.42
42:e:244:ASN:O	42:e:249:MET:SD	2.78	0.42
42:e:397:ALA:C	42:e:399:SER:H	2.27	0.42
42:e:416:GLN:O	42:e:420:MET:HG3	2.19	0.42
44:c:857:LEU:HD22	46:3f:340:LEU:CB	2.50	0.42
45:a:69:GLU:OE2	45:a:69:GLU:HA	2.19	0.42
45:a:475:ALA:HB2	45:a:482:VAL:HG12	2.02	0.42
1:S2:194:C:H2'	1:S2:195:C:N1	2.35	0.42
1:S2:557:U:H2'	1:S2:558:G:C8	2.55	0.42
1:S2:1308:U:HO2'	1:S2:1309:C:P	2.42	0.42
1:S2:1621:U:O2'	1:S2:1622:U:H2'	2.20	0.42
1:S2:1678:A2M:HM'3	1:S2:1678:A2M:H1'	1.70	0.42
27:Sg:262:GLU:C	27:Sg:262:GLU:CD	2.88	0.42
30:SM:72:HIS:HB3	30:SM:74:ILE:HD13	2.02	0.42
31:SU:20:ILE:CD1	31:SU:98:VAL:HG11	2.50	0.42
37:D:163:LEU:C	37:D:163:LEU:HD12	2.45	0.42
42:e:235:LEU:HD12	42:e:236:PHE:H	1.84	0.42
44:c:374:ILE:HA	44:c:377:ASN:OD1	2.18	0.42
44:c:742:LYS:HA	45:a:340:ARG:CD	2.50	0.42
48:h:350:TYR:O	48:h:351:ASN:C	2.61	0.42
1:S2:71:G:H22	13:SG:170:ARG:HH21	1.68	0.41
1:S2:512:A2M:H1'	1:S2:512:A2M:HM'3	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1088:U:H4'	1:S2:1089:G:OP2	2.19	0.41
1:S2:1265:A:H5'	1:S2:1266:C:OP2	2.20	0.41
1:S2:1567:G:C6	33:SS:82:TRP:CG	3.08	0.41
9:SV:16:LYS:H	12:SC:259:THR:HG21	1.85	0.41
9:SV:66:ASP:OD1	9:SV:66:ASP:C	2.62	0.41
13:SG:105:ASN:OD1	13:SG:105:ASN:C	2.61	0.41
14:SJ:29:LEU:HD23	20:Se:42:PHE:HE2	1.84	0.41
23:SF:204:ARG:CZ	28:Sc:60:GLU:CD	2.93	0.41
42:e:362:MET:CE	42:e:363:THR:O	2.68	0.41
44:c:649:GLY:HA2	44:c:670:GLN:CB	2.50	0.41
45:a:229:HIS:O	45:a:233:ARG:HG2	2.20	0.41
45:a:532:LYS:HZ1	46:3f:280:GLN:CB	2.33	0.41
1:S2:568:C:C4	1:S2:583:A:N7	2.88	0.41
1:S2:668:A2M:H5''	1:S2:1198:G:H4'	2.02	0.41
1:S2:1074:C:C2	1:S2:1075:C:C5	3.08	0.41
1:S2:1588:A:H2'	1:S2:1589:A:C8	2.54	0.41
7:SI:149:TYR:O	7:SI:153:LYS:HG2	2.20	0.41
8:SL:52:GLU:OE2	8:SL:52:GLU:O	2.38	0.41
18:SY:54:VAL:HG22	18:SY:76:TYR:HB2	2.02	0.41
26:Sd:5:GLN:OE1	26:Sd:5:GLN:O	2.38	0.41
35:SP:12:PHE:C	35:SP:13:ARG:HE	2.28	0.41
39:F:187:MET:HG2	39:F:188:ARG:HD2	2.03	0.41
44:c:368:GLU:O	44:c:371:ILE:HG13	2.19	0.41
44:c:425:LEU:HD12	44:c:425:LEU:N	2.34	0.41
45:a:368:ILE:HD12	45:a:368:ILE:O	2.21	0.41
24:Sf:103:LEU:HD12	24:Sf:103:LEU:C	2.45	0.41
36:SZ:69:THR:O	36:SZ:70:PRO:C	2.62	0.41
37:D:132:GLN:O	37:D:136:TRP:HB2	2.19	0.41
40:G:25:U:C4	40:G:26:2MG:N2	2.89	0.41
42:e:253:ILE:HA	42:e:256:TYR:CD2	2.56	0.41
43:d:380:VAL:HG23	43:d:390:PHE:CD1	2.54	0.41
44:c:111:ALA:HB2	44:c:156:ILE:HD13	2.02	0.41
44:c:611:ARG:HG3	44:c:611:ARG:HH11	1.85	0.41
1:S2:329:G:C4'	1:S2:330:G:OP1	2.68	0.41
1:S2:393:U:OP2	44:c:146:ARG:NH2	2.53	0.41
1:S2:529:A:N6	1:S2:555:A:H61	2.15	0.41
1:S2:577:U:C4	1:S2:578:C:C5	3.08	0.41
1:S2:1616:U:O2	1:S2:1661:A:H2	2.04	0.41
5:SB:69:VAL:HG13	5:SB:74:LEU:HD11	2.02	0.41
10:SX:17:ARG:NE	10:SX:17:ARG:HA	2.35	0.41
22:SD:162:ASP:N	22:SD:163:PRO:CD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Sg:60:ARG:HH11	27:Sg:60:ARG:HB3	1.85	0.41
27:Sg:232:GLY:O	27:Sg:257:LYS:HE2	2.21	0.41
27:Sg:251:ALA:HB1	27:Sg:286:CYS:HB3	2.03	0.41
31:SU:40:ILE:HD12	31:SU:50:VAL:HG11	2.01	0.41
38:E:67:VAL:HG23	38:E:67:VAL:O	2.20	0.41
38:E:155:ALA:HB3	38:E:185:ILE:HD13	2.03	0.41
38:E:295:GLU:HB2	38:E:361:VAL:HG22	2.01	0.41
42:e:272:GLN:CD	42:e:272:GLN:N	2.78	0.41
44:c:453:GLU:HA	44:c:456:THR:HG22	2.01	0.41
44:c:677:ILE:O	44:c:678:ASN:C	2.63	0.41
44:c:777:THR:HA	44:c:780:VAL:HG22	2.03	0.41
45:a:55:LEU:HD21	45:a:71:LEU:CD2	2.50	0.41
45:a:174:TYR:CE2	45:a:175:HIS:CD2	3.09	0.41
45:a:222:ASN:C	45:a:222:ASN:OD1	2.63	0.41
1:S2:634:A:C2	1:S2:635:G:C5	3.09	0.41
1:S2:746:C:H2'	1:S2:747:U:O4'	2.20	0.41
1:S2:1291:A:C6	1:S2:1302:G:C6	3.08	0.41
5:SB:7:LYS:O	5:SB:8:ARG:HG2	2.20	0.41
5:SB:154:SER:O	5:SB:154:SER:OG	2.39	0.41
7:SI:36:THR:HG23	7:SI:57:ALA:O	2.21	0.41
12:SC:167:ARG:HB3	12:SC:177:PRO:HB2	2.03	0.41
14:SJ:136:ARG:O	14:SJ:157:ILE:HD12	2.21	0.41
27:Sg:94:THR:OG1	27:Sg:96:THR:HG22	2.21	0.41
34:ST:107:LEU:HB3	34:ST:113:VAL:HG12	2.02	0.41
35:SP:54:HIS:O	35:SP:58:LYS:HG2	2.19	0.41
37:D:48:LEU:HD12	37:D:48:LEU:HA	1.96	0.41
38:E:142:MET:HE2	38:E:451:TRP:CD1	2.54	0.41
44:c:683:GLU:HG3	44:c:687:LEU:HD12	2.02	0.41
45:a:74:TYR:O	45:a:78:CYS:HB2	2.21	0.41
45:a:379:VAL:HG12	45:a:379:VAL:O	2.20	0.41
1:S2:1122:A:C6	1:S2:1123:C:C5	3.09	0.41
1:S2:1303:C:O2	1:S2:1303:C:O4'	2.37	0.41
1:S2:1308:U:C2'	1:S2:1309:C:O5'	2.69	0.41
17:SW:125:ILE:HG23	17:SW:125:ILE:O	2.19	0.41
29:SK:24:LYS:HA	29:SK:66:HIS:CD2	2.56	0.41
32:SQ:41:MET:HE2	32:SQ:41:MET:HB2	1.98	0.41
32:SQ:128:GLU:OE2	32:SQ:137:ALA:HB1	2.21	0.41
33:SS:84:LEU:HD11	33:SS:95:TYR:HB3	2.02	0.41
33:SS:141:ARG:O	33:SS:142:ARG:C	2.64	0.41
37:D:191:ILE:O	37:D:238:THR:HA	2.20	0.41
43:d:380:VAL:HG22	43:d:381:MET:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:d:396:LEU:HD13	43:d:449:LEU:HD22	2.03	0.41
44:c:497:GLU:HA	44:c:560:ARG:CZ	2.50	0.41
45:a:52:LEU:HD23	45:a:52:LEU:C	2.45	0.41
45:a:86:LEU:O	45:a:89:VAL:HG12	2.21	0.41
45:a:320:THR:HG21	45:a:384:VAL:HG23	2.02	0.41
1:S2:166:A2M:HM'3	1:S2:166:A2M:H1'	1.70	0.41
1:S2:799:U:H5'	6:SH:109:ARG:HB3	2.03	0.41
1:S2:884:C:C2	1:S2:885:U:O4	2.74	0.41
1:S2:1134:G:H2'	1:S2:1135:C:C6	2.55	0.41
1:S2:1383:A2M:H1'	1:S2:1383:A2M:HM'3	1.72	0.41
1:S2:1797:U:H2'	1:S2:1798:C:C6	2.56	0.41
6:SH:145:ARG:HE	17:SW:49:GLU:HB3	1.86	0.41
18:SY:17:LEU:H	18:SY:17:LEU:HD22	1.86	0.41
32:SQ:105:LYS:HA	32:SQ:108:ILE:HG22	2.03	0.41
33:SS:21:ASP:OD1	33:SS:21:ASP:C	2.62	0.41
35:SP:115:TYR:HB2	35:SP:118:GLU:OE1	2.20	0.41
37:D:190:LYS:O	37:D:190:LYS:HD3	2.21	0.41
43:d:25:PHE:O	43:d:25:PHE:CG	2.74	0.41
43:d:301:ASP:HB3	43:d:309:PRO:HG3	2.03	0.41
44:c:470:VAL:O	44:c:474:LYS:HG2	2.20	0.41
45:a:295:THR:HG22	45:a:359:LEU:CD1	2.51	0.41
1:S2:560:A:C2'	1:S2:561:A:O5'	2.69	0.41
1:S2:1634:A:H2'	1:S2:1635:C:O4'	2.21	0.41
1:S2:1661:A:H8	26:Sd:14:PHE:HB2	1.86	0.41
4:SA:42:LYS:HG3	4:SA:46:ILE:O	2.20	0.41
13:SG:159:ARG:HE	13:SG:171:THR:HG23	1.86	0.41
14:SJ:110:LEU:HD22	14:SJ:142:VAL:HG11	2.02	0.41
26:Sd:31:ILE:HD11	26:Sd:36:LEU:HD13	2.02	0.41
43:d:80:PHE:O	43:d:80:PHE:HD1	2.04	0.41
43:d:80:PHE:CD1	43:d:80:PHE:C	2.98	0.41
44:c:548:MET:HE1	44:c:572:HIS:CA	2.51	0.41
44:c:578:LEU:HD12	44:c:615:GLN:OE1	2.21	0.41
44:c:804:MET:CE	44:c:841:THR:OG1	2.68	0.41
44:c:825:MET:HE2	44:c:830:GLU:OE1	2.21	0.41
45:a:438:ARG:HD3	45:a:438:ARG:HA	1.92	0.41
1:S2:15:U:H2'	1:S2:16:G:O4'	2.20	0.41
1:S2:92:A:H4'	1:S2:93:PSU:OP2	2.19	0.41
1:S2:1010:G:H2'	1:S2:1011:A:H8	1.86	0.41
1:S2:1311:C:O2'	29:SK:6:LYS:CG	2.69	0.41
1:S2:1344:A:H4'	1:S2:1345:G:OP1	2.21	0.41
1:S2:1605:G:H2'	1:S2:1606:G:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1823:A:O3'	1:S2:1824:A:O4'	2.39	0.41
1:S2:1839:U:H2'	1:S2:1840:U:C6	2.56	0.41
1:S2:1864:U:H5'	11:Sa:79:ILE:HD11	2.02	0.41
3:SE:145:ARG:CZ	3:SE:162:ILE:HD11	2.51	0.41
4:SA:58:LEU:HD22	4:SA:161:ILE:CG2	2.51	0.41
4:SA:201:LEU:HD13	4:SA:201:LEU:C	2.46	0.41
5:SB:139:CYS:HB2	5:SB:172:MET:SD	2.60	0.41
5:SB:231:LEU:C	5:SB:231:LEU:HD13	2.46	0.41
7:SI:107:THR:OG1	7:SI:108:PRO:HD3	2.21	0.41
9:SV:13:VAL:O	9:SV:13:VAL:CG2	2.69	0.41
12:SC:95:ASP:OD1	12:SC:95:ASP:C	2.63	0.41
14:SJ:125:HIS:CD2	14:SJ:129:LEU:HD13	2.56	0.41
15:SN:22:VAL:CG1	15:SN:66:VAL:HA	2.51	0.41
17:SW:103:VAL:CG2	17:SW:129:PHE:HE2	2.33	0.41
19:Sb:37:CYS:HB3	19:Sb:38:PRO:HD2	2.02	0.41
20:Se:53:LYS:HD2	20:Se:57:ALA:HB1	2.03	0.41
22:SD:113:LEU:HD21	22:SD:117:ARG:NE	2.35	0.41
23:SF:25:THR:O	23:SF:28:VAL:HG22	2.21	0.41
23:SF:77:MET:HG3	23:SF:77:MET:O	2.21	0.41
27:Sg:60:ARG:HH12	32:SQ:97:GLN:NE2	2.19	0.41
27:Sg:140:TYR:CD1	27:Sg:140:TYR:C	2.99	0.41
27:Sg:312:VAL:O	27:Sg:312:VAL:HG23	2.20	0.41
30:SM:58:GLU:HB2	30:SM:61:TYR:HB3	2.01	0.41
32:SQ:63:PHE:O	32:SQ:66:VAL:HG12	2.21	0.41
32:SQ:105:LYS:C	32:SQ:105:LYS:HD2	2.46	0.41
35:SP:44:ARG:HG2	35:SP:84:ILE:CD1	2.50	0.41
35:SP:83:MET:HB3	35:SP:116:LEU:HD22	2.02	0.41
38:E:193:ASP:HA	39:F:187:MET:HE2	2.03	0.41
41:H:75:ASP:O	41:H:76:ILE:HD12	2.20	0.41
42:e:270:ARG:HH11	42:e:273:VAL:HG22	1.86	0.41
44:c:60:LEU:HD23	44:c:105:PHE:HE1	1.85	0.41
44:c:548:MET:SD	44:c:572:HIS:HD2	2.44	0.41
44:c:804:MET:HE1	44:c:841:THR:OG1	2.21	0.41
45:a:58:CYS:SG	45:a:67:ALA:HB2	2.61	0.41
45:a:284:TRP:HB2	45:a:292:HIS:ND1	2.36	0.41
47:m:322:TYR:CB	47:m:332:VAL:HA	2.51	0.41
48:h:51:LYS:O	48:h:55:GLU:CB	2.68	0.41
1:S2:194:C:H2'	1:S2:195:C:C6	2.56	0.41
1:S2:674:C:H2'	1:S2:675:U:C6	2.56	0.41
1:S2:1036:A:C5	1:S2:1037:G:C8	3.09	0.41
1:S2:1520:G:H4'	1:S2:1521:C:OP2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:SA:212:LYS:HA	4:SA:215:GLN:HG2	2.03	0.41
7:SI:103:LEU:HD22	7:SI:170:LYS:HB3	2.02	0.41
14:SJ:50:LEU:HD12	14:SJ:51:ALA:N	2.35	0.41
14:SJ:114:VAL:HG11	14:SJ:126:ALA:HB1	2.02	0.41
18:SY:25:ILE:HG21	18:SY:44:LEU:HD11	2.02	0.41
22:SD:20:GLU:HG3	29:SK:64:TRP:CD2	2.56	0.41
22:SD:115:VAL:HG23	22:SD:116:ARG:N	2.35	0.41
25:SR:40:ILE:O	25:SR:40:ILE:HG22	2.20	0.41
44:c:510:THR:O	44:c:510:THR:CG2	2.69	0.41
44:c:844:MET:HG3	44:c:846:ARG:HD3	2.03	0.41
1:S2:375:U:OP2	8:SL:59:LYS:HE2	2.21	0.40
1:S2:562:U:O3'	1:S2:563:G:O4'	2.39	0.40
4:SA:207:PRO:HA	4:SA:210:ILE:HD12	2.04	0.40
6:SH:7:LYS:O	6:SH:8:ILE:HB	2.22	0.40
7:SI:161:LEU:O	7:SI:165:GLN:HG2	2.22	0.40
11:Sa:46:GLU:O	11:Sa:50:VAL:HG23	2.20	0.40
16:SO:53:ILE:HD13	16:SO:90:ILE:HG13	2.03	0.40
31:SU:40:ILE:HD11	31:SU:89:ILE:HD12	2.03	0.40
32:SQ:31:LEU:HD11	32:SQ:33:LYS:HG3	2.04	0.40
41:H:2:PRO:HD2	41:H:7:LYS:HB2	2.04	0.40
44:c:62:ASN:O	44:c:66:THR:HG23	2.22	0.40
44:c:742:LYS:HA	45:a:340:ARG:HD3	2.03	0.40
45:a:372:ASN:OD1	45:a:372:ASN:C	2.62	0.40
45:a:416:GLU:OE1	45:a:416:GLU:CA	2.69	0.40
1:S2:28:U:H2'	1:S2:29:G:H8	1.86	0.40
1:S2:167:G:H3'	1:S2:168:C:H5''	2.03	0.40
1:S2:1007:C:H2'	1:S2:1008:A:O4'	2.20	0.40
1:S2:1401:A:H2'	1:S2:1402:A:C8	2.56	0.40
1:S2:1401:A:H2'	1:S2:1402:A:H8	1.86	0.40
1:S2:1549:U:H2'	1:S2:1550:G:O4'	2.21	0.40
5:SB:77:ASP:OD1	5:SB:77:ASP:N	2.54	0.40
7:SI:10:LYS:HB3	8:SL:136:LYS:HZ1	1.85	0.40
7:SI:62:VAL:HA	7:SI:77:ARG:HA	2.03	0.40
11:Sa:53:ILE:HD13	11:Sa:53:ILE:HA	1.92	0.40
12:SC:199:PRO:HD2	12:SC:223:TYR:OH	2.21	0.40
16:SO:24:GLY:O	16:SO:25:GLU:C	2.64	0.40
18:SY:36:PRO:HD2	18:SY:39:GLU:OE2	2.22	0.40
24:Sf:142:GLY:C	24:Sf:143:LYS:HG3	2.46	0.40
31:SU:36:CYS:O	31:SU:40:ILE:HG12	2.22	0.40
33:SS:30:ILE:CD1	33:SS:41:ALA:HB1	2.50	0.40
36:SZ:74:SER:HA	36:SZ:79:ILE:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:d:41:LYS:O	44:c:613:MET:HE2	2.22	0.40
44:c:105:PHE:O	44:c:109:ILE:CD1	2.69	0.40
45:a:98:GLU:O	45:a:102:GLU:HG2	2.22	0.40
45:a:565:HIS:CD2	45:a:565:HIS:C	2.98	0.40
45:a:570:ALA:HB3	45:a:573:GLN:HA	2.03	0.40
1:S2:438:G:H5''	1:S2:438:G:N3	2.36	0.40
1:S2:544:G:H2'	1:S2:545:A:H4'	2.03	0.40
1:S2:986:G:C5	16:SO:137:SER:HA	2.57	0.40
4:SA:77:ILE:HD12	4:SA:133:PRO:HG3	2.03	0.40
10:SX:139:GLU:OE1	10:SX:140:ARG:N	2.54	0.40
14:SJ:121:LYS:O	14:SJ:122:SER:CB	2.69	0.40
17:SW:46:TYR:CE2	17:SW:129:PHE:CD1	3.10	0.40
17:SW:91:ASN:OD1	17:SW:91:ASN:C	2.64	0.40
18:SY:101:LYS:N	18:SY:101:LYS:HD2	2.37	0.40
18:SY:103:SER:OG	18:SY:106:GLN:HG2	2.21	0.40
30:SM:21:VAL:HG21	30:SM:123:VAL:HG21	2.03	0.40
37:D:138:PHE:CD2	37:D:152:ALA:HB3	2.56	0.40
37:D:223:MET:O	37:D:223:MET:CG	2.68	0.40
38:E:62:SER:HG	38:E:132:PHE:HE1	1.67	0.40
38:E:203:GLN:OE1	38:E:203:GLN:HA	2.21	0.40
42:e:237:LEU:HD23	42:e:240:PRO:HG2	2.03	0.40
43:d:37:ASP:OD1	44:c:590:LEU:HD11	2.22	0.40
44:c:651:LEU:HD11	44:c:667:ARG:NE	2.36	0.40
45:a:384:VAL:HG12	45:a:386:GLU:H	1.85	0.40
45:a:459:VAL:CG1	45:a:462:VAL:HG12	2.52	0.40
45:a:462:VAL:HG22	45:a:466:GLN:HB2	2.02	0.40
45:a:537:ILE:O	45:a:540:ALA:HB2	2.21	0.40
1:S2:160:U:O2'	1:S2:161:U:H3'	2.21	0.40
1:S2:528:A:H2'	1:S2:529:A:C8	2.56	0.40
1:S2:1440:C:H2'	1:S2:1441:U:C6	2.56	0.40
1:S2:1845:A:H2'	1:S2:1846:G:C8	2.57	0.40
3:SE:92:ILE:HG21	18:SY:17:LEU:HD11	2.04	0.40
4:SA:22:GLY:C	4:SA:24:HIS:H	2.30	0.40
4:SA:143:PRO:HA	4:SA:158:ASP:OD2	2.21	0.40
5:SB:9:LEU:C	5:SB:9:LEU:HD23	2.46	0.40
6:SH:39:GLN:O	6:SH:43:LEU:HD13	2.20	0.40
13:SG:207:ALA:O	13:SG:211:LYS:HG3	2.21	0.40
14:SJ:135:ILE:HG22	14:SJ:157:ILE:HD11	2.02	0.40
14:SJ:157:ILE:HD12	14:SJ:157:ILE:HA	1.94	0.40
22:SD:74:GLN:OE1	22:SD:74:GLN:C	2.65	0.40
22:SD:136:VAL:HG13	22:SD:152:PHE:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Sg:110:SER:CB	27:Sg:153:CYS:HA	2.51	0.40
32:SQ:52:LEU:O	32:SQ:53:GLU:C	2.64	0.40
37:D:8:PHE:HB2	37:D:38:GLU:O	2.21	0.40
37:D:180:ILE:O	37:D:183:ARG:O	2.39	0.40
38:E:47:ILE:HG22	38:E:157:LEU:HA	2.03	0.40
41:H:77:ILE:HD12	41:H:77:ILE:O	2.22	0.40
42:e:261:VAL:O	42:e:267:VAL:HG11	2.22	0.40
44:c:159:TYR:O	44:c:159:TYR:CG	2.74	0.40
44:c:464:PRO:O	44:c:469:TYR:HD2	2.03	0.40
45:a:51:MET:CE	45:a:74:TYR:HB2	2.51	0.40
45:a:318:MET:SD	45:a:318:MET:C	3.04	0.40
45:a:429:PRO:O	45:a:432:GLN:HG2	2.20	0.40
47:m:336:HIS:O	47:m:337:SER:C	2.64	0.40
1:S2:385:G:H3'	8:SL:136:LYS:HB2	2.03	0.40
1:S2:439:A:O2'	1:S2:440:G:H5'	2.22	0.40
1:S2:520:A:H5''	14:SJ:12:THR:HG23	2.04	0.40
1:S2:1012:A:H2'	1:S2:1013:U:O4'	2.22	0.40
4:SA:1:MET:HB2	4:SA:56:GLU:O	2.21	0.40
5:SB:190:PRO:HB2	45:a:18:PHE:CE1	2.56	0.40
12:SC:63:VAL:HG23	12:SC:64:THR:HG23	2.03	0.40
18:SY:24:VAL:HG12	18:SY:72:PHE:HD1	1.87	0.40
35:SP:31:GLU:HA	35:SP:31:GLU:OE2	2.22	0.40
35:SP:94:VAL:HG11	35:SP:116:LEU:HD21	2.03	0.40
40:G:20:A:N6	40:G:57:G:H2'	2.37	0.40
41:H:77:ILE:HD12	41:H:77:ILE:C	2.47	0.40
42:e:261:VAL:O	42:e:267:VAL:CG1	2.69	0.40
43:d:41:LYS:HE3	43:d:55:TYR:HB2	2.04	0.40
44:c:684:CYS:CB	44:c:765:VAL:HG11	2.52	0.40
45:a:15:ALA:HB2	45:a:31:LEU:CD2	2.50	0.40
45:a:375:VAL:HG13	45:a:376:ARG:N	2.36	0.40
45:a:412:ASN:OD1	45:a:416:GLU:OE2	2.40	0.40
45:a:439:LEU:CD2	45:a:459:VAL:CG2	2.99	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	
2	Ln	22/25 (88%)	22 (100%)	0	0	100	100
3	SE	260/263 (99%)	251 (96%)	9 (4%)	0	100	100
4	SA	217/295 (74%)	211 (97%)	6 (3%)	0	100	100
5	SB	219/264 (83%)	207 (94%)	11 (5%)	1 (0%)	24	60
6	SH	187/194 (96%)	172 (92%)	15 (8%)	0	100	100
7	SI	204/208 (98%)	195 (96%)	9 (4%)	0	100	100
8	SL	152/158 (96%)	141 (93%)	11 (7%)	0	100	100
9	SV	81/83 (98%)	75 (93%)	6 (7%)	0	100	100
10	SX	139/143 (97%)	133 (96%)	6 (4%)	0	100	100
11	Sa	100/115 (87%)	91 (91%)	9 (9%)	0	100	100
12	SC	218/293 (74%)	210 (96%)	8 (4%)	0	100	100
13	SG	232/249 (93%)	227 (98%)	5 (2%)	0	100	100
14	SJ	180/194 (93%)	170 (94%)	9 (5%)	1 (1%)	21	56
15	SN	148/151 (98%)	143 (97%)	5 (3%)	0	100	100
16	SO	132/151 (87%)	120 (91%)	12 (9%)	0	100	100
17	SW	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
18	SY	122/133 (92%)	118 (97%)	4 (3%)	0	100	100
19	Sb	81/84 (96%)	75 (93%)	6 (7%)	0	100	100
20	Se	57/133 (43%)	54 (95%)	3 (5%)	0	100	100
22	SD	225/243 (93%)	216 (96%)	9 (4%)	0	100	100
23	SF	187/204 (92%)	177 (95%)	9 (5%)	1 (0%)	24	60
24	Sf	61/156 (39%)	53 (87%)	7 (12%)	1 (2%)	7	34
25	SR	129/135 (96%)	124 (96%)	5 (4%)	0	100	100
26	Sd	53/56 (95%)	50 (94%)	3 (6%)	0	100	100
27	Sg	312/317 (98%)	296 (95%)	16 (5%)	0	100	100
28	Sc	63/69 (91%)	55 (87%)	7 (11%)	1 (2%)	7	34
29	SK	95/165 (58%)	89 (94%)	6 (6%)	0	100	100
30	SM	116/132 (88%)	103 (89%)	11 (10%)	2 (2%)	7	32
31	SU	100/119 (84%)	94 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	SQ	139/146 (95%)	128 (92%)	11 (8%)	0	100	100
33	SS	143/152 (94%)	136 (95%)	7 (5%)	0	100	100
34	ST	140/145 (97%)	137 (98%)	3 (2%)	0	100	100
35	SP	132/145 (91%)	122 (92%)	9 (7%)	1 (1%)	16	50
36	SZ	71/125 (57%)	68 (96%)	3 (4%)	0	100	100
37	D	292/315 (93%)	270 (92%)	20 (7%)	2 (1%)	18	53
38	E	470/472 (100%)	447 (95%)	21 (4%)	2 (0%)	30	65
39	F	14/333 (4%)	11 (79%)	3 (21%)	0	100	100
41	H	109/144 (76%)	96 (88%)	11 (10%)	2 (2%)	6	31
42	e	380/445 (85%)	338 (89%)	41 (11%)	1 (0%)	36	70
43	d	408/548 (74%)	369 (90%)	39 (10%)	0	100	100
44	c	636/913 (70%)	586 (92%)	50 (8%)	0	100	100
45	a	588/1382 (42%)	527 (90%)	61 (10%)	0	100	100
46	3f	251/357 (70%)	218 (87%)	29 (12%)	4 (2%)	7	34
47	m	348/374 (93%)	285 (82%)	58 (17%)	5 (1%)	9	36
48	h	313/352 (89%)	265 (85%)	46 (15%)	2 (1%)	21	56
49	k	209/218 (96%)	194 (93%)	13 (6%)	2 (1%)	12	45
50	l	307/564 (54%)	291 (95%)	16 (5%)	0	100	100
All	All	9169/11992 (76%)	8480 (92%)	661 (7%)	28 (0%)	37	70

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
30	SM	45	ARG
30	SM	80	ASP
35	SP	138	SER
37	D	200	TYR
41	H	17	ASN
46	3f	258	SER
46	3f	259	PRO
46	3f	262	VAL
47	m	40	VAL
47	m	295	ASP
48	h	95	ASP
48	h	209	HIS
5	SB	22	VAL

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Mol	Chain	Res	Type
47	m	29	ILE
47	m	292	ILE
37	D	4	LEU
38	E	274	LEU
14	SJ	3	VAL
42	e	202	SER
46	3f	260	ASN
41	H	28	PHE
23	SF	79	HIS
24	Sf	128	ALA
28	Sc	61	SER
38	E	324	GLU
49	k	207	PHE
47	m	267	GLY
49	k	205	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Ln	23/24 (96%)	23 (100%)	0	100	100
3	SE	224/225 (100%)	219 (98%)	5 (2%)	45	74
4	SA	182/243 (75%)	181 (100%)	1 (0%)	81	89
5	SB	202/231 (87%)	197 (98%)	5 (2%)	42	72
6	SH	169/174 (97%)	166 (98%)	3 (2%)	51	77
7	SI	178/180 (99%)	173 (97%)	5 (3%)	38	70
8	SL	138/142 (97%)	136 (99%)	2 (1%)	59	80
9	SV	67/67 (100%)	64 (96%)	3 (4%)	24	59
10	SX	113/115 (98%)	109 (96%)	4 (4%)	32	65
11	Sa	89/98 (91%)	86 (97%)	3 (3%)	32	66
12	SC	186/225 (83%)	183 (98%)	3 (2%)	55	79
13	SG	204/218 (94%)	201 (98%)	3 (2%)	57	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	SJ	161/168 (96%)	159 (99%)	2 (1%)	63	82
15	SN	130/131 (99%)	129 (99%)	1 (1%)	73	86
16	SO	105/118 (89%)	100 (95%)	5 (5%)	23	57
17	SW	112/113 (99%)	111 (99%)	1 (1%)	70	85
18	SY	108/115 (94%)	101 (94%)	7 (6%)	15	47
19	Sb	75/76 (99%)	74 (99%)	1 (1%)	61	81
20	Se	48/104 (46%)	47 (98%)	1 (2%)	47	75
22	SD	190/202 (94%)	183 (96%)	7 (4%)	30	64
23	SF	159/170 (94%)	157 (99%)	2 (1%)	61	81
24	Sf	56/140 (40%)	55 (98%)	1 (2%)	51	77
25	SR	119/122 (98%)	118 (99%)	1 (1%)	73	86
26	Sd	48/49 (98%)	47 (98%)	1 (2%)	47	75
27	Sg	272/275 (99%)	264 (97%)	8 (3%)	37	70
28	Sc	58/62 (94%)	56 (97%)	2 (3%)	32	66
29	SK	88/136 (65%)	86 (98%)	2 (2%)	44	74
30	SM	98/108 (91%)	95 (97%)	3 (3%)	35	68
31	SU	94/107 (88%)	92 (98%)	2 (2%)	47	75
32	SQ	117/121 (97%)	113 (97%)	4 (3%)	32	66
33	SS	126/132 (96%)	121 (96%)	5 (4%)	28	62
34	ST	112/114 (98%)	111 (99%)	1 (1%)	70	85
35	SP	120/130 (92%)	115 (96%)	5 (4%)	26	61
36	SZ	65/103 (63%)	61 (94%)	4 (6%)	16	49
37	D	264/280 (94%)	259 (98%)	5 (2%)	50	76
38	E	397/397 (100%)	388 (98%)	9 (2%)	44	74
39	F	16/304 (5%)	15 (94%)	1 (6%)	16	48
41	H	94/123 (76%)	93 (99%)	1 (1%)	65	83
42	e	206/406 (51%)	198 (96%)	8 (4%)	28	62
43	d	200/494 (40%)	190 (95%)	10 (5%)	22	56
44	c	563/811 (69%)	540 (96%)	23 (4%)	27	61
45	a	528/1259 (42%)	514 (97%)	14 (3%)	39	71
47	m	49/335 (15%)	46 (94%)	3 (6%)	17	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	6553/9147 (72%)	6376 (97%)	177 (3%)	40 71

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	SE	87	MET
3	SE	90	ILE
3	SE	115	THR
3	SE	192	ILE
3	SE	220	THR
4	SA	75	SER
5	SB	26	SER
5	SB	29	ASP
5	SB	48	LEU
5	SB	95	ASN
5	SB	191	ASP
6	SH	17	ASP
6	SH	40	LEU
6	SH	193	GLN
7	SI	7	ASN
7	SI	46	VAL
7	SI	100	CYS
7	SI	130	THR
7	SI	184	ARG
8	SL	22	ARG
8	SL	25	LEU
9	SV	51	LYS
9	SV	56	CYS
9	SV	74	LYS
10	SX	8	ARG
10	SX	73	GLN
10	SX	88	ASP
10	SX	118	VAL
11	Sa	19	GLN
11	Sa	60	ASP
11	Sa	69	VAL
12	SC	86	LEU
12	SC	230	THR
12	SC	248	TYR
13	SG	36	VAL
13	SG	102	VAL
13	SG	219	GLU

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Mol	Chain	Res	Type
14	SJ	97	ILE
14	SJ	179	LYS
15	SN	14	SER
16	SO	26	ASN
16	SO	40	THR
16	SO	56	VAL
16	SO	80	ASP
16	SO	88	LEU
17	SW	81	VAL
18	SY	21	LYS
18	SY	40	ILE
18	SY	54	VAL
18	SY	55	ILE
18	SY	78	SER
18	SY	109	GLU
18	SY	125	VAL
19	Sb	57	VAL
20	Se	36	MET
22	SD	26	THR
22	SD	37	VAL
22	SD	38	GLU
22	SD	46	THR
22	SD	47	GLU
22	SD	113	LEU
22	SD	142	LEU
23	SF	65	GLN
23	SF	195	GLU
24	Sf	145	CYS
25	SR	117	LEU
26	Sd	8	TRP
27	Sg	63	SER
27	Sg	90	TRP
27	Sg	111	VAL
27	Sg	117	ASN
27	Sg	127	LYS
27	Sg	154	VAL
27	Sg	189	ILE
27	Sg	240	CYS
28	Sc	50	VAL
28	Sc	52	GLU
29	SK	20	VAL
29	SK	45	VAL

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Mol	Chain	Res	Type
30	SM	54	SER
30	SM	91	LEU
30	SM	118	SER
31	SU	63	ILE
31	SU	107	GLU
32	SQ	10	VAL
32	SQ	25	CYS
32	SQ	32	ILE
32	SQ	127	CYS
33	SS	2	SER
33	SS	43	VAL
33	SS	95	TYR
33	SS	109	GLU
33	SS	134	GLN
34	ST	87	VAL
35	SP	20	VAL
35	SP	28	MET
35	SP	37	TYR
35	SP	57	LEU
35	SP	118	GLU
36	SZ	50	PHE
36	SZ	69	THR
36	SZ	90	GLU
36	SZ	107	VAL
37	D	5	SER
37	D	11	HIS
37	D	99	GLU
37	D	103	THR
37	D	239	THR
38	E	14	HIS
38	E	47	ILE
38	E	135	CYS
38	E	236	CYS
38	E	296	VAL
38	E	319	VAL
38	E	339	VAL
38	E	435	THR
38	E	450	HIS
39	F	187	MET
41	H	34	GLU
42	e	231	ASN
42	e	242	TYR

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Mol	Chain	Res	Type
42	e	274	LEU
42	e	275	LYS
42	e	309	GLN
42	e	314	GLU
42	e	315	CYS
42	e	318	VAL
43	d	69	TYR
43	d	77	GLU
43	d	292	SER
43	d	318	TYR
43	d	375	CYS
43	d	393	ILE
43	d	426	LYS
43	d	428	ASN
43	d	452	VAL
43	d	461	SER
44	c	64	ILE
44	c	338	GLN
44	c	401	CYS
44	c	408	LEU
44	c	440	VAL
44	c	445	LEU
44	c	465	HIS
44	c	548	MET
44	c	563	ARG
44	c	591	MET
44	c	701	HIS
44	c	718	LEU
44	c	720	VAL
44	c	741	SER
44	c	751	THR
44	c	779	LEU
44	c	785	GLU
44	c	793	PHE
44	c	799	TYR
44	c	802	ILE
44	c	820	SER
44	c	844	MET
44	c	845	HIS
45	a	125	GLU
45	a	152	PHE
45	a	161	LEU

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Mol	Chain	Res	Type
45	a	243	MET
45	a	332	THR
45	a	342	LEU
45	a	387	VAL
45	a	398	PHE
45	a	402	LYS
45	a	404	CYS
45	a	410	VAL
45	a	412	ASN
45	a	449	SER
45	a	450	ILE
47	m	323	CYS
47	m	349	GLN
47	m	350	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
3	SE	50	ASN
3	SE	157	ASN
4	SA	29	ASN
4	SA	169	HIS
5	SB	101	HIS
5	SB	186	ASN
7	SI	52	ASN
10	SX	16	HIS
10	SX	77	ASN
12	SC	172	ASN
12	SC	235	ASN
12	SC	267	GLN
12	SC	272	HIS
13	SG	81	HIS
14	SJ	125	HIS
16	SO	26	ASN
16	SO	113	GLN
18	SY	89	HIS
22	SD	101	GLN
22	SD	159	HIS
23	SF	149	GLN
23	SF	165	ASN
27	Sg	64	HIS
29	SK	61	GLN

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Mol	Chain	Res	Type
29	SK	66	HIS
30	SM	19	GLN
30	SM	48	HIS
30	SM	75	ASN
35	SP	137	HIS
36	SZ	45	ASN
37	D	289	GLN
38	E	173	HIS
38	E	325	HIS
38	E	396	GLN
38	E	450	HIS
41	H	33	GLN
41	H	44	ASN
42	e	231	ASN
44	c	338	GLN
44	c	575	HIS
44	c	674	HIS
45	a	109	GLN
45	a	110	GLN
45	a	200	ASN
45	a	257	HIS
45	a	425	GLN
45	a	426	GLN
45	a	518	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S2	1713/1869 (91%)	353 (20%)	9 (0%)
21	B	27/50 (54%)	17 (62%)	1 (3%)
40	G	72/75 (96%)	17 (23%)	0
All	All	1812/1994 (90%)	387 (21%)	10 (0%)

All (387) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S2	4	C
1	S2	17	C
1	S2	26	U
1	S2	33	G
1	S2	41	G

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Mol	Chain	Res	Type
1	S2	42	A
1	S2	44	U
1	S2	45	A
1	S2	46	A
1	S2	56	G
1	S2	59	U
1	S2	62	G
1	S2	67	C
1	S2	68	A
1	S2	71	G
1	S2	73	C
1	S2	75	G
1	S2	76	U
1	S2	77	A
1	S2	103	A
1	S2	113	G
1	S2	114	G
1	S2	115	U
1	S2	126	G
1	S2	140	C
1	S2	143	U
1	S2	149	A
1	S2	155	G
1	S2	162	C
1	S2	163	U
1	S2	166	A2M
1	S2	168	C
1	S2	175	A
1	S2	182	C
1	S2	184	G
1	S2	197	U
1	S2	198	U
1	S2	200	G
1	S2	202	G
1	S2	203	G
1	S2	204	G
1	S2	207	G
1	S2	209	A
1	S2	288	G
1	S2	293	C
1	S2	294	U
1	S2	302	A

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Mol	Chain	Res	Type
1	S2	306	C
1	S2	307	G
1	S2	308	G
1	S2	309	G
1	S2	319	C
1	S2	325	C
1	S2	326	C
1	S2	327	G
1	S2	328	U
1	S2	329	G
1	S2	330	G
1	S2	331	C
1	S2	347	G
1	S2	351	G
1	S2	360	A
1	S2	362	C
1	S2	364	A
1	S2	368	U
1	S2	369	C
1	S2	370	G
1	S2	385	G
1	S2	386	C
1	S2	407	G
1	S2	408	A
1	S2	409	C
1	S2	438	G
1	S2	448	A
1	S2	450	C
1	S2	452	G
1	S2	462	OMC
1	S2	464	A
1	S2	471	G
1	S2	472	C
1	S2	473	A
1	S2	474	G
1	S2	476	A
1	S2	482	G
1	S2	483	C
1	S2	487	U
1	S2	488	U
1	S2	492	C
1	S2	493	A

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Mol	Chain	Res	Type
1	S2	508	A
1	S2	532	C
1	S2	535	G
1	S2	536	A
1	S2	537	C
1	S2	538	U
1	S2	540	U
1	S2	543	C
1	S2	544	G
1	S2	545	A
1	S2	546	G
1	S2	547	G
1	S2	552	G
1	S2	553	U
1	S2	555	A
1	S2	558	G
1	S2	559	G
1	S2	563	G
1	S2	564	A
1	S2	576	A2M
1	S2	583	A
1	S2	587	A
1	S2	589	G
1	S2	591	U
1	S2	592	C
1	S2	593	C
1	S2	598	G
1	S2	604	A
1	S2	607	U
1	S2	608	C
1	S2	614	C
1	S2	617	G
1	S2	628	A
1	S2	643	A
1	S2	655	A
1	S2	660	C
1	S2	663	C
1	S2	668	A2M
1	S2	669	A
1	S2	671	A
1	S2	672	A
1	S2	673	G

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Mol	Chain	Res	Type
1	S2	688	U
1	S2	689	U
1	S2	692	G
1	S2	694	G
1	S2	695	C
1	S2	696	G
1	S2	731	G
1	S2	732	U
1	S2	733	C
1	S2	735	C
1	S2	736	C
1	S2	737	G
1	S2	738	C
1	S2	747	U
1	S2	748	C
1	S2	749	U
1	S2	750	C
1	S2	751	G
1	S2	752	G
1	S2	753	C
1	S2	788	G
1	S2	789	G
1	S2	790	C
1	S2	791	C
1	S2	794	A
1	S2	796	G
1	S2	797	C
1	S2	798	G
1	S2	799	U
1	S2	800	U
1	S2	811	A
1	S2	821	G
1	S2	822	PSU
1	S2	823	U
1	S2	827	A
1	S2	830	A
1	S2	835	C
1	S2	836	G
1	S2	837	A
1	S2	838	G
1	S2	839	C
1	S2	841	G

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Mol	Chain	Res	Type
1	S2	842	C
1	S2	847	A
1	S2	867	OMG
1	S2	870	A
1	S2	872	A
1	S2	874	G
1	S2	878	G
1	S2	883	U
1	S2	885	U
1	S2	888	U
1	S2	889	U
1	S2	890	U
1	S2	891	G
1	S2	892	U
1	S2	893	U
1	S2	894	G
1	S2	896	U
1	S2	897	U
1	S2	898	U
1	S2	899	U
1	S2	900	C
1	S2	903	A
1	S2	904	A
1	S2	905	C
1	S2	906	U
1	S2	913	A
1	S2	919	A
1	S2	920	A
1	S2	922	A
1	S2	933	G
1	S2	943	U
1	S2	969	U
1	S2	971	G
1	S2	990	A
1	S2	992	A
1	S2	1002	U
1	S2	1017	U
1	S2	1023	A
1	S2	1027	A
1	S2	1028	A
1	S2	1061	U
1	S2	1062	A

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Mol	Chain	Res	Type
1	S2	1081	U
1	S2	1083	A
1	S2	1085	C
1	S2	1089	G
1	S2	1096	G
1	S2	1109	C
1	S2	1114	U
1	S2	1116	C
1	S2	1119	A
1	S2	1121	G
1	S2	1133	A
1	S2	1138	C
1	S2	1139	C
1	S2	1150	A
1	S2	1153	C
1	S2	1154	U
1	S2	1166	G
1	S2	1195	A
1	S2	1207	G
1	S2	1208	A
1	S2	1215	C
1	S2	1216	C
1	S2	1217	A
1	S2	1221	G
1	S2	1224	G
1	S2	1242	U
1	S2	1243	U
1	S2	1251	A
1	S2	1253	A
1	S2	1256	G
1	S2	1257	G
1	S2	1258	A
1	S2	1259	A
1	S2	1264	C
1	S2	1274	G
1	S2	1275	G
1	S2	1286	G
1	S2	1301	A
1	S2	1302	G
1	S2	1306	U
1	S2	1307	U
1	S2	1308	U

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Mol	Chain	Res	Type
1	S2	1309	C
1	S2	1311	C
1	S2	1312	G
1	S2	1314	U
1	S2	1317	C
1	S2	1322	G
1	S2	1343	U
1	S2	1348	G
1	S2	1371	U
1	S2	1372	U
1	S2	1378	A
1	S2	1382	A
1	S2	1418	C
1	S2	1419	C
1	S2	1420	G
1	S2	1421	A
1	S2	1422	G
1	S2	1423	C
1	S2	1424	G
1	S2	1429	G
1	S2	1434	C
1	S2	1435	C
1	S2	1436	C
1	S2	1437	C
1	S2	1438	A
1	S2	1442	OMU
1	S2	1454	A
1	S2	1462	U
1	S2	1463	U
1	S2	1487	A
1	S2	1489	A
1	S2	1490	OMG
1	S2	1495	G
1	S2	1497	G
1	S2	1498	A
1	S2	1509	U
1	S2	1521	C
1	S2	1533	A
1	S2	1534	C
1	S2	1544	C
1	S2	1553	C
1	S2	1556	A

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Mol	Chain	Res	Type
1	S2	1570	G
1	S2	1574	C
1	S2	1579	A
1	S2	1580	A
1	S2	1586	U
1	S2	1588	A
1	S2	1601	A
1	S2	1606	G
1	S2	1618	C
1	S2	1621	U
1	S2	1623	A
1	S2	1646	C
1	S2	1648	G
1	S2	1654	G
1	S2	1663	A
1	S2	1665	G
1	S2	1671	G
1	S2	1680	G
1	S2	1715	A
1	S2	1721	U
1	S2	1722	G
1	S2	1729	U
1	S2	1744	G
1	S2	1745	A
1	S2	1751	C
1	S2	1753	C
1	S2	1755	C
1	S2	1757	G
1	S2	1758	G
1	S2	1760	G
1	S2	1761	U
1	S2	1773	C
1	S2	1774	C
1	S2	1775	U
1	S2	1777	G
1	S2	1780	G
1	S2	1782	G
1	S2	1783	C
1	S2	1786	U
1	S2	1806	A
1	S2	1824	A
1	S2	1825	A

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Mol	Chain	Res	Type
1	S2	1826	G
1	S2	1829	G
1	S2	1831	A
1	S2	1835	A
1	S2	1837	G
1	S2	1838	U
1	S2	1849	G
1	S2	1851	MA6
1	S2	1861	G
1	S2	1862	G
1	S2	1863	A
1	S2	1865	C
21	B	-8	A
21	B	-7	C
21	B	-5	G
21	B	-4	A
21	B	-3	C
21	B	4	G
21	B	5	A
21	B	6	A
21	B	7	U
21	B	8	A
21	B	10	C
21	B	11	U
21	B	12	G
21	B	15	U
21	B	16	C
21	B	17	C
21	B	18	U
40	G	5	A
40	G	8	G
40	G	9	U
40	G	10	1MG
40	G	11[1]	2MG
40	G	17	C
40	G	19	G
40	G	20	A
40	G	48	5MC
40	G	49	G
40	G	52	G
40	G	54	A
40	G	59	A

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Mol	Chain	Res	Type
40	G	60	A
40	G	74	C
40	G	75	C
40	G	76	A

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	S2	324	C
1	S2	329	G
1	S2	563	G
1	S2	1257	G
1	S2	1308	U
1	S2	1316	C
1	S2	1433	C
1	S2	1520	G
1	S2	1824	A
21	B	-4	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	OMU	S2	1288	1	19,22,23	0.33	0	26,31,34	0.42	0
1	PSU	S2	609	1	18,21,22	0.49	0	22,30,33	0.62	0
40	1MG	G	10	40	22,26,27	0.29	0	33,39,42	0.64	1 (3%)
1	OMU	S2	354	1	19,22,23	0.31	0	26,31,34	0.59	0
1	B8N	S2	1248	1	24,29,30	0.61	0	29,42,45	0.62	0
1	OMG	S2	644	1	23,26,27	0.30	0	33,38,41	0.41	0
1	PSU	S2	1186	1	18,21,22	0.50	0	22,30,33	0.59	0
1	PSU	S2	966	1	18,21,22	0.55	0	22,30,33	0.54	0
1	OMG	S2	1490	52,1	23,26,27	0.34	0	33,38,41	0.33	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PSU	S2	1367	1	18,21,22	0.53	0	22,30,33	0.53	0
1	A2M	S2	576	1	22,25,26	0.09	0	31,36,39	0.29	0
1	PSU	S2	218	1	18,21,22	0.47	0	22,30,33	0.60	0
1	PSU	S2	1692	1	18,21,22	0.58	0	22,30,33	0.56	0
40	T6A	G	37	40	31,34,35	0.45	0	44,49,52	0.63	1 (2%)
1	PSU	S2	63	1	18,21,22	0.51	0	22,30,33	0.62	0
1	A2M	S2	1678	1	22,25,26	0.10	0	31,36,39	0.26	0
1	MA6	S2	1850	1	23,26,27	0.32	0	34,38,41	0.60	1 (2%)
40	2MG	G	26	40	23,26,27	0.34	0	32,38,41	0.37	0
1	PSU	S2	1004	1	18,21,22	0.50	0	22,30,33	0.57	0
1	PSU	S2	822	1	18,21,22	0.63	1 (5%)	22,30,33	0.50	0
1	PSU	S2	1643	52,1	18,21,22	0.59	0	22,30,33	0.56	0
1	PSU	S2	93	1	18,21,22	0.52	0	22,30,33	0.56	0
1	OMG	S2	509	52,1	23,26,27	0.34	0	33,38,41	0.46	0
1	PSU	S2	109	1	18,21,22	0.55	0	22,30,33	0.55	0
1	OMC	S2	517	1	19,22,23	0.31	0	26,31,34	0.43	0
1	PSU	S2	814	1	18,21,22	0.50	0	22,30,33	0.57	0
1	PSU	S2	296	1	18,21,22	0.54	0	22,30,33	0.54	0
1	UY1	S2	1326	52,1	19,22,23	0.43	0	22,31,34	0.43	0
1	PSU	S2	1046	1	18,21,22	0.53	0	22,30,33	0.53	0
1	A2M	S2	668	1	22,25,26	0.12	0	31,36,39	0.31	0
1	A2M	S2	159	1	22,25,26	0.11	0	31,36,39	0.23	0
1	4AC	S2	1842	1	21,24,25	0.32	0	29,34,37	0.29	0
1	PSU	S2	1596	1	18,21,22	0.55	0	22,30,33	0.52	0
1	PSU	S2	1360	51,1	18,21,22	0.57	0	22,30,33	0.63	0
1	PSU	S2	1244	1	18,21,22	0.53	0	22,30,33	0.55	0
1	PSU	S2	366	1	18,21,22	0.54	0	22,30,33	0.53	0
40	5MC	G	48	40	18,22,23	0.53	0	26,32,35	0.56	0
1	PSU	S2	119	1	18,21,22	0.52	0	22,30,33	0.58	0
1	PSU	S2	406	1	18,21,22	0.52	0	22,30,33	0.60	0
1	A2M	S2	590	1	22,25,26	0.11	0	31,36,39	0.31	0
1	OMG	S2	1328	51,1	23,26,27	0.32	0	33,38,41	0.40	0
1	A2M	S2	484	1	22,25,26	0.08	0	31,36,39	0.19	0
1	OMC	S2	1391	1	19,22,23	0.31	0	26,31,34	0.44	0
1	PSU	S2	572	1	18,21,22	0.54	0	22,30,33	0.54	0
1	OMU	S2	428	1	19,22,23	0.26	0	26,31,34	0.45	0
1	OMC	S2	462	1	19,22,23	0.29	0	26,31,34	0.41	0
1	PSU	S2	1625	1	18,21,22	0.54	0	22,30,33	0.58	0
1	A2M	S2	1031	1	22,25,26	0.10	0	31,36,39	0.23	0
1	A2M	S2	468	1	22,25,26	0.09	0	31,36,39	0.31	0
1	OMC	S2	1272	1	19,22,23	0.29	0	26,31,34	0.37	0
40	1MA	G	58	40	21,25,26	0.46	0	31,37,40	0.73	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PSU	S2	1056	1	18,21,22	0.54	0	22,30,33	0.55	0
1	4AC	S2	1337	1	21,24,25	0.33	0	29,34,37	0.35	0
1	PSU	S2	801	1	18,21,22	0.52	0	22,30,33	0.56	0
1	PSU	S2	918	1	18,21,22	0.46	0	22,30,33	0.37	0
1	PSU	S2	1445	1	18,21,22	0.55	0	22,30,33	0.56	0
1	PSU	S2	667	52,1	18,21,22	0.59	0	22,30,33	0.52	0
1	OMG	S2	601	1	23,26,27	0.32	0	33,38,41	0.32	0
1	A2M	S2	99	52,1	22,25,26	0.09	0	31,36,39	0.29	0
1	OMG	S2	683	1	23,26,27	0.32	0	33,38,41	0.46	0
1	OMU	S2	172	1	19,22,23	0.27	0	26,31,34	0.54	0
1	OMG	S2	867	1	23,26,27	0.31	0	33,38,41	0.31	0
1	PSU	S2	815	1	18,21,22	0.48	0	22,30,33	0.59	0
34	NMM	ST	67	34	9,11,12	0.64	0	6,12,14	1.75	2 (33%)
1	PSU	S2	1174	1	18,21,22	0.54	0	22,30,33	0.57	0
1	OMU	S2	1442	52,1	19,22,23	0.30	0	26,31,34	0.40	0
1	6MZ	S2	1832	52,51,1	22,25,26	0.13	0	30,36,39	0.28	0
1	PSU	S2	863	1	18,21,22	0.57	0	22,30,33	0.52	0
1	PSU	S2	649	1	18,21,22	0.53	0	22,30,33	0.64	0
1	PSU	S2	1232	1	18,21,22	0.54	0	22,30,33	0.54	0
1	PSU	S2	866	1	18,21,22	0.53	0	22,30,33	0.56	0
1	PSU	S2	100	1	18,21,22	0.49	0	22,30,33	0.58	0
1	OMG	S2	1447	1	23,26,27	0.30	0	33,38,41	0.41	0
1	PSU	S2	1347	1	18,21,22	0.56	0	22,30,33	0.55	0
1	OMC	S2	1703	52,1	19,22,23	0.29	0	26,31,34	0.51	0
1	PSU	S2	34	1	18,21,22	0.49	0	22,30,33	0.60	0
1	PSU	S2	651	1	18,21,22	0.53	0	22,30,33	0.58	0
1	PSU	S2	300	1	18,21,22	0.52	0	22,30,33	0.57	0
1	PSU	S2	1136	1	18,21,22	0.52	0	22,30,33	0.57	0
1	OMU	S2	1804	1	19,22,23	0.31	0	26,31,34	0.47	0
16	IAS	SO	138	16	6,7,8	1.05	0	6,8,10	1.66	3 (50%)
1	OMC	S2	174	1	19,22,23	0.29	0	26,31,34	0.42	0
1	PSU	S2	1045	1	18,21,22	0.49	0	22,30,33	0.62	0
1	OMU	S2	116	1	19,22,23	0.26	0	26,31,34	0.44	0
1	PSU	S2	36	1	18,21,22	0.53	0	22,30,33	0.53	0
1	PSU	S2	1177	1	18,21,22	0.54	0	22,30,33	0.56	0
1	PSU	S2	686	1	18,21,22	0.53	0	22,30,33	0.55	0
1	PSU	S2	105	1	18,21,22	0.49	0	22,30,33	0.58	0
1	A2M	S2	166	1	22,25,26	0.10	0	31,36,39	0.35	0
1	PSU	S2	681	1	18,21,22	0.55	0	22,30,33	0.55	0
1	A2M	S2	1383	1	22,25,26	0.08	0	31,36,39	0.48	0
1	A2M	S2	27	1	22,25,26	0.10	0	31,36,39	0.23	0
1	A2M	S2	512	1	22,25,26	0.09	0	31,36,39	0.50	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MA6	S2	1851	1	23,26,27	0.33	0	34,38,41	0.66	1 (2%)
1	PSU	S2	1003	1	18,21,22	0.54	0	22,30,33	0.54	0
1	PSU	S2	1238	1	18,21,22	0.53	0	22,30,33	0.55	0
40	H2U	G	47	40	18,21,22	0.31	0	21,30,33	0.45	0
1	OMU	S2	121	1	19,22,23	0.30	0	26,31,34	0.50	0
1	OMG	S2	436	1	23,26,27	0.35	0	33,38,41	0.48	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	S2	1288	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	609	1	-	0/7/25/26	0/2/2/2
40	1MG	G	10	40	-	2/7/25/26	0/3/3/3
1	OMU	S2	354	1	-	0/9/27/28	0/2/2/2
1	B8N	S2	1248	1	-	2/16/34/35	0/2/2/2
1	OMG	S2	644	1	-	1/9/27/28	0/3/3/3
1	PSU	S2	1186	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	966	1	-	0/7/25/26	0/2/2/2
1	OMG	S2	1490	52,1	-	2/9/27/28	0/3/3/3
1	PSU	S2	1367	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	576	1	-	3/9/27/28	0/3/3/3
1	PSU	S2	218	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1692	1	-	0/7/25/26	0/2/2/2
40	T6A	G	37	40	-	0/23/41/42	0/3/3/3
1	PSU	S2	63	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	1678	1	-	1/9/27/28	0/3/3/3
1	MA6	S2	1850	1	-	0/11/29/30	0/3/3/3
40	2MG	G	26	40	-	4/9/27/28	0/3/3/3
1	PSU	S2	1004	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	822	1	-	1/7/25/26	0/2/2/2
1	PSU	S2	1643	52,1	-	0/7/25/26	0/2/2/2
1	PSU	S2	93	1	-	0/7/25/26	0/2/2/2
1	OMG	S2	509	52,1	-	0/9/27/28	0/3/3/3
1	PSU	S2	109	1	-	0/7/25/26	0/2/2/2
1	OMC	S2	517	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	814	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	296	1	-	0/7/25/26	0/2/2/2
1	UY1	S2	1326	52,1	-	2/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	S2	1046	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	668	1	-	3/9/27/28	0/3/3/3
1	A2M	S2	159	1	-	3/9/27/28	0/3/3/3
1	4AC	S2	1842	1	-	0/11/29/30	0/2/2/2
1	PSU	S2	1596	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1360	51,1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1244	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	366	1	-	2/7/25/26	0/2/2/2
40	5MC	G	48	40	-	3/7/25/26	0/2/2/2
1	PSU	S2	119	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	406	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	590	1	-	3/9/27/28	0/3/3/3
1	OMG	S2	1328	51,1	-	0/9/27/28	0/3/3/3
1	A2M	S2	484	1	-	0/9/27/28	0/3/3/3
1	OMC	S2	1391	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	572	1	-	0/7/25/26	0/2/2/2
1	OMU	S2	428	1	-	4/9/27/28	0/2/2/2
1	OMC	S2	462	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	1625	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	1031	1	-	1/9/27/28	0/3/3/3
1	A2M	S2	468	1	-	1/9/27/28	0/3/3/3
1	OMC	S2	1272	1	-	0/9/27/28	0/2/2/2
40	1MA	G	58	40	-	0/7/25/26	0/3/3/3
1	PSU	S2	1056	1	-	0/7/25/26	0/2/2/2
1	4AC	S2	1337	1	-	0/11/29/30	0/2/2/2
1	PSU	S2	801	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	918	1	-	2/7/25/26	0/2/2/2
1	PSU	S2	1445	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	667	52,1	-	2/7/25/26	0/2/2/2
1	OMG	S2	601	1	-	0/9/27/28	0/3/3/3
1	A2M	S2	99	52,1	-	0/9/27/28	0/3/3/3
1	OMG	S2	683	1	-	0/9/27/28	0/3/3/3
1	OMU	S2	172	1	-	0/9/27/28	0/2/2/2
1	OMG	S2	867	1	-	2/9/27/28	0/3/3/3
1	PSU	S2	815	1	-	0/7/25/26	0/2/2/2
34	NMM	ST	67	34	-	0/9/11/13	-
1	PSU	S2	1174	1	-	0/7/25/26	0/2/2/2
1	OMU	S2	1442	52,1	-	1/9/27/28	0/2/2/2
1	6MZ	S2	1832	52,51,1	-	2/9/27/28	0/3/3/3
1	PSU	S2	863	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	S2	649	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1232	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	866	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	100	1	-	0/7/25/26	0/2/2/2
1	OMG	S2	1447	1	-	2/9/27/28	0/3/3/3
1	PSU	S2	1347	1	-	0/7/25/26	0/2/2/2
1	OMC	S2	1703	52,1	-	0/9/27/28	0/2/2/2
1	PSU	S2	34	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	651	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	300	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1136	1	-	0/7/25/26	0/2/2/2
1	OMU	S2	1804	1	-	2/9/27/28	0/2/2/2
16	IAS	SO	138	16	-	1/7/7/8	-
1	OMC	S2	174	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	1045	1	-	0/7/25/26	0/2/2/2
1	OMU	S2	116	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	36	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1177	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	686	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	105	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	166	1	-	3/9/27/28	0/3/3/3
1	PSU	S2	681	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	1383	1	-	1/9/27/28	0/3/3/3
1	A2M	S2	27	1	-	1/9/27/28	0/3/3/3
1	A2M	S2	512	1	-	1/9/27/28	0/3/3/3
1	MA6	S2	1851	1	-	3/11/29/30	0/3/3/3
1	PSU	S2	1003	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1238	1	-	0/7/25/26	0/2/2/2
40	H2U	G	47	40	-	3/7/38/39	0/2/2/2
1	OMU	S2	121	1	-	0/9/27/28	0/2/2/2
1	OMG	S2	436	1	-	0/9/27/28	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	822	PSU	O4'-C1'	-2.13	1.40	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	ST	67	NMM	NE-CZ-NH2	-3.23	116.52	119.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	G	10	1MG	C6-C5-C4	-2.67	117.02	119.97
40	G	37	T6A	C12-N11-C10	2.65	126.36	121.94
1	S2	1850	MA6	C2-N1-C6	2.40	117.42	111.75
1	S2	1851	MA6	C2-N1-C6	2.35	117.31	111.75
34	ST	67	NMM	NE-CZ-NH1	2.34	124.65	120.26
16	SO	138	IAS	OD1-CG-CB	-2.30	118.74	125.43
16	SO	138	IAS	OXT-C-O	-2.18	119.15	124.09
40	G	58	1MA	N1-C6-N6	2.13	125.19	119.77
1	S2	512	A2M	C2'-C3'-C4'	-2.06	97.51	101.99
16	SO	138	IAS	OXT-C-CA	2.04	120.34	113.38

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	S2	27	A2M	C1'-C2'-O2'-CM'
1	S2	166	A2M	C1'-C2'-O2'-CM'
1	S2	428	OMU	C2'-C1'-N1-C2
1	S2	428	OMU	C2'-C1'-N1-C6
1	S2	468	A2M	C1'-C2'-O2'-CM'
1	S2	512	A2M	C1'-C2'-O2'-CM'
1	S2	576	A2M	C1'-C2'-O2'-CM'
1	S2	668	A2M	C1'-C2'-O2'-CM'
1	S2	918	PSU	C2'-C1'-C5-C6
1	S2	1031	A2M	C1'-C2'-O2'-CM'
1	S2	1326	UY1	C2'-C1'-C5-C6
1	S2	1383	A2M	C1'-C2'-O2'-CM'
1	S2	1442	OMU	C1'-C2'-O2'-CM2
1	S2	1490	OMG	O4'-C4'-C5'-O5'
1	S2	1678	A2M	C1'-C2'-O2'-CM'
1	S2	1832	6MZ	N1-C6-N6-C9
1	S2	1851	MA6	O4'-C4'-C5'-O5'
16	SO	138	IAS	CA-CB-CG-OD1
40	G	10	1MG	O4'-C4'-C5'-O5'
40	G	26	2MG	O4'-C1'-N9-C8
40	G	26	2MG	O4'-C1'-N9-C4
40	G	26	2MG	N1-C2-N2-CM2
40	G	26	2MG	N3-C2-N2-CM2
40	G	47	H2U	C2'-C1'-N1-C2
1	S2	166	A2M	O4'-C4'-C5'-O5'
1	S2	576	A2M	O4'-C4'-C5'-O5'
1	S2	576	A2M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	S2	1447	OMG	C3'-C4'-C5'-O5'
1	S2	1851	MA6	C3'-C4'-C5'-O5'
40	G	48	5MC	O4'-C4'-C5'-O5'
40	G	48	5MC	C3'-C4'-C5'-O5'
40	G	47	H2U	C2'-C1'-N1-C6
1	S2	159	A2M	O4'-C4'-C5'-O5'
1	S2	159	A2M	C3'-C4'-C5'-O5'
1	S2	166	A2M	C3'-C4'-C5'-O5'
1	S2	1447	OMG	O4'-C4'-C5'-O5'
1	S2	428	OMU	O4'-C1'-N1-C6
1	S2	428	OMU	O4'-C1'-N1-C2
1	S2	867	OMG	C4'-C5'-O5'-P
1	S2	1832	6MZ	C5-C6-N6-C9
1	S2	644	OMG	C4'-C5'-O5'-P
1	S2	1490	OMG	C4'-C5'-O5'-P
1	S2	1804	OMU	C3'-C4'-C5'-O5'
1	S2	1851	MA6	C4'-C5'-O5'-P
40	G	48	5MC	C4'-C5'-O5'-P
40	G	47	H2U	O4'-C1'-N1-C2
1	S2	867	OMG	C3'-C4'-C5'-O5'
1	S2	366	PSU	O4'-C1'-C5-C4
1	S2	667	PSU	O4'-C1'-C5-C4
1	S2	822	PSU	O4'-C1'-C5-C4
1	S2	1248	B8N	O4'-C1'-C5-C4
1	S2	159	A2M	C3'-C2'-O2'-CM'
1	S2	590	A2M	O4'-C1'-N9-C8
40	G	10	1MG	C3'-C4'-C5'-O5'
1	S2	366	PSU	O4'-C1'-C5-C6
1	S2	667	PSU	O4'-C1'-C5-C6
1	S2	918	PSU	O4'-C1'-C5-C6
1	S2	1248	B8N	O4'-C1'-C5-C6
1	S2	1326	UY1	O4'-C1'-C5-C6
1	S2	1804	OMU	O4'-C4'-C5'-O5'
1	S2	590	A2M	C2'-C1'-N9-C8
1	S2	668	A2M	C2'-C1'-N9-C8
1	S2	668	A2M	O4'-C4'-C5'-O5'
1	S2	590	A2M	C2'-C1'-N9-C4

There are no ring outliers.

28 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	S2	354	OMU	1	0
1	S2	576	A2M	4	0
1	S2	1678	A2M	2	0
1	S2	1850	MA6	4	0
40	G	26	2MG	1	0
1	S2	93	PSU	1	0
1	S2	814	PSU	2	0
1	S2	668	A2M	3	0
1	S2	159	A2M	2	0
1	S2	1842	4AC	1	0
1	S2	484	A2M	3	0
1	S2	428	OMU	2	0
1	S2	462	OMC	1	0
1	S2	1031	A2M	1	0
1	S2	468	A2M	2	0
1	S2	1337	4AC	1	0
1	S2	99	A2M	1	0
1	S2	815	PSU	2	0
1	S2	1174	PSU	1	0
1	S2	1442	OMU	2	0
1	S2	1832	6MZ	4	0
1	S2	116	OMU	2	0
1	S2	166	A2M	6	0
1	S2	1383	A2M	1	0
1	S2	27	A2M	5	0
1	S2	512	A2M	3	0
1	S2	1851	MA6	3	0
1	S2	121	OMU	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 111 ligands modelled in this entry, 109 are monoatomic - leaving 2 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	$\# Z  > 2$
55	MET	E	502	-	6,7,8	0.48	0	2,7,9	0.13	0
54	GNP	E	501	-	33,34,34	2.23	5 (15%)	46,54,54	1.48	3 (6%)

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
55	MET	E	502	-	-	2/5/6/8	-
54	GNP	E	501	-	-	5/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	E	501	GNP	PB-O3A	8.12	1.69	1.59
54	E	501	GNP	PG-N3B	6.53	1.80	1.63
54	E	501	GNP	PG-O1G	4.67	1.53	1.46
54	E	501	GNP	PB-O1B	3.10	1.51	1.46
54	E	501	GNP	PB-O2B	-2.15	1.51	1.56

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	E	501	GNP	O1G-PG-N3B	-7.18	101.20	111.77
54	E	501	GNP	O2B-PB-O1B	4.80	119.98	109.92
54	E	501	GNP	O2G-PG-O3G	2.30	113.77	107.64

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	E	501	GNP	PB-N3B-PG-O1G
54	E	501	GNP	PG-N3B-PB-O1B
54	E	501	GNP	C4'-C5'-O5'-PA
54	E	501	GNP	O4'-C4'-C5'-O5'
55	E	502	MET	C-CA-CB-CG
54	E	501	GNP	C3'-C4'-C5'-O5'

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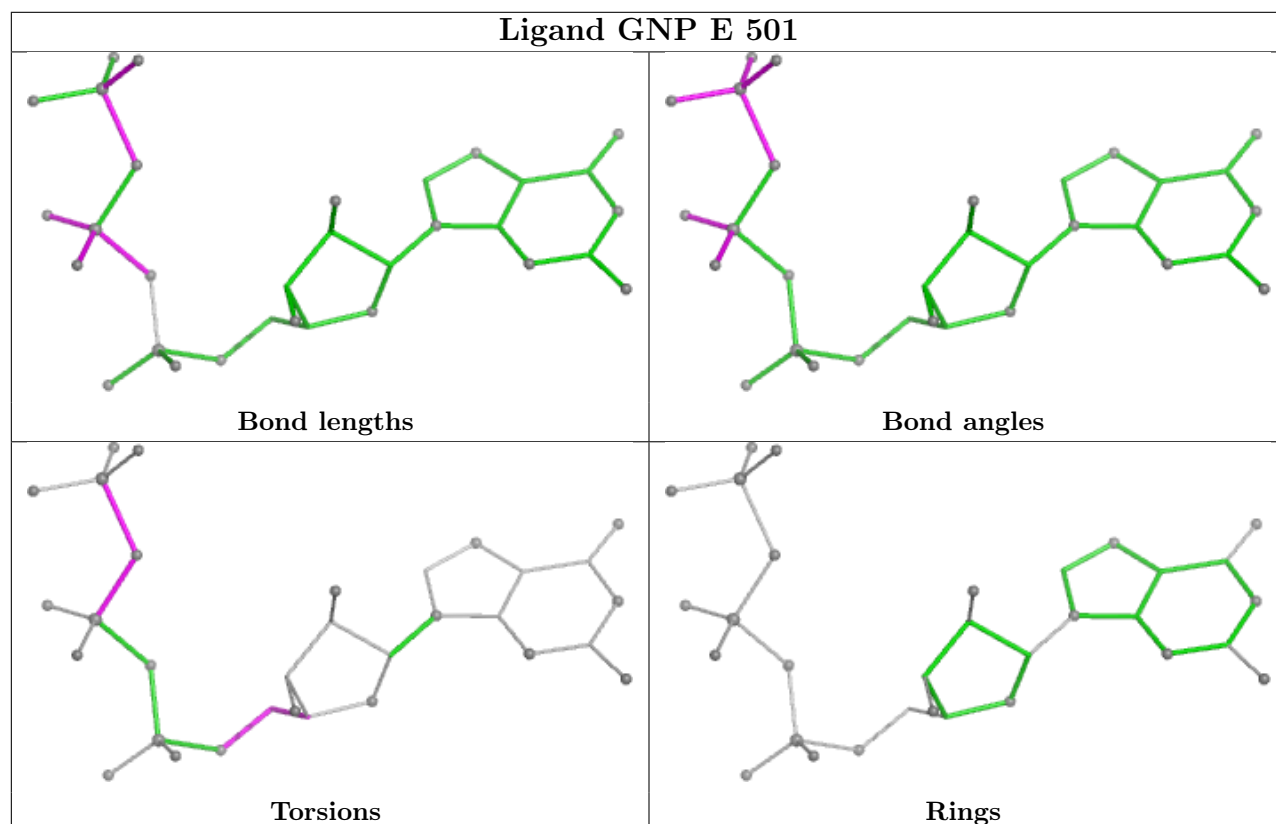
Mol	Chain	Res	Type	Atoms
55	E	502	MET	CB-CG-SD-CE

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	E	502	MET	1	0

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
16	SO	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	SO	136:PRO	C	137:SER	N	1.14

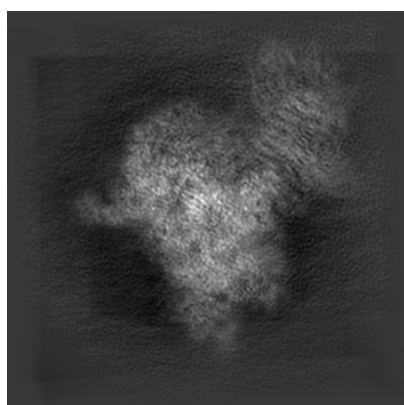
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-57010. These allow visual inspection of the internal detail of the map and identification of artifacts.

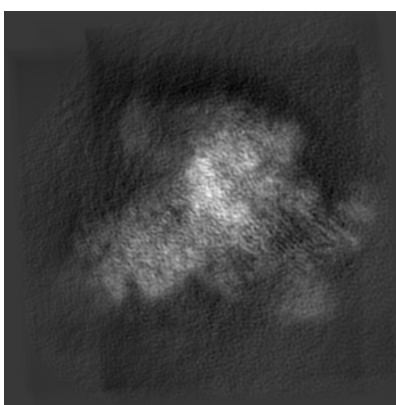
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

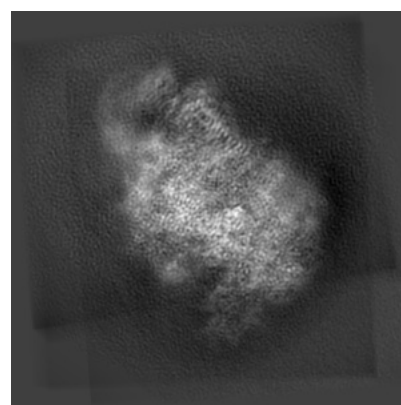
#### 6.1.1 Primary map



X



Y

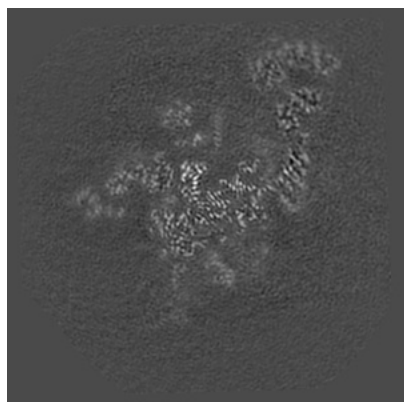


Z

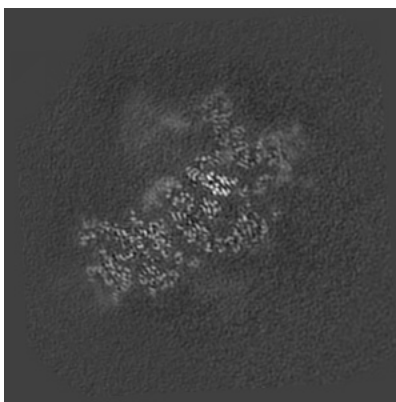
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

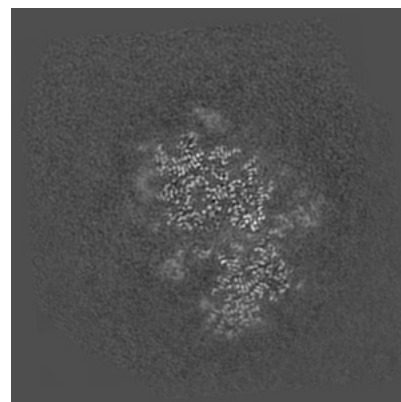
#### 6.2.1 Primary map



X Index: 260



Y Index: 260

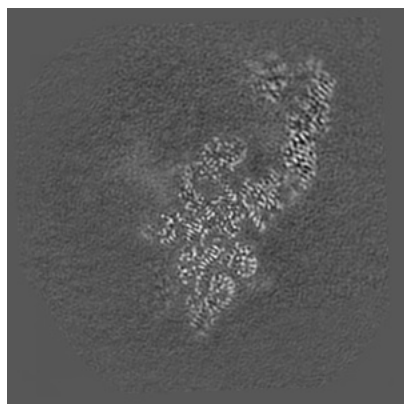


Z Index: 260

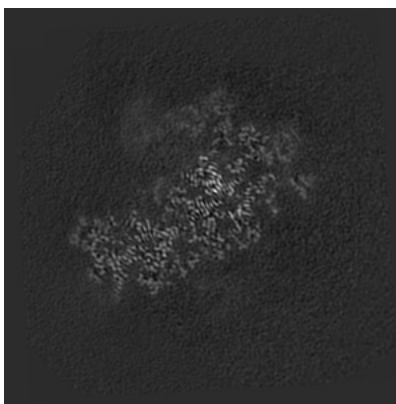
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

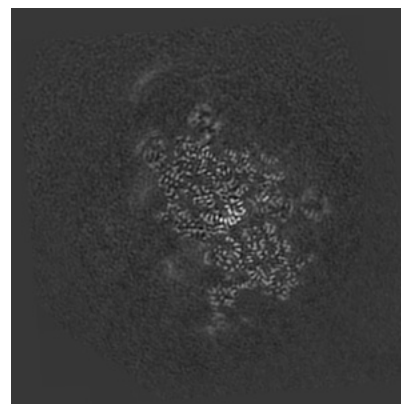
### 6.3.1 Primary map



X Index: 233



Y Index: 253

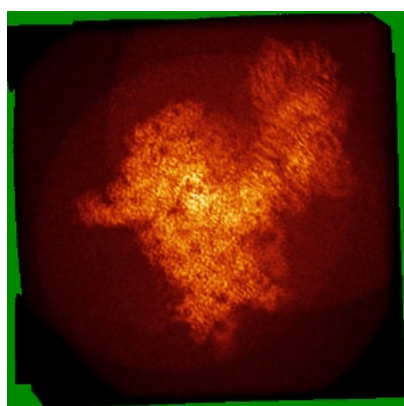


Z Index: 279

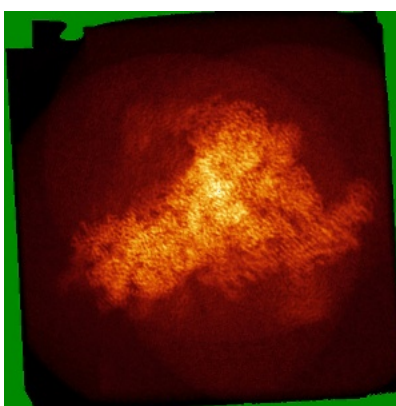
The images above show the largest variance slices of the map in three orthogonal directions.

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

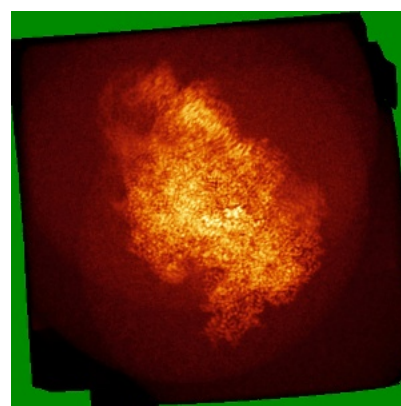
### 6.4.1 Primary map



X



Y

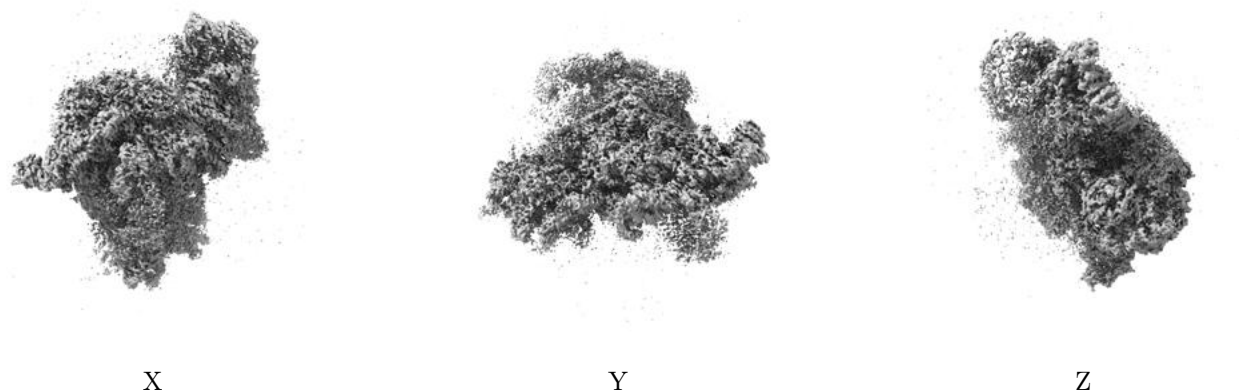


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.88. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

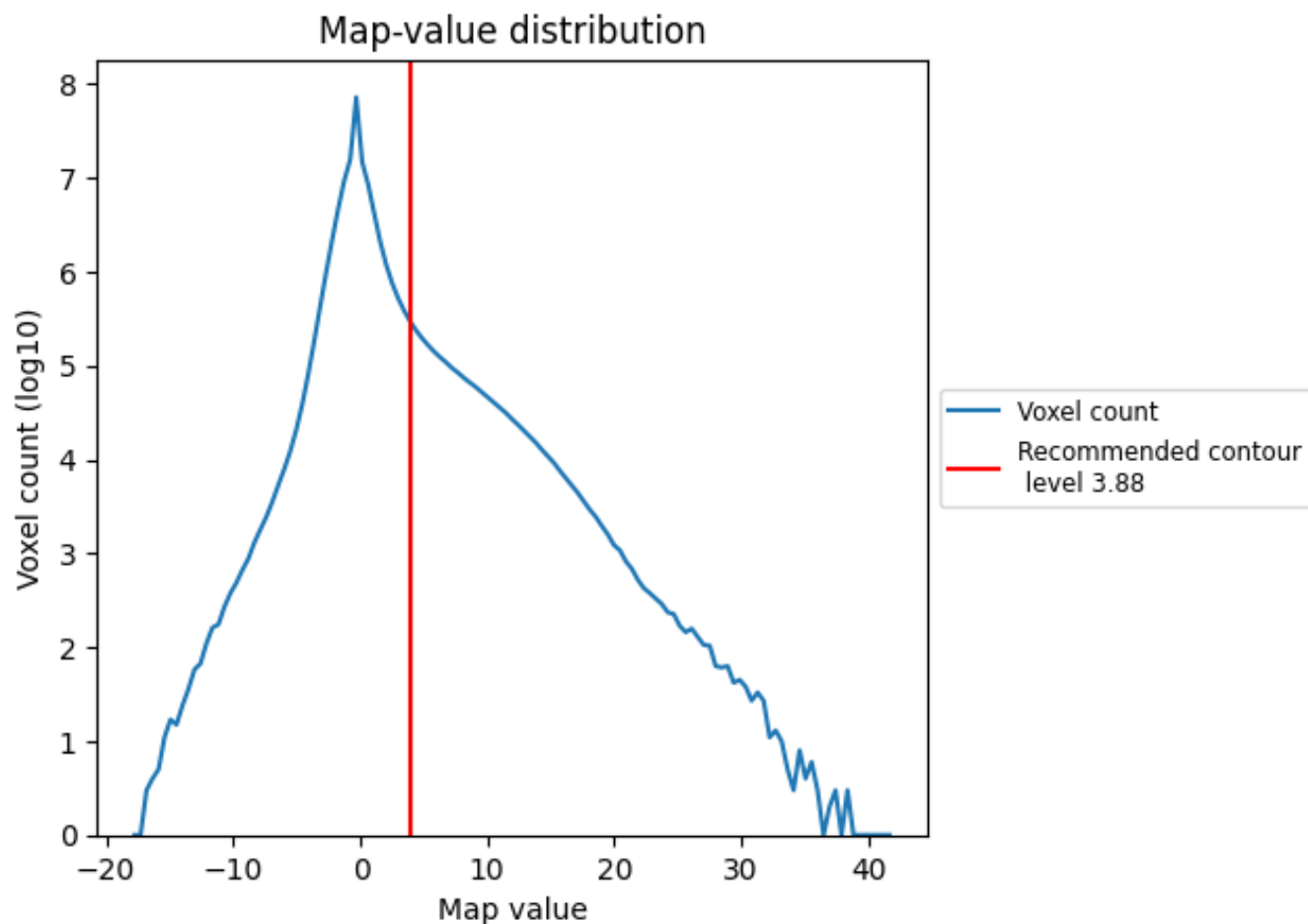
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

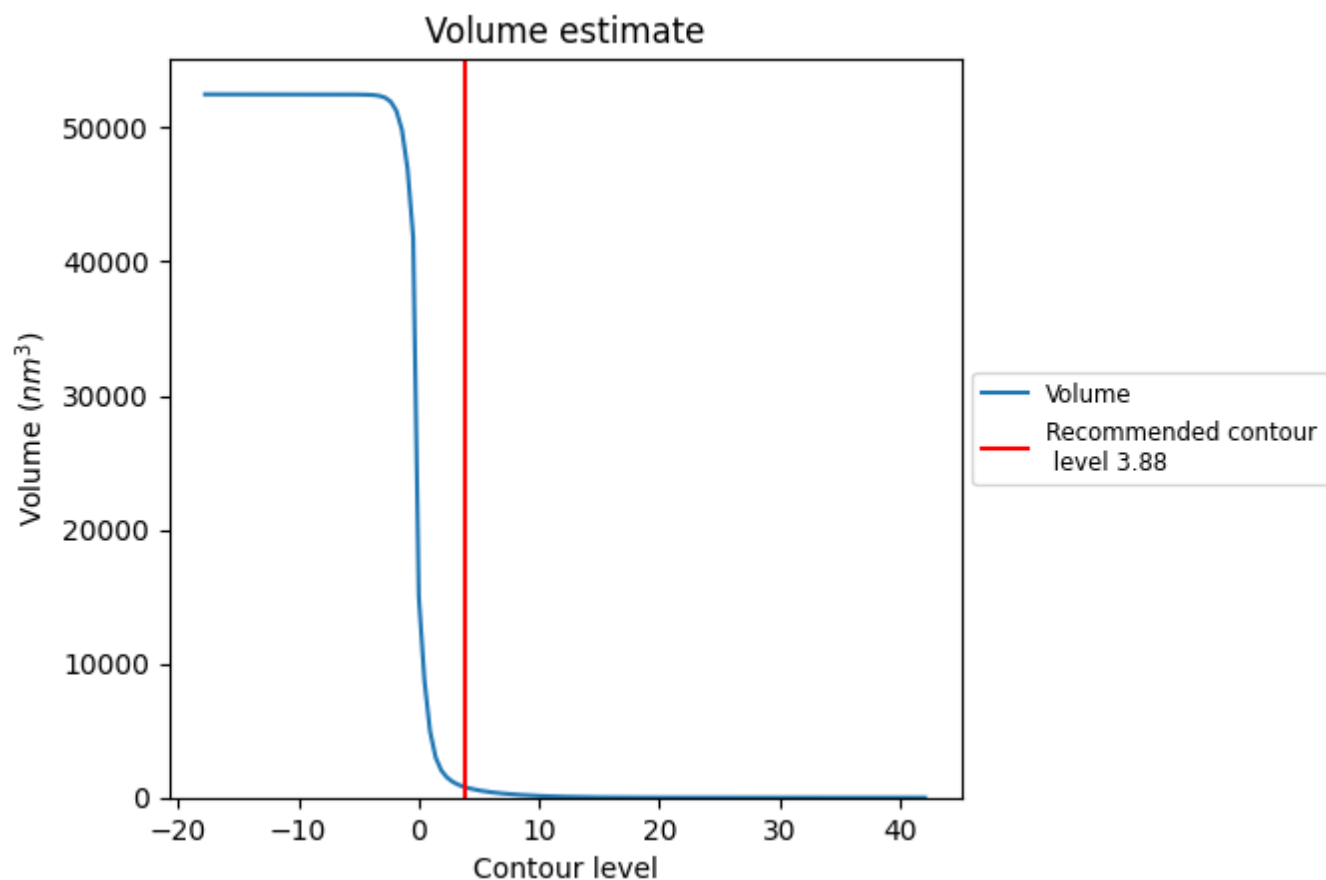
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

## 7.2 Volume estimate [i](#)

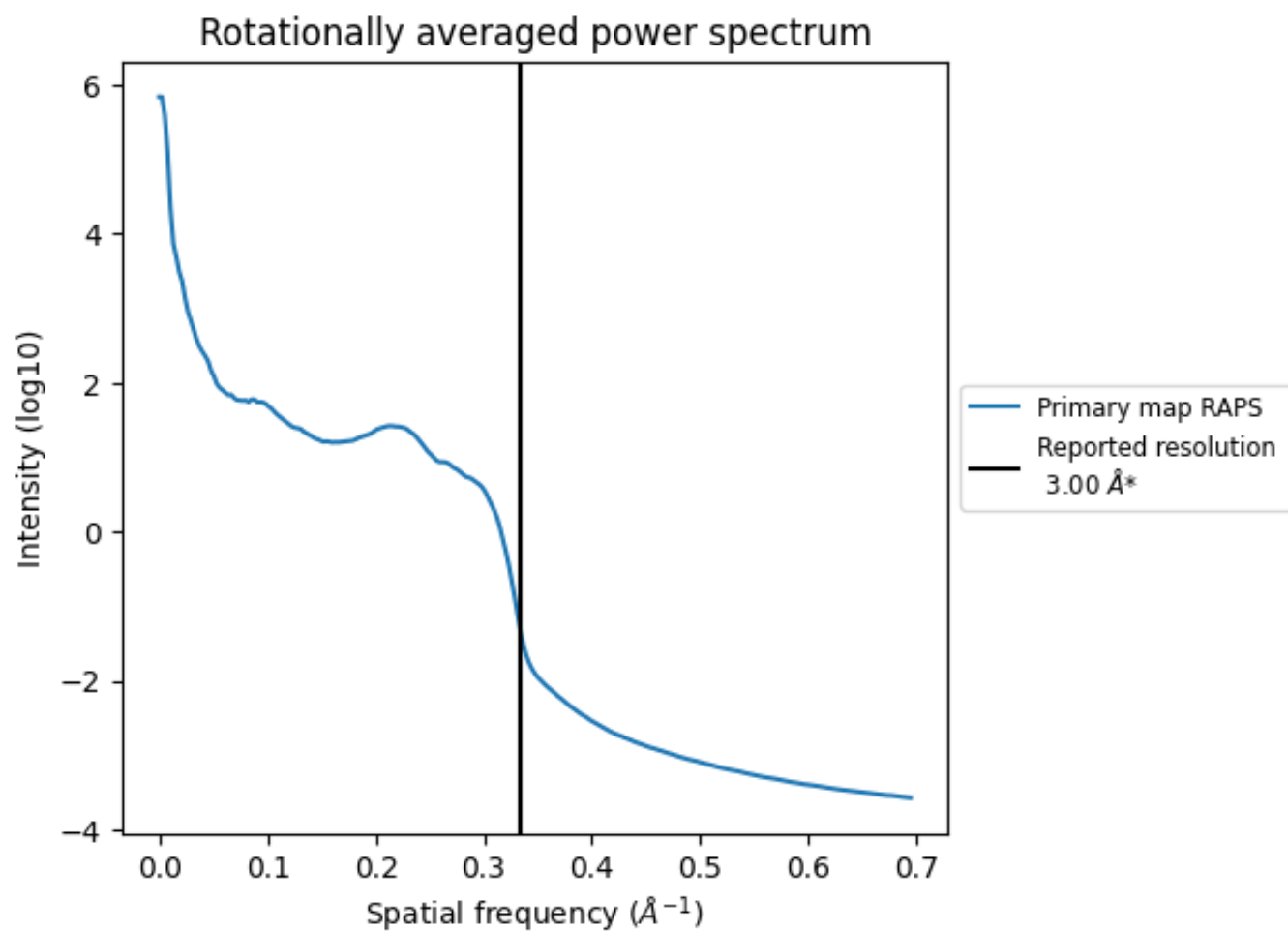


The volume at the recommended contour level is 774 nm<sup>3</sup>; this corresponds to an approximate mass of 699 kDa.

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



### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.333 Å<sup>-1</sup>

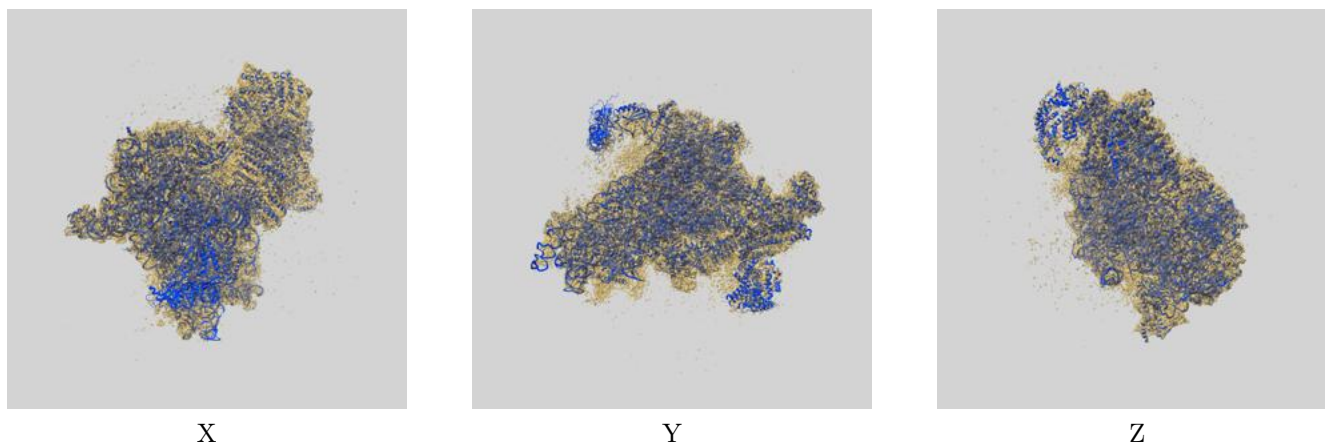
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

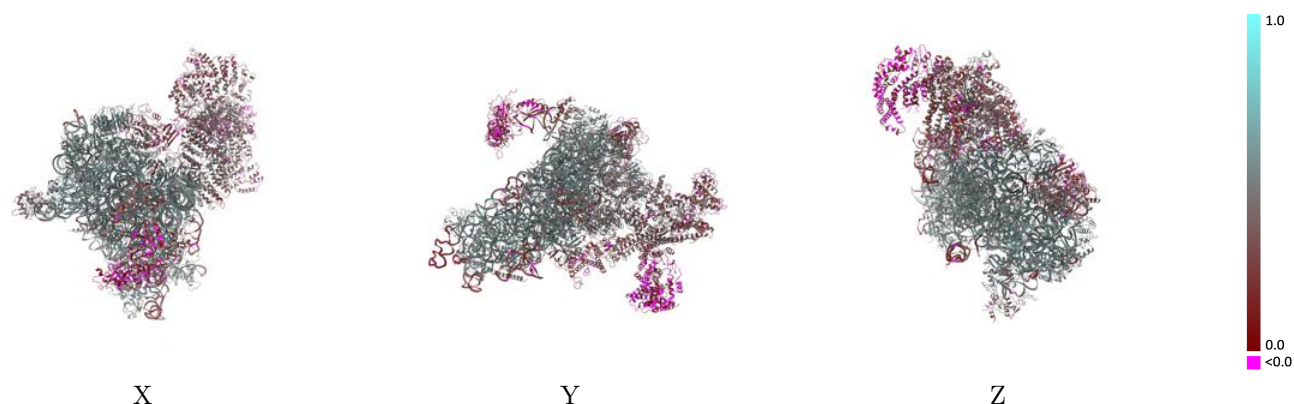
This section contains information regarding the fit between EMDB map EMD-57010 and PDB model 28ZY. Per-residue inclusion information can be found in section [3](#) on page [15](#).

### 9.1 Map-model overlay [i](#)



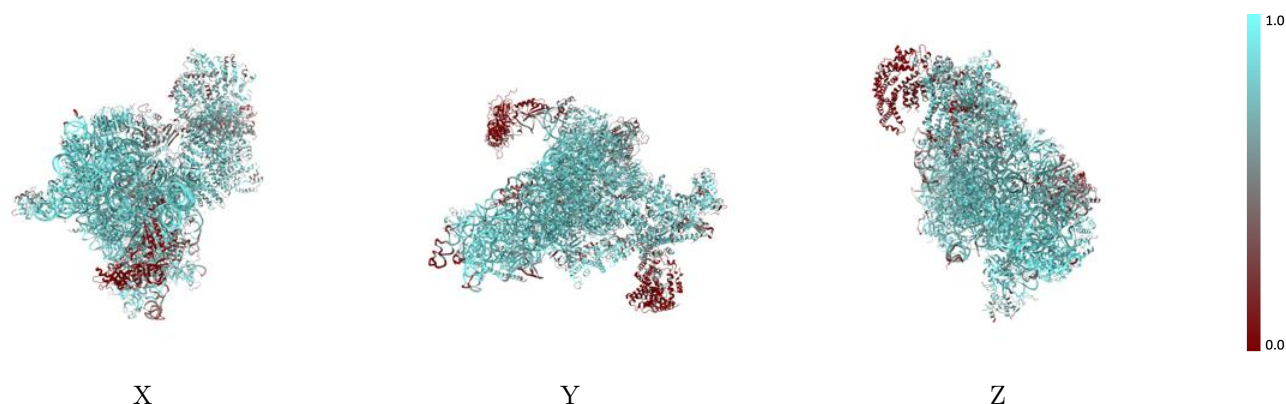
The images above show the 3D surface view of the map at the recommended contour level 3.88 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



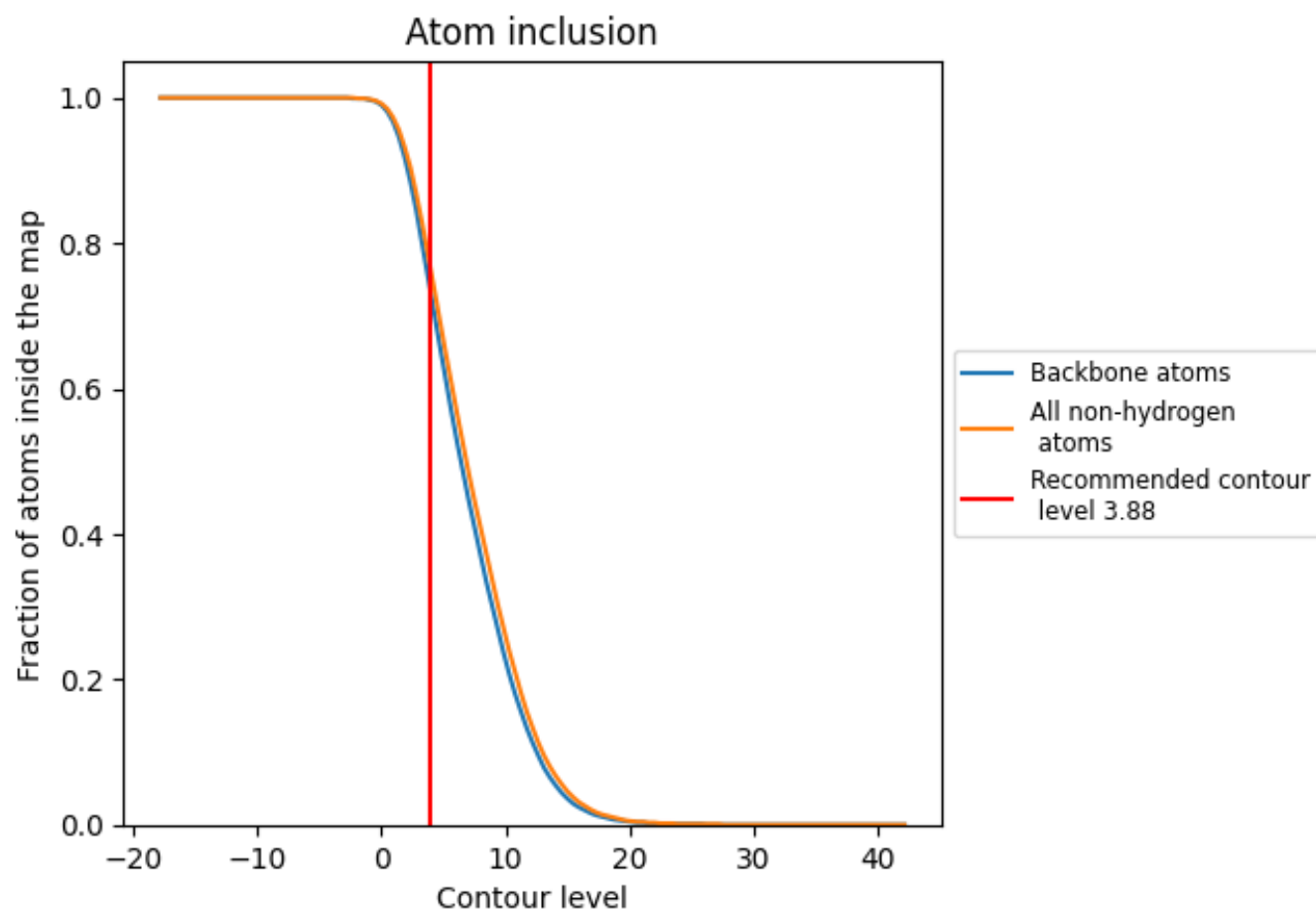
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.88).







































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 74% of all backbone atoms, 77% 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 (3.88) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7740	 0.4480
3f	 0.6790	 0.3320
B	 0.7010	 0.3220
D	 0.4760	 0.3430
E	 0.0360	 0.1250
F	 0.0000	 0.0630
G	 0.7680	 0.3470
H	 0.8060	 0.4690
Ln	 0.8370	 0.5140
S2	 0.9050	 0.5050
SA	 0.8350	 0.5160
SB	 0.8420	 0.5070
SC	 0.8740	 0.5400
SD	 0.8460	 0.5190
SE	 0.8940	 0.5510
SF	 0.8830	 0.5450
SG	 0.8050	 0.5000
SH	 0.7360	 0.4660
SI	 0.8510	 0.5160
SJ	 0.8390	 0.5160
SK	 0.8510	 0.5250
SL	 0.8500	 0.5340
SM	 0.6070	 0.3850
SN	 0.8680	 0.5310
SO	 0.8460	 0.5160
SP	 0.8380	 0.5180
SQ	 0.8980	 0.5560
SR	 0.8130	 0.5110
SS	 0.8540	 0.5430
ST	 0.8740	 0.5390
SU	 0.7960	 0.5050
SV	 0.8360	 0.5220
SW	 0.9120	 0.5630
SX	 0.9090	 0.5530
SY	 0.8570	 0.5300



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Chain	Atom inclusion	Q-score
SZ	 0.8630	 0.5230
Sa	 0.8810	 0.5340
Sb	 0.8750	 0.5140
Sc	 0.8870	 0.5090
Sd	 0.9210	 0.5640
Se	 0.7480	 0.4980
Sf	 0.6870	 0.4100
Sg	 0.8410	 0.5140
a	 0.6960	 0.3620
c	 0.6890	 0.3710
d	 0.6050	 0.3170
e	 0.6550	 0.2820
h	 0.6380	 0.2950
k	 0.1180	 0.0820
l	 0.1890	 0.0980
m	 0.6780	 0.3070