



Full wwPDB EM Validation Report ⓘ

Jun 18, 2026 – 10:17 am BST

PDB ID : 28ZX / pdb_000028zx
EMDB ID : EMD-57009
Title : human 48S PIC with mRNA (Kozak_1)
Authors : von Loeffelholz, O.; Barchet, C.; Klaholz, B.
Deposited on : 2026-03-03
Resolution : 2.80 Å (reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

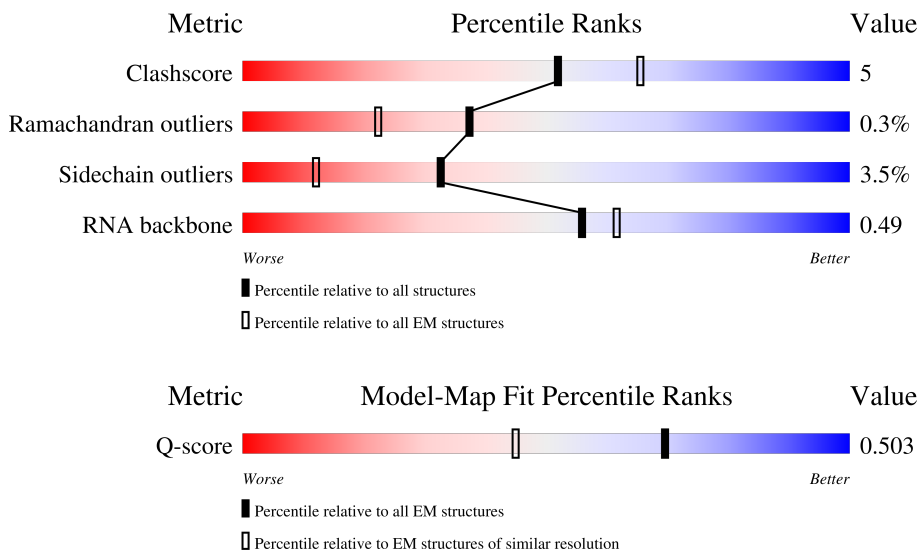
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.80 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.




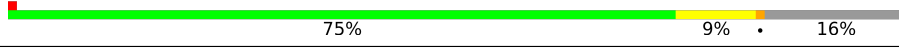
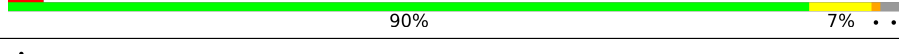
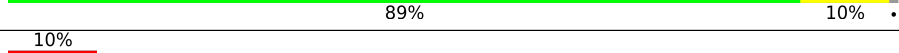
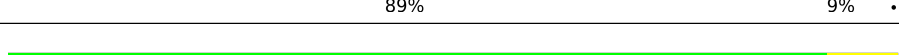
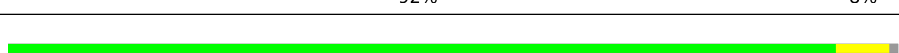
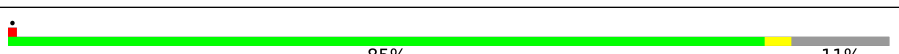



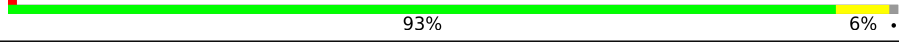

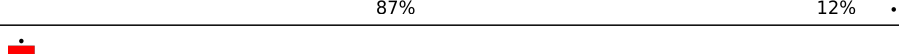

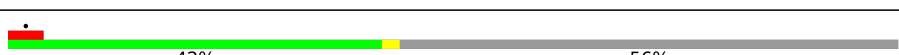
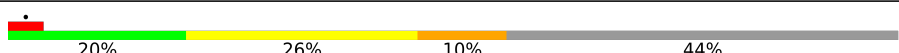




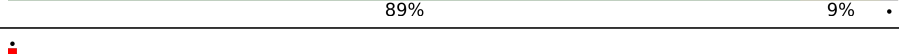
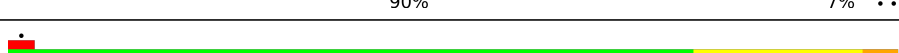



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11806 (2.30 - 3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

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

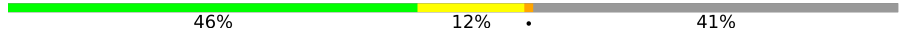

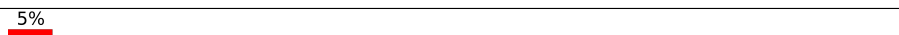
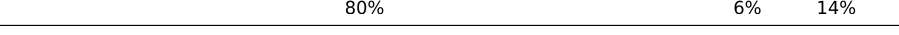


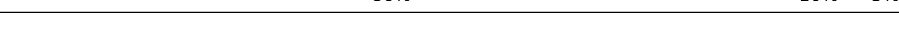



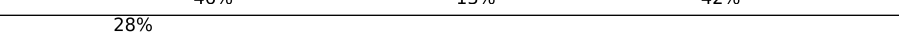



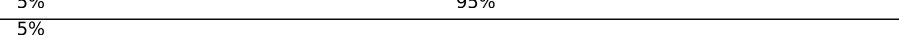



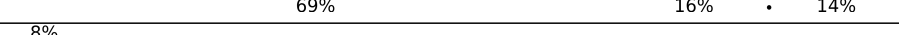


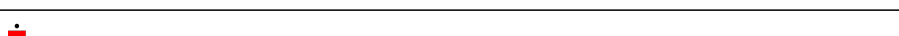
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Mol	Chain	Length	Quality of chain
4	SA	295	 66% 8% 26%
5	SB	264	 75% 9% 16%
6	SH	194	 90% 7% ..
7	SI	208	 89% 10% .
8	SL	158	 10% 89% 9% .
9	SV	83	 92% 8%
10	SX	143	 93% 6% .
11	Sa	115	 85% . 11%
12	SC	293	 67% 8% . 25%
13	SG	249	 88% 6% 6%
14	SJ	194	 85% 9% 6%
15	SN	151	 93% 6% .
16	SO	151	 74% 15% . 10%
17	SW	130	 87% 12% .
18	SY	133	 89% 5% 7%
19	Sb	84	 83% 15% .
20	Se	133	 42% . 56%
21	B	50	 20% 26% 10% 44%
22	SD	243	 84% 10% 7%
23	SF	204	 82% 9% . 7%
24	Sf	156	 31% 8% . 60%
25	SR	135	 80% 16% ..
26	Sd	56	 89% 9% .
27	Sg	317	 90% 7% ..
28	Sc	69	 77% 19% .

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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 [i](#)

There are 56 unique types of molecules in this entry. The entry contains 108811 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
			Total	C	N	O	S		
17	SW	129	1034	659	193	176	6	0	0

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

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

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

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

- 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_Kozak.

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
			Total	C	N	O	S		
27	Sg	314	2440	1537	425	466	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	Sc	69	546	330	110	103	3	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 40 is a RNA chain called initiator tRNA.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	H	113	Total	C	N	O	S	0	0
			910	565	174	166	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	SF	1	Total	K	0
			1	1	
51	Sd	1	Total	K	0
			1	1	

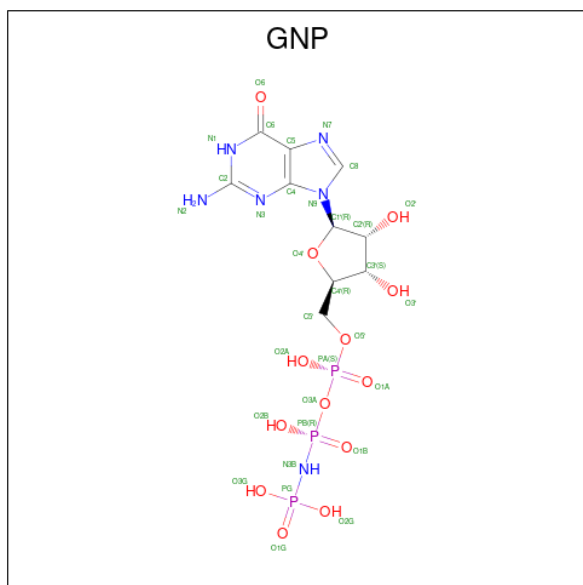
- Molecule 52 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
52	S2	80	Total	Mg	0
			80	80	
52	Sa	1	Total	Mg	0
			1	1	
52	SN	1	Total	Mg	0
			1	1	
52	B	3	Total	Mg	0
			3	3	
52	H	1	Total	Mg	0
			1	1	

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

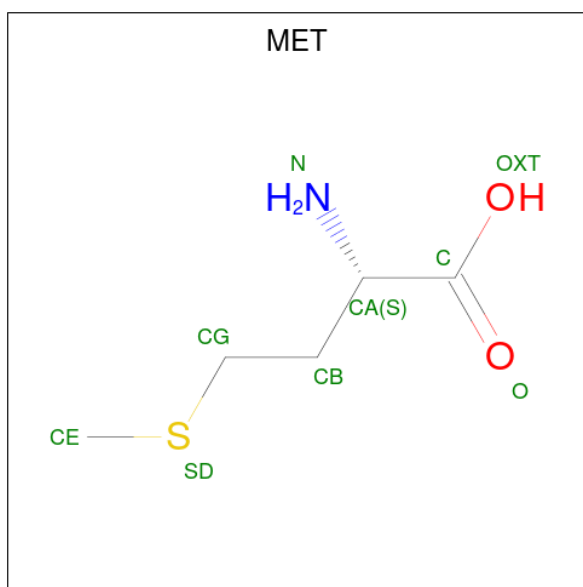
Mol	Chain	Residues	Atoms		AltConf
53	Sa	1	Total	Zn	0
			1	1	
53	Sf	1	Total	Zn	0
			1	1	
53	Sd	1	Total	Zn	0
			1	1	

- 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	

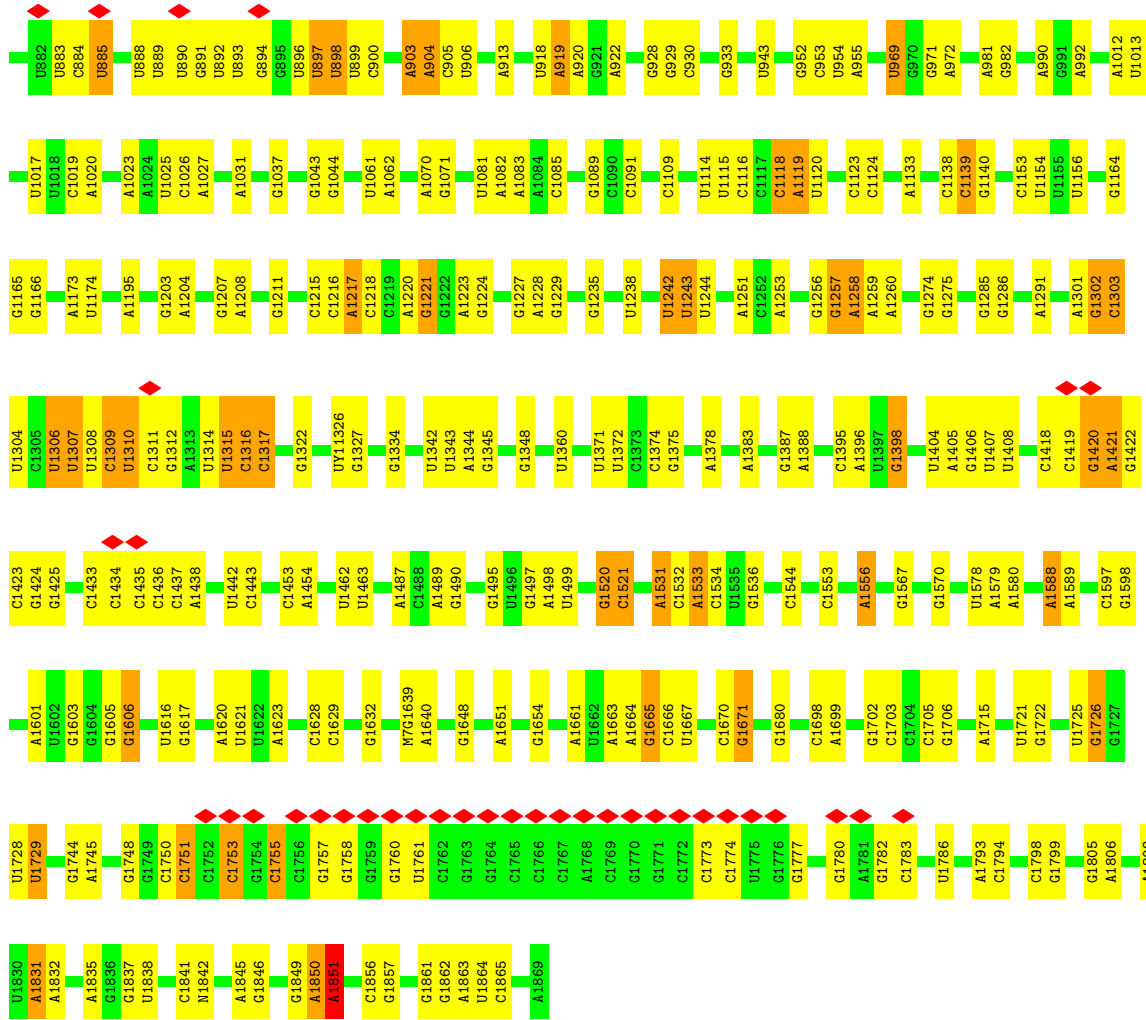
- Molecule 55 is METHIONINE (CCD ID: MET) (formula: $C_5H_{11}NO_2S$).



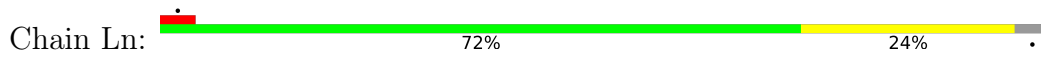
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
55	E	1	8	5	1	1	1	0

- Molecule 56 is water.

Mol	Chain	Residues	Atoms		AltConf
56	S2	345	Total	O	0
			345	345	
56	SE	2	Total	O	0
			2	2	
56	SB	1	Total	O	0
			1	1	
56	SL	2	Total	O	0
			2	2	
56	Sa	3	Total	O	0
			3	3	
56	SN	4	Total	O	0
			4	4	
56	SO	3	Total	O	0
			3	3	
56	SS	1	Total	O	0
			1	1	
56	ST	2	Total	O	0
			2	2	



- Molecule 2: 60S ribosomal protein L41

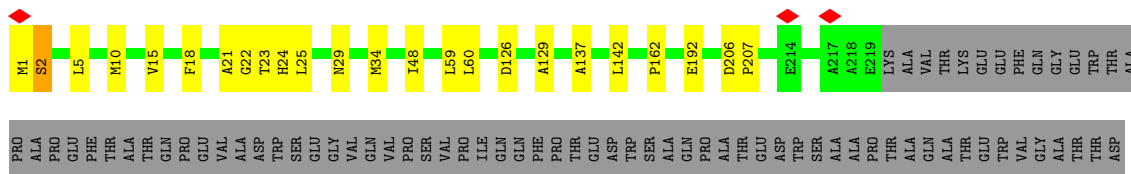


- Molecule 3: Small ribosomal subunit protein eS4, X isoform



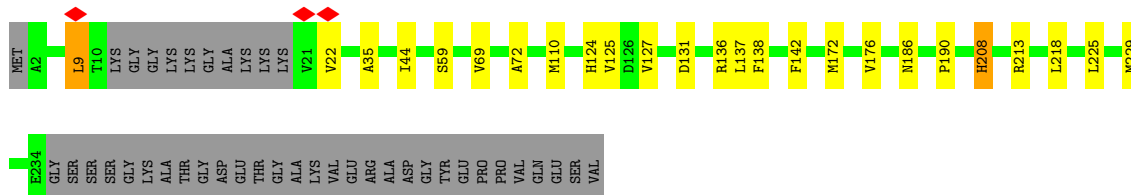
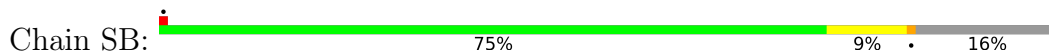
- Molecule 4: 40S ribosomal protein SA



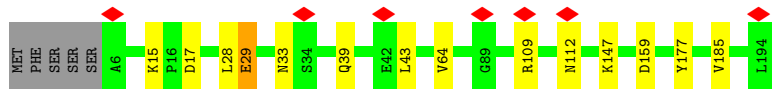
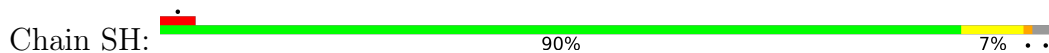


TRP
SER

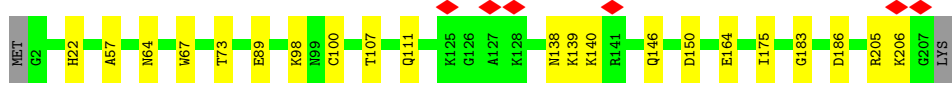
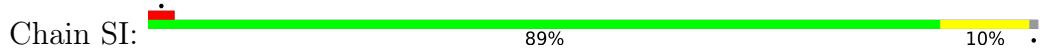
- Molecule 5: 40S ribosomal protein S3a



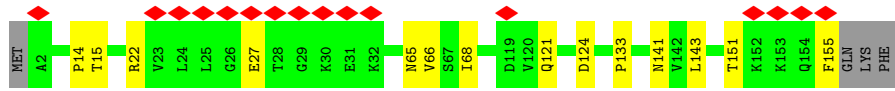
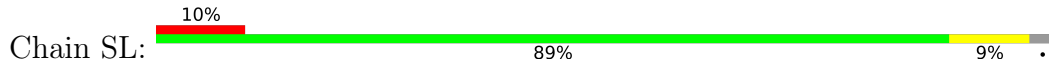
- Molecule 6: 40S ribosomal protein S7



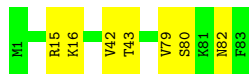
- Molecule 7: 40S ribosomal protein S8



- Molecule 8: Small ribosomal subunit protein uS17




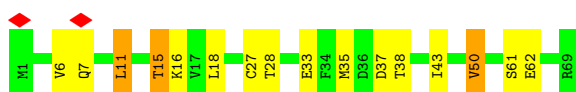
- Molecule 9: 40S ribosomal protein S21



- Molecule 10: 40S ribosomal protein S23

- Molecule 28: 40S ribosomal protein S28

Chain Sc:  77% 19%




- Molecule 29: 40S ribosomal protein S10

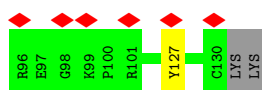
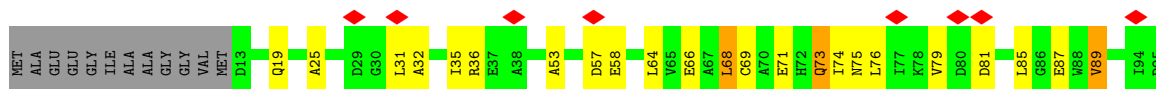
Chain SK:  46% 12% 41%




GLU
ALA
ASP
ARG
THR
TYR
ARG
SER
ALA
VAL
PRO
PRO
GLY
ALA
ASP
LYS
LYS
ALA
ALA
ALA
ALA
GLY
SER
ALA
THR
PHE
GLN
PHE
ARG
GLY
GLY
PHE
GLY
ARG
GLY
ARG
GLY
GLY
GLN
PRO
PRO
PRO
GLN

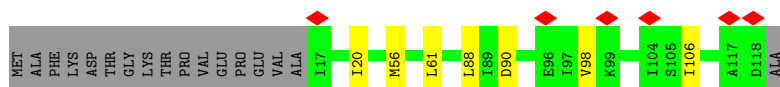
- Molecule 30: 40S ribosomal protein S12

Chain SM:  11% 71% 16% 11%




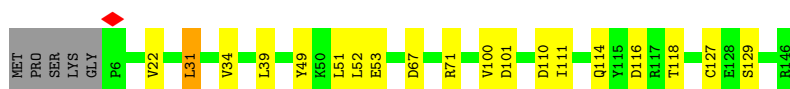
- Molecule 31: 40S ribosomal protein S20

Chain SU:  5% 80% 6% 14%




- Molecule 32: 40S ribosomal protein S16

Chain SQ:  84% 12%

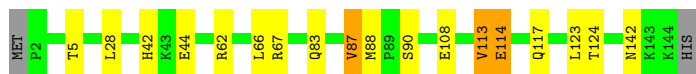
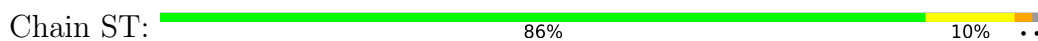


- Molecule 33: 40S ribosomal protein S18

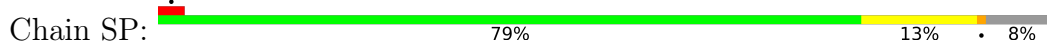
Chain SS:  86% 10% 5%



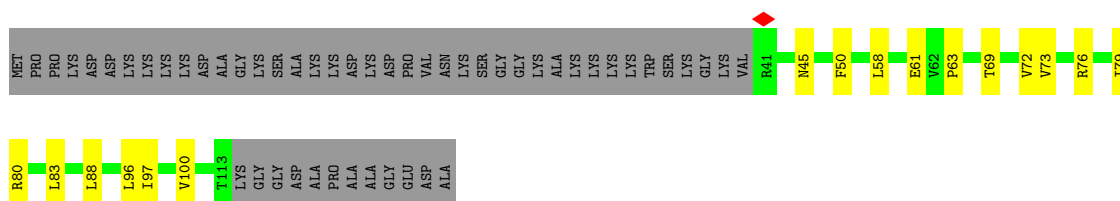
- Molecule 34: Small ribosomal subunit protein eS19



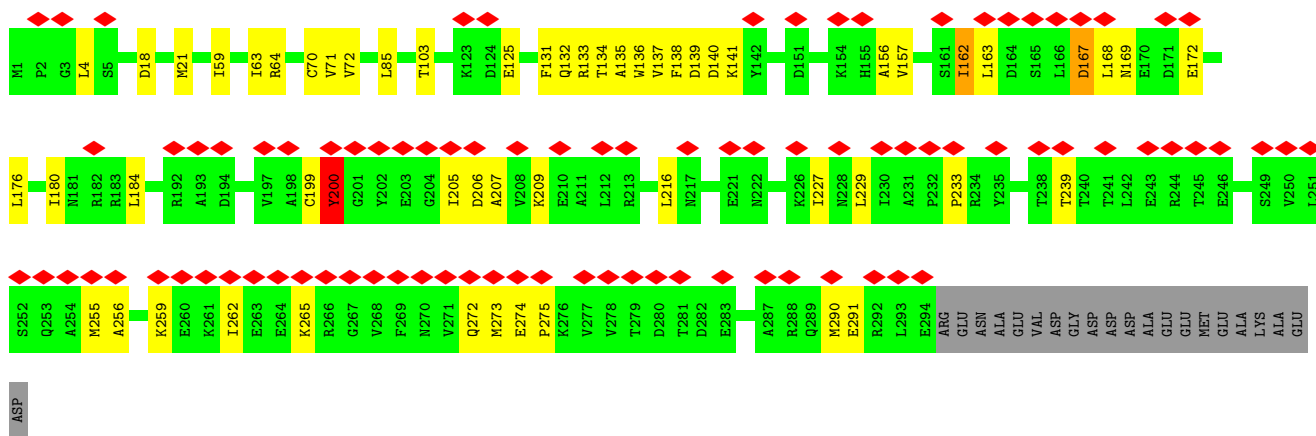
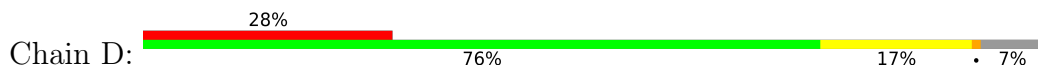
- Molecule 35: 40S ribosomal protein S15



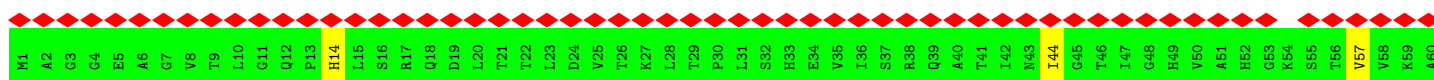
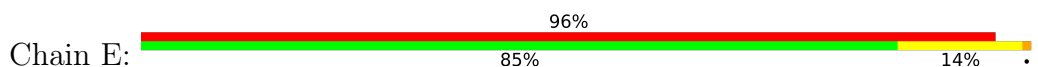
- Molecule 36: Small ribosomal subunit protein eS25



- Molecule 37: Eukaryotic translation initiation factor 2 subunit 1

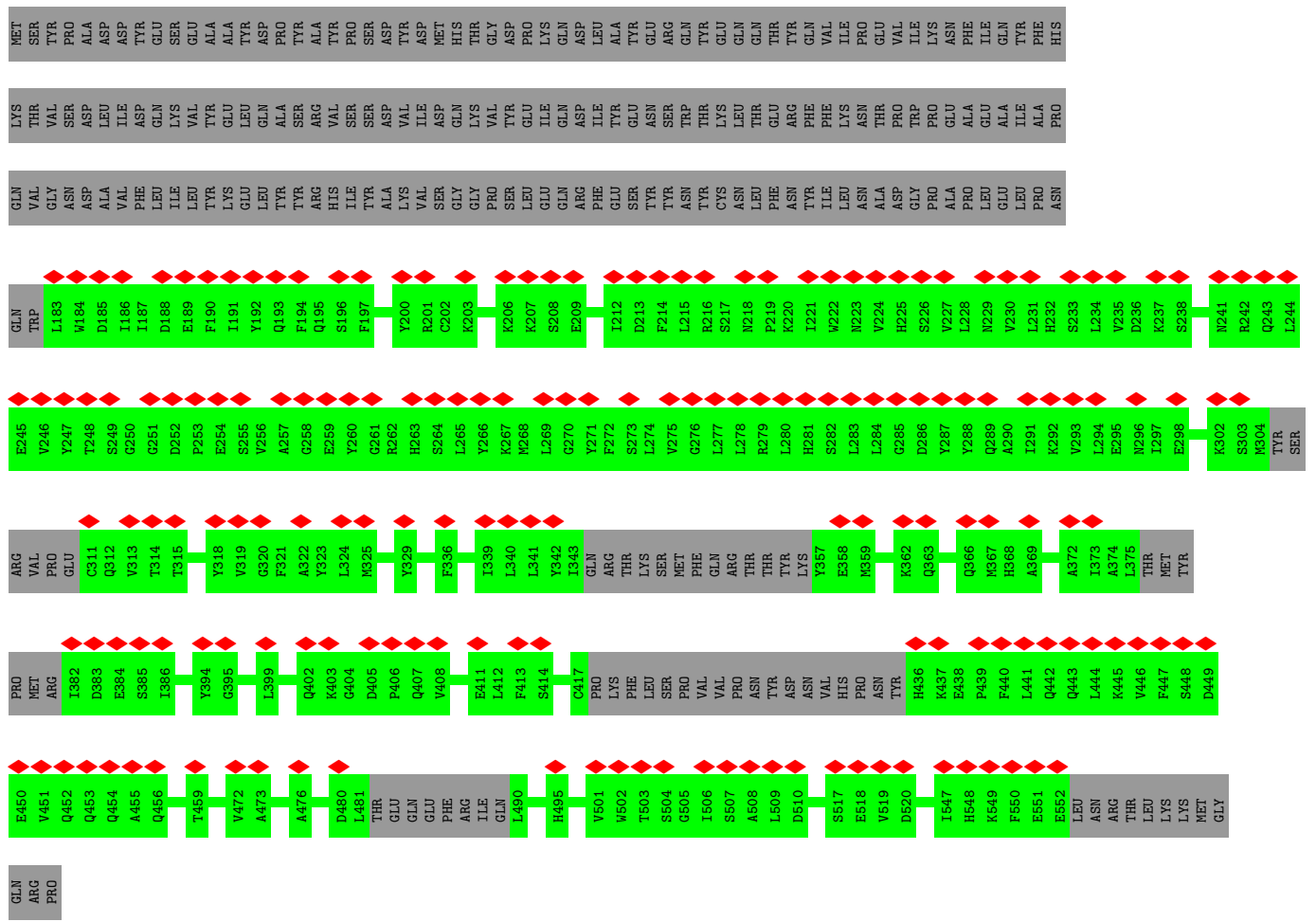


- Molecule 38: Eukaryotic translation initiation factor 2 subunit 3





• Molecule 50: Eukaryotic translation initiation factor 3 subunit L



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39433	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	47.435	Depositor
Minimum map value	-25.167	Depositor
Average map value	0.034	Depositor
Map value standard deviation	1.632	Depositor
Recommended contour level	4.66	Depositor
Map size (\AA)	374.40002, 374.40002, 374.40002	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.72, 0.72, 0.72	Depositor

5 Model quality i

5.1 Standard geometry i

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

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	0.26	0/39125	0.28	0/60957
2	Ln	0.21	0/231	0.32	0/294
3	SE	0.20	0/2118	0.29	0/2849
4	SA	0.22	0/1764	0.33	0/2396
5	SB	0.21	0/1832	0.33	0/2449
6	SH	0.16	0/1546	0.30	0/2071
7	SI	0.19	0/1715	0.34	0/2287
8	SL	0.20	0/1280	0.28	0/1712
9	SV	0.21	0/643	0.27	0/860
10	SX	0.20	0/1116	0.29	0/1490
11	Sa	0.22	0/836	0.28	0/1121
12	SC	0.22	0/1746	0.29	0/2358
13	SG	0.17	0/1926	0.30	0/2563
14	SJ	0.19	0/1537	0.30	0/2052
15	SN	0.19	0/1232	0.28	0/1656
16	SO	0.31	1/1020 (0.1%)	0.37	0/1366
17	SW	0.23	0/1051	0.33	0/1406
18	SY	0.18	0/1031	0.27	0/1370
19	Sb	0.21	0/665	0.30	0/891
20	Se	0.21	0/474	0.29	0/623
21	B	0.17	0/664	0.30	0/1031
22	SD	0.19	0/1793	0.27	0/2414
23	SF	0.21	0/1516	0.31	0/2037
24	Sf	0.14	0/525	0.35	0/695
25	SR	0.19	0/1078	0.31	0/1447
26	Sd	0.22	0/470	0.30	0/623
27	Sg	0.19	0/2497	0.32	0/3399
28	Sc	0.24	0/548	0.43	0/733
29	SK	0.22	0/840	0.40	0/1133
30	SM	0.17	0/916	0.46	1/1233 (0.1%)
31	SU	0.19	0/821	0.32	0/1103

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	SQ	0.22	0/1142	0.36	0/1528
33	SS	0.19	0/1216	0.30	0/1628
34	ST	0.20	0/1119	0.29	0/1498
35	SP	0.20	0/1126	0.35	0/1505
36	SZ	0.18	0/591	0.35	0/794
37	D	0.16	0/2400	0.36	0/3235
38	E	0.12	0/3643	0.29	0/4929
39	F	0.13	0/144	0.32	0/191
40	G	0.21	0/1600	0.25	0/2492
41	H	0.17	0/921	0.37	0/1224
42	e	0.17	0/2672	0.41	0/3647
43	d	0.16	0/2821	0.37	0/3852
44	c	0.24	0/5284	0.40	0/7123
45	a	0.23	0/4891	0.44	0/6615
46	3f	0.14	0/1269	0.32	0/1762
47	m	0.15	0/1926	0.38	0/2669
48	h	0.16	0/1569	0.39	0/2183
49	k	0.09	0/1055	0.24	0/1469
50	l	0.11	0/1575	0.26	0/2187
All	All	0.22	1/111520 (0.0%)	0.32	1/159150 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	SO	136	PRO	C-N	7.09	1.43	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	SM	73	GLN	CA-CB-CG	5.42	124.94	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	S2	36955	0	18670	226	0
2	Ln	230	0	276	3	0
3	SE	2076	0	2177	8	0
4	SA	1727	0	1729	22	0
5	SB	1806	0	1888	18	0
6	SH	1523	0	1622	6	0
7	SI	1686	0	1772	12	0
8	SL	1258	0	1332	10	0
9	SV	636	0	637	6	0
10	SX	1098	0	1167	4	0
11	Sa	821	0	870	3	0
12	SC	1709	0	1797	15	0
13	SG	1903	0	2068	12	0
14	SJ	1512	0	1629	9	0
15	SN	1208	0	1293	2	0
16	SO	1016	0	1038	17	0
17	SW	1034	0	1080	11	0
18	SY	1014	0	1082	3	0
19	Sb	651	0	672	9	0
20	Se	468	0	519	1	0
21	B	594	0	304	5	0
22	SD	1765	0	1865	18	0
23	SF	1495	0	1549	13	0
24	Sf	515	0	523	9	0
25	SR	1064	0	1118	16	0
26	Sd	459	0	448	1	0
27	Sg	2440	0	2396	16	0
28	Sc	546	0	577	11	0
29	SK	816	0	841	14	0
30	SM	906	0	921	22	0
31	SU	811	0	877	4	0
32	SQ	1124	0	1193	10	0
33	SS	1198	0	1261	7	0
34	ST	1113	0	1145	12	0
35	SP	1103	0	1156	14	0
36	SZ	585	0	640	10	0
37	D	2367	0	2411	39	0
38	E	3585	0	3736	40	0
39	F	143	0	144	0	0
40	G	1623	0	828	9	0
41	H	910	0	936	13	0
42	e	2635	0	2207	65	0
43	d	2778	0	2143	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	c	5197	0	5201	158	0
45	a	4799	0	4830	146	0
46	3f	1272	0	564	3	0
47	m	1917	0	1096	27	0
48	h	1571	0	683	7	0
49	k	1057	0	475	1	0
50	l	1581	0	689	0	0
51	S2	17	0	0	0	0
51	SF	1	0	0	0	0
51	Sd	1	0	0	0	0
52	B	3	0	0	0	0
52	H	1	0	0	0	0
52	S2	80	0	0	0	0
52	SN	1	0	0	0	0
52	Sa	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	0	0
56	S2	345	0	0	2	0
56	SB	1	0	0	0	0
56	SE	2	0	0	0	0
56	SL	2	0	0	0	0
56	SN	4	0	0	0	0
56	SO	3	0	0	0	0
56	SS	1	0	0	0	0
56	ST	2	0	0	0	0
56	Sa	3	0	0	0	0
All	All	108811	0	86096	1046	0

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

All (1046) 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)
4:SA:1:MET:HE3	4:SA:60:LEU:HD13	1.46	0.98
1:S2:166:A2M:H5'	1:S2:166:A2M:H8	1.51	0.93
47:m:46:ILE:O	47:m:50:ASP:CB	2.26	0.83
1:S2:165:G:H2'	1:S2:166:A2M:H5''	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:a:157:TYR:O	45:a:161:LEU:HD22	1.83	0.77
1:S2:846:G:C6	3:SE:19:MET:HE3	2.22	0.75
44:c:684:CYS:SG	44:c:765:VAL:HG21	2.28	0.74
44:c:358:VAL:HG13	44:c:371:ILE:HD11	1.68	0.74
1:S2:512:A2M:H4'	1:S2:576:A2M:H2	1.69	0.74
5:SB:142:PHE:HB2	5:SB:208:HIS:CE1	2.24	0.73
45:a:332:THR:O	45:a:332:THR:HG22	1.87	0.73
47:m:320:MET:HA	47:m:320:MET:HE2	1.71	0.72
30:SM:79:VAL:HG11	30:SM:85:LEU:HB2	1.72	0.72
1:S2:165:G:C2'	1:S2:166:A2M:H5''	2.20	0.72
44:c:113:LEU:HD23	44:c:145:ILE:HD11	1.72	0.71
1:S2:1850:MA6:H103	1:S2:1851:MA6:H102	1.71	0.71
5:SB:142:PHE:HB2	5:SB:208:HIS:HE1	1.56	0.71
40:G:10:1MG:H5''	40:G:46:M7G:H81	1.72	0.71
43:d:447:LEU:HD11	43:d:473:PRO:HA	1.73	0.71
1:S2:166:A2M:H8	1:S2:166:A2M:C5'	2.21	0.69
42:e:399:SER:O	42:e:404:VAL:HG22	1.92	0.69
37:D:21:MET:HA	37:D:21:MET:HE2	1.73	0.69
44:c:646:LEU:HD12	44:c:648:GLN:NE2	2.07	0.69
38:E:411:LEU:HD13	38:E:412:SER:N	2.08	0.69
45:a:191:LYS:HG2	45:a:245:LEU:HD11	1.73	0.69
44:c:448:VAL:HG21	44:c:486:VAL:HG21	1.74	0.68
44:c:718:LEU:HD11	45:a:344:MET:SD	2.33	0.68
34:ST:114:GLU:HG2	34:ST:124:THR:HG23	1.75	0.67
43:d:319:ILE:HG22	43:d:395:THR:HG21	1.75	0.67
37:D:63:ILE:HD12	37:D:64:ARG:N	2.10	0.67
4:SA:1:MET:CE	4:SA:60:LEU:HD13	2.21	0.67
32:SQ:116:ASP:OD1	32:SQ:118:THR:HG22	1.94	0.67
38:E:411:LEU:HD13	38:E:412:SER:H	1.60	0.67
22:SD:93:THR:HG23	22:SD:93:THR:O	1.95	0.66
1:S2:1315:U:H4'	29:SK:2:LEU:HD22	1.76	0.66
44:c:106:TYR:HA	44:c:109:ILE:HD12	1.79	0.65
1:S2:99:A2M:O5'	1:S2:99:A2M:H8	1.97	0.65
31:SU:56:MET:HE1	31:SU:88:LEU:HD22	1.79	0.65
15:SN:33:VAL:HG21	15:SN:66:VAL:HG11	1.79	0.64
42:e:208:LEU:HD11	42:e:246:ILE:CG2	2.27	0.64
43:d:28:MET:CE	44:c:591:MET:HE1	2.28	0.64
45:a:243:MET:HB3	45:a:245:LEU:HD12	1.78	0.64
5:SB:125:VAL:HG22	5:SB:172:MET:HE3	1.80	0.64
44:c:455:PHE:CD2	44:c:479:VAL:HG21	2.32	0.64
45:a:437:LEU:HD12	45:a:437:LEU:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:E:155:ALA:HB2	38:E:182:LEU:HD13	1.81	0.63
45:a:446:ILE:HG23	45:a:447:TYR:HD1	1.63	0.63
1:S2:1229:G:H21	34:ST:87:VAL:CG2	2.12	0.63
37:D:63:ILE:HD12	37:D:64:ARG:H	1.61	0.62
44:c:646:LEU:HD13	44:c:646:LEU:O	1.99	0.62
45:a:331:ILE:C	45:a:333:PRO:HD3	2.23	0.62
43:d:364:LYS:N	43:d:364:LYS:HE2	2.13	0.62
44:c:424:ILE:C	44:c:425:LEU:HD12	2.24	0.62
4:SA:18:PHE:CD1	4:SA:23:THR:HG21	2.34	0.62
45:a:401:LEU:H	45:a:401:LEU:HD23	1.63	0.62
1:S2:1841:C:H2'	1:S2:1842:4AC:H6	1.82	0.62
44:c:832:MET:HE3	44:c:843:VAL:HG22	1.80	0.62
42:e:208:LEU:HD11	42:e:246:ILE:HG21	1.82	0.62
44:c:679:LEU:HD13	44:c:679:LEU:O	1.98	0.61
28:Sc:18:LEU:HD11	28:Sc:43:ILE:HD12	1.81	0.61
45:a:390:LEU:HD12	45:a:410:VAL:HG21	1.81	0.61
45:a:52:LEU:HD23	45:a:52:LEU:C	2.26	0.61
47:m:127:LEU:O	47:m:131:ALA:HB3	2.00	0.61
1:S2:1404:U:C5	31:SU:88:LEU:HD21	2.36	0.61
38:E:454:ILE:C	38:E:454:ILE:HD12	2.25	0.61
37:D:136:TRP:HA	37:D:139:ASP:HB2	1.82	0.61
40:G:46:M7G:H4'	40:G:47:H2U:OP1	2.01	0.60
44:c:548:MET:HE1	44:c:572:HIS:HA	1.82	0.60
37:D:59:ILE:HD12	37:D:59:ILE:H	1.66	0.60
45:a:229:HIS:HB3	45:a:259:LEU:HD11	1.83	0.60
1:S2:483:C:O2'	1:S2:484:A2M:H5'	2.01	0.60
45:a:283:PHE:CE2	45:a:355:LEU:HD21	2.36	0.60
45:a:92:ALA:O	45:a:96:MET:HE3	2.01	0.60
1:S2:575:A:H3'	1:S2:576:A2M:H5''	1.84	0.59
1:S2:168:C:O2	13:SG:133:LEU:HD12	2.02	0.59
23:SF:41:VAL:HG23	23:SF:42:LYS:HG3	1.85	0.59
1:S2:529:A:H61	1:S2:555:A:H61	1.51	0.59
1:S2:1750:C:H2'	1:S2:1751:C:C1'	2.33	0.59
44:c:64:ILE:HG13	44:c:109:ILE:HD11	1.85	0.58
42:e:273:VAL:HG23	42:e:274:LEU:N	2.18	0.58
16:SO:65:ASP:O	16:SO:65:ASP:OD1	2.20	0.58
30:SM:25:ALA:HB3	30:SM:31:LEU:HD21	1.86	0.58
43:d:458:LYS:HD2	43:d:458:LYS:O	2.04	0.58
45:a:279:VAL:HG12	45:a:295:THR:HG21	1.85	0.58
45:a:283:PHE:CZ	45:a:355:LEU:HD21	2.38	0.58
1:S2:1698:C:O2	21:B:8:A:N6	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:m:324:LYS:C	47:m:325:ILE:HD12	2.29	0.57
44:c:510:THR:O	44:c:510:THR:HG22	2.05	0.57
37:D:59:ILE:O	37:D:63:ILE:HG13	2.03	0.57
45:a:411:LEU:HD12	45:a:428:VAL:HG23	1.87	0.57
45:a:101:THR:HG21	45:a:153:LEU:HD13	1.85	0.57
1:S2:1442:OMU:O5'	1:S2:1442:OMU:H6	2.04	0.57
45:a:290:LEU:HA	45:a:329:ILE:HD12	1.86	0.57
45:a:230:LEU:HD13	45:a:230:LEU:O	2.04	0.57
44:c:756:ILE:HG22	44:c:756:ILE:O	2.05	0.57
1:S2:1091:C:HO2'	17:SW:2:VAL:N	2.02	0.56
42:e:261:VAL:HG11	42:e:274:LEU:HG	1.86	0.56
43:d:411:GLN:OE1	43:d:411:GLN:C	2.49	0.56
45:a:549:GLN:O	45:a:553:ALA:HB3	2.04	0.56
16:SO:56:VAL:HG22	16:SO:81:VAL:HG13	1.86	0.56
24:Sf:106:TYR:HB2	30:SM:64:LEU:HD21	1.87	0.56
45:a:167:ASN:OD1	45:a:170:VAL:HG22	2.06	0.56
37:D:233:PRO:HB3	38:E:346:THR:HG23	1.87	0.56
44:c:86:LEU:HD11	44:c:106:TYR:CE1	2.39	0.56
44:c:822:ILE:O	44:c:826:ILE:HG12	2.05	0.56
45:a:55:LEU:HD13	45:a:93:TYR:HB2	1.88	0.56
32:SQ:100:VAL:HG23	32:SQ:101:ASP:N	2.20	0.56
1:S2:159:A2M:H2	1:S2:468:A2M:O4'	2.05	0.56
45:a:450:ILE:HD13	45:a:455:LEU:HD13	1.87	0.56
30:SM:73:GLN:O	30:SM:73:GLN:OE1	2.24	0.56
44:c:555:ILE:HG21	44:c:568:ALA:HB3	1.86	0.56
44:c:718:LEU:HB2	44:c:738:VAL:HG23	1.88	0.56
44:c:788:LEU:HD23	44:c:792:LEU:HD23	1.88	0.55
44:c:625:LEU:H	44:c:625:LEU:HD12	1.71	0.55
47:m:324:LYS:O	47:m:325:ILE:HD12	2.05	0.55
11:Sa:44:ILE:HG23	11:Sa:45:VAL:HG13	1.88	0.55
44:c:684:CYS:HA	44:c:733:MET:CE	2.37	0.55
45:a:371:ILE:C	45:a:371:ILE:HD12	2.31	0.55
44:c:700:ALA:HB2	44:c:793:PHE:CG	2.41	0.55
45:a:338:ILE:O	45:a:342:LEU:HD22	2.07	0.55
1:S2:1235:G:H21	35:SP:135:ALA:HA	1.71	0.55
35:SP:110:GLU:N	35:SP:110:GLU:OE2	2.40	0.55
47:m:333:VAL:HG13	47:m:334:VAL:H	1.72	0.55
28:Sc:35:MET:HE3	28:Sc:35:MET:HA	1.88	0.55
30:SM:64:LEU:HD13	30:SM:68:LEU:HD23	1.88	0.55
45:a:374:MET:HA	45:a:374:MET:HE3	1.88	0.55
23:SF:25:THR:HG22	23:SF:109:LEU:HD13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:SM:73:GLN:O	30:SM:73:GLN:CD	2.49	0.55
16:SO:21:VAL:HG23	16:SO:22:ALA:N	2.22	0.55
42:e:233:ILE:HG23	42:e:234:ASP:N	2.22	0.55
43:d:42:VAL:HG23	44:c:610:ASN:OD1	2.07	0.55
43:d:369:ILE:O	43:d:369:ILE:HG13	2.06	0.55
45:a:55:LEU:HD11	45:a:71:LEU:HD21	1.89	0.55
1:S2:1425:G:H21	34:ST:5:THR:CG2	2.20	0.54
38:E:69:PHE:O	38:E:73:LEU:HD22	2.07	0.54
42:e:399:SER:HB3	42:e:404:VAL:HG13	1.88	0.54
43:d:33:PHE:HB3	44:c:591:MET:HA	1.89	0.54
1:S2:71:G:H22	13:SG:170:ARG:HH12	1.54	0.54
42:e:362:MET:HE1	42:e:367:ALA:N	2.22	0.54
1:S2:121:OMU:HM22	1:S2:122:G:O4'	2.08	0.54
1:S2:1388:A:H61	22:SD:161:GLY:HA3	1.71	0.54
16:SO:56:VAL:HG23	16:SO:77:ALA:HB1	1.89	0.54
28:Sc:37:ASP:O	28:Sc:38:THR:HG22	2.06	0.54
45:a:203:MET:HA	45:a:203:MET:HE2	1.90	0.54
45:a:570:ALA:HB3	45:a:573:GLN:HA	1.90	0.54
1:S2:952:G:H21	16:SO:52:THR:HG21	1.72	0.54
16:SO:21:VAL:HG23	16:SO:22:ALA:H	1.73	0.54
16:SO:85:CYS:HB2	16:SO:124:MET:HE1	1.88	0.54
47:m:197:ALA:HB1	47:m:200:ALA:HB3	1.90	0.54
47:m:333:VAL:HG13	47:m:334:VAL:N	2.23	0.54
36:SZ:72:VAL:O	36:SZ:76:ARG:HG2	2.08	0.54
45:a:109:GLN:HA	45:a:112:VAL:HG22	1.89	0.54
38:E:264:VAL:HG12	38:E:264:VAL:O	2.08	0.54
42:e:229:ARG:O	42:e:232:ILE:HG22	2.08	0.54
44:c:105:PHE:O	44:c:109:ILE:HD12	2.07	0.54
45:a:378:ASN:ND2	45:a:381:GLN:HG2	2.23	0.54
44:c:424:ILE:HD11	44:c:437:PRO:HB2	1.90	0.54
17:SW:37:PHE:O	17:SW:40:VAL:HG12	2.08	0.54
43:d:40:GLY:O	43:d:41:LYS:HD2	2.07	0.54
45:a:105:LYS:HG3	45:a:149:TRP:CD1	2.43	0.53
1:S2:121:OMU:H6	1:S2:121:OMU:O5'	2.09	0.53
16:SO:85:CYS:CB	16:SO:124:MET:HE1	2.38	0.53
35:SP:137:HIS:O	35:SP:138:SER:CB	2.55	0.53
45:a:432:GLN:HA	45:a:435:THR:HG22	1.90	0.53
45:a:446:ILE:HG23	45:a:447:TYR:CD1	2.42	0.53
4:SA:1:MET:HE1	9:SV:79:VAL:HG23	1.91	0.53
45:a:318:MET:SD	45:a:318:MET:C	2.91	0.53
44:c:555:ILE:HG21	44:c:568:ALA:CB	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:a:519:ILE:HD12	45:a:519:ILE:N	2.24	0.53
44:c:733:MET:SD	44:c:733:MET:C	2.92	0.53
44:c:826:ILE:HD12	44:c:832:MET:HB2	1.91	0.53
23:SF:126:THR:HG21	28:Sc:27:CYS:SG	2.48	0.53
42:e:249:MET:HE2	42:e:281:ILE:HG23	1.90	0.53
44:c:735:GLU:HA	44:c:738:VAL:HG12	1.90	0.53
1:S2:1227:G:C2	1:S2:1228:A:C8	2.97	0.53
1:S2:1442:OMU:HM22	1:S2:1443:C:O4'	2.09	0.53
34:ST:108:GLU:HG3	34:ST:113:VAL:HG23	1.90	0.53
43:d:39:LEU:O	44:c:613:MET:HE1	2.09	0.53
1:S2:116:OMU:H6	1:S2:116:OMU:O5'	2.09	0.53
42:e:345:CYS:SG	42:e:393:MET:HE2	2.49	0.52
44:c:512:TYR:CD2	44:c:675:LEU:HD11	2.43	0.52
41:H:30:GLU:H	41:H:33:GLN:HB2	1.75	0.52
45:a:237:LEU:HD11	45:a:253:VAL:HG23	1.92	0.52
1:S2:1665:G:C8	34:ST:88:MET:HE3	2.45	0.52
5:SB:136:ARG:HB2	5:SB:218:LEU:HD21	1.91	0.52
45:a:571:ARG:N	46:3f:107:GLU:O	2.41	0.52
47:m:331:LYS:O	47:m:331:LYS:HD3	2.08	0.52
47:m:322:TYR:HB3	47:m:332:VAL:HA	1.91	0.52
13:SG:7:PHE:CD2	13:SG:10:THR:HG22	2.45	0.52
19:Sb:53:VAL:HG13	19:Sb:53:VAL:O	2.09	0.52
36:SZ:96:LEU:HD23	36:SZ:96:LEU:H	1.75	0.52
12:SC:211:LYS:O	12:SC:215:MET:HG3	2.10	0.52
38:E:185:ILE:HD12	38:E:185:ILE:O	2.10	0.52
44:c:64:ILE:HG23	44:c:109:ILE:HG12	1.90	0.52
1:S2:860:G:N2	17:SW:107:SER:HG	2.07	0.52
8:SL:66:VAL:HG11	8:SL:141:ASN:HD22	1.74	0.52
37:D:216:LEU:HB2	37:D:227:ILE:HD13	1.91	0.52
36:SZ:73:VAL:HG21	36:SZ:88:LEU:HD11	1.92	0.51
37:D:21:MET:HE2	37:D:21:MET:CA	2.38	0.51
38:E:182:LEU:HD22	38:E:185:ILE:HG23	1.91	0.51
34:ST:142:ASN:C	34:ST:142:ASN:OD1	2.53	0.51
37:D:167:ASP:O	37:D:167:ASP:OD1	2.29	0.51
43:d:400:ASP:HB2	43:d:457:VAL:HG13	1.91	0.51
1:S2:903:A:C6	1:S2:904:A:N6	2.78	0.51
1:S2:1395:C:O2'	1:S2:1396:A:H5'	2.11	0.51
37:D:229:LEU:N	37:D:229:LEU:HD23	2.25	0.51
44:c:445:LEU:HD12	44:c:498:GLU:HB2	1.91	0.51
45:a:467:LEU:O	45:a:471:ILE:HG12	2.10	0.51
1:S2:1383:A2M:H4'	22:SD:156:LEU:CD2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:G:10:1MG:H5''	40:G:46:M7G:C8	2.39	0.51
1:S2:2:A:O4'	1:S2:418:A:C8	2.64	0.51
42:e:392:VAL:HG13	42:e:392:VAL:O	2.10	0.51
43:d:21:VAL:N	43:d:22:PRO:CD	2.73	0.51
45:a:322:VAL:O	45:a:326:THR:HG22	2.11	0.51
1:S2:468:A2M:HM'2	1:S2:469:A:O4'	2.11	0.51
11:Sa:45:VAL:HG12	16:SO:116:LEU:HD23	1.93	0.51
41:H:99:GLU:OE2	41:H:99:GLU:HA	2.11	0.51
1:S2:928:G:H2'	1:S2:929:G:C8	2.46	0.51
13:SG:103:ASP:OD1	13:SG:103:ASP:C	2.53	0.51
44:c:358:VAL:HG13	44:c:371:ILE:CD1	2.39	0.51
44:c:500:CYS:SG	44:c:564:ILE:HG21	2.50	0.51
45:a:563:LYS:HD3	45:a:568:ILE:HG12	1.93	0.51
43:d:378:ASP:HB2	43:d:393:ILE:HG22	1.92	0.51
45:a:128:LEU:HD12	45:a:128:LEU:H	1.76	0.51
1:S2:575:A:C3'	1:S2:576:A2M:H5''	2.41	0.51
8:SL:27:GLU:HA	8:SL:27:GLU:OE1	2.10	0.50
21:B:12:G:H21	21:B:13:A:N6	2.09	0.50
27:Sg:199:THR:HG21	27:Sg:239:LEU:O	2.12	0.50
38:E:270:GLU:HA	38:E:270:GLU:OE2	2.11	0.50
42:e:288:TYR:C	42:e:290:ASP:H	2.20	0.50
44:c:499:VAL:HA	44:c:502:ILE:HG22	1.94	0.50
44:c:821:ILE:O	44:c:825:MET:HG3	2.12	0.50
1:S2:884:C:C2	1:S2:885:U:O4	2.65	0.50
14:SJ:120:ALA:HB2	14:SJ:129:LEU:HD12	1.93	0.50
44:c:668:ARG:CZ	44:c:668:ARG:O	2.59	0.50
1:S2:1082:A:P	56:S2:2008:HOH:O	2.68	0.50
44:c:102:VAL:HG11	44:c:152:PHE:HD2	1.75	0.50
1:S2:501:C:H2'	1:S2:501:C:O2	2.12	0.50
44:c:778:MET:SD	44:c:778:MET:C	2.94	0.50
47:m:331:LYS:HD3	47:m:331:LYS:C	2.36	0.50
1:S2:29:G:H2'	1:S2:30:C:C6	2.47	0.50
4:SA:206:ASP:OD1	4:SA:207:PRO:HD2	2.12	0.50
30:SM:19:GLN:C	30:SM:19:GLN:OE1	2.54	0.50
42:e:377:ASN:OD1	42:e:377:ASN:C	2.55	0.50
45:a:378:ASN:ND2	45:a:378:ASN:O	2.40	0.50
45:a:447:TYR:CD2	45:a:450:ILE:HD12	2.47	0.50
45:a:519:ILE:HD12	45:a:519:ILE:H	1.75	0.50
45:a:521:ASN:HA	45:a:524:THR:HG23	1.94	0.50
29:SK:9:ILE:HD12	29:SK:10:ALA:N	2.26	0.49
42:e:205:LEU:HD21	43:d:26:ARG:HG3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:d:311:ASN:HA	43:d:314:MET:HG3	1.94	0.49
44:c:651:LEU:HD11	44:c:667:ARG:HD2	1.94	0.49
36:SZ:63:PRO:HA	36:SZ:97:ILE:HD11	1.93	0.49
37:D:134:THR:O	37:D:137:VAL:HG12	2.12	0.49
38:E:373:ILE:HG23	38:E:458:GLN:O	2.12	0.49
45:a:548:GLU:O	45:a:549:GLN:C	2.54	0.49
42:e:290:ASP:HB3	42:e:293:THR:CG2	2.42	0.49
42:e:413:PHE:O	42:e:417:MET:HG2	2.12	0.49
43:d:28:MET:SD	44:c:591:MET:HE1	2.52	0.49
1:S2:1223:A:O2'	1:S2:1651:A:H4'	2.11	0.49
40:G:11[1]:2MG:HN2	40:G:45:G:H21	1.59	0.49
45:a:519:ILE:O	45:a:522:GLN:HG3	2.12	0.49
8:SL:14:PRO:C	8:SL:15:THR:HG23	2.36	0.49
19:Sb:46:VAL:HG12	19:Sb:54:VAL:HG11	1.94	0.49
25:SR:14:ARG:O	25:SR:18:GLU:HG3	2.11	0.49
42:e:399:SER:HA	42:e:403:GLN:H	1.76	0.49
44:c:412:LEU:HD21	44:c:489:TYR:CE1	2.48	0.49
44:c:709:MET:HE3	44:c:712:LYS:HA	1.93	0.49
45:a:26:PRO:O	45:a:30:VAL:HG13	2.12	0.49
14:SJ:88:ASP:OD1	14:SJ:89:GLU:N	2.46	0.49
42:e:233:ILE:HG23	42:e:234:ASP:H	1.78	0.49
1:S2:1164:G:O2'	1:S2:1165:G:H5'	2.12	0.49
9:SV:79:VAL:HG12	9:SV:80:SER:O	2.13	0.49
38:E:294:ILE:N	38:E:294:ILE:HD12	2.28	0.49
42:e:404:VAL:HG23	42:e:405:ILE:N	2.27	0.49
45:a:195:ARG:O	45:a:199:ASP:OD1	2.31	0.49
47:m:312:VAL:HA	47:m:322:TYR:OH	2.13	0.49
1:S2:1374:C:H2'	1:S2:1375:G:O4'	2.13	0.49
44:c:451:MET:CE	44:c:479:VAL:HG13	2.43	0.49
9:SV:16:LYS:H	12:SC:259:THR:HG21	1.76	0.49
35:SP:13:ARG:HB3	35:SP:13:ARG:CZ	2.43	0.49
37:D:199:CYS:O	37:D:200:TYR:C	2.55	0.49
41:H:85:GLN:C	41:H:85:GLN:OE1	2.55	0.49
42:e:208:LEU:CD1	42:e:246:ILE:HG21	2.42	0.49
38:E:57:VAL:HG13	38:E:226:ALA:HB2	1.95	0.49
44:c:627:LYS:HA	44:c:693:LEU:HD11	1.95	0.49
45:a:380:LEU:O	45:a:383:VAL:HG22	2.12	0.49
45:a:384:VAL:HG13	45:a:385:PRO:HD2	1.94	0.49
1:S2:865:A:C2'	1:S2:866:PSU:H5''	2.43	0.48
13:SG:29:GLU:O	13:SG:29:GLU:HG3	2.13	0.48
25:SR:99:ASP:OD1	25:SR:100:PRO:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:a:30:VAL:O	45:a:33:ASP:OD1	2.31	0.48
1:S2:918:PSU:O2'	1:S2:919:A:C8	2.63	0.48
7:SI:64:ASN:OD1	7:SI:73:THR:HG22	2.12	0.48
7:SI:107:THR:O	7:SI:111:GLN:HG2	2.13	0.48
27:Sg:197:THR:HG23	27:Sg:239:LEU:HD22	1.95	0.48
44:c:719:ARG:HA	45:a:344:MET:HE1	1.94	0.48
44:c:789:ARG:O	44:c:793:PHE:CD2	2.66	0.48
47:m:322:TYR:HA	47:m:333:VAL:HG12	1.95	0.48
1:S2:659:G:H21	10:SX:17:ARG:NH2	2.11	0.48
25:SR:100:PRO:O	25:SR:104:GLU:HG2	2.13	0.48
29:SK:11:ILE:HG22	29:SK:35:LEU:HD13	1.95	0.48
38:E:404:LEU:HD22	38:E:445:ARG:HG2	1.94	0.48
42:e:374:LEU:O	42:e:374:LEU:HD23	2.12	0.48
44:c:762:ASN:O	44:c:767:ASP:HB2	2.13	0.48
1:S2:1556:A:H2'	1:S2:1556:A:N3	2.28	0.48
5:SB:110:MET:HE2	5:SB:213:ARG:HD2	1.96	0.48
30:SM:66:GLU:HA	30:SM:69:CYS:SG	2.53	0.48
42:e:295:PHE:CG	42:e:311:LYS:HG2	2.48	0.48
47:m:345:GLN:CD	47:m:345:GLN:C	2.81	0.48
1:S2:796:G:H2'	1:S2:797:C:C5'	2.43	0.48
4:SA:23:THR:HG22	4:SA:23:THR:O	2.13	0.48
43:d:314:MET:SD	43:d:314:MET:C	2.96	0.48
1:S2:562:U:H2'	1:S2:563:G:C8	2.49	0.48
43:d:39:LEU:HD12	44:c:595:GLN:OE1	2.14	0.48
1:S2:1588:A:H2'	1:S2:1589:A:C8	2.48	0.48
32:SQ:100:VAL:CG2	32:SQ:101:ASP:N	2.77	0.48
45:a:43:TRP:CD1	45:a:46:ILE:HG22	2.48	0.48
45:a:98:GLU:OE1	45:a:157:TYR:OH	2.31	0.48
37:D:21:MET:HE1	37:D:70:CYS:SG	2.52	0.48
44:c:455:PHE:CZ	44:c:459:MET:HE3	2.49	0.48
44:c:682:LEU:HD23	44:c:682:LEU:O	2.14	0.48
45:a:278:LYS:HA	45:a:281:THR:HG22	1.96	0.48
1:S2:4:C:H4'	12:SC:207:ALA:HB2	1.95	0.48
1:S2:563:G:HO2'	1:S2:564:A:P	2.36	0.48
1:S2:969:U:C5	5:SB:9:LEU:HD21	2.48	0.48
1:S2:1383:A2M:H4'	22:SD:156:LEU:HD22	1.94	0.48
33:SS:51:ASP:OD1	33:SS:51:ASP:O	2.31	0.48
44:c:86:LEU:C	44:c:86:LEU:HD13	2.38	0.48
44:c:548:MET:HE1	44:c:571:CYS:C	2.38	0.48
45:a:113:LEU:HD21	45:a:138:GLN:HA	1.96	0.48
45:a:291:PHE:O	45:a:295:THR:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1238:PSU:O4	1:S2:1242:U:H5	1.97	0.48
1:S2:1578:U:H2'	1:S2:1578:U:O2	2.13	0.48
1:S2:1698:C:C2	21:B:8:A:N6	2.81	0.48
30:SM:53:ALA:HA	30:SM:79:VAL:HG12	1.94	0.48
33:SS:112:GLU:OE2	33:SS:112:GLU:HA	2.13	0.48
42:e:361:ASN:O	42:e:362:MET:HB3	2.14	0.48
45:a:372:ASN:HA	45:a:375:VAL:HG12	1.95	0.48
45:a:411:LEU:HD21	45:a:431:LEU:HD23	1.95	0.48
47:m:327:GLN:O	47:m:327:GLN:HG2	2.14	0.48
1:S2:15:U:H2'	1:S2:16:G:O4'	2.14	0.47
1:S2:121:OMU:HM23	3:SE:144:ALA:HB3	1.96	0.47
1:S2:354:OMU:H1'	1:S2:354:OMU:HM23	1.60	0.47
1:S2:1220:A:H2'	1:S2:1221:G:O4'	2.14	0.47
3:SE:139:LEU:HD12	3:SE:139:LEU:C	2.39	0.47
37:D:167:ASP:OD1	37:D:167:ASP:C	2.57	0.47
1:S2:118:C:H1'	1:S2:445:A:C5	2.49	0.47
1:S2:1639:M7G:H2'	1:S2:1640:A:C8	2.49	0.47
24:Sf:108:VAL:HG12	24:Sf:114:ILE:HG22	1.95	0.47
42:e:235:LEU:HD23	42:e:239:GLN:HG3	1.95	0.47
42:e:251:PRO:O	42:e:255:ARG:HG3	2.14	0.47
44:c:589:MET:HA	44:c:589:MET:HE2	1.96	0.47
5:SB:72:ALA:HB3	16:SO:128:ARG:HH21	1.78	0.47
6:SH:29:GLU:O	6:SH:33:ASN:OD1	2.32	0.47
22:SD:162:ASP:N	22:SD:163:PRO:CD	2.77	0.47
36:SZ:61:GLU:N	36:SZ:61:GLU:OE2	2.47	0.47
47:m:60:VAL:O	47:m:61:GLU:C	2.57	0.47
1:S2:749:U:H3	1:S2:750:C:H41	1.61	0.47
34:ST:87:VAL:O	34:ST:87:VAL:HG13	2.15	0.47
47:m:320:MET:HE1	47:m:335:SER:O	2.15	0.47
1:S2:860:G:H21	17:SW:107:SER:HG	1.60	0.47
25:SR:20:TYR:CD2	25:SR:38:ILE:HD13	2.50	0.47
45:a:15:ALA:CB	45:a:31:LEU:HD21	2.44	0.47
45:a:15:ALA:HB2	45:a:31:LEU:HD21	1.95	0.47
1:S2:1037:G:H4'	1:S2:1845:A:H4'	1.97	0.47
5:SB:225:LEU:O	5:SB:229:MET:HG2	2.15	0.47
21:B:-4:A:H2	23:SF:133:THR:HG1	1.59	0.47
23:SF:62:ARG:HG3	23:SF:62:ARG:HH11	1.79	0.47
44:c:465:HIS:HB2	45:a:143:ARG:HD2	1.97	0.47
44:c:626:THR:CB	44:c:693:LEU:HD21	2.44	0.47
45:a:307:ARG:HG3	45:a:309:ASN:H	1.79	0.47
45:a:416:GLU:O	45:a:417:GLN:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:a:568:ILE:HG13	45:a:568:ILE:O	2.15	0.47
1:S2:1217:A:H2'	1:S2:1218:C:C6	2.50	0.47
8:SL:65:ASN:CG	8:SL:65:ASN:O	2.58	0.47
37:D:184:LEU:O	37:D:184:LEU:HG	2.15	0.47
43:d:364:LYS:HE2	43:d:364:LYS:H	1.80	0.47
1:S2:1661:A:C8	26:Sd:14:PHE:CD1	3.03	0.47
1:S2:1798:C:H2'	1:S2:1799:G:O4'	2.15	0.47
12:SC:59:GLU:OE2	12:SC:59:GLU:HA	2.15	0.47
28:Sc:62:GLU:OE2	28:Sc:62:GLU:O	2.33	0.47
32:SQ:110:ASP:OD1	32:SQ:111:ILE:N	2.48	0.47
37:D:157:VAL:HG12	37:D:180:ILE:HG22	1.95	0.47
38:E:61:ILE:HG12	38:E:232:ILE:HG23	1.96	0.47
42:e:304:ASP:N	42:e:304:ASP:OD1	2.48	0.47
42:e:362:MET:HE1	42:e:366:GLU:C	2.40	0.47
42:e:364:PRO:HA	42:e:367:ALA:HB3	1.96	0.47
43:d:80:PHE:O	43:d:81:GLN:HG3	2.15	0.47
45:a:468:GLU:O	45:a:472:VAL:HG22	2.15	0.47
47:m:327:GLN:O	47:m:328:THR:C	2.58	0.47
1:S2:813:A:C5	1:S2:814:PSU:C6	3.03	0.47
1:S2:846:G:C5	3:SE:19:MET:HE3	2.50	0.47
1:S2:953:C:H2'	1:S2:954:U:O4'	2.15	0.47
8:SL:22:ARG:HA	8:SL:22:ARG:NE	2.30	0.47
22:SD:109:LEU:HD12	22:SD:184:ILE:HD11	1.97	0.47
34:ST:113:VAL:HG12	34:ST:123:LEU:HD12	1.97	0.47
42:e:249:MET:O	42:e:250:CYS:C	2.58	0.47
43:d:314:MET:SD	43:d:315:GLU:N	2.88	0.47
43:d:380:VAL:HG22	43:d:381:MET:H	1.80	0.47
45:a:320:THR:HG21	45:a:384:VAL:HG23	1.97	0.47
1:S2:1666:C:H2'	1:S2:1667:U:O4'	2.13	0.46
37:D:209:LYS:HE3	38:E:274:LEU:HB2	1.97	0.46
1:S2:455:A:H2'	1:S2:456:C:H6	1.80	0.46
1:S2:1531:A:H2'	1:S2:1532:C:C6	2.50	0.46
24:Sf:103:LEU:HD11	30:SM:36:ARG:HD3	1.98	0.46
32:SQ:31:LEU:HB3	32:SQ:67:ASP:OD1	2.14	0.46
37:D:205:ILE:HG23	37:D:206:ASP:N	2.30	0.46
41:H:33:GLN:HB3	41:H:78:LEU:HD11	1.97	0.46
43:d:69:TYR:N	43:d:69:TYR:CD1	2.81	0.46
1:S2:461:U:O2'	1:S2:462:OMC:P	2.73	0.46
1:S2:1705:C:H2'	1:S2:1706:G:C8	2.50	0.46
1:S2:1728:U:H2'	1:S2:1729:U:O4'	2.15	0.46
13:SG:10:THR:HG23	13:SG:12:CYS:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:a:549:GLN:NE2	45:a:550:HIS:H	2.12	0.46
1:S2:533:A:H61	1:S2:550:C:H42	1.62	0.46
1:S2:1303:C:O2	1:S2:1303:C:O4'	2.32	0.46
29:SK:6:LYS:O	29:SK:9:ILE:HD12	2.15	0.46
31:SU:61:LEU:HD12	31:SU:61:LEU:N	2.31	0.46
34:ST:62:ARG:NH2	34:ST:66:LEU:HD11	2.31	0.46
36:SZ:45:ASN:C	36:SZ:45:ASN:OD1	2.59	0.46
42:e:208:LEU:C	42:e:208:LEU:HD13	2.40	0.46
43:d:69:TYR:OH	44:c:591:MET:HE3	2.15	0.46
1:S2:793:G:N2	1:S2:795:A:H61	2.13	0.46
4:SA:18:PHE:O	4:SA:22:GLY:O	2.33	0.46
38:E:295:GLU:HB2	38:E:361:VAL:HG22	1.97	0.46
44:c:412:LEU:HD21	44:c:489:TYR:CD1	2.51	0.46
44:c:626:THR:OG1	44:c:693:LEU:HD21	2.16	0.46
17:SW:28:ARG:HB3	17:SW:29:PRO:HD3	1.98	0.46
40:G:10:1MG:C5'	40:G:46:M7G:H81	2.43	0.46
4:SA:1:MET:HE2	4:SA:60:LEU:HD22	1.98	0.46
17:SW:37:PHE:O	17:SW:41:MET:HG3	2.16	0.46
35:SP:62:LYS:O	35:SP:66:GLU:HG2	2.16	0.46
44:c:113:LEU:HD23	44:c:145:ILE:CD1	2.42	0.46
1:S2:1228:A:H2'	1:S2:1229:G:C8	2.51	0.46
1:S2:1387:G:H21	25:SR:8:THR:HG21	1.80	0.46
3:SE:18:TRP:HH2	3:SE:31:PRO:HD3	1.81	0.46
38:E:141:LEU:HD23	38:E:141:LEU:O	2.16	0.46
38:E:403:VAL:O	38:E:404:LEU:HD23	2.16	0.46
42:e:303:PHE:HD2	42:e:347:ILE:HD11	1.81	0.46
43:d:314:MET:HA	43:d:317:THR:HG22	1.98	0.46
1:S2:1229:G:H21	34:ST:87:VAL:HG21	1.80	0.46
6:SH:39:GLN:OE1	6:SH:39:GLN:N	2.48	0.46
13:SG:126:ASP:OD1	13:SG:126:ASP:N	2.49	0.46
16:SO:56:VAL:HG22	16:SO:81:VAL:CG1	2.45	0.46
27:Sg:87:LEU:HB2	27:Sg:101:PHE:HB2	1.97	0.46
40:G:71:C:C4	40:G:72:U:C5	3.04	0.46
44:c:354:LEU:O	44:c:358:VAL:HG23	2.16	0.46
44:c:757:ILE:HG22	44:c:757:ILE:O	2.16	0.46
1:S2:1406:G:H2'	1:S2:1407:U:H6	1.81	0.46
9:SV:42:VAL:HG13	9:SV:43:THR:N	2.31	0.46
29:SK:35:LEU:HB3	29:SK:40:VAL:HG22	1.96	0.46
35:SP:52:LYS:HD3	35:SP:80:LEU:HD21	1.97	0.46
37:D:141:LYS:HD3	37:D:141:LYS:C	2.41	0.46
42:e:235:LEU:HD23	42:e:239:GLN:CG	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:a:237:LEU:HD12	45:a:252:ALA:HB3	1.97	0.46
45:a:446:ILE:HD12	45:a:514:MET:HE1	1.98	0.46
1:S2:1025:U:H2'	1:S2:1026:C:O4'	2.17	0.45
1:S2:1119:A:H2'	1:S2:1120:U:O4'	2.16	0.45
1:S2:1598:G:H2'	36:SZ:80:ARG:HG2	1.97	0.45
7:SI:64:ASN:O	7:SI:186:ASP:HB2	2.16	0.45
12:SC:146:GLU:CD	22:SD:120:TYR:HH	2.23	0.45
35:SP:138:SER:HA	41:H:3:LYS:HD3	1.98	0.45
42:e:399:SER:HA	42:e:403:GLN:HB2	1.98	0.45
44:c:512:TYR:CE2	44:c:675:LEU:HD21	2.52	0.45
44:c:549:GLU:OE2	44:c:549:GLU:HA	2.16	0.45
44:c:756:ILE:O	44:c:757:ILE:HD13	2.15	0.45
1:S2:1405:A:H2'	1:S2:1406:G:O4'	2.16	0.45
13:SG:157:VAL:HG22	13:SG:176:ILE:HD11	1.97	0.45
34:ST:42:HIS:HB2	34:ST:83:GLN:HA	1.98	0.45
1:S2:871:U:O2'	1:S2:872:A:H4'	2.16	0.45
4:SA:137:ALA:HB1	4:SA:142:LEU:HB3	1.98	0.45
42:e:235:LEU:HD12	42:e:236:PHE:H	1.80	0.45
44:c:64:ILE:HG13	44:c:109:ILE:CD1	2.46	0.45
44:c:370:VAL:O	44:c:374:ILE:HG23	2.16	0.45
44:c:673:PHE:HA	44:c:676:HIS:CE1	2.52	0.45
44:c:684:CYS:HA	44:c:733:MET:HE3	1.97	0.45
44:c:712:LYS:CD	44:c:712:LYS:C	2.90	0.45
45:a:43:TRP:CD1	45:a:43:TRP:C	2.94	0.45
1:S2:587:A:H5'	1:S2:592:C:H41	1.82	0.45
1:S2:1031:A2M:HM'3	1:S2:1031:A2M:H1'	1.67	0.45
3:SE:139:LEU:HD23	3:SE:150:PRO:HB3	1.99	0.45
43:d:447:LEU:HD21	43:d:473:PRO:HG3	1.98	0.45
1:S2:544:G:H2'	1:S2:545:A:H4'	1.97	0.45
1:S2:590:A2M:HM'2	1:S2:591:U:P	2.56	0.45
1:S2:1851:MA6:H5''	2:Ln:1:MET:HE3	1.98	0.45
16:SO:136:PRO:CB	16:SO:139:SER:HB3	2.47	0.45
27:Sg:180:ALA:O	27:Sg:181:ASN:CG	2.60	0.45
29:SK:90:VAL:HG22	29:SK:91:PRO:HD2	1.97	0.45
33:SS:50:ILE:HD12	33:SS:67:VAL:CG1	2.47	0.45
38:E:408:ILE:HG22	38:E:441:ILE:HG13	1.98	0.45
42:e:261:VAL:HG21	42:e:270:ARG:HD2	1.97	0.45
44:c:489:TYR:CD2	44:c:490:LEU:HD12	2.52	0.45
44:c:831:LEU:HD22	44:c:846:ARG:HG3	1.98	0.45
45:a:230:LEU:HD12	45:a:271:LEU:CD2	2.47	0.45
45:a:535:GLU:O	45:a:539:PRO:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:158:A:H2'	1:S2:159:A2M:O4'	2.17	0.45
1:S2:581:U:H4'	18:SY:66:GLY:HA2	1.97	0.45
1:S2:1203:G:H2'	1:S2:1204:A:C8	2.52	0.45
1:S2:1396:A:O2'	1:S2:1398:G:N7	2.43	0.45
12:SC:127:PHE:CD2	12:SC:141:VAL:HG22	2.52	0.45
30:SM:76:LEU:O	30:SM:127:TYR:CZ	2.69	0.45
38:E:89:TYR:OH	38:E:111:ASP:HA	2.16	0.45
1:S2:918:PSU:O2'	1:S2:919:A:O5'	2.34	0.45
1:S2:1793:A:C2	1:S2:1794:C:C5	3.05	0.45
5:SB:190:PRO:HD3	45:a:17:GLU:OE1	2.17	0.45
37:D:134:THR:O	37:D:138:PHE:CD2	2.70	0.45
37:D:256:ALA:O	37:D:259:LYS:HG2	2.16	0.45
47:m:316:VAL:HG23	47:m:320:MET:O	2.17	0.45
1:S2:481:C:H2'	1:S2:482:G:O4'	2.16	0.45
1:S2:563:G:C2	1:S2:564:A:C8	3.05	0.45
1:S2:981:A:H2'	1:S2:982:G:C8	2.51	0.45
1:S2:1258:A:P	56:S2:2050:HOH:O	2.73	0.45
1:S2:1605:G:H2'	1:S2:1606:G:O4'	2.16	0.45
1:S2:1856:C:H2'	1:S2:1857:G:C8	2.51	0.45
8:SL:151:THR:HG21	8:SL:155:PHE:CZ	2.52	0.45
17:SW:5:ASN:HB3	17:SW:8:ALA:HB3	1.99	0.45
27:Sg:121:VAL:HG21	27:Sg:165:ILE:HD12	1.98	0.45
42:e:252:HIS:O	42:e:256:TYR:CD2	2.69	0.45
44:c:358:VAL:HA	44:c:374:ILE:HD11	1.98	0.45
45:a:186:LEU:HD11	45:a:239:SER:HA	1.98	0.45
45:a:295:THR:HG22	45:a:359:LEU:CD1	2.46	0.45
1:S2:194:C:H2'	1:S2:195:C:C1'	2.46	0.45
1:S2:815:PSU:C4	1:S2:816:A:C8	3.05	0.45
4:SA:10:MET:SD	4:SA:15:VAL:HG22	2.57	0.45
5:SB:35:ALA:HB2	5:SB:44:ILE:HD13	1.99	0.45
43:d:289:LEU:HD12	43:d:317:THR:HA	1.98	0.45
44:c:363:GLU:OE2	44:c:363:GLU:HA	2.16	0.45
44:c:368:GLU:HA	44:c:371:ILE:HG22	1.99	0.45
44:c:580:SER:HA	44:c:619:CYS:SG	2.57	0.45
45:a:109:GLN:NE2	45:a:110:GLN:HG2	2.32	0.45
1:S2:443:U:H2'	1:S2:444:G:O4'	2.17	0.45
1:S2:653:A:H2'	1:S2:654:A:O4'	2.18	0.45
1:S2:1285:G:C2	30:SM:58:GLU:OE2	2.70	0.45
12:SC:266:TYR:O	12:SC:270:THR:HG23	2.17	0.45
19:Sb:10:PRO:HG2	19:Sb:15:GLU:OE1	2.17	0.45
27:Sg:78:ALA:HB2	27:Sg:92:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:SM:79:VAL:HG13	30:SM:81:ASP:H	1.82	0.45
43:d:37:ASP:OD1	44:c:590:LEU:HD11	2.16	0.45
44:c:815:LEU:HD13	44:c:815:LEU:O	2.17	0.45
46:3f:261:ARG:O	46:3f:262:VAL:CB	2.64	0.45
1:S2:376:A:H2'	1:S2:377:G:O4'	2.17	0.44
1:S2:1453:C:H4'	25:SR:49:LYS:HA	1.99	0.44
5:SB:9:LEU:C	5:SB:9:LEU:HD23	2.42	0.44
25:SR:38:ILE:HD12	25:SR:38:ILE:O	2.17	0.44
25:SR:99:ASP:OD1	25:SR:100:PRO:CD	2.66	0.44
37:D:132:GLN:O	37:D:133:ARG:C	2.60	0.44
38:E:421:LYS:O	38:E:422:ALA:HB3	2.17	0.44
45:a:230:LEU:HD13	45:a:230:LEU:C	2.41	0.44
45:a:385:PRO:HA	45:a:388:LYS:HB2	1.99	0.44
48:h:350:TYR:O	48:h:351:ASN:C	2.60	0.44
13:SG:7:PHE:HD2	13:SG:10:THR:HG22	1.81	0.44
30:SM:31:LEU:O	30:SM:32:ALA:C	2.58	0.44
38:E:175:ALA:O	38:E:179:ILE:HG13	2.17	0.44
42:e:407:LYS:HG3	42:e:408:THR:N	2.32	0.44
44:c:691:MET:HE1	44:c:756:ILE:HD12	2.00	0.44
45:a:283:PHE:O	45:a:287:GLY:O	2.36	0.44
1:S2:1499:U:H4'	22:SD:176:LEU:HD13	2.00	0.44
1:S2:1809:A:H2'	1:S2:1810:U:C6	2.52	0.44
5:SB:127:VAL:HG13	5:SB:176:VAL:HG11	1.99	0.44
28:Sc:15:THR:O	28:Sc:16:LYS:C	2.60	0.44
30:SM:75:ASN:C	30:SM:76:LEU:HD22	2.43	0.44
43:d:44:ASP:OD2	43:d:49:THR:HG23	2.18	0.44
43:d:455:TYR:CE1	43:d:464:VAL:HG23	2.51	0.44
44:c:570:LEU:HD21	44:c:594:LEU:HD13	1.98	0.44
1:S2:140:C:H42	1:S2:313:A:H61	1.65	0.44
19:Sb:37:CYS:SG	19:Sb:63:LEU:HD21	2.58	0.44
23:SF:142:SER:HB3	28:Sc:50:VAL:HG22	2.00	0.44
24:Sf:100:LEU:HD12	24:Sf:101:ALA:N	2.33	0.44
37:D:168:LEU:HD22	37:D:172:GLU:OE2	2.18	0.44
41:H:31:ASP:OD1	41:H:32:GLY:N	2.50	0.44
45:a:555:THR:O	45:a:559:LYS:HD2	2.17	0.44
48:h:225:ALA:HA	48:h:229:GLU:CB	2.48	0.44
18:SY:105:LYS:O	18:SY:109:GLU:HG3	2.17	0.44
23:SF:90:VAL:O	23:SF:93:VAL:HG12	2.18	0.44
31:SU:20:ILE:HD11	31:SU:98:VAL:HG21	1.99	0.44
38:E:156:LEU:HD23	38:E:186:LEU:HB2	2.00	0.44
43:d:202:TYR:HA	43:d:328:LEU:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:d:380:VAL:HG23	43:d:390:PHE:CD1	2.52	0.44
44:c:643:LYS:HE2	44:c:650:LEU:HD12	1.99	0.44
44:c:781:ARG:O	44:c:785:GLU:OE1	2.35	0.44
45:a:51:MET:HE1	45:a:70:GLY:O	2.17	0.44
1:S2:216:C:C2	1:S2:217:A:C8	3.06	0.44
1:S2:640:A:H2'	1:S2:641:A:C8	2.52	0.44
29:SK:9:ILE:O	29:SK:13:GLU:HG3	2.17	0.44
37:D:140:ASP:OD1	37:D:140:ASP:C	2.60	0.44
42:e:212:THR:HA	42:e:242:TYR:CE1	2.53	0.44
42:e:243:LEU:HD23	42:e:243:LEU:O	2.17	0.44
43:d:203:ASP:CB	43:d:329:ARG:HE	2.30	0.44
43:d:296:ASN:HB3	43:d:297:GLU:OE2	2.18	0.44
44:c:857:LEU:C	44:c:857:LEU:HD23	2.43	0.44
27:Sg:144:ASP:O	27:Sg:145:GLU:HG2	2.18	0.44
37:D:157:VAL:HG12	37:D:180:ILE:CG2	2.48	0.44
44:c:548:MET:HE1	44:c:571:CYS:O	2.17	0.44
45:a:343:ASP:OD1	45:a:343:ASP:C	2.61	0.44
45:a:518:GLN:HA	45:a:521:ASN:OD1	2.18	0.44
1:S2:512:A2M:H5'	1:S2:576:A2M:N1	2.33	0.44
1:S2:1725:U:H2'	1:S2:1726:G:O4'	2.16	0.44
1:S2:1753:C:H2'	1:S2:1755:C:H41	1.82	0.44
6:SH:177:TYR:CD2	6:SH:185:VAL:HG21	2.53	0.44
24:Sf:109:ASP:OD1	24:Sf:113:LYS:HB2	2.17	0.44
27:Sg:126:ASP:OD1	27:Sg:128:THR:HG22	2.18	0.44
43:d:25:PHE:O	43:d:25:PHE:CG	2.70	0.44
44:c:60:LEU:O	44:c:64:ILE:HG12	2.17	0.44
44:c:117:LEU:HD21	44:c:141:LEU:HD23	2.00	0.44
44:c:383:TYR:OH	44:c:451:MET:HB2	2.18	0.44
44:c:823:SER:HA	44:c:826:ILE:HG12	1.98	0.44
48:h:222:SER:HA	48:h:229:GLU:CB	2.48	0.44
1:S2:99:A2M:HM'3	1:S2:99:A2M:H1'	1.88	0.44
1:S2:194:C:H2'	1:S2:195:C:O4'	2.17	0.44
1:S2:1019:C:H2'	1:S2:1020:A:O4'	2.18	0.44
1:S2:1309:C:HO2'	1:S2:1310:U:P	2.41	0.44
12:SC:70:VAL:HG21	12:SC:93:ILE:HG23	2.00	0.44
23:SF:33:ILE:HD11	28:Sc:11:LEU:HD23	1.99	0.44
27:Sg:101:PHE:CD1	27:Sg:101:PHE:N	2.86	0.44
37:D:176:LEU:HD23	37:D:176:LEU:O	2.18	0.44
38:E:44:ILE:HD13	38:E:130:VAL:HG13	2.00	0.44
42:e:273:VAL:HA	42:e:277:LEU:HD13	2.00	0.44
43:d:297:GLU:O	43:d:297:GLU:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:d:452:VAL:HG13	43:d:464:VAL:C	2.43	0.44
45:a:306:MET:SD	45:a:306:MET:C	3.00	0.44
45:a:368:ILE:O	45:a:368:ILE:HG22	2.18	0.44
45:a:429:PRO:O	45:a:432:GLN:HG2	2.18	0.44
47:m:331:LYS:O	47:m:331:LYS:CG	2.66	0.44
1:S2:484:A2M:O5'	1:S2:484:A2M:H8	2.18	0.43
1:S2:495:U:H2'	1:S2:496:C:O4'	2.17	0.43
1:S2:746:C:H2'	1:S2:747:U:C1'	2.47	0.43
1:S2:1291:A:C6	1:S2:1302:G:C6	3.06	0.43
16:SO:24:GLY:C	16:SO:25:GLU:HG3	2.42	0.43
17:SW:125:ILE:HG23	17:SW:125:ILE:O	2.17	0.43
38:E:254:PRO:HG2	38:E:360:ALA:HB2	2.00	0.43
44:c:67:ILE:O	44:c:71:MET:HG3	2.18	0.43
44:c:691:MET:HE1	44:c:756:ILE:CD1	2.48	0.43
45:a:112:VAL:O	45:a:115:ILE:HG13	2.18	0.43
45:a:471:ILE:CG2	45:a:482:VAL:HG11	2.48	0.43
48:h:154:PRO:C	48:h:161:SER:HA	2.43	0.43
1:S2:747:U:H3	1:S2:748:C:H41	1.65	0.43
1:S2:1334:G:O3'	22:SD:183:GLY:HA3	2.18	0.43
12:SC:199:PRO:HG3	14:SJ:58:ARG:HD2	2.00	0.43
19:Sb:34:ASP:HB2	19:Sb:43:ILE:CG2	2.48	0.43
22:SD:93:THR:O	22:SD:93:THR:CG2	2.62	0.43
42:e:356:LEU:HD21	42:e:371:ILE:HG13	2.01	0.43
42:e:368:GLU:O	42:e:372:VAL:HG23	2.18	0.43
43:d:21:VAL:HG12	43:d:22:PRO:HD3	2.01	0.43
45:a:122:GLN:O	45:a:122:GLN:CG	2.65	0.43
45:a:549:GLN:CD	45:a:550:HIS:H	2.26	0.43
49:k:212:SER:O	49:k:216:SER:C	2.61	0.43
1:S2:528:A:H2'	1:S2:529:A:C8	2.53	0.43
1:S2:969:U:H5	5:SB:9:LEU:HD21	1.83	0.43
1:S2:1229:G:H21	34:ST:87:VAL:HG22	1.83	0.43
28:Sc:33:GLU:OE1	43:d:296:ASN:ND2	2.51	0.43
32:SQ:39:LEU:HD22	32:SQ:51:LEU:HB3	1.98	0.43
37:D:207:ALA:HB1	37:D:265:LYS:HD2	1.99	0.43
42:e:215:ILE:HB	42:e:242:TYR:OH	2.17	0.43
44:c:848:GLU:OE1	44:c:852:GLN:N	2.50	0.43
1:S2:102:A:H4'	1:S2:104:A:C8	2.53	0.43
1:S2:172:OMU:H6	1:S2:314:U:O2'	2.18	0.43
1:S2:641:A:H2'	1:S2:642:U:O4'	2.18	0.43
1:S2:1520:G:H4'	1:S2:1521:C:OP2	2.18	0.43
5:SB:35:ALA:HB2	5:SB:44:ILE:CD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:SX:4:CYS:HB2	10:SX:9:THR:HG21	2.00	0.43
14:SJ:79:ARG:HA	14:SJ:82:VAL:HG22	2.00	0.43
37:D:209:LYS:HE3	38:E:274:LEU:CB	2.49	0.43
42:e:355:MET:SD	42:e:355:MET:C	3.01	0.43
42:e:397:ALA:C	42:e:399:SER:H	2.25	0.43
45:a:35:MET:HA	45:a:35:MET:HE3	2.01	0.43
1:S2:833:C:H2'	1:S2:834:C:C6	2.53	0.43
5:SB:142:PHE:CB	5:SB:208:HIS:HE1	2.28	0.43
27:Sg:236:ILE:HG12	27:Sg:252:THR:HG22	2.01	0.43
33:SS:62:ASP:O	33:SS:65:GLU:HG3	2.18	0.43
33:SS:80:PRO:HB2	33:SS:82:TRP:CE3	2.53	0.43
35:SP:21:ASP:OD2	35:SP:23:ASP:OD1	2.36	0.43
1:S2:1260:A:C2	1:S2:1620:A:C4	3.07	0.43
1:S2:1388:A:H61	22:SD:161:GLY:CA	2.31	0.43
21:B:4:G:H2'	21:B:5:A:C8	2.53	0.43
27:Sg:87:LEU:HD21	27:Sg:122:SER:HB3	2.00	0.43
29:SK:18:GLU:O	29:SK:93:THR:HG23	2.19	0.43
41:H:31:ASP:OD1	41:H:31:ASP:C	2.61	0.43
44:c:117:LEU:HD11	44:c:141:LEU:HG	2.01	0.43
44:c:141:LEU:O	44:c:142:ARG:C	2.61	0.43
44:c:422:GLU:OE1	44:c:437:PRO:HA	2.18	0.43
44:c:677:ILE:O	44:c:678:ASN:C	2.59	0.43
44:c:840:GLN:OE1	44:c:842:VAL:HG23	2.18	0.43
45:a:147:THR:N	45:a:148:PRO:CD	2.82	0.43
45:a:390:LEU:HD12	45:a:410:VAL:CG2	2.48	0.43
45:a:516:SER:C	45:a:517:GLU:HG3	2.42	0.43
1:S2:166:A2M:H5'	1:S2:166:A2M:C8	2.35	0.43
3:SE:139:LEU:HD12	3:SE:139:LEU:O	2.19	0.43
7:SI:205:ARG:HG3	7:SI:206:LYS:N	2.32	0.43
41:H:34:GLU:O	41:H:78:LEU:HD12	2.18	0.43
42:e:277:LEU:O	42:e:281:ILE:HD13	2.18	0.43
44:c:756:ILE:O	44:c:756:ILE:CG2	2.67	0.43
44:c:792:LEU:HD11	44:c:802:ILE:HD13	2.01	0.43
44:c:831:LEU:C	44:c:832:MET:SD	3.01	0.43
47:m:127:LEU:O	47:m:131:ALA:CB	2.67	0.43
1:S2:648:A:N3	10:SX:45:SER:OG	2.52	0.43
1:S2:1616:U:H2'	1:S2:1617:G:O4'	2.18	0.43
4:SA:34:MET:HE1	4:SA:162:PRO:HB3	2.00	0.43
17:SW:53:ILE:HD13	19:Sb:24:LEU:HD11	2.00	0.43
19:Sb:53:VAL:O	19:Sb:53:VAL:CG1	2.67	0.43
24:Sf:117:LEU:HD22	24:Sf:117:LEU:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Sg:197:THR:HG21	27:Sg:238:ALA:HA	1.99	0.43
37:D:131:PHE:O	37:D:132:GLN:C	2.62	0.43
41:H:86:ASP:O	41:H:88:LYS:N	2.52	0.43
42:e:362:MET:SD	42:e:362:MET:C	3.01	0.43
44:c:80:LEU:O	44:c:84:GLU:CD	2.62	0.43
44:c:451:MET:HE3	44:c:479:VAL:HG22	2.01	0.43
44:c:597:ASN:OD1	44:c:597:ASN:O	2.37	0.43
44:c:626:THR:HB	44:c:693:LEU:HD21	2.00	0.43
45:a:538:LYS:HB2	45:a:539:PRO:HD3	2.00	0.43
1:S2:116:OMU:HM22	1:S2:117:C:O4'	2.19	0.43
1:S2:198:U:H2'	1:S2:199:C:H2'	2.00	0.43
4:SA:22:GLY:C	4:SA:24:HIS:H	2.27	0.43
4:SA:192:GLU:C	4:SA:192:GLU:OE1	2.62	0.43
7:SI:138:ASN:OD1	7:SI:138:ASN:N	2.51	0.43
14:SJ:47:LYS:HG3	14:SJ:102:ILE:HD12	2.01	0.43
38:E:199:GLN:O	38:E:202:GLU:HG3	2.19	0.43
43:d:311:ASN:OD1	43:d:312:LEU:N	2.52	0.43
44:c:832:MET:HE1	44:c:843:VAL:HG13	2.01	0.43
45:a:15:ALA:O	45:a:19:LEU:HG	2.19	0.43
47:m:325:ILE:CG2	47:m:326:ASP:N	2.82	0.43
47:m:347:TRP:N	47:m:347:TRP:CD1	2.87	0.43
1:S2:203:G:H2'	1:S2:204:G:C8	2.54	0.43
1:S2:1043:G:H2'	1:S2:1044:G:O4'	2.19	0.43
12:SC:167:ARG:HB3	12:SC:177:PRO:HB2	2.00	0.43
22:SD:223:ILE:HD11	27:Sg:189:ILE:HD11	2.01	0.43
23:SF:78:MET:O	23:SF:79:HIS:HB2	2.18	0.43
32:SQ:22:VAL:HG11	32:SQ:71:ARG:NH2	2.34	0.43
38:E:296:VAL:HG22	38:E:358:LEU:HD12	2.01	0.43
41:H:24:ARG:O	41:H:25:GLU:C	2.60	0.43
44:c:159:TYR:O	44:c:159:TYR:CG	2.71	0.43
45:a:305:GLU:CD	45:a:305:GLU:C	2.87	0.43
45:a:384:VAL:HG12	45:a:386:GLU:H	1.84	0.43
25:SR:34:VAL:O	25:SR:38:ILE:HG13	2.19	0.42
33:SS:17:ASN:O	33:SS:17:ASN:CG	2.62	0.42
33:SS:84:LEU:N	33:SS:84:LEU:HD22	2.34	0.42
43:d:57:ASN:ND2	44:c:593:HIS:ND1	2.67	0.42
44:c:603:PRO:N	44:c:604:PRO:CD	2.82	0.42
45:a:269:PRO:C	45:a:271:LEU:H	2.26	0.42
45:a:361:LEU:N	45:a:361:LEU:HD23	2.33	0.42
45:a:378:ASN:HD21	45:a:381:GLN:CD	2.25	0.42
1:S2:194:C:H2'	1:S2:195:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:441:C:H2'	1:S2:442:C:C6	2.55	0.42
1:S2:1118:C:O2'	1:S2:1119:A:O5'	2.38	0.42
1:S2:1223:A:OP1	23:SF:79:HIS:HA	2.20	0.42
22:SD:61:GLU:C	22:SD:62:LYS:HG3	2.44	0.42
28:Sc:6:VAL:HG13	28:Sc:7:GLN:N	2.33	0.42
30:SM:71:GLU:OE2	30:SM:71:GLU:C	2.62	0.42
36:SZ:69:THR:O	36:SZ:73:VAL:HG23	2.19	0.42
37:D:290:MET:SD	37:D:290:MET:C	3.02	0.42
38:E:75:ARG:O	38:E:77:ILE:HG23	2.18	0.42
42:e:270:ARG:HH11	42:e:273:VAL:HG22	1.83	0.42
42:e:299:LEU:HD11	42:e:340:ILE:HA	2.01	0.42
44:c:646:LEU:HD12	44:c:648:GLN:CD	2.44	0.42
45:a:283:PHE:CD2	45:a:291:PHE:HB3	2.54	0.42
45:a:519:ILE:H	45:a:519:ILE:CD1	2.32	0.42
47:m:48:ALA:C	47:m:50:ASP:H	2.26	0.42
48:h:208:SER:O	48:h:209:HIS:CB	2.67	0.42
1:S2:572:PSU:H5''	18:SY:60:PHE:O	2.19	0.42
1:S2:1520:G:H2'	1:S2:1520:G:N3	2.34	0.42
1:S2:1597:C:H4'	1:S2:1603:G:O6	2.20	0.42
23:SF:73:THR:O	23:SF:89:THR:HG21	2.18	0.42
35:SP:44:ARG:HG2	35:SP:84:ILE:HD12	2.02	0.42
43:d:28:MET:O	43:d:29:PRO:C	2.63	0.42
44:c:497:GLU:HA	44:c:560:ARG:CZ	2.49	0.42
44:c:567:CYS:SG	44:c:605:VAL:HG22	2.59	0.42
44:c:733:MET:SD	44:c:734:ARG:N	2.92	0.42
44:c:832:MET:CE	44:c:843:VAL:HG22	2.46	0.42
45:a:237:LEU:HD21	45:a:253:VAL:HG22	2.01	0.42
1:S2:865:A:H2'	1:S2:866:PSU:H5''	2.02	0.42
1:S2:1243:U:H2'	1:S2:1244:PSU:O4'	2.20	0.42
22:SD:72:VAL:HG22	29:SK:22:VAL:HG22	2.01	0.42
38:E:158:LEU:HD11	38:E:190:ASN:HB2	2.00	0.42
44:c:81:GLU:O	44:c:84:GLU:HG2	2.19	0.42
44:c:726:LEU:HD21	45:a:286:SER:OG	2.20	0.42
45:a:25:GLN:HB3	45:a:26:PRO:HD3	2.02	0.42
45:a:358:LEU:HD23	45:a:359:LEU:HD23	2.01	0.42
1:S2:1304:U:O2	1:S2:1304:U:O4'	2.37	0.42
29:SK:5:LYS:O	29:SK:9:ILE:HG13	2.19	0.42
38:E:174:LEU:O	38:E:178:GLU:HG2	2.19	0.42
44:c:552:CYS:O	44:c:556:TYR:CD2	2.73	0.42
44:c:602:ASP:HB2	44:c:604:PRO:HD2	2.02	0.42
45:a:86:LEU:O	45:a:89:VAL:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:a:416:GLU:O	45:a:417:GLN:C	2.62	0.42
45:a:482:VAL:O	45:a:482:VAL:CG1	2.67	0.42
1:S2:321:C:O2	1:S2:321:C:H2'	2.19	0.42
1:S2:614:C:H2'	1:S2:626:G:C8	2.55	0.42
1:S2:1316:C:O2'	1:S2:1317:C:P	2.77	0.42
4:SA:1:MET:N	4:SA:59:LEU:HB2	2.33	0.42
8:SL:68:ILE:HG12	8:SL:143:LEU:HD21	2.01	0.42
23:SF:102:LEU:HD21	36:SZ:100:VAL:HG21	2.02	0.42
36:SZ:79:ILE:HB	36:SZ:83:LEU:HD23	2.01	0.42
37:D:262:ILE:HG12	37:D:265:LYS:HZ3	1.84	0.42
43:d:380:VAL:HG22	43:d:381:MET:N	2.35	0.42
44:c:666:GLU:OE2	44:c:666:GLU:HA	2.19	0.42
44:c:850:THR:HG21	45:a:502:ARG:HE	1.85	0.42
1:S2:563:G:O2'	1:S2:564:A:P	2.77	0.42
1:S2:1831:A:O2'	1:S2:1832:6MZ:H5'1	2.19	0.42
4:SA:21:ALA:HB2	25:SR:91:LEU:HD22	2.00	0.42
19:Sb:65:GLN:O	19:Sb:65:GLN:HG3	2.18	0.42
29:SK:37:ASP:OD1	29:SK:37:ASP:N	2.51	0.42
42:e:288:TYR:C	42:e:290:ASP:N	2.75	0.42
44:c:682:LEU:HD23	44:c:682:LEU:C	2.44	0.42
45:a:567:ARG:HB2	45:a:573:GLN:HB2	2.02	0.42
4:SA:18:PHE:HD1	4:SA:23:THR:HG21	1.79	0.42
16:SO:78:ALA:HB3	16:SO:118:ALA:HB3	2.01	0.42
30:SM:71:GLU:C	30:SM:71:GLU:CD	2.88	0.42
35:SP:15:PHE:CZ	35:SP:109:PRO:O	2.73	0.42
37:D:132:GLN:HA	37:D:136:TRP:CE3	2.55	0.42
42:e:355:MET:HE3	42:e:356:LEU:N	2.35	0.42
44:c:673:PHE:HA	44:c:676:HIS:ND1	2.34	0.42
45:a:439:LEU:CD2	45:a:459:VAL:CG2	2.97	0.42
4:SA:1:MET:SD	9:SV:79:VAL:CG2	3.08	0.42
7:SI:139:LYS:H	7:SI:139:LYS:CD	2.32	0.42
14:SJ:24:ARG:O	14:SJ:28:GLU:HG3	2.20	0.42
40:G:35:A:H4'	41:H:7:LYS:HD3	2.02	0.42
42:e:255:ARG:HG2	42:e:292:ILE:CG2	2.50	0.42
43:d:296:ASN:O	43:d:297:GLU:OE2	2.38	0.42
45:a:482:VAL:O	45:a:482:VAL:HG13	2.19	0.42
46:3f:179:ILE:CB	46:3f:183:SER:CB	2.97	0.42
1:S2:525:A:H5''	20:Se:32:ALA:CB	2.50	0.42
1:S2:903:A:H2'	1:S2:904:A:C8	2.55	0.42
1:S2:1012:A:H2'	1:S2:1013:U:O4'	2.20	0.42
1:S2:1173:A:H2'	1:S2:1174:PSU:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1533:A:H2	1:S2:1536:G:N3	2.17	0.42
7:SI:67:TRP:O	7:SI:67:TRP:CD1	2.73	0.42
13:SG:23:LYS:O	13:SG:24:LEU:HB2	2.19	0.42
14:SJ:152:ASP:OD1	14:SJ:153:SER:N	2.53	0.42
22:SD:136:VAL:HG22	22:SD:152:PHE:HB2	2.02	0.42
25:SR:73:LEU:O	25:SR:73:LEU:HD23	2.20	0.42
42:e:244:ASN:O	42:e:249:MET:SD	2.78	0.42
44:c:379:ILE:HG21	44:c:447:LEU:HD13	2.02	0.42
1:S2:206:G:H3'	1:S2:207:G:H5''	2.02	0.41
1:S2:1070:A:H2'	1:S2:1071:G:O4'	2.19	0.41
1:S2:1326:UY1:O3'	1:S2:1326:UY1:CM2	2.68	0.41
1:S2:1344:A:H4'	1:S2:1345:G:OP1	2.20	0.41
1:S2:1567:G:H21	1:S2:1628:C:H4'	1.85	0.41
44:c:556:TYR:CZ	44:c:569:ILE:HD12	2.55	0.41
1:S2:433:A:H5''	7:SI:22:HIS:HB3	2.01	0.41
1:S2:897:U:H5''	1:S2:898:U:OP2	2.20	0.41
1:S2:1257:G:H4'	1:S2:1258:A:O5'	2.20	0.41
1:S2:1306:U:H2'	1:S2:1307:U:OP1	2.20	0.41
7:SI:98:LYS:O	7:SI:175:ILE:O	2.38	0.41
9:SV:16:LYS:N	12:SC:259:THR:HG21	2.35	0.41
25:SR:79:GLU:OE2	25:SR:79:GLU:C	2.63	0.41
30:SM:31:LEU:HD13	30:SM:89:VAL:CG2	2.50	0.41
30:SM:73:GLN:C	30:SM:74:ILE:HD13	2.45	0.41
32:SQ:49:TYR:O	32:SQ:53:GLU:HG2	2.20	0.41
38:E:187:ILE:HG21	38:E:221:ILE:HG12	2.02	0.41
42:e:243:LEU:HD23	42:e:243:LEU:C	2.45	0.41
43:d:72:PHE:HA	44:c:600:HIS:O	2.19	0.41
44:c:464:PRO:HA	44:c:469:TYR:CD2	2.55	0.41
1:S2:468:A2M:HM'3	1:S2:468:A2M:H1'	1.92	0.41
1:S2:808:A:H2	1:S2:855:G:H22	1.68	0.41
1:S2:929:G:H2'	1:S2:930:C:O4'	2.19	0.41
1:S2:1139:C:O2	1:S2:1139:C:O4'	2.37	0.41
1:S2:1217:A:H2'	1:S2:1218:C:H6	1.86	0.41
1:S2:1406:G:H2'	1:S2:1407:U:C6	2.55	0.41
25:SR:57:LEU:HD13	25:SR:69:ILE:HD11	2.02	0.41
42:e:273:VAL:HG23	42:e:274:LEU:H	1.84	0.41
44:c:347:ARG:HA	44:c:350:GLN:HG2	2.00	0.41
44:c:779:LEU:O	44:c:783:ILE:HG12	2.20	0.41
45:a:11:ALA:HB2	45:a:34:VAL:HG21	2.02	0.41
45:a:481:GLN:OE1	45:a:499:TYR:CG	2.74	0.41
1:S2:27:A2M:H1'	1:S2:27:A2M:HM'3	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:383:G:O2'	8:SL:133:PRO:O	2.38	0.41
1:S2:525:A:C2	1:S2:526:A:C5	3.08	0.41
17:SW:69:LEU:HD21	17:SW:72:CYS:SG	2.61	0.41
37:D:133:ARG:HD2	37:D:167:ASP:OD1	2.21	0.41
40:G:43:G:H2'	40:G:44:A:C8	2.55	0.41
42:e:362:MET:CE	42:e:366:GLU:HB3	2.50	0.41
44:c:349:ALA:HA	44:c:352:GLU:HG2	2.02	0.41
44:c:520:GLN:O	44:c:521:ARG:HB3	2.20	0.41
44:c:660:GLN:N	44:c:660:GLN:OE1	2.53	0.41
44:c:684:CYS:SG	44:c:733:MET:HE2	2.60	0.41
45:a:521:ASN:O	45:a:524:THR:HG23	2.21	0.41
1:S2:648:A:H4'	10:SX:104:GLY:O	2.20	0.41
5:SB:124:HIS:HA	5:SB:137:LEU:O	2.20	0.41
8:SL:121:GLN:O	8:SL:124:ASP:OD2	2.38	0.41
22:SD:161:GLY:O	22:SD:164:VAL:HG12	2.21	0.41
27:Sg:181:ASN:OD1	27:Sg:181:ASN:C	2.63	0.41
35:SP:44:ARG:HG2	35:SP:84:ILE:CD1	2.50	0.41
42:e:299:LEU:O	42:e:299:LEU:HD23	2.20	0.41
44:c:735:GLU:HA	44:c:738:VAL:CG1	2.51	0.41
44:c:825:MET:O	44:c:828:ASN:O	2.39	0.41
45:a:19:LEU:HD21	45:a:57:LEU:HD11	2.03	0.41
45:a:153:LEU:HD22	45:a:184:PHE:CE1	2.56	0.41
1:S2:796:G:H3'	1:S2:797:C:H5'	2.02	0.41
1:S2:1383:A2M:H1'	1:S2:1383:A2M:HM'3	1.85	0.41
4:SA:48:ILE:CG2	25:SR:105:MET:HE2	2.51	0.41
6:SH:159:ASP:OD1	6:SH:159:ASP:C	2.63	0.41
8:SL:22:ARG:HB3	8:SL:27:GLU:HG3	2.03	0.41
12:SC:94:ILE:HG13	12:SC:159:LYS:O	2.20	0.41
16:SO:34:PHE:CD1	16:SO:34:PHE:C	2.96	0.41
22:SD:119:CYS:SG	22:SD:138:VAL:HG21	2.61	0.41
30:SM:73:GLN:O	30:SM:74:ILE:HD13	2.21	0.41
32:SQ:34:VAL:O	32:SQ:34:VAL:HG23	2.19	0.41
42:e:235:LEU:O	42:e:236:PHE:C	2.62	0.41
42:e:281:ILE:O	42:e:282:GLN:C	2.64	0.41
44:c:422:GLU:CD	44:c:437:PRO:HA	2.46	0.41
44:c:425:LEU:HD12	44:c:425:LEU:N	2.35	0.41
44:c:511:TYR:O	44:c:574:TYR:HD1	2.03	0.41
44:c:696:PRO:HA	44:c:790:THR:HG22	2.01	0.41
45:a:175:HIS:HE2	45:a:229:HIS:CE1	2.39	0.41
45:a:295:THR:HG22	45:a:359:LEU:HD11	2.03	0.41
47:m:322:TYR:CB	47:m:332:VAL:HA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:m:343:GLY:O	47:m:347:TRP:CD1	2.74	0.41
1:S2:1123:C:C4	1:S2:1124:C:C5	3.08	0.41
1:S2:1628:C:H2'	1:S2:1629:C:C6	2.56	0.41
1:S2:1670:C:H2'	1:S2:1671:G:O4'	2.20	0.41
22:SD:99:ILE:HG23	22:SD:173:ARG:NH2	2.35	0.41
23:SF:135:ARG:O	23:SF:136:ARG:HB2	2.20	0.41
43:d:41:LYS:H	44:c:613:MET:CE	2.33	0.41
44:c:55:LYS:O	44:c:58:GLU:HG3	2.20	0.41
45:a:12:LEU:HB2	45:a:50:ILE:HD11	2.03	0.41
45:a:437:LEU:HD11	45:a:507:ILE:HD12	2.01	0.41
45:a:540:ALA:HA	45:a:544:GLN:CB	2.51	0.41
1:S2:166:A2M:HM'3	1:S2:166:A2M:H1'	1.85	0.41
1:S2:526:A:C2	1:S2:560:A:C2	3.09	0.41
1:S2:571:U:C2	1:S2:572:PSU:C6	3.09	0.41
1:S2:576:A2M:H1'	1:S2:576:A2M:HM'3	1.79	0.41
1:S2:841:G:O2'	1:S2:842:C:P	2.79	0.41
1:S2:1228:A:H2'	1:S2:1229:G:H8	1.85	0.41
7:SI:57:ALA:HB2	7:SI:183:GLY:HA2	2.02	0.41
7:SI:164:GLU:C	7:SI:164:GLU:OE2	2.63	0.41
11:Sa:26:CYS:SG	11:Sa:28:ARG:HB2	2.61	0.41
14:SJ:93:LYS:HD3	14:SJ:93:LYS:HA	1.91	0.41
32:SQ:52:LEU:O	32:SQ:53:GLU:C	2.63	0.41
37:D:272:GLN:HB3	37:D:273:MET:SD	2.60	0.41
40:G:26:2MG:C5	40:G:27:C:C6	3.09	0.41
43:d:37:ASP:OD1	43:d:37:ASP:C	2.62	0.41
1:S2:456:C:C2	1:S2:457:C:C5	3.09	0.41
1:S2:569:A:H2'	1:S2:570:C:O4'	2.20	0.41
1:S2:1420:G:O2'	1:S2:1421:A:O4'	2.39	0.41
1:S2:1702:G:H2'	1:S2:1703:OMC:O4'	2.21	0.41
1:S2:1845:A:H2'	1:S2:1846:G:C8	2.55	0.41
2:Ln:2:ARG:HB3	2:Ln:5:TRP:CD1	2.56	0.41
3:SE:139:LEU:HD23	3:SE:150:PRO:CB	2.51	0.41
16:SO:63:LYS:HD3	16:SO:63:LYS:N	2.36	0.41
25:SR:98:VAL:HG13	25:SR:102:THR:HB	2.02	0.41
27:Sg:176:VAL:HG22	27:Sg:186:THR:HG22	2.02	0.41
29:SK:8:ARG:HD2	29:SK:12:TYR:CZ	2.56	0.41
35:SP:13:ARG:HB3	35:SP:13:ARG:NH1	2.36	0.41
38:E:266:LYS:HD2	38:E:266:LYS:HA	1.88	0.41
43:d:445:GLU:C	43:d:446:TYR:HD1	2.29	0.41
44:c:375:LYS:O	44:c:379:ILE:HD13	2.21	0.41
44:c:683:GLU:OE1	44:c:683:GLU:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:a:122:GLN:O	45:a:122:GLN:CD	2.64	0.41
45:a:265:LYS:HB2	45:a:266:PRO:HD2	2.03	0.41
45:a:321:ARG:HE	45:a:423:GLU:HG3	1.86	0.41
45:a:482:VAL:HG23	45:a:493:PHE:CE1	2.55	0.41
1:S2:84:A:N3	1:S2:150:A:O2'	2.50	0.41
1:S2:662:G:H5'	1:S2:1156:U:O2	2.21	0.41
1:S2:955:A:N7	1:S2:969:U:C5	2.89	0.41
1:S2:1139:C:H2'	1:S2:1140:G:O4'	2.21	0.41
4:SA:1:MET:HG2	4:SA:60:LEU:HB2	2.02	0.41
6:SH:147:LYS:HA	17:SW:49:GLU:OE1	2.21	0.41
12:SC:275:LYS:HG3	12:SC:276:THR:HG23	2.02	0.41
14:SJ:125:HIS:HA	14:SJ:128:VAL:HG22	2.03	0.41
15:SN:101:HIS:CE1	15:SN:105:ASN:OD1	2.73	0.41
28:Sc:62:GLU:OE2	28:Sc:62:GLU:C	2.64	0.41
29:SK:40:VAL:O	29:SK:40:VAL:HG23	2.20	0.41
30:SM:57:ASP:OD1	30:SM:57:ASP:N	2.54	0.41
38:E:195:VAL:HG13	38:E:199:GLN:HB3	2.02	0.41
42:e:116:TYR:O	42:e:117:LEU:CB	2.68	0.41
42:e:399:SER:N	42:e:400:PRO:HD2	2.36	0.41
43:d:54:ARG:O	43:d:54:ARG:HG2	2.21	0.41
44:c:105:PHE:O	44:c:109:ILE:CD1	2.68	0.41
44:c:548:MET:SD	44:c:572:HIS:HD2	2.44	0.41
44:c:680:GLU:OE1	44:c:680:GLU:HA	2.21	0.41
45:a:446:ILE:CD1	45:a:514:MET:HE1	2.51	0.41
1:S2:202:G:H3'	1:S2:203:G:H5''	2.03	0.40
4:SA:126:ASP:HB3	4:SA:129:ALA:HB3	2.03	0.40
5:SB:186:ASN:O	45:a:17:GLU:OE1	2.38	0.40
38:E:454:ILE:HD12	38:E:455:GLY:N	2.36	0.40
44:c:507:ILE:O	44:c:511:TYR:HB3	2.21	0.40
44:c:607:ILE:HG13	44:c:608:LEU:N	2.36	0.40
45:a:80:GLN:HA	45:a:83:ILE:HG13	2.02	0.40
45:a:101:THR:HG22	45:a:149:TRP:HB3	2.03	0.40
45:a:153:LEU:HD21	45:a:157:TYR:HE2	1.86	0.40
45:a:448:GLN:OE1	47:m:325:ILE:HD11	2.21	0.40
45:a:507:ILE:O	45:a:508:GLY:C	2.64	0.40
1:S2:76:U:H3'	1:S2:77:A:C5'	2.51	0.40
1:S2:481:C:H2'	1:S2:482:G:C1'	2.51	0.40
1:S2:568:C:H2'	1:S2:569:A:O4'	2.20	0.40
24:Sf:125:GLU:OE2	24:Sf:125:GLU:HA	2.21	0.40
27:Sg:142:VAL:O	27:Sg:142:VAL:HG23	2.21	0.40
37:D:156:ALA:HB2	37:D:162:ILE:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:E:273:ASP:O	38:E:274:LEU:C	2.64	0.40
41:H:54:GLY:C	41:H:55:VAL:HG23	2.45	0.40
44:c:114:GLU:HG3	44:c:149:ASN:OD1	2.20	0.40
44:c:453:GLU:HA	44:c:456:THR:HG22	2.03	0.40
44:c:573:ILE:HD13	44:c:589:MET:HE2	2.03	0.40
44:c:792:LEU:HD13	44:c:792:LEU:HA	1.93	0.40
44:c:828:ASN:O	44:c:829:GLU:HG2	2.21	0.40
45:a:384:VAL:CG1	45:a:385:PRO:HD2	2.51	0.40
48:h:187:LEU:HA	48:h:191:ASN:CB	2.50	0.40
1:S2:160:U:O2'	1:S2:161:U:H3'	2.22	0.40
1:S2:796:G:H2'	1:S2:797:C:H5'	2.03	0.40
1:S2:1407:U:H2'	1:S2:1408:U:C6	2.57	0.40
1:S2:1606:G:N2	1:S2:1632:G:H1'	2.37	0.40
6:SH:112:ASN:OD1	6:SH:112:ASN:O	2.38	0.40
13:SG:145:PHE:CB	13:SG:147:LEU:HD13	2.52	0.40
16:SO:90:ILE:HG22	16:SO:124:MET:HE3	2.03	0.40
29:SK:26:ASP:OD1	29:SK:26:ASP:C	2.64	0.40
38:E:207:ILE:O	38:E:211:VAL:HG22	2.22	0.40
42:e:236:PHE:O	42:e:238:TYR:N	2.54	0.40
43:d:404:CYS:O	43:d:405:ASN:C	2.64	0.40
44:c:342:LYS:O	44:c:345:THR:HG22	2.22	0.40
44:c:739:ALA:HB1	44:c:755:PHE:CE2	2.56	0.40
45:a:31:LEU:O	45:a:35:MET:HG2	2.21	0.40
45:a:172:ARG:CZ	45:a:228:MET:CE	2.98	0.40
45:a:301:HIS:HB2	45:a:376:ARG:NH2	2.37	0.40
45:a:428:VAL:CG1	45:a:429:PRO:HD3	2.51	0.40
1:S2:71:G:H22	13:SG:170:ARG:NH1	2.20	0.40
1:S2:71:G:C5	1:S2:72:C:H1'	2.57	0.40
1:S2:682:U:H2'	1:S2:683:OMG:O4'	2.22	0.40
1:S2:1316:C:HO2'	1:S2:1317:C:P	2.45	0.40
1:S2:1639:M7G:H5'1	1:S2:1639:M7G:C8	2.52	0.40
2:Ln:21:ARG:O	2:Ln:21:ARG:HD2	2.22	0.40
4:SA:2:SER:O	4:SA:5:LEU:HB2	2.22	0.40
12:SC:191:VAL:HG11	12:SC:236:PHE:HA	2.03	0.40
35:SP:137:HIS:O	35:SP:138:SER:HB2	2.20	0.40
38:E:369:THR:HG21	38:E:465:ILE:HD12	2.03	0.40
38:E:408:ILE:HG22	38:E:441:ILE:HD11	2.02	0.40
1:S2:1828:C:H2'	1:S2:1829:G:O4'	2.21	0.40
4:SA:24:HIS:O	4:SA:25:LEU:HB2	2.21	0.40
5:SB:138:PHE:O	5:SB:213:ARG:N	2.55	0.40
7:SI:146:GLN:O	7:SI:150:ASP:OD1	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:SC:271:ASP:O	12:SC:274:VAL:HG12	2.21	0.40
19:Sb:35:VAL:HG23	19:Sb:63:LEU:HD22	2.04	0.40
24:Sf:103:LEU:O	24:Sf:103:LEU:HD12	2.22	0.40
24:Sf:121:CYS:HB3	24:Sf:132:MET:SD	2.62	0.40
25:SR:26:ASN:OD1	25:SR:26:ASN:N	2.55	0.40
30:SM:35:ILE:HG23	30:SM:36:ARG:N	2.36	0.40
35:SP:23:ASP:OD1	35:SP:23:ASP:N	2.53	0.40
37:D:134:THR:OG1	37:D:135:ALA:N	2.54	0.40
37:D:274:GLU:HB3	37:D:275:PRO:HD2	2.03	0.40
37:D:290:MET:SD	37:D:291:GLU:N	2.95	0.40
41:H:47:LEU:HD23	41:H:61:ILE:HD11	2.04	0.40
42:e:220:PHE:HB2	42:e:225:HIS:CE1	2.57	0.40
42:e:289:LYS:C	42:e:291:PRO:HD3	2.47	0.40
43:d:424:GLU:O	43:d:428:ASN:OD1	2.40	0.40
44:c:474:LYS:HE3	45:a:125:GLU:OE1	2.22	0.40
45:a:417:GLN:N	45:a:418:PRO:HD3	2.37	0.40
48:h:94:PHE:O	48:h:95:ASP:CB	2.70	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%)	21 (96%)	1 (4%)	0	100	100
3	SE	260/263 (99%)	251 (96%)	9 (4%)	0	100	100
4	SA	217/295 (74%)	207 (95%)	10 (5%)	0	100	100
5	SB	219/264 (83%)	210 (96%)	8 (4%)	1 (0%)	24	55
6	SH	187/194 (96%)	170 (91%)	17 (9%)	0	100	100
7	SI	204/208 (98%)	191 (94%)	13 (6%)	0	100	100
8	SL	152/158 (96%)	143 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	SV	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
10	SX	139/143 (97%)	133 (96%)	6 (4%)	0	100	100
11	Sa	100/115 (87%)	94 (94%)	6 (6%)	0	100	100
12	SC	218/293 (74%)	217 (100%)	1 (0%)	0	100	100
13	SG	232/249 (93%)	225 (97%)	7 (3%)	0	100	100
14	SJ	180/194 (93%)	171 (95%)	8 (4%)	1 (1%)	21	51
15	SN	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
16	SO	132/151 (87%)	119 (90%)	13 (10%)	0	100	100
17	SW	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
18	SY	122/133 (92%)	120 (98%)	2 (2%)	0	100	100
19	Sb	81/84 (96%)	76 (94%)	5 (6%)	0	100	100
20	Se	57/133 (43%)	53 (93%)	4 (7%)	0	100	100
22	SD	225/243 (93%)	214 (95%)	11 (5%)	0	100	100
23	SF	187/204 (92%)	175 (94%)	10 (5%)	2 (1%)	11	36
24	Sf	61/156 (39%)	48 (79%)	13 (21%)	0	100	100
25	SR	129/135 (96%)	127 (98%)	2 (2%)	0	100	100
26	Sd	53/56 (95%)	50 (94%)	3 (6%)	0	100	100
27	Sg	312/317 (98%)	292 (94%)	20 (6%)	0	100	100
28	Sc	67/69 (97%)	56 (84%)	11 (16%)	0	100	100
29	SK	95/165 (58%)	88 (93%)	7 (7%)	0	100	100
30	SM	116/132 (88%)	105 (90%)	11 (10%)	0	100	100
31	SU	100/119 (84%)	97 (97%)	3 (3%)	0	100	100
32	SQ	139/146 (95%)	127 (91%)	12 (9%)	0	100	100
33	SS	143/152 (94%)	138 (96%)	5 (4%)	0	100	100
34	ST	140/145 (97%)	136 (97%)	4 (3%)	0	100	100
35	SP	132/145 (91%)	120 (91%)	11 (8%)	1 (1%)	16	44
36	SZ	71/125 (57%)	68 (96%)	3 (4%)	0	100	100
37	D	292/315 (93%)	262 (90%)	28 (10%)	2 (1%)	18	47
38	E	470/472 (100%)	435 (93%)	34 (7%)	1 (0%)	43	72
39	F	14/333 (4%)	12 (86%)	2 (14%)	0	100	100
41	H	111/144 (77%)	99 (89%)	9 (8%)	3 (3%)	4	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	e	380/445 (85%)	324 (85%)	56 (15%)	0	100	100
43	d	408/548 (74%)	366 (90%)	42 (10%)	0	100	100
44	c	636/913 (70%)	579 (91%)	57 (9%)	0	100	100
45	a	588/1382 (42%)	524 (89%)	64 (11%)	0	100	100
46	3f	251/357 (70%)	209 (83%)	38 (15%)	4 (2%)	7	27
47	m	348/374 (93%)	274 (79%)	69 (20%)	5 (1%)	9	30
48	h	313/352 (89%)	252 (80%)	59 (19%)	2 (1%)	21	51
49	k	209/218 (96%)	189 (90%)	18 (9%)	2 (1%)	12	38
50	l	307/564 (54%)	287 (94%)	20 (6%)	0	100	100
All	All	9175/11992 (76%)	8398 (92%)	753 (8%)	24 (0%)	37	66

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	SB	22	VAL
35	SP	138	SER
37	D	200	TYR
46	3f	258	SER
46	3f	259	PRO
47	m	40	VAL
47	m	295	ASP
48	h	95	ASP
48	h	209	HIS
41	H	87	ASN
46	3f	262	VAL
47	m	29	ILE
47	m	292	ILE
37	D	4	LEU
38	E	274	LEU
41	H	55	VAL
49	k	207	PHE
14	SJ	3	VAL
46	3f	260	ASN
41	H	31	ASP
47	m	266	LEU
23	SF	79	HIS
23	SF	136	ARG
49	k	205	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Ln	23/24 (96%)	21 (91%)	2 (9%)	9	30
3	SE	224/225 (100%)	220 (98%)	4 (2%)	51	82
4	SA	182/243 (75%)	180 (99%)	2 (1%)	65	87
5	SB	202/231 (87%)	197 (98%)	5 (2%)	42	76
6	SH	169/174 (97%)	162 (96%)	7 (4%)	27	62
7	SI	178/180 (99%)	175 (98%)	3 (2%)	53	83
8	SL	138/142 (97%)	138 (100%)	0	100	100
9	SV	67/67 (100%)	65 (97%)	2 (3%)	36	72
10	SX	113/115 (98%)	110 (97%)	3 (3%)	39	74
11	Sa	89/98 (91%)	89 (100%)	0	100	100
12	SC	186/225 (83%)	182 (98%)	4 (2%)	45	78
13	SG	204/218 (94%)	202 (99%)	2 (1%)	68	88
14	SJ	161/168 (96%)	160 (99%)	1 (1%)	78	92
15	SN	130/131 (99%)	125 (96%)	5 (4%)	29	64
16	SO	105/118 (89%)	99 (94%)	6 (6%)	18	49
17	SW	112/113 (99%)	110 (98%)	2 (2%)	51	82
18	SY	108/115 (94%)	106 (98%)	2 (2%)	50	81
19	Sb	75/76 (99%)	74 (99%)	1 (1%)	61	86
20	Se	48/104 (46%)	46 (96%)	2 (4%)	26	61
22	SD	190/202 (94%)	187 (98%)	3 (2%)	55	83
23	SF	159/170 (94%)	156 (98%)	3 (2%)	50	81
24	Sf	56/140 (40%)	53 (95%)	3 (5%)	20	51
25	SR	119/122 (98%)	113 (95%)	6 (5%)	22	54
26	Sd	48/49 (98%)	44 (92%)	4 (8%)	10	32
27	Sg	272/275 (99%)	262 (96%)	10 (4%)	30	65
28	Sc	62/62 (100%)	57 (92%)	5 (8%)	11	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	SK	88/136 (65%)	84 (96%)	4 (4%)	24	58
30	SM	98/108 (91%)	95 (97%)	3 (3%)	35	70
31	SU	94/107 (88%)	92 (98%)	2 (2%)	47	79
32	SQ	117/121 (97%)	113 (97%)	4 (3%)	32	68
33	SS	126/132 (96%)	121 (96%)	5 (4%)	28	63
34	ST	112/114 (98%)	105 (94%)	7 (6%)	16	45
35	SP	120/130 (92%)	115 (96%)	5 (4%)	26	61
36	SZ	65/103 (63%)	63 (97%)	2 (3%)	35	70
37	D	264/280 (94%)	251 (95%)	13 (5%)	22	55
38	E	397/397 (100%)	384 (97%)	13 (3%)	33	69
39	F	16/304 (5%)	15 (94%)	1 (6%)	16	45
41	H	95/123 (77%)	91 (96%)	4 (4%)	26	61
42	e	206/406 (51%)	192 (93%)	14 (7%)	14	42
43	d	200/494 (40%)	184 (92%)	16 (8%)	11	34
44	c	563/811 (69%)	537 (95%)	26 (5%)	24	58
45	a	528/1259 (42%)	508 (96%)	20 (4%)	29	64
47	m	49/335 (15%)	48 (98%)	1 (2%)	48	80
All	All	6558/9147 (72%)	6331 (96%)	227 (4%)	32	67

All (227) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Ln	10	MET
2	Ln	20	MET
3	SE	19	MET
3	SE	60	GLU
3	SE	165	GLU
3	SE	220	THR
4	SA	2	SER
4	SA	29	ASN
5	SB	9	LEU
5	SB	59	SER
5	SB	69	VAL
5	SB	131	ASP
5	SB	208	HIS
6	SH	15	LYS

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Mol	Chain	Res	Type
6	SH	17	ASP
6	SH	28	LEU
6	SH	29	GLU
6	SH	43	LEU
6	SH	64	VAL
6	SH	109	ARG
7	SI	89	GLU
7	SI	100	CYS
7	SI	140	LYS
9	SV	15	ARG
9	SV	82	ASN
10	SX	64	SER
10	SX	96	GLU
10	SX	99	GLU
12	SC	80	GLU
12	SC	104	ASP
12	SC	146	GLU
12	SC	274	VAL
13	SG	168	LYS
13	SG	197	GLN
14	SJ	123	ILE
15	SN	14	SER
15	SN	22	VAL
15	SN	48	SER
15	SN	57	SER
15	SN	103	GLU
16	SO	51	GLU
16	SO	56	VAL
16	SO	63	LYS
16	SO	86	LYS
16	SO	91	THR
16	SO	103	ASN
17	SW	81	VAL
17	SW	111	MET
18	SY	54	VAL
18	SY	96	LEU
19	Sb	81	ARG
20	Se	1	LYS
20	Se	46	VAL
22	SD	31	GLU
22	SD	45	ARG
22	SD	142	LEU

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Mol	Chain	Res	Type
23	SF	34	SER
23	SF	36	GLN
23	SF	175	ASP
24	Sf	110	GLU
24	Sf	117	LEU
24	Sf	130	VAL
25	SR	5	ARG
25	SR	8	THR
25	SR	66	VAL
25	SR	77	GLU
25	SR	85	VAL
25	SR	105	MET
26	Sd	3	HIS
26	Sd	8	TRP
26	Sd	25	SER
26	Sd	48	LYS
27	Sg	63	SER
27	Sg	139	LYS
27	Sg	145	GLU
27	Sg	165	ILE
27	Sg	176	VAL
27	Sg	177	TRP
27	Sg	186	THR
27	Sg	197	THR
27	Sg	229	THR
27	Sg	309	VAL
28	Sc	11	LEU
28	Sc	15	THR
28	Sc	28	THR
28	Sc	50	VAL
28	Sc	61	SER
29	SK	2	LEU
29	SK	45	VAL
29	SK	58	VAL
29	SK	76	ILE
30	SM	68	LEU
30	SM	87	GLU
30	SM	89	VAL
31	SU	90	ASP
31	SU	106	ILE
32	SQ	31	LEU
32	SQ	114	GLN

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Mol	Chain	Res	Type
32	SQ	127	CYS
32	SQ	129	SER
33	SS	36	VAL
33	SS	43	VAL
33	SS	44	VAL
33	SS	83	PHE
33	SS	85	ASN
34	ST	28	LEU
34	ST	44	GLU
34	ST	87	VAL
34	ST	90	SER
34	ST	113	VAL
34	ST	114	GLU
34	ST	117	GLN
35	SP	16	THR
35	SP	26	LEU
35	SP	27	ASP
35	SP	31	GLU
35	SP	140	ARG
36	SZ	50	PHE
36	SZ	58	LEU
37	D	18	ASP
37	D	71	VAL
37	D	72	VAL
37	D	85	LEU
37	D	103	THR
37	D	125	GLU
37	D	162	ILE
37	D	163	LEU
37	D	167	ASP
37	D	169	ASN
37	D	200	TYR
37	D	239	THR
37	D	255	MET
38	E	14	HIS
38	E	140	ILE
38	E	141	LEU
38	E	152	MET
38	E	185	ILE
38	E	192	ILE
38	E	296	VAL
38	E	336	LEU

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Mol	Chain	Res	Type
38	E	337	ILE
38	E	348	CYS
38	E	405	MET
38	E	434	CYS
38	E	461	ARG
39	F	176	TYR
41	H	22	GLU
41	H	33	GLN
41	H	81	LEU
41	H	96	ASN
42	e	202	SER
42	e	219	LEU
42	e	225	HIS
42	e	231	ASN
42	e	242	TYR
42	e	249	MET
42	e	274	LEU
42	e	292	ILE
42	e	297	GLU
42	e	299	LEU
42	e	309	GLN
42	e	318	VAL
42	e	402	GLN
42	e	422	ILE
43	d	30	TYR
43	d	69	TYR
43	d	76	ASP
43	d	77	GLU
43	d	292	SER
43	d	294	THR
43	d	296	ASN
43	d	318	TYR
43	d	361	ARG
43	d	375	CYS
43	d	389	SER
43	d	393	ILE
43	d	403	HIS
43	d	404	CYS
43	d	426	LYS
43	d	430	TYR
44	c	84	GLU
44	c	155	HIS

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Mol	Chain	Res	Type
44	c	329	VAL
44	c	356	LEU
44	c	378	ILE
44	c	391	THR
44	c	401	CYS
44	c	408	LEU
44	c	411	ILE
44	c	423	ASN
44	c	548	MET
44	c	552	CYS
44	c	591	MET
44	c	648	GLN
44	c	691	MET
44	c	718	LEU
44	c	720	VAL
44	c	741	SER
44	c	779	LEU
44	c	799	TYR
44	c	815	LEU
44	c	820	SER
44	c	830	GLU
44	c	844	MET
44	c	845	HIS
44	c	858	GLN
45	a	29	ASP
45	a	96	MET
45	a	113	LEU
45	a	152	PHE
45	a	161	LEU
45	a	184	PHE
45	a	235	VAL
45	a	237	LEU
45	a	280	SER
45	a	344	MET
45	a	361	LEU
45	a	378	ASN
45	a	387	VAL
45	a	398	PHE
45	a	404	CYS
45	a	438	ARG
45	a	468	GLU
45	a	488	SER

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Mol	Chain	Res	Type
45	a	504	ASP
45	a	516	SER
47	m	316	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
3	SE	112	HIS
3	SE	216	ASN
4	SA	132	GLN
5	SB	76	ASN
5	SB	149	GLN
7	SI	99	ASN
8	SL	13	GLN
12	SC	113	GLN
12	SC	136	HIS
15	SN	90	HIS
16	SO	26	ASN
18	SY	63	HIS
18	SY	89	HIS
22	SD	101	GLN
23	SF	149	GLN
23	SF	165	ASN
23	SF	179	ASN
25	SR	127	ASN
27	Sg	20	GLN
27	Sg	188	HIS
31	SU	47	ASN
31	SU	92	HIS
32	SQ	77	HIS
32	SQ	97	GLN
33	SS	10	GLN
34	ST	10	ASN
35	SP	114	HIS
37	D	40	ASN
38	E	292	GLN
38	E	396	GLN
42	e	225	HIS
43	d	57	ASN
43	d	416	GLN
44	c	149	ASN
44	c	670	GLN

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Mol	Chain	Res	Type
44	c	676	HIS
45	a	200	ASN
45	a	257	HIS
45	a	378	ASN
45	a	518	GLN
45	a	560	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S2	1713/1869 (91%)	342 (19%)	13 (0%)
21	B	27/50 (54%)	17 (62%)	1 (3%)
40	G	72/75 (96%)	16 (22%)	1 (1%)
All	All	1812/1994 (90%)	375 (20%)	15 (0%)

All (375) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S2	2	A
1	S2	4	C
1	S2	17	C
1	S2	26	U
1	S2	33	G
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

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Mol	Chain	Res	Type
1	S2	143	U
1	S2	155	G
1	S2	166	A2M
1	S2	168	C
1	S2	175	A
1	S2	184	G
1	S2	192	C
1	S2	196	C
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	294	U
1	S2	306	C
1	S2	307	G
1	S2	308	G
1	S2	309	G
1	S2	319	C
1	S2	321	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

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Mol	Chain	Res	Type
1	S2	436	OMG
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	482	G
1	S2	487	U
1	S2	488	U
1	S2	492	C
1	S2	493	A
1	S2	502	C
1	S2	525	A
1	S2	531	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	548	C
1	S2	552	G
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

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Mol	Chain	Res	Type
1	S2	598	G
1	S2	607	U
1	S2	608	C
1	S2	614	C
1	S2	615	C
1	S2	617	G
1	S2	627	U
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
1	S2	688	U
1	S2	692	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	796	G
1	S2	797	C
1	S2	798	G

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Mol	Chain	Res	Type
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	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
1	S2	842	C
1	S2	847	A
1	S2	866	PSU
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

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Mol	Chain	Res	Type
1	S2	922	A
1	S2	933	G
1	S2	943	U
1	S2	969	U
1	S2	971	G
1	S2	972	A
1	S2	990	A
1	S2	992	A
1	S2	1017	U
1	S2	1023	A
1	S2	1027	A
1	S2	1061	U
1	S2	1062	A
1	S2	1081	U
1	S2	1083	A
1	S2	1085	C
1	S2	1089	G
1	S2	1109	C
1	S2	1114	U
1	S2	1115	U
1	S2	1116	C
1	S2	1118	C
1	S2	1119	A
1	S2	1133	A
1	S2	1138	C
1	S2	1139	C
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	1211	G
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

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Mol	Chain	Res	Type
1	S2	1256	G
1	S2	1257	G
1	S2	1258	A
1	S2	1259	A
1	S2	1274	G
1	S2	1275	G
1	S2	1286	G
1	S2	1301	A
1	S2	1302	G
1	S2	1303	C
1	S2	1306	U
1	S2	1307	U
1	S2	1308	U
1	S2	1309	C
1	S2	1310	U
1	S2	1311	C
1	S2	1312	G
1	S2	1314	U
1	S2	1315	U
1	S2	1317	C
1	S2	1322	G
1	S2	1327	G
1	S2	1343	U
1	S2	1348	G
1	S2	1371	U
1	S2	1372	U
1	S2	1378	A
1	S2	1398	G
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	1434	C
1	S2	1435	C
1	S2	1436	C
1	S2	1437	C
1	S2	1438	A
1	S2	1454	A
1	S2	1462	U

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Mol	Chain	Res	Type
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	1521	C
1	S2	1531	A
1	S2	1533	A
1	S2	1534	C
1	S2	1544	C
1	S2	1553	C
1	S2	1556	A
1	S2	1570	G
1	S2	1579	A
1	S2	1580	A
1	S2	1588	A
1	S2	1601	A
1	S2	1606	G
1	S2	1621	U
1	S2	1623	A
1	S2	1648	G
1	S2	1654	G
1	S2	1663	A
1	S2	1664	A
1	S2	1665	G
1	S2	1671	G
1	S2	1680	G
1	S2	1699	A
1	S2	1715	A
1	S2	1721	U
1	S2	1722	G
1	S2	1726	G
1	S2	1729	U
1	S2	1744	G
1	S2	1745	A
1	S2	1748	G
1	S2	1751	C
1	S2	1753	C
1	S2	1755	C
1	S2	1757	G

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Mol	Chain	Res	Type
1	S2	1758	G
1	S2	1760	G
1	S2	1761	U
1	S2	1773	C
1	S2	1774	C
1	S2	1777	G
1	S2	1780	G
1	S2	1782	G
1	S2	1783	C
1	S2	1786	U
1	S2	1805	G
1	S2	1806	A
1	S2	1824	A
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	1864	U
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	7	U
21	B	8	A
21	B	9	A
21	B	10	C
21	B	12	G
21	B	14	C
21	B	15	U
21	B	16	C
21	B	17	C
21	B	18	U

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Mol	Chain	Res	Type
40	G	5	A
40	G	8	G
40	G	9	U
40	G	11[1]	2MG
40	G	12	C
40	G	17	C
40	G	20	A
40	G	21	A
40	G	48	5MC
40	G	49	G
40	G	54	A
40	G	59	A
40	G	73	A
40	G	74	C
40	G	75	C
40	G	76	A

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	S2	324	C
1	S2	329	G
1	S2	563	G
1	S2	866	PSU
1	S2	905	C
1	S2	1114	U
1	S2	1257	G
1	S2	1308	U
1	S2	1309	C
1	S2	1316	C
1	S2	1342	U
1	S2	1433	C
1	S2	1520	G
21	B	-5	G
40	G	73	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	PSU	S2	1136	1	18,21,22	0.57	0	22,30,33	0.55	0
1	PSU	S2	1445	1	18,21,22	0.58	0	22,30,33	0.56	0
1	B8N	S2	1248	1	24,29,30	0.60	0	29,42,45	0.64	0
1	4AC	S2	1337	1	21,24,25	0.34	0	29,34,37	0.42	0
1	A2M	S2	512	1	22,25,26	0.11	0	31,36,39	0.41	0
1	OMU	S2	1288	1	19,22,23	0.30	0	26,31,34	0.42	0
1	PSU	S2	36	1	18,21,22	0.56	0	22,30,33	0.52	0
1	OMG	S2	1490	1,52	23,26,27	0.38	0	33,38,41	0.37	0
1	OMC	S2	462	1	19,22,23	0.32	0	26,31,34	0.40	0
1	PSU	S2	667	1	18,21,22	0.65	1 (5%)	22,30,33	0.52	0
1	PSU	S2	1045	1	18,21,22	0.51	0	22,30,33	0.60	0
1	PSU	S2	1186	1	18,21,22	0.51	0	22,30,33	0.60	0
1	OMG	S2	683	1	23,26,27	0.34	0	33,38,41	0.45	0
34	NMM	ST	67	34	9,11,12	0.62	0	6,12,14	1.72	2 (33%)
1	PSU	S2	366	1	18,21,22	0.54	0	22,30,33	0.53	0
1	PSU	S2	1046	1	18,21,22	0.58	0	22,30,33	0.54	0
1	PSU	S2	1232	1	18,21,22	0.55	0	22,30,33	0.54	0
40	1MA	G	58	40	21,25,26	0.49	0	31,37,40	0.72	1 (3%)
1	PSU	S2	966	1	18,21,22	0.54	0	22,30,33	0.53	0
1	PSU	S2	866	1	18,21,22	0.56	0	22,30,33	0.60	0
1	A2M	S2	159	1	22,25,26	0.11	0	31,36,39	0.23	0
1	PSU	S2	300	1	18,21,22	0.55	0	22,30,33	0.53	0
1	OMU	S2	172	1	19,22,23	0.27	0	26,31,34	0.51	0
1	OMC	S2	517	1	19,22,23	0.32	0	26,31,34	0.46	0
1	PSU	S2	609	1	18,21,22	0.54	0	22,30,33	0.61	0
1	PSU	S2	1056	1	18,21,22	0.56	0	22,30,33	0.57	0
1	A2M	S2	668	1	22,25,26	0.14	0	31,36,39	0.32	0
1	A2M	S2	468	1	22,25,26	0.10	0	31,36,39	0.35	0
1	PSU	S2	1347	1	18,21,22	0.59	0	22,30,33	0.56	0
1	PSU	S2	63	1	18,21,22	0.51	0	22,30,33	0.56	0
1	PSU	S2	801	1	18,21,22	0.52	0	22,30,33	0.53	0
1	PSU	S2	34	1	18,21,22	0.54	0	22,30,33	0.57	0
1	OMG	S2	436	1	23,26,27	0.38	0	33,38,41	0.44	0
1	PSU	S2	296	1	18,21,22	0.55	0	22,30,33	0.55	0
1	PSU	S2	681	1	18,21,22	0.59	0	22,30,33	0.53	0
1	PSU	S2	1360	1,51	18,21,22	0.57	0	22,30,33	0.63	1 (4%)
1	A2M	S2	1031	1	22,25,26	0.11	0	31,36,39	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	2MG	G	26	40	23,26,27	0.33	0	32,38,41	0.35	0
1	PSU	S2	406	1	18,21,22	0.53	0	22,30,33	0.56	0
1	OMC	S2	174	1	19,22,23	0.29	0	26,31,34	0.39	0
1	PSU	S2	1367	1	18,21,22	0.56	0	22,30,33	0.58	0
1	OMU	S2	116	1	19,22,23	0.30	0	26,31,34	0.42	0
1	PSU	S2	863	1	18,21,22	0.57	0	22,30,33	0.54	0
1	PSU	S2	1004	1	18,21,22	0.57	0	22,30,33	0.57	0
1	PSU	S2	822	1	18,21,22	0.60	1 (5%)	22,30,33	0.58	1 (4%)
1	A2M	S2	99	1,52	22,25,26	0.10	0	31,36,39	0.29	0
1	PSU	S2	572	1	18,21,22	0.55	0	22,30,33	0.55	0
1	PSU	S2	1596	1	18,21,22	0.55	0	22,30,33	0.55	0
1	MA6	S2	1850	1	23,26,27	0.33	0	34,38,41	0.61	1 (2%)
1	OMU	S2	428	1	19,22,23	0.26	0	26,31,34	0.43	0
1	OMC	S2	1703	1,52	19,22,23	0.30	0	26,31,34	0.43	0
1	PSU	S2	100	1,52	18,21,22	0.50	0	22,30,33	0.58	0
1	OMG	S2	601	1	23,26,27	0.35	0	33,38,41	0.34	0
1	OMU	S2	121	1	19,22,23	0.33	0	26,31,34	0.49	0
1	PSU	S2	1238	1	18,21,22	0.56	0	22,30,33	0.59	0
1	PSU	S2	686	1	18,21,22	0.53	0	22,30,33	0.55	0
1	PSU	S2	1643	1,52	18,21,22	0.61	0	22,30,33	0.53	0
40	1MG	G	10	40	22,26,27	0.30	0	33,39,42	0.62	1 (3%)
1	A2M	S2	576	1	22,25,26	0.09	0	31,36,39	0.28	0
1	PSU	S2	105	1	18,21,22	0.54	0	22,30,33	0.57	0
1	PSU	S2	815	1	18,21,22	0.50	0	22,30,33	0.59	0
1	OMC	S2	1391	1	19,22,23	0.32	0	26,31,34	0.46	0
1	OMU	S2	354	1	19,22,23	0.34	0	26,31,34	0.54	0
1	PSU	S2	651	1	18,21,22	0.56	0	22,30,33	0.56	0
1	PSU	S2	649	1	18,21,22	0.54	0	22,30,33	0.62	0
1	OMG	S2	509	1,52	23,26,27	0.36	0	33,38,41	0.47	0
1	A2M	S2	590	1	22,25,26	0.11	0	31,36,39	0.30	0
1	OMU	S2	1804	1	19,22,23	0.30	0	26,31,34	0.41	0
1	A2M	S2	1383	1	22,25,26	0.11	0	31,36,39	0.53	0
1	OMG	S2	1328	1,51	23,26,27	0.34	0	33,38,41	0.40	0
1	4AC	S2	1842	1	21,24,25	0.33	0	29,34,37	0.29	0
1	PSU	S2	1625	1	18,21,22	0.55	0	22,30,33	0.60	0
1	OMU	S2	1442	1,52	19,22,23	0.33	0	26,31,34	0.41	0
1	A2M	S2	1678	1	22,25,26	0.11	0	31,36,39	0.26	0
1	PSU	S2	93	1	18,21,22	0.55	0	22,30,33	0.55	0
1	PSU	S2	918	1	18,21,22	0.48	0	22,30,33	0.39	0
1	OMG	S2	1447	1	23,26,27	0.34	0	33,38,41	0.39	0
1	PSU	S2	1003	1	18,21,22	0.60	0	22,30,33	0.54	0
1	PSU	S2	814	1	18,21,22	0.54	0	22,30,33	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	5MC	G	48	40	18,22,23	0.55	0	26,32,35	0.57	0
1	PSU	S2	1244	1	18,21,22	0.55	0	22,30,33	0.56	0
1	PSU	S2	119	1	18,21,22	0.54	0	22,30,33	0.56	0
1	PSU	S2	109	1	18,21,22	0.54	0	22,30,33	0.54	0
1	6MZ	S2	1832	1,52,51	22,25,26	0.15	0	30,36,39	0.30	0
1	UY1	S2	1326	1,52	19,22,23	0.40	0	22,31,34	0.49	0
1	PSU	S2	1177	1	18,21,22	0.54	0	22,30,33	0.57	0
1	MA6	S2	1851	1	23,26,27	0.37	0	34,38,41	0.66	1 (2%)
1	A2M	S2	166	1	22,25,26	0.11	0	31,36,39	0.42	0
1	OMC	S2	1272	1	19,22,23	0.33	0	26,31,34	0.38	0
1	OMG	S2	867	1	23,26,27	0.31	0	33,38,41	0.31	0
1	A2M	S2	484	1	22,25,26	0.09	0	31,36,39	0.23	0
16	IAS	SO	138	16	6,7,8	1.03	0	6,8,10	1.65	3 (50%)
40	T6A	G	37	40	31,34,35	0.46	0	44,49,52	0.53	0
1	PSU	S2	218	1	18,21,22	0.52	0	22,30,33	0.57	0
1	OMG	S2	644	1	23,26,27	0.32	0	33,38,41	0.42	0
1	A2M	S2	27	1	22,25,26	0.10	0	31,36,39	0.28	0
1	PSU	S2	1692	1	18,21,22	0.57	0	22,30,33	0.53	0
40	H2U	G	47	40	18,21,22	0.33	0	21,30,33	0.53	0
1	PSU	S2	1174	1	18,21,22	0.56	0	22,30,33	0.59	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	PSU	S2	1136	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1445	1	-	0/7/25/26	0/2/2/2
1	B8N	S2	1248	1	-	0/16/34/35	0/2/2/2
1	4AC	S2	1337	1	-	0/11/29/30	0/2/2/2
1	A2M	S2	512	1	-	0/9/27/28	0/3/3/3
1	OMU	S2	1288	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	36	1	-	0/7/25/26	0/2/2/2
1	OMG	S2	1490	1,52	-	2/9/27/28	0/3/3/3
1	OMC	S2	462	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	667	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1045	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1186	1	-	0/7/25/26	0/2/2/2
1	OMG	S2	683	1	-	0/9/27/28	0/3/3/3
34	NMM	ST	67	34	-	0/9/11/13	-
1	PSU	S2	366	1	-	1/7/25/26	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	PSU	S2	1232	1	-	0/7/25/26	0/2/2/2
40	1MA	G	58	40	-	0/7/25/26	0/3/3/3
1	PSU	S2	966	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	866	1	-	3/7/25/26	0/2/2/2
1	A2M	S2	159	1	-	3/9/27/28	0/3/3/3
1	PSU	S2	300	1	-	0/7/25/26	0/2/2/2
1	OMU	S2	172	1	-	1/9/27/28	0/2/2/2
1	OMC	S2	517	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	609	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1056	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	468	1	-	0/9/27/28	0/3/3/3
1	PSU	S2	1347	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	63	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	801	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	34	1	-	0/7/25/26	0/2/2/2
1	OMG	S2	436	1	-	2/9/27/28	0/3/3/3
1	PSU	S2	296	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	681	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1360	1,51	-	0/7/25/26	0/2/2/2
1	A2M	S2	1031	1	-	1/9/27/28	0/3/3/3
40	2MG	G	26	40	-	4/9/27/28	0/3/3/3
1	PSU	S2	406	1	-	0/7/25/26	0/2/2/2
1	OMC	S2	174	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	1367	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	863	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1004	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	822	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	99	1,52	-	0/9/27/28	0/3/3/3
1	PSU	S2	572	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1596	1	-	0/7/25/26	0/2/2/2
1	MA6	S2	1850	1	-	0/11/29/30	0/3/3/3
1	OMU	S2	428	1	-	4/9/27/28	0/2/2/2
1	OMC	S2	1703	1,52	-	0/9/27/28	0/2/2/2
1	PSU	S2	100	1,52	-	0/7/25/26	0/2/2/2
1	OMG	S2	601	1	-	0/9/27/28	0/3/3/3
1	OMU	S2	121	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	1238	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	686	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	S2	1643	1,52	-	0/7/25/26	0/2/2/2
40	1MG	G	10	40	-	2/7/25/26	0/3/3/3
1	A2M	S2	576	1	-	3/9/27/28	0/3/3/3
1	PSU	S2	105	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	815	1	-	0/7/25/26	0/2/2/2
1	OMC	S2	1391	1	-	0/9/27/28	0/2/2/2
1	OMU	S2	354	1	-	1/9/27/28	0/2/2/2
1	PSU	S2	651	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	649	1	-	0/7/25/26	0/2/2/2
1	OMG	S2	509	1,52	-	0/9/27/28	0/3/3/3
1	A2M	S2	590	1	-	3/9/27/28	0/3/3/3
1	OMU	S2	1804	1	-	0/9/27/28	0/2/2/2
1	A2M	S2	1383	1	-	2/9/27/28	0/3/3/3
1	OMG	S2	1328	1,51	-	0/9/27/28	0/3/3/3
1	4AC	S2	1842	1	-	0/11/29/30	0/2/2/2
1	PSU	S2	1625	1	-	0/7/25/26	0/2/2/2
1	OMU	S2	1442	1,52	-	0/9/27/28	0/2/2/2
1	A2M	S2	1678	1	-	0/9/27/28	0/3/3/3
1	PSU	S2	93	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	918	1	-	1/7/25/26	0/2/2/2
1	OMG	S2	1447	1	-	2/9/27/28	0/3/3/3
1	PSU	S2	1003	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	814	1	-	0/7/25/26	0/2/2/2
40	5MC	G	48	40	-	2/7/25/26	0/2/2/2
1	PSU	S2	1244	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	119	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	109	1	-	0/7/25/26	0/2/2/2
1	6MZ	S2	1832	1,52,51	-	2/9/27/28	0/3/3/3
1	UY1	S2	1326	1,52	-	3/9/27/28	0/2/2/2
1	PSU	S2	1177	1	-	0/7/25/26	0/2/2/2
1	MA6	S2	1851	1	-	2/11/29/30	0/3/3/3
1	A2M	S2	166	1	-	2/9/27/28	0/3/3/3
1	OMC	S2	1272	1	-	0/9/27/28	0/2/2/2
1	OMG	S2	867	1	-	2/9/27/28	0/3/3/3
1	A2M	S2	484	1	-	0/9/27/28	0/3/3/3
16	IAS	SO	138	16	-	1/7/7/8	-
40	T6A	G	37	40	-	2/23/41/42	0/3/3/3
1	PSU	S2	218	1	-	0/7/25/26	0/2/2/2
1	OMG	S2	644	1	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	S2	27	1	-	1/9/27/28	0/3/3/3
1	PSU	S2	1692	1	-	0/7/25/26	0/2/2/2
40	H2U	G	47	40	-	3/7/38/39	0/2/2/2
1	PSU	S2	1174	1	-	0/7/25/26	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	822	PSU	O4'-C1'	-2.08	1.41	1.43
1	S2	667	PSU	O4'-C1'	-2.07	1.41	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	-3.25	116.50	119.48
40	G	10	1MG	C6-C5-C4	-2.62	117.07	119.97
1	S2	1850	MA6	C2-N1-C6	2.36	117.33	111.75
34	ST	67	NMM	NE-CZ-NH1	2.35	124.65	120.26
1	S2	1851	MA6	C2-N1-C6	2.33	117.25	111.75
16	SO	138	IAS	OD1-CG-CB	-2.30	118.72	125.43
40	G	58	1MA	N1-C6-N6	2.24	125.46	119.77
16	SO	138	IAS	OXT-C-O	-2.15	119.20	124.09
1	S2	1360	PSU	O4'-C1'-C2'	2.07	108.06	105.14
1	S2	822	PSU	O4'-C1'-C2'	2.05	108.03	105.14
16	SO	138	IAS	OXT-C-CA	2.03	120.31	113.38

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	S2	27	A2M	C1'-C2'-O2'-CM'
1	S2	159	A2M	C3'-C4'-C5'-O5'
1	S2	166	A2M	C1'-C2'-O2'-CM'
1	S2	354	OMU	C1'-C2'-O2'-CM2
1	S2	428	OMU	C2'-C1'-N1-C2
1	S2	428	OMU	C2'-C1'-N1-C6
1	S2	436	OMG	O4'-C4'-C5'-O5'
1	S2	436	OMG	C3'-C4'-C5'-O5'
1	S2	576	A2M	C1'-C2'-O2'-CM'
1	S2	668	A2M	C1'-C2'-O2'-CM'
1	S2	867	OMG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	S2	867	OMG	C3'-C4'-C5'-O5'
1	S2	1031	A2M	C1'-C2'-O2'-CM'
1	S2	1326	UY1	C2'-C1'-C5-C6
1	S2	1326	UY1	C1'-C2'-O2'-CM2
1	S2	1383	A2M	C1'-C2'-O2'-CM'
1	S2	1832	6MZ	C5-C6-N6-C9
1	S2	1832	6MZ	N1-C6-N6-C9
16	SO	138	IAS	CA-CB-CG-OD1
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	37	T6A	C14-C12-C13-ODB
40	G	47	H2U	C2'-C1'-N1-C2
1	S2	159	A2M	O4'-C4'-C5'-O5'
1	S2	576	A2M	O4'-C4'-C5'-O5'
1	S2	576	A2M	C3'-C4'-C5'-O5'
1	S2	866	PSU	O4'-C4'-C5'-O5'
1	S2	1490	OMG	O4'-C4'-C5'-O5'
1	S2	1851	MA6	O4'-C4'-C5'-O5'
40	G	48	5MC	O4'-C4'-C5'-O5'
1	S2	1447	OMG	C3'-C4'-C5'-O5'
1	S2	1851	MA6	C3'-C4'-C5'-O5'
40	G	48	5MC	C3'-C4'-C5'-O5'
1	S2	172	OMU	C3'-C2'-O2'-CM2
40	G	47	H2U	C2'-C1'-N1-C6
1	S2	866	PSU	C3'-C4'-C5'-O5'
1	S2	1447	OMG	O4'-C4'-C5'-O5'
40	G	37	T6A	C14-C12-C13-ODA
1	S2	644	OMG	C4'-C5'-O5'-P
1	S2	1490	OMG	C4'-C5'-O5'-P
1	S2	428	OMU	O4'-C1'-N1-C6
1	S2	166	A2M	O4'-C4'-C5'-O5'
1	S2	366	PSU	O4'-C1'-C5-C4
1	S2	866	PSU	O4'-C1'-C5-C4
1	S2	159	A2M	C3'-C2'-O2'-CM'
1	S2	428	OMU	O4'-C1'-N1-C2
1	S2	590	A2M	C2'-C1'-N9-C4
1	S2	590	A2M	C2'-C1'-N9-C8
1	S2	668	A2M	C2'-C1'-N9-C8
40	G	10	1MG	C2'-C1'-N9-C8
1	S2	1383	A2M	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
40	G	10	1MG	O4'-C4'-C5'-O5'
1	S2	918	PSU	O4'-C1'-C5-C6
1	S2	1326	UY1	O4'-C1'-C5-C6
1	S2	590	A2M	O4'-C1'-N9-C8
1	S2	668	A2M	O4'-C4'-C5'-O5'
40	G	47	H2U	O4'-C1'-N1-C2

There are no ring outliers.

35 monomers are involved in 58 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	S2	512	A2M	2	0
1	S2	462	OMC	1	0
1	S2	683	OMG	1	0
1	S2	866	PSU	2	0
1	S2	159	A2M	2	0
1	S2	172	OMU	1	0
1	S2	468	A2M	3	0
1	S2	1031	A2M	1	0
40	G	26	2MG	1	0
1	S2	116	OMU	2	0
1	S2	99	A2M	2	0
1	S2	572	PSU	2	0
1	S2	1850	MA6	1	0
1	S2	1703	OMC	1	0
1	S2	121	OMU	3	0
1	S2	1238	PSU	1	0
40	G	10	1MG	3	0
1	S2	576	A2M	5	0
1	S2	815	PSU	1	0
1	S2	354	OMU	1	0
1	S2	590	A2M	1	0
1	S2	1383	A2M	3	0
1	S2	1842	4AC	1	0
1	S2	1442	OMU	2	0
1	S2	918	PSU	2	0
1	S2	814	PSU	1	0
1	S2	1244	PSU	1	0
1	S2	1832	6MZ	1	0
1	S2	1326	UY1	1	0
1	S2	1851	MA6	2	0
1	S2	166	A2M	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	S2	484	A2M	2	0
1	S2	27	A2M	1	0
40	G	47	H2U	1	0
1	S2	1174	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 110 ligands modelled in this entry, 108 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
54	GNP	E	501	-	33,34,34	2.24	6 (18%)	46,54,54	1.47	4 (8%)
55	MET	E	502	-	6,7,8	0.48	0	2,7,9	0.18	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
54	GNP	E	501	-	-	4/18/38/38	0/3/3/3
55	MET	E	502	-	-	1/5/6/8	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	E	501	GNP	PB-O3A	8.05	1.69	1.59
54	E	501	GNP	PG-N3B	6.60	1.80	1.63
54	E	501	GNP	PG-O1G	4.68	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	E	501	GNP	PB-O1B	3.15	1.51	1.46
54	E	501	GNP	PB-O2B	-2.19	1.50	1.56
54	E	501	GNP	PB-N3B	2.03	1.68	1.63

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	E	501	GNP	O1G-PG-N3B	-7.30	101.01	111.77
54	E	501	GNP	O2B-PB-O1B	4.51	119.37	109.92
54	E	501	GNP	O2G-PG-O3G	2.30	113.76	107.64
54	E	501	GNP	O3A-PB-N3B	-2.20	100.49	106.59

There are no chirality outliers.

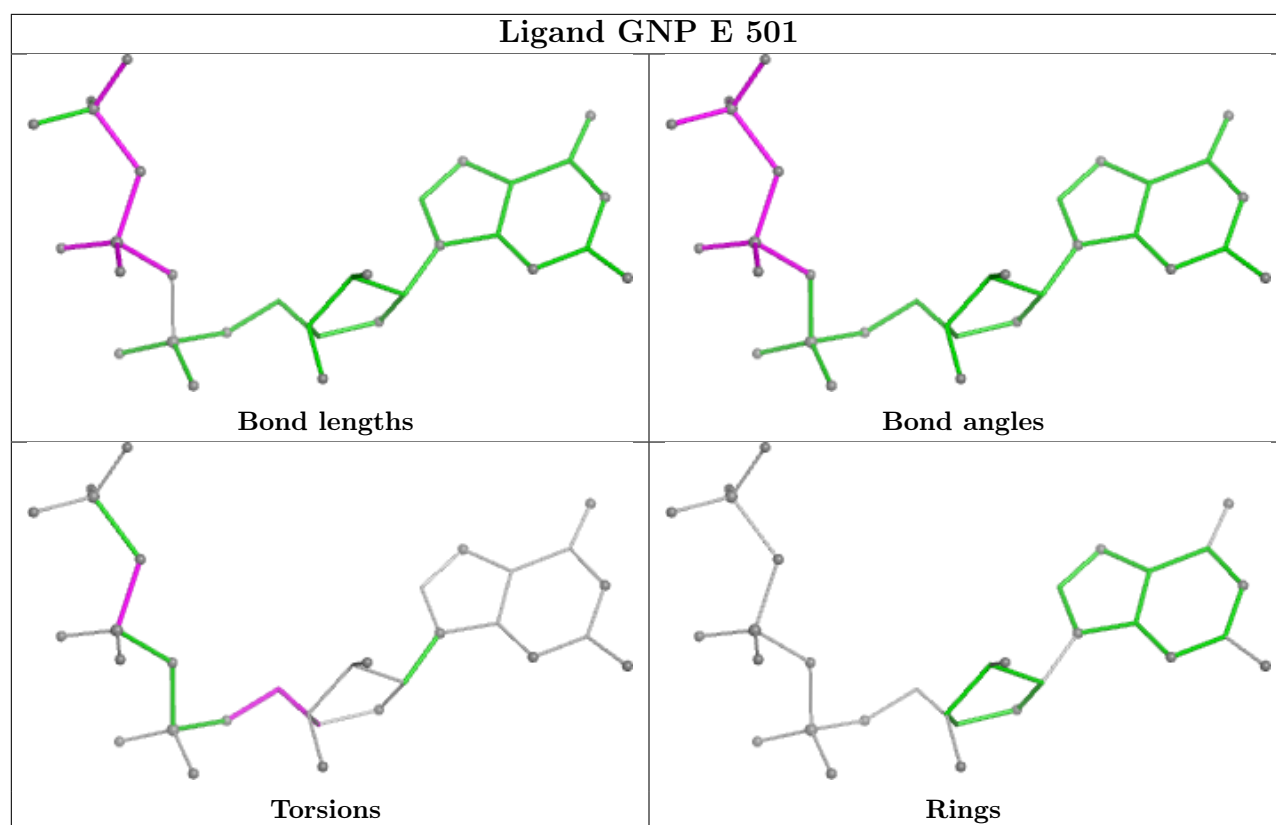
All (5) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

There are no chain breaks in this entry.

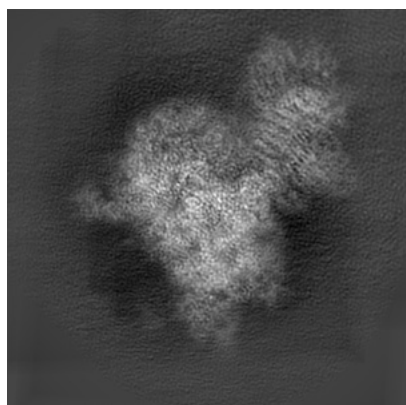
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-57009. These allow visual inspection of the internal detail of the map and identification of artifacts.

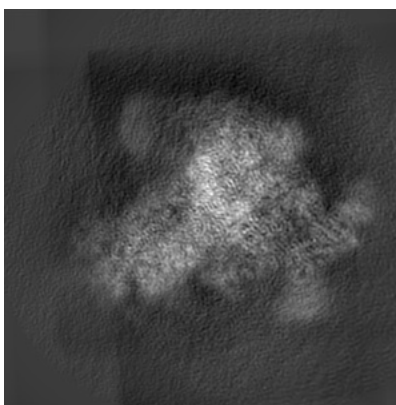
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

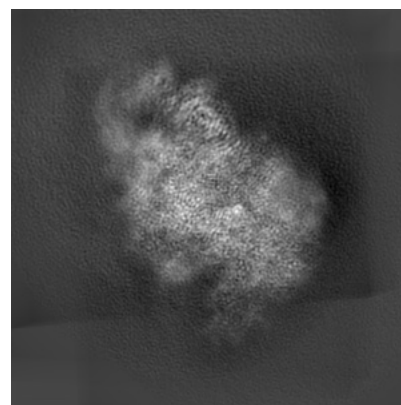
6.1.1 Primary map



X



Y

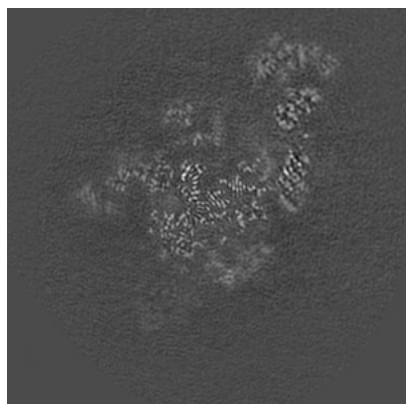


Z

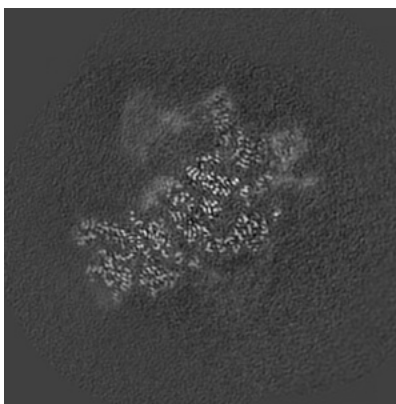
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

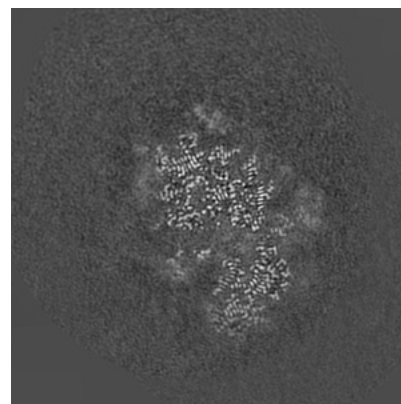
6.2.1 Primary map



X Index: 260



Y Index: 260

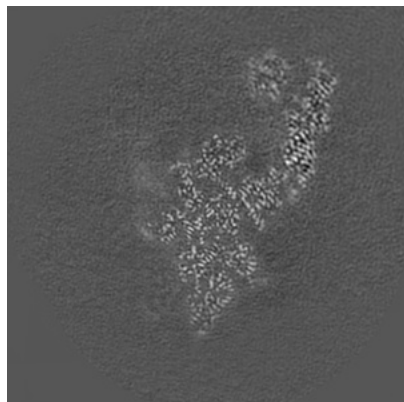


Z Index: 260

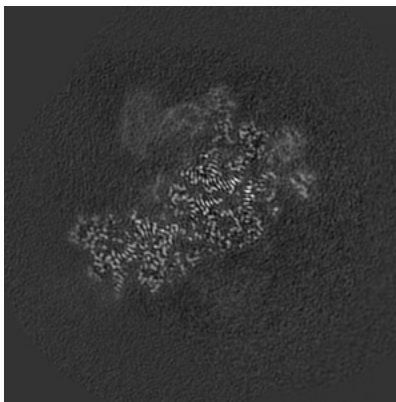
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

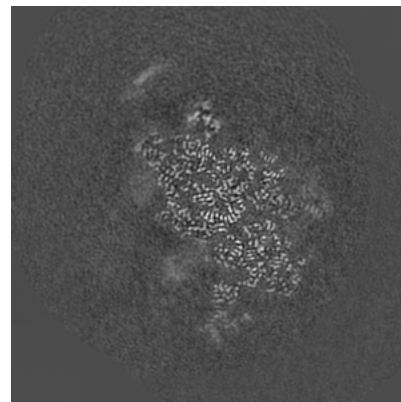
6.3.1 Primary map



X Index: 232



Y Index: 254

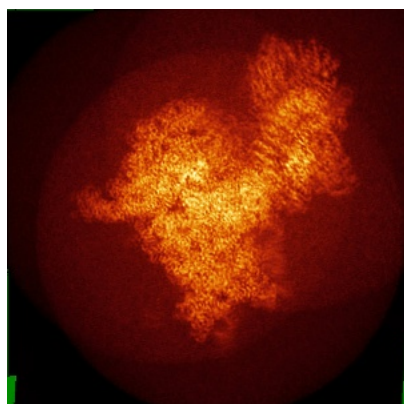


Z Index: 279

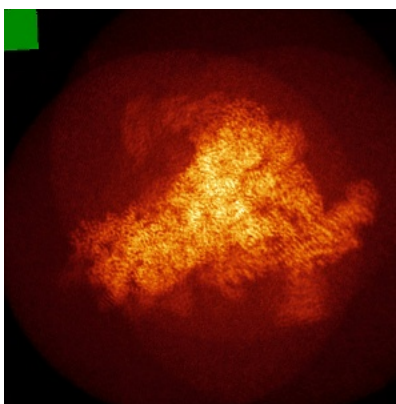
The images above show the largest variance slices of the map in three orthogonal directions.

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

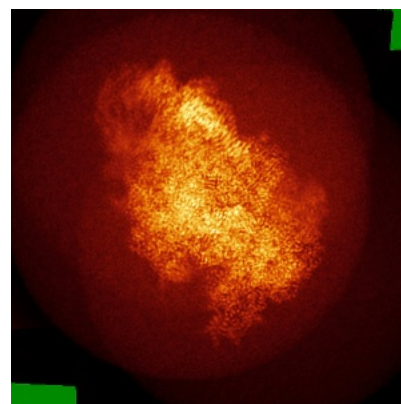
6.4.1 Primary map



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

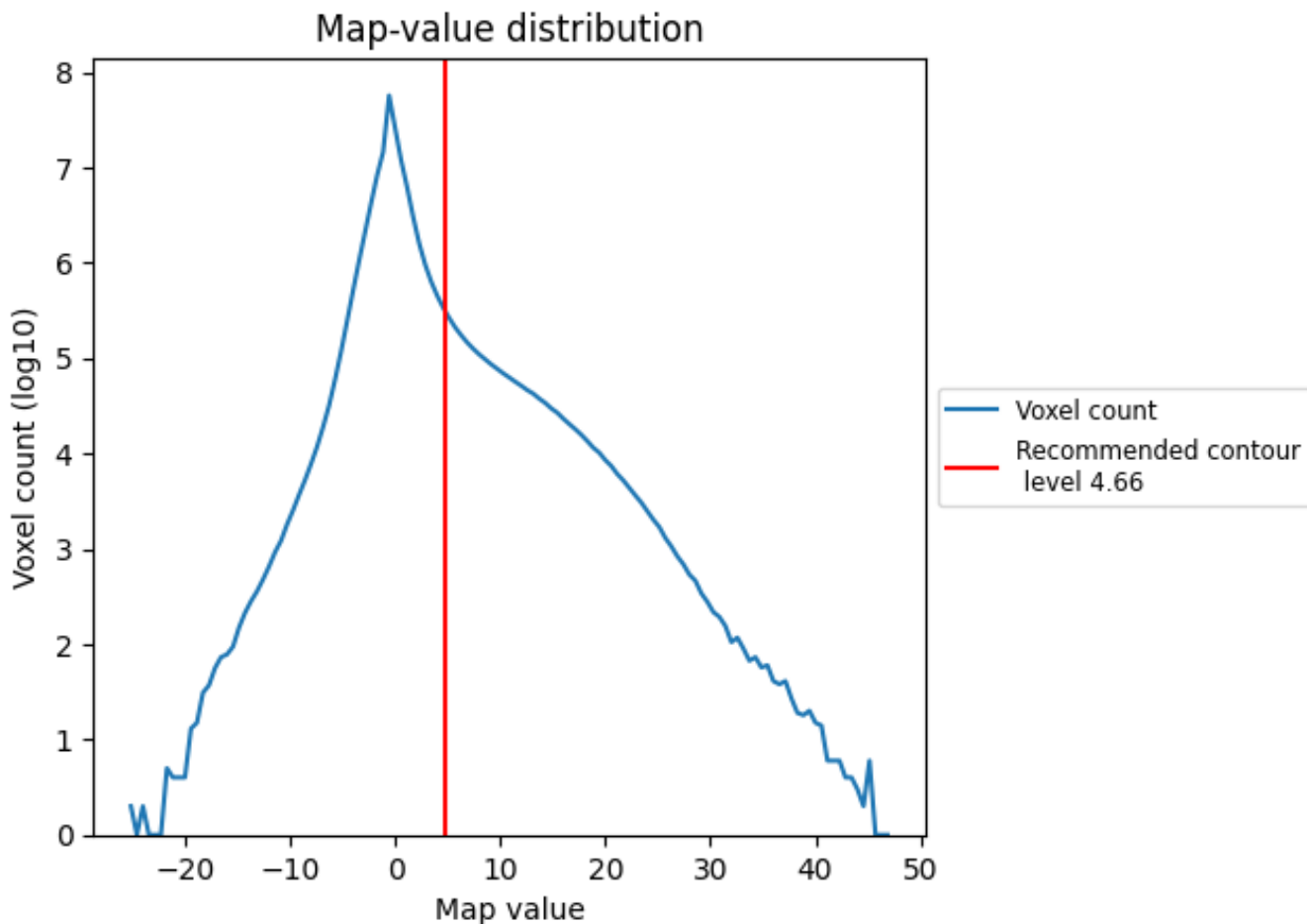
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

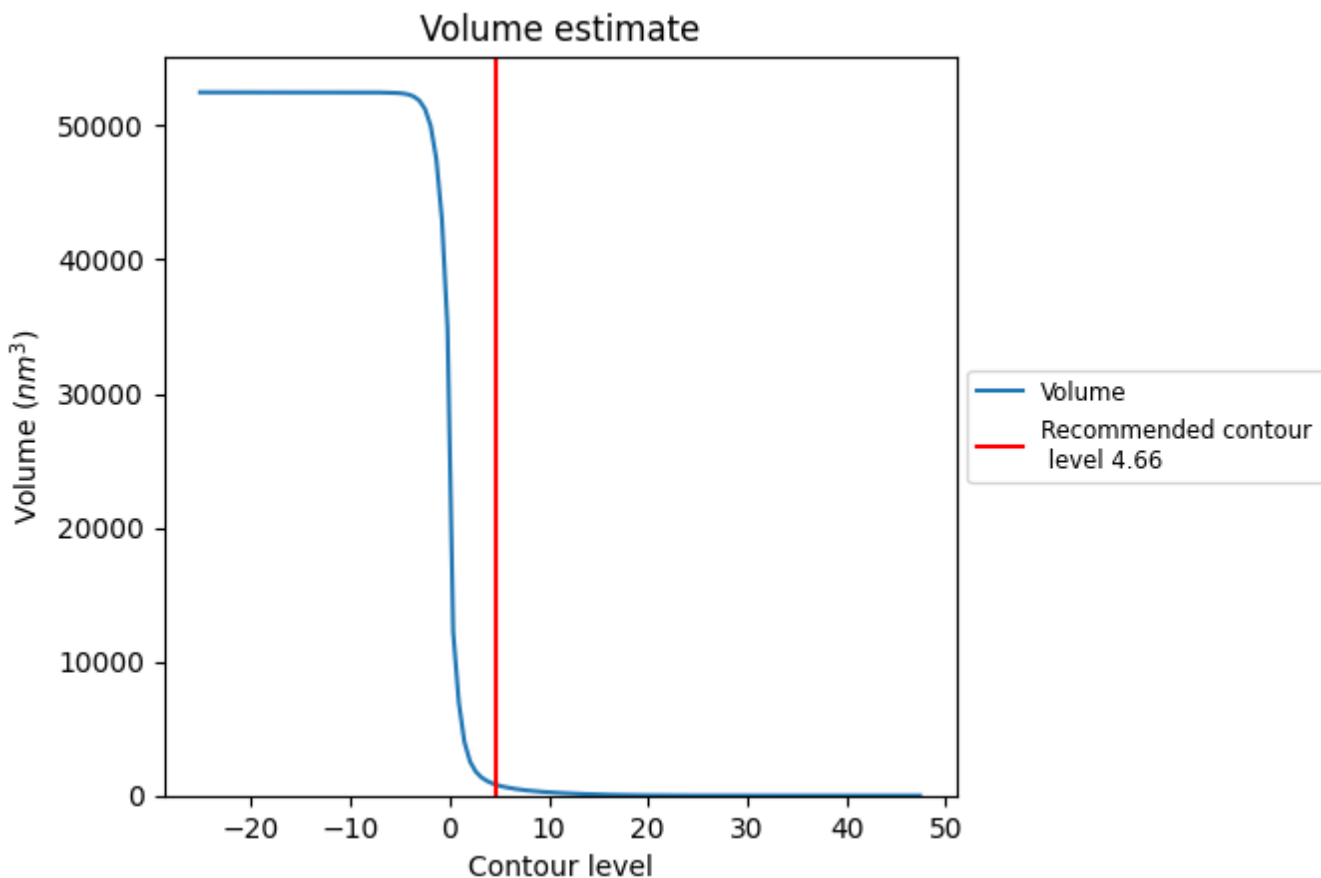
This section contains the results of statistical analysis of the map.

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.

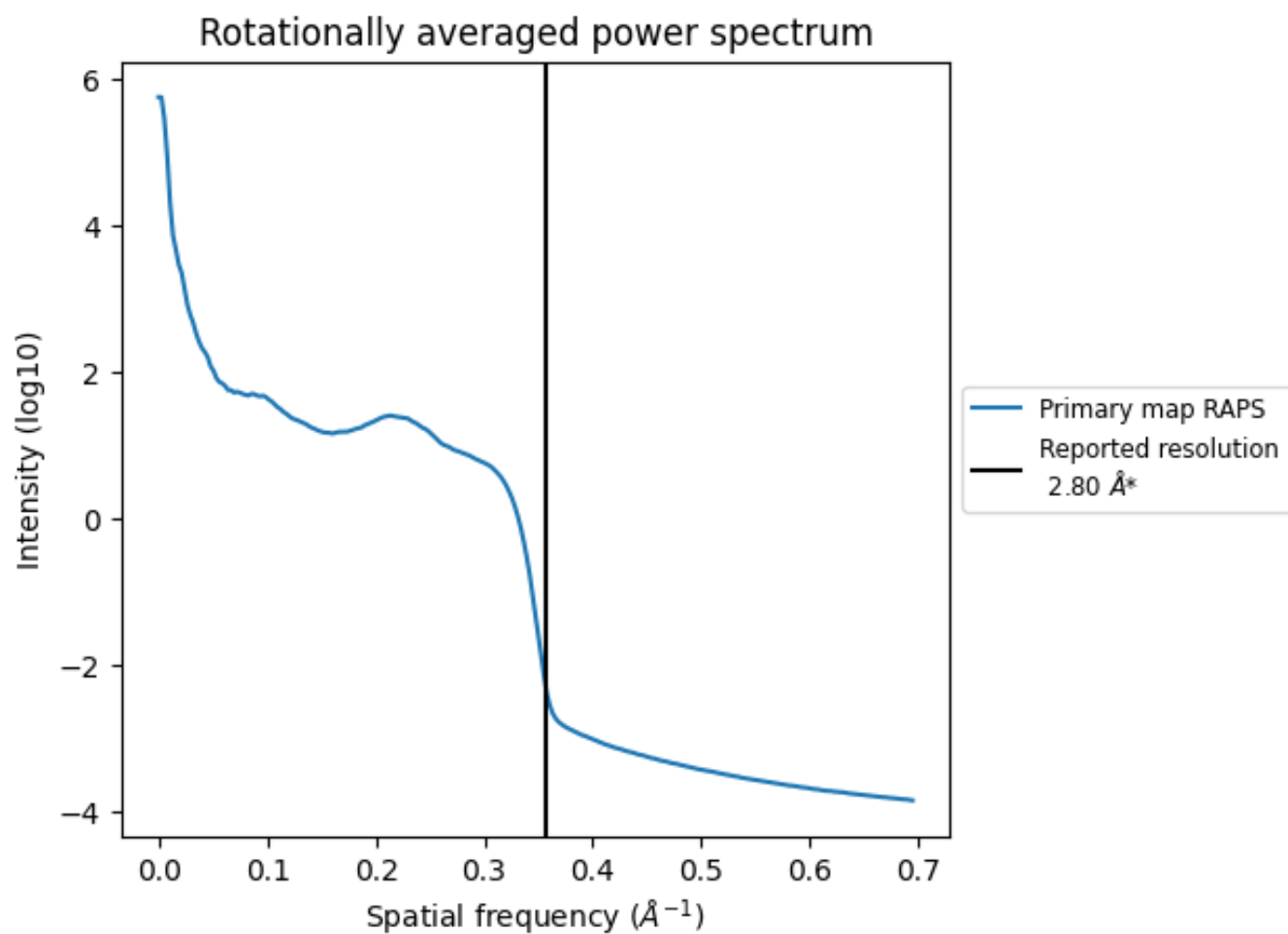
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 819 nm³; this corresponds to an approximate mass of 740 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

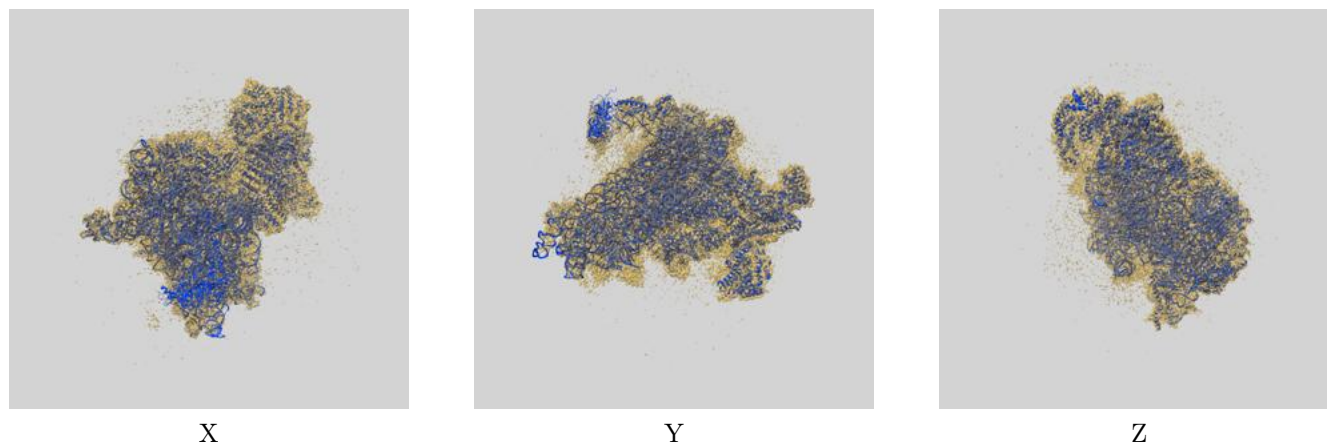
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

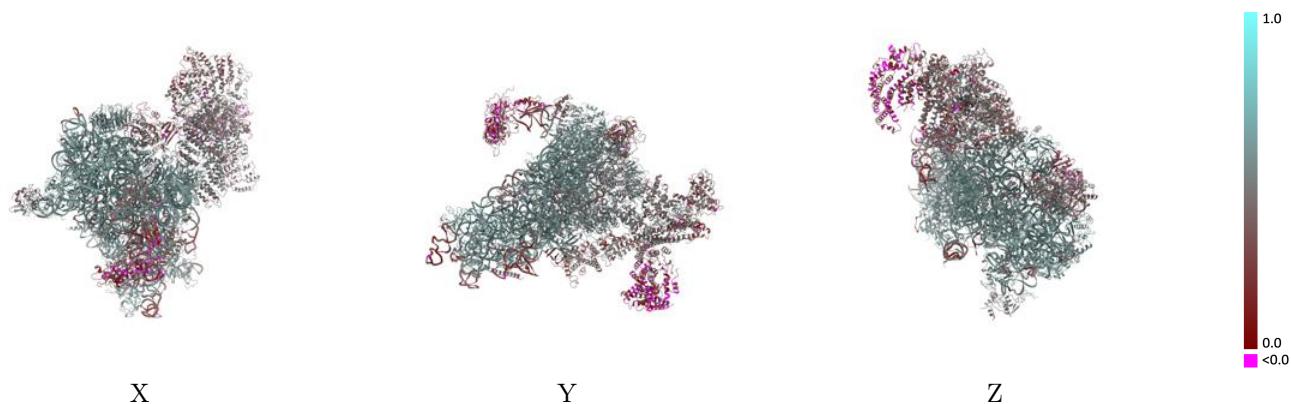
This section contains information regarding the fit between EMDB map EMD-57009 and PDB model 28ZX. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



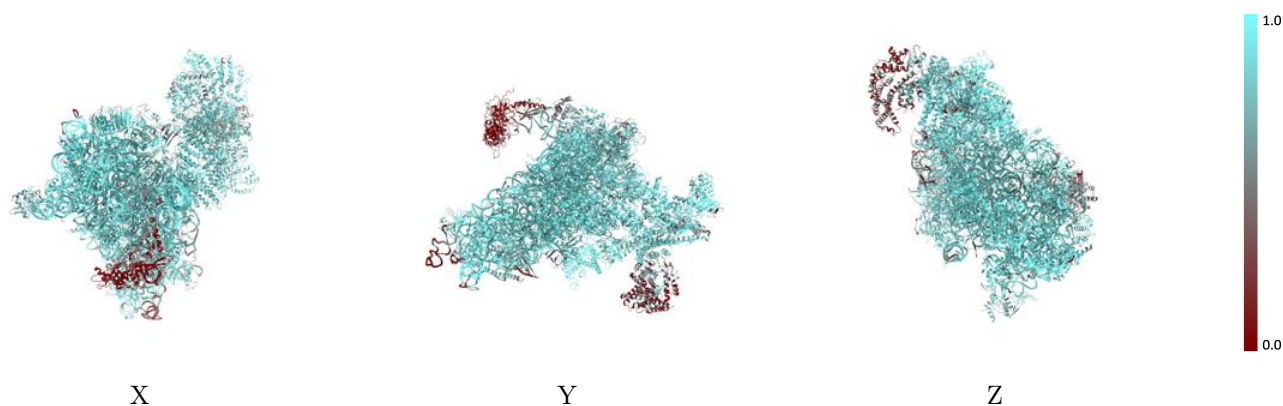
The images above show the 3D surface view of the map at the recommended contour level 4.66 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



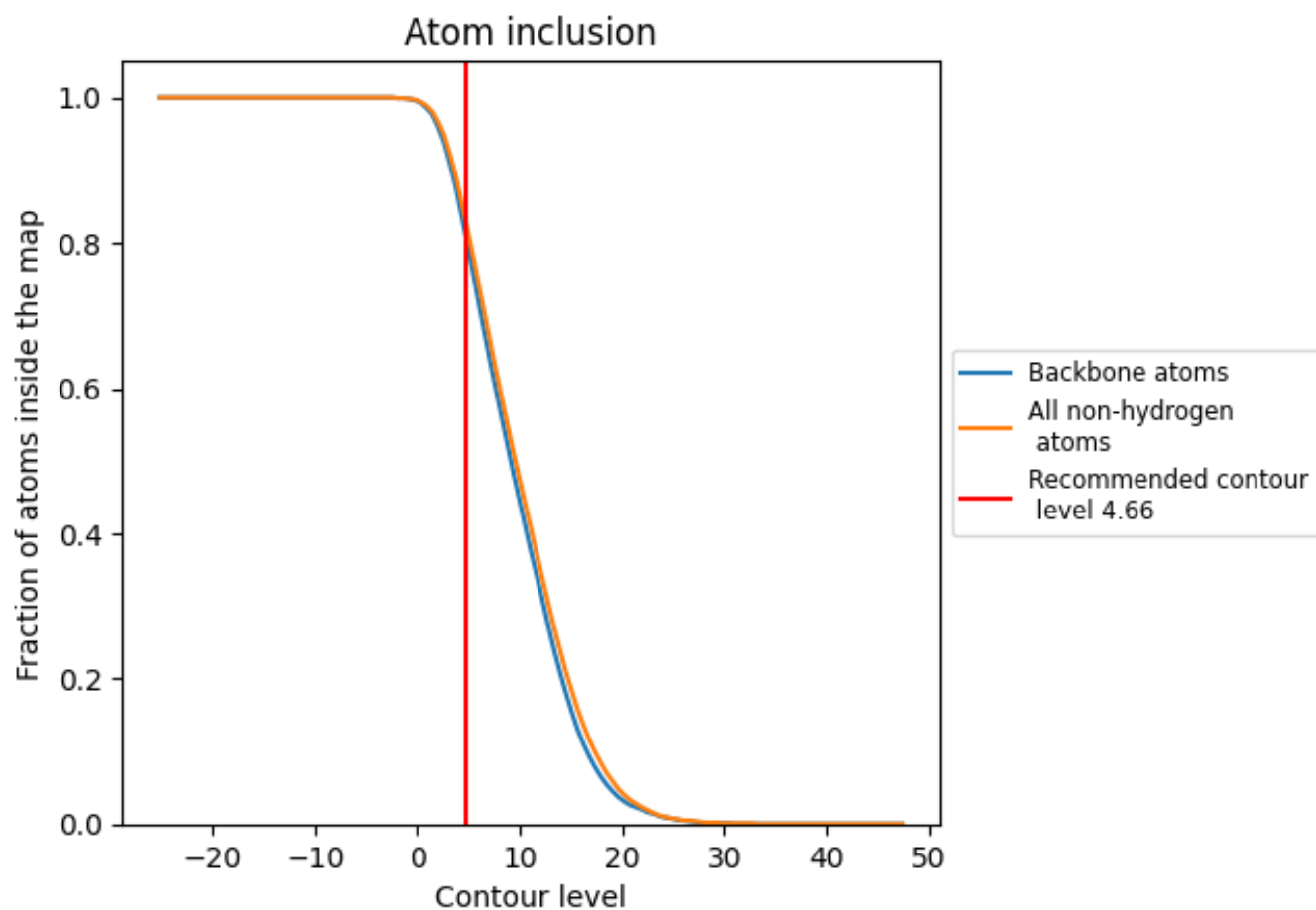
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.66).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 84% 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 (4.66) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8360	 0.5030
3f	 0.8300	 0.3790
B	 0.7570	 0.4140
D	 0.5620	 0.3960
E	 0.0780	 0.1880
F	 0.0580	 0.2550
G	 0.8140	 0.4140
H	 0.7660	 0.4790
Ln	 0.8760	 0.5560
S2	 0.9230	 0.5520
SA	 0.9050	 0.5780
SB	 0.8950	 0.5710
SC	 0.9320	 0.6010
SD	 0.8710	 0.5660
SE	 0.9170	 0.5930
SF	 0.9050	 0.5920
SG	 0.8240	 0.5450
SH	 0.8330	 0.5250
SI	 0.8620	 0.5600
SJ	 0.9030	 0.5830
SK	 0.8910	 0.5730
SL	 0.8580	 0.5710
SM	 0.6680	 0.4500
SN	 0.9040	 0.5770
SO	 0.8970	 0.5800
SP	 0.8550	 0.5670
SQ	 0.9310	 0.5960
SR	 0.8810	 0.5670
SS	 0.8620	 0.5800
ST	 0.9050	 0.5840
SU	 0.8290	 0.5480
SV	 0.8950	 0.5900
SW	 0.9480	 0.6050
SX	 0.9410	 0.6000
SY	 0.8940	 0.5800



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Chain	Atom inclusion	Q-score
SZ	 0.8670	 0.5660
Sa	 0.9060	 0.5770
Sb	 0.9230	 0.5670
Sc	 0.8450	 0.5510
Sd	 0.9460	 0.6050
Se	 0.8570	 0.5590
Sf	 0.7150	 0.4990
Sg	 0.8890	 0.5490
a	 0.8410	 0.4330
c	 0.8630	 0.4510
d	 0.7850	 0.3900
e	 0.8250	 0.3700
h	 0.7780	 0.3520
k	 0.3550	 0.1660
l	 0.4420	 0.1780
m	 0.8490	 0.3710