



Full wwPDB EM Validation Report ⓘ

Jun 19, 2026 – 07:05 am BST

PDB ID : 8PPL / pdb_00008ppl
EMDB ID : EMD-17805
Title : MERS-CoV Nsp1 bound to the human 43S pre-initiation complex
Authors : Schubert, K.; Karousis, E.D.; Ban, I.; Lapointe, C.P.; Leibundgut, M.; Baeumlin, E.; Kummerant, E.; Scaiola, A.; Schoenhut, T.; Ziegelmueller, J.; Puglisi, J.D.; Muehlemann, O.; Ban, N.
Deposited on : 2023-07-07
Resolution : 2.65 Å(reported)
Based on initial models : 6ZOK, 6ZOL

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:

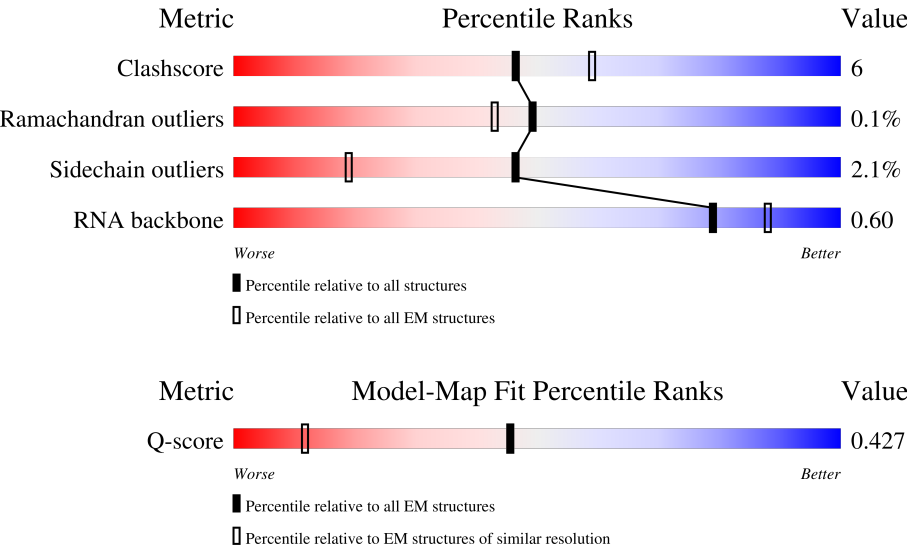
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.65 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	9050 (2.15 - 3.15)

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	I3	218	100% 67% 30% .
2	I4	357	74% 53% 21% . 25%
3	I5	564	65% 45% 20% . 34%

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Mol	Chain	Length	Quality of chain
4	I6	374	
5	I8	352	
6	Io	320	
7	Ip	113	
8	Iq	144	
9	Ir	315	
10	Is	333	
11	It	472	
12	Iu	1382	
13	Iv	445	
14	Iw	75	
15	Ix	548	
16	Iy	913	
17	A2	1869	
18	AA	295	
19	AB	264	
20	AC	293	
21	AD	243	
22	AE	263	
23	AF	204	
24	AG	249	
25	AH	194	
26	AI	208	
27	AJ	194	
28	AK	165	

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Mol	Chain	Length	Quality of chain
29	AL	158	 6% 92% ..
30	AM	132	 19% 76% 17% 7%
31	AN	151	 89% 9% .
32	AO	151	 78% 11% 11%
33	AP	145	 81% 10% 10%
34	AQ	146	 84% 12% ..
35	AR	135	 89% 10% ..
36	AS	152	 84% 11% 5%
37	AT	145	 91% 8% .
38	AU	119	 75% 10% 15%
39	AV	83	 96% ..
40	AW	130	 88% 11% .
41	AX	143	 91% 8% .
42	AY	133	 77% 16% 7%
43	AZ	125	 45% 12% 42%
44	Aa	115	 77% 10% 12%
45	Ab	84	 92% 6% ..
46	Ac	69	 6% 68% 26% 6%
47	Ad	56	 88% 11% .
48	Ae	133	 42% 56%
49	Af	156	 29% 19% 53%
50	Ag	317	 76% 22% .
51	Ah	25	 12% 84% 16%
52	Aj	216	 12% 87%

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 118236 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Eukaryotic translation initiation factor 3 subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I3	217	Total	C	N	O	S	0	0
			1750	1116	288	334	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I4	268	Total	C	N	O	S	0	0
			2087	1315	355	405	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I5	372	Total	C	N	O	S	0	0
			3111	2011	520	563	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I6	345	Total	C	N	O	S	0	0
			2751	1753	464	517	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I8	318	Total	C	N	O	S	0	0
			2594	1641	444	494	15		

- Molecule 6 is a protein called Eukaryotic translation initiation factor 3 subunit G.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	Io	77	Total	C	N	O	0	0
			616	389	111	116		

- Molecule 7 is a protein called Eukaryotic translation initiation factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Ip	105	Total	C	N	O	S	0	0
			797	501	145	149	2		

- Molecule 8 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Iq	103	Total	C	N	O	S	0	0
			835	525	148	158	4		

- Molecule 9 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Ir	293	Total	C	N	O	S	0	0
			2368	1486	415	454	13		

- Molecule 10 is a protein called Eukaryotic translation initiation factor 2 subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Is	159	Total	C	N	O	S	0	0
			1288	813	238	228	9		

- Molecule 11 is a protein called Eukaryotic translation initiation factor 2 subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	It	451	Total	C	N	O	S	0	0
			3445	2191	605	632	17		

- Molecule 12 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Iu	587	Total	C	N	O	S	0	0
			4830	3048	869	891	22		

- Molecule 13 is a protein called Eukaryotic translation initiation factor 3 subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Iv	430	Total	C	N	O	S	0	0
			3553	2272	602	658	21		

- Molecule 14 is a RNA chain called Met-tRNAⁱ(Met).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Iw	75	Total	C	N	O	P	0	0
			1624	728	299	522	75		

- Molecule 15 is a protein called Eukaryotic translation initiation factor 3 subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Ix	455	Total	C	N	O	S	0	0
			3680	2311	640	707	22		

- Molecule 16 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Iy	633	Total	C	N	O	S	0	0
			4949	3102	886	928	33		

- Molecule 17 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	A2	1780	Total	C	N	O	P	0	0
			38049	17008	6822	12439	1780		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AA	216	Total	C	N	O	S	0	0
			1708	1085	299	316	8		

- Molecule 19 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AB	224	Total	C	N	O	S	0	0
			1815	1152	328	321	14		

- Molecule 20 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AC	218	Total	C	N	O	S	1	0
			1698	1099	292	297	10		

- Molecule 21 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AD	225	Total	C	N	O	S	0	0
			1752	1117	315	313	7		

- Molecule 22 is a protein called 40S ribosomal protein S4, X isoform.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AF	192	Total	C	N	O	S	0	0
			1517	948	287	275	7		

- Molecule 24 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AG	240	Total	C	N	O	S	0	0
			1945	1212	393	333	7		

- Molecule 25 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AH	188	Total	C	N	O	S	0	0
			1515	966	279	269	1		

- Molecule 26 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AI	205	Total	C	N	O	S	0	0
			1682	1056	331	290	5		

- Molecule 27 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AJ	180	Total	C	N	O	S	0	0
			1499	955	300	242	2		

- Molecule 28 is a protein called 40S ribosomal protein S10.

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

- Molecule 29 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AL	151	Total	C	N	O	S	0	0
			1229	782	230	211	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	AM	123	Total	C	N	O	S	0	0
			953	598	169	177	9		

- Molecule 31 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	AN	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 32 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	AO	135	Total	C	N	O	S	0	0
			1010	618	198	188	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AO	138	IAS	ASP	modified residue	UNP P62263

- Molecule 33 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	AP	131	Total	C	N	O	S	0	0
			1075	682	204	182	7		

- Molecule 34 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	AQ	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 35 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	AR	134	Total	C	N	O	S	0	0
			1082	680	201	197	4		

- Molecule 36 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	AS	145	Total	C	N	O	S	0	0
			1200	753	242	204	1		

- Molecule 37 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	AT	144	Total	C	N	O	S	0	0
			1123	704	217	199	3		

- Molecule 38 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	AU	101	Total	C	N	O	S	0	0
			803	504	153	142	4		

- Molecule 39 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	AV	83	Total	C	N	O	S	0	0
			639	395	117	122	5		

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

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

- Molecule 41 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	AX	141	Total	C	N	O	S	2	0
			1112	703	222	184	3		

- Molecule 42 is a protein called 40S ribosomal protein S24.

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

- Molecule 43 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	AZ	72	Total	C	N	O	S	0	0
			574	368	104	101	1		

- Molecule 44 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Aa	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 45 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Ab	83	Total	C	N	O	S	0	0
			650	408	121	114	7		

- Molecule 46 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Ac	65	Total	C	N	O	S	0	0
			512	311	103	96	2		

- Molecule 47 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Ad	55	Total	C	N	O	S	0	0
			458	286	94	73	5		

- Molecule 48 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Ae	59	Total	C	N	O	S	0	0
			467	290	102	74	1		

- Molecule 49 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Af	74	Total	C	N	O	S	0	0
			610	385	117	101	7		

- Molecule 50 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 51 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Ah	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 52 is a protein called Host translation inhibitor nsp1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Aj	29	Total	C	N	O	S	0	0
			227	145	36	44	2		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Aj	-22	MET	-	initiating methionine	UNP K9N7C7
Aj	-21	ALA	-	expression tag	UNP K9N7C7
Aj	-20	ASP	-	expression tag	UNP K9N7C7
Aj	-19	TYR	-	expression tag	UNP K9N7C7
Aj	-18	LYS	-	expression tag	UNP K9N7C7
Aj	-17	ASP	-	expression tag	UNP K9N7C7
Aj	-16	HIS	-	expression tag	UNP K9N7C7
Aj	-15	ASP	-	expression tag	UNP K9N7C7
Aj	-14	GLY	-	expression tag	UNP K9N7C7
Aj	-13	ASP	-	expression tag	UNP K9N7C7
Aj	-12	TYR	-	expression tag	UNP K9N7C7
Aj	-11	LYS	-	expression tag	UNP K9N7C7

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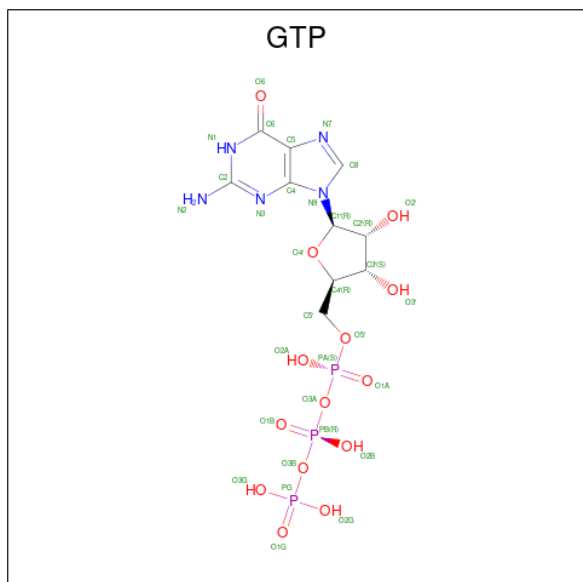
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Chain	Residue	Modelled	Actual	Comment	Reference
Aj	-10	ASP	-	expression tag	UNP K9N7C7
Aj	-9	HIS	-	expression tag	UNP K9N7C7
Aj	-8	ASP	-	expression tag	UNP K9N7C7
Aj	-7	ILE	-	expression tag	UNP K9N7C7
Aj	-6	ASP	-	expression tag	UNP K9N7C7
Aj	-5	TYR	-	expression tag	UNP K9N7C7
Aj	-4	LYS	-	expression tag	UNP K9N7C7
Aj	-3	ASP	-	expression tag	UNP K9N7C7
Aj	-2	ASP	-	expression tag	UNP K9N7C7
Aj	-1	ASP	-	expression tag	UNP K9N7C7
Aj	0	ASP	-	expression tag	UNP K9N7C7
Aj	1	LYS	-	expression tag	UNP K9N7C7

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

Mol	Chain	Residues	Atoms	AltConf
53	Is	1	Total Zn 1 1	0
53	Aa	1	Total Zn 1 1	0
53	Ad	1	Total Zn 1 1	0
53	Af	1	Total Zn 1 1	0

- Molecule 54 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

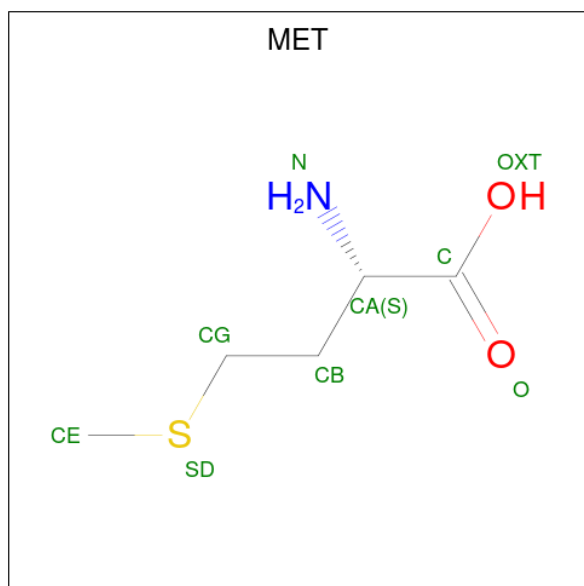


Mol	Chain	Residues	Atoms					AltConf
54	It	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
55	It	1	Total	Mg	0
			1	1	
55	A2	110	Total	Mg	0
			110	110	
55	AG	1	Total	Mg	0
			1	1	
55	AS	2	Total	Mg	0
			2	2	
55	AT	1	Total	Mg	0
			1	1	
55	AX	1	Total	Mg	0
			1	1	

- Molecule 56 is METHIONINE (CCD ID: MET) (formula: C₅H₁₁NO₂S).



Mol	Chain	Residues	Atoms					AltConf
56	Iw	1	Total	C	N	O	S	0
			8	5	1	1	1	

- Molecule 57 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

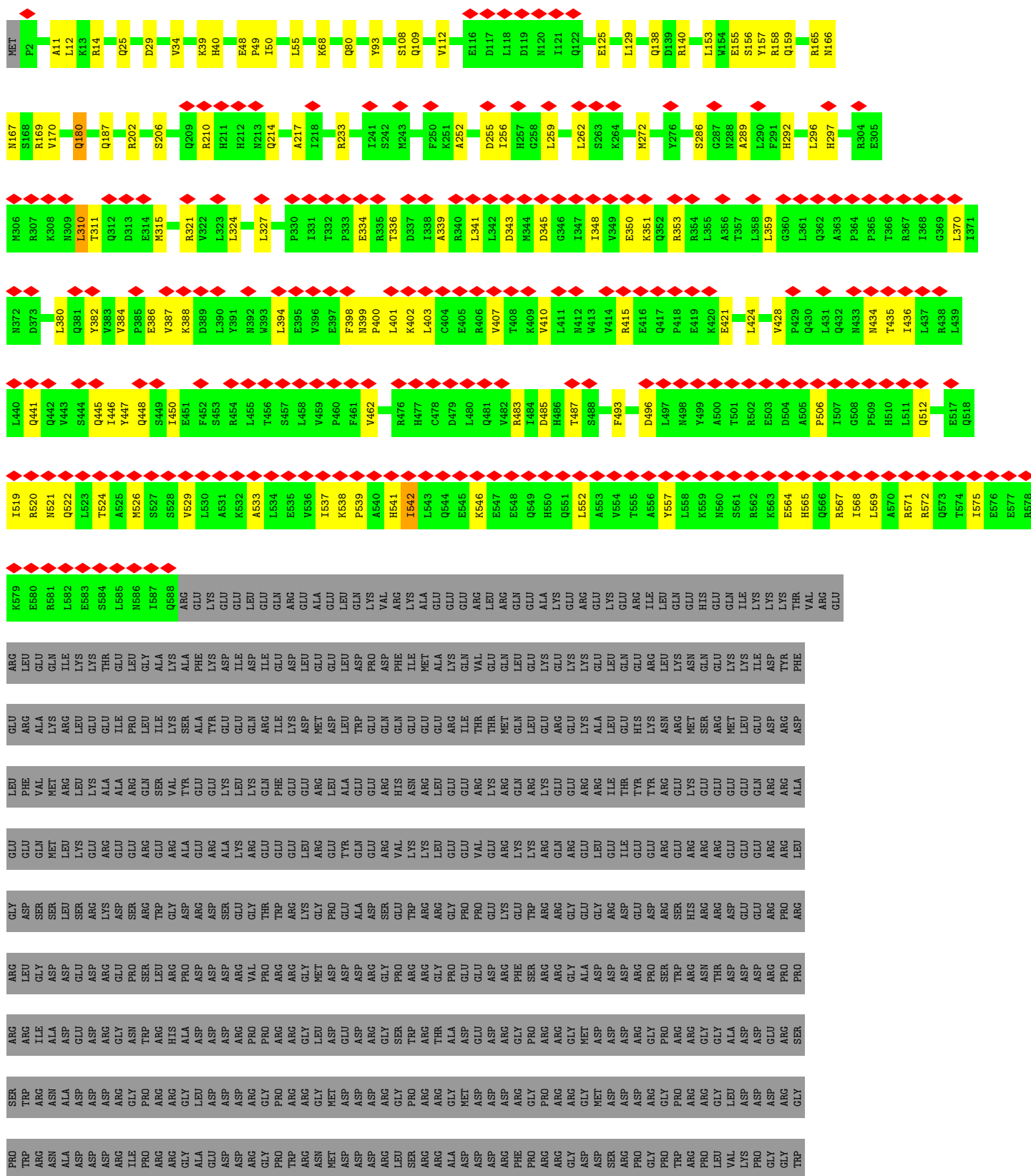
Mol	Chain	Residues	Atoms		AltConf
57	Iw	2	Total 2	X 2	0
57	A2	122	Total 122	X 122	0
57	AJ	1	Total 1	X 1	0
57	AN	1	Total 1	X 1	0
57	AO	2	Total 2	X 2	0
57	Ad	1	Total 1	X 1	0

- Molecule 58 is water.

Mol	Chain	Residues	Atoms		AltConf
58	It	2	Total 2	O 2	0

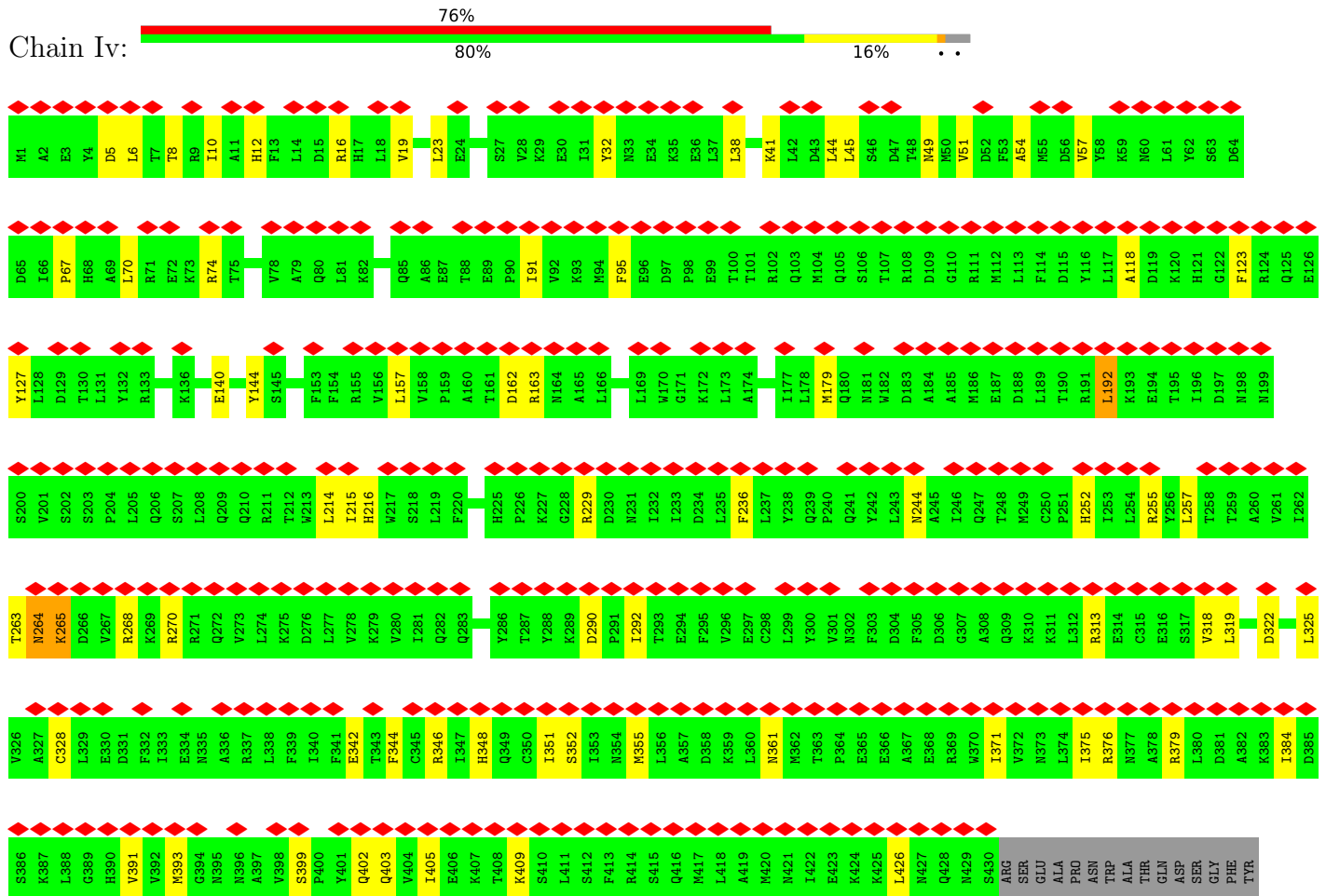




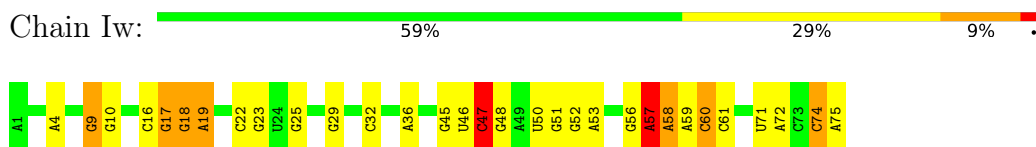


[illegible]

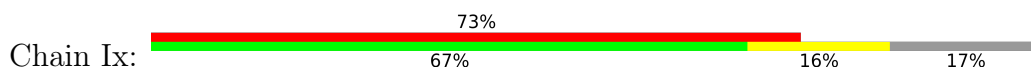
- Molecule 13: Eukaryotic translation initiation factor 3 subunit E

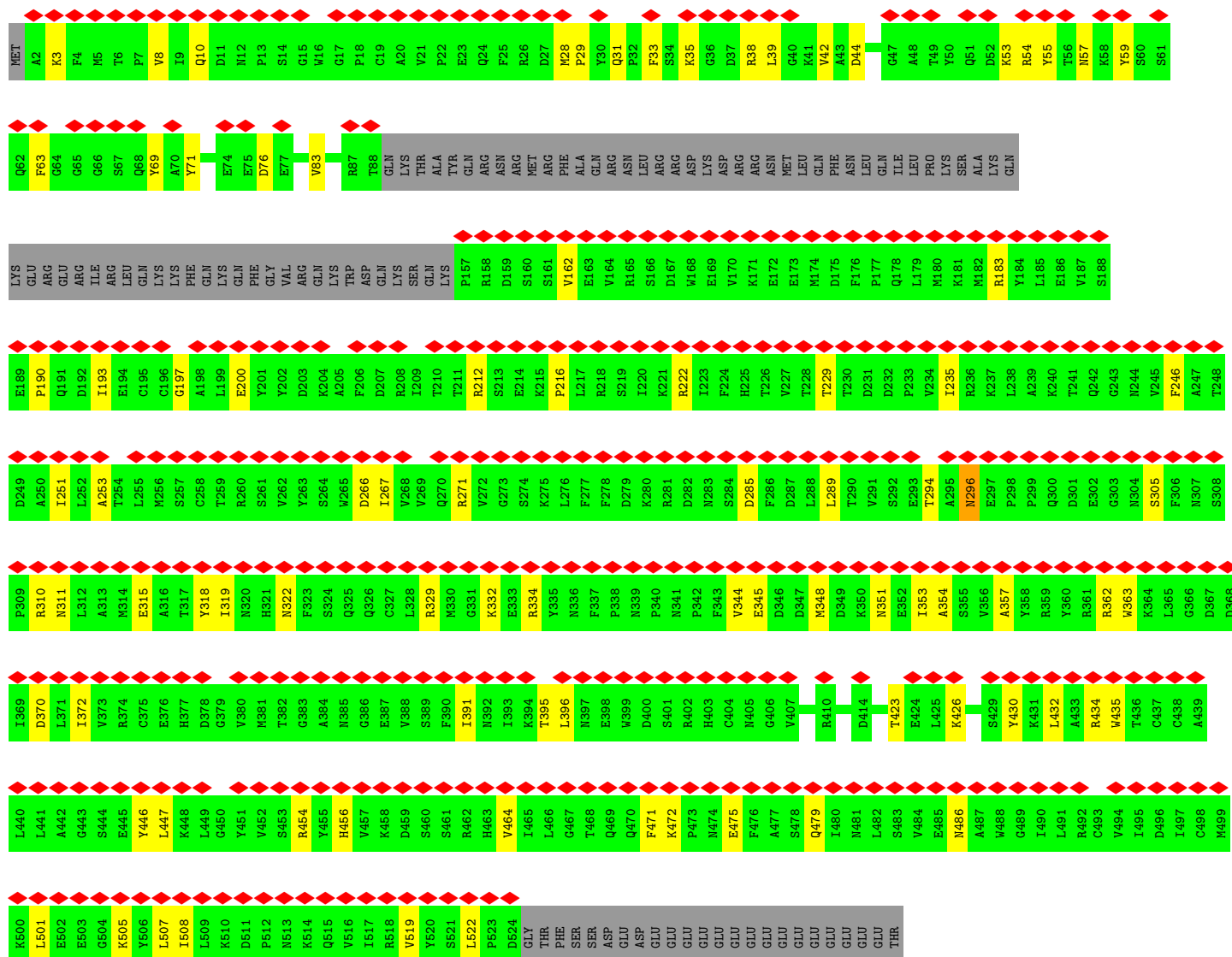


- Molecule 14: Met-tRNAⁱ(Met)

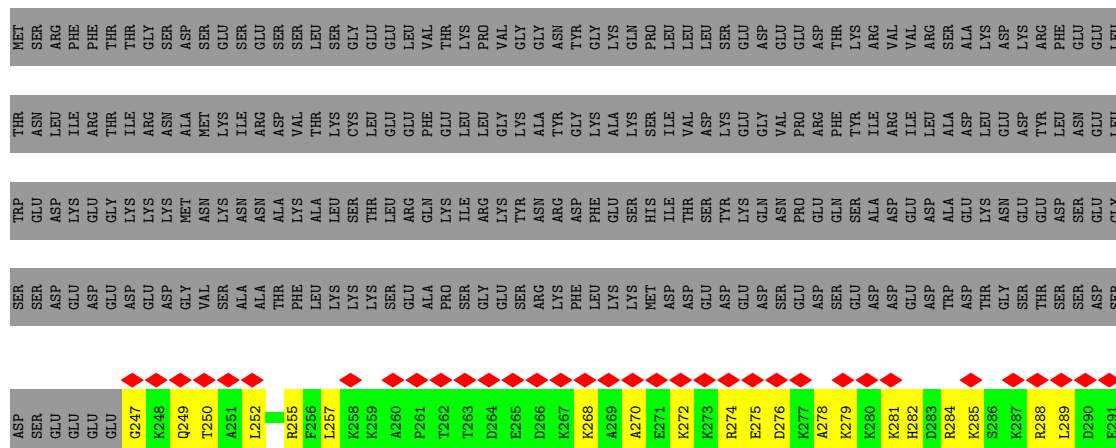


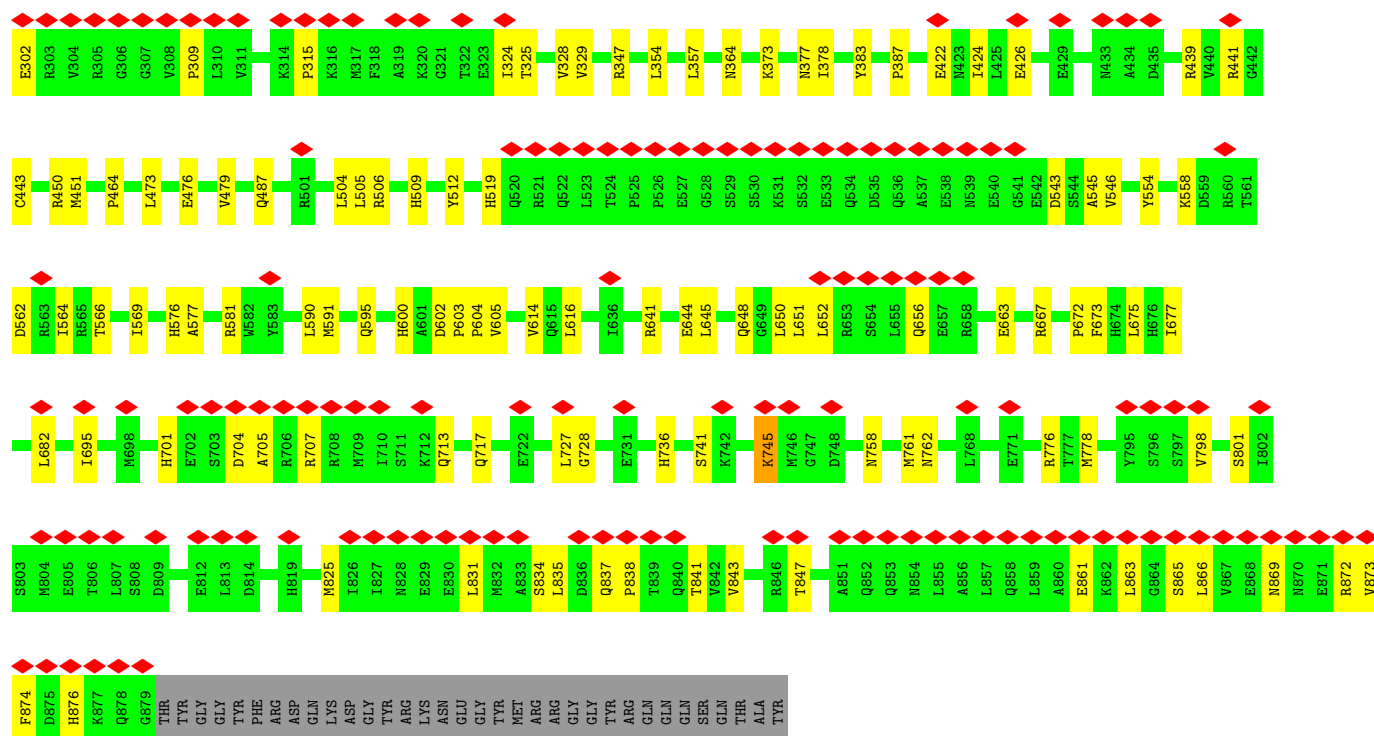
- Molecule 15: Eukaryotic translation initiation factor 3 subunit D





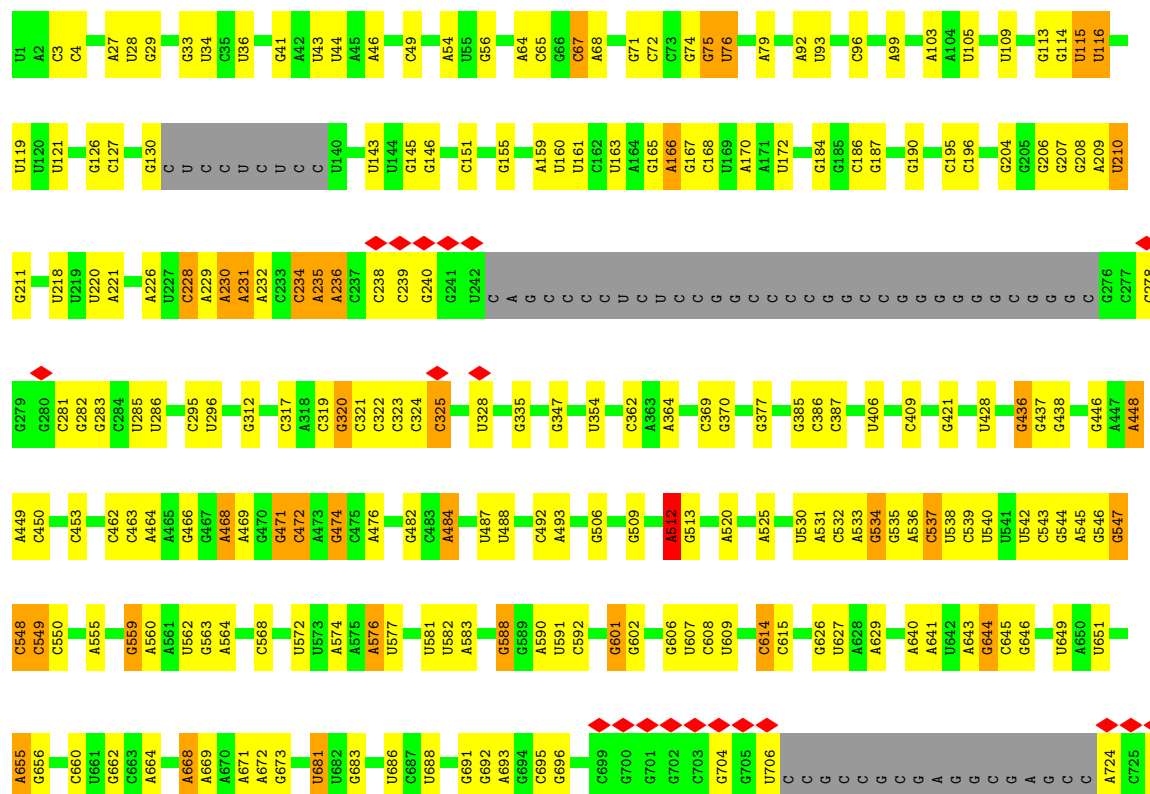
● Molecule 16: Eukaryotic translation initiation factor 3 subunit C



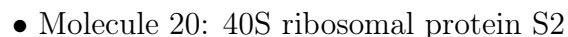


Molecule 17: 18S rRNA

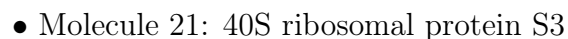
Chain A2: 64% 27% 5%



A horizontal bar chart showing the distribution of responses for the question 'How often do you use the app?'. The bar is divided into three segments: a large green segment representing 75%, a smaller yellow segment representing 10%, and a small grey segment representing 15%. A legend on the right side of the chart identifies these segments: green for '75%', yellow for '10%', and grey for '15%'. The chart is titled 'How often do you use the app?' and is part of a larger survey analysis.



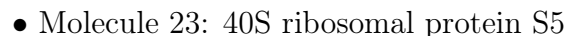
Response	Percentage
Yes	66%
No	8%
Don't know	26%



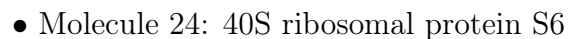
Response	Percentage
Yes, the U.S. is a democracy	83%
No, the U.S. is not a democracy	9%
Don't know	7%



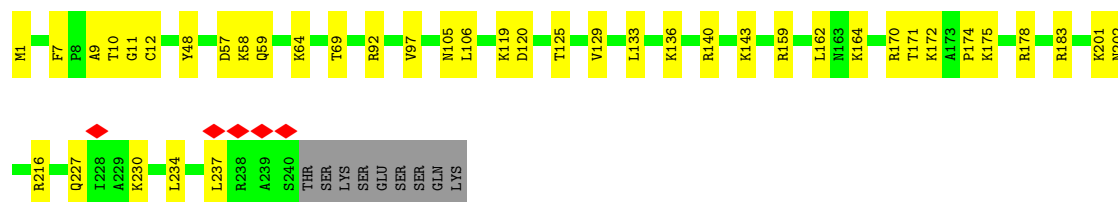
Response	Percentage
Yes, it is a crisis	90%
No, it is not a crisis	9%



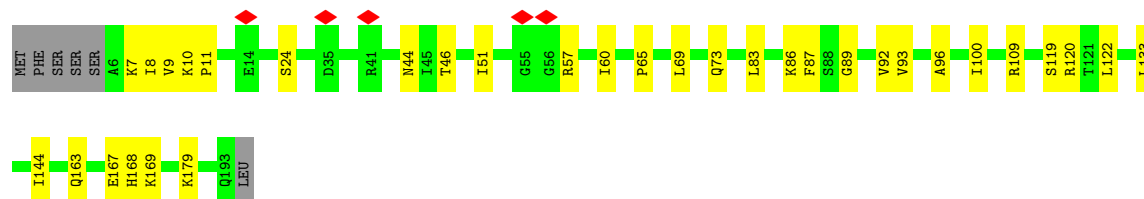
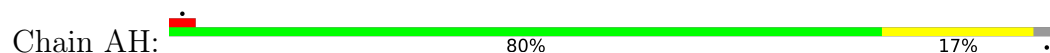
Response	Percentage
Yes	83%
No	11%
Don't know	6%



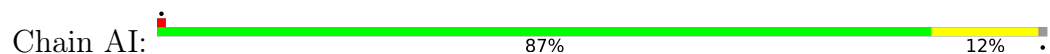
Frequency	Percentage
Often	80%
Sometimes	16%
Rarely	4%



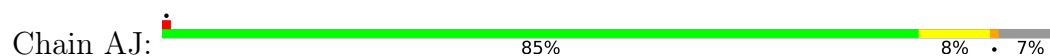
- Molecule 25: 40S ribosomal protein S7



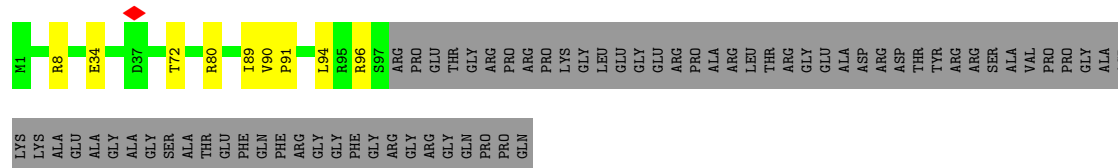
- Molecule 26: 40S ribosomal protein S8



- Molecule 27: 40S ribosomal protein S9



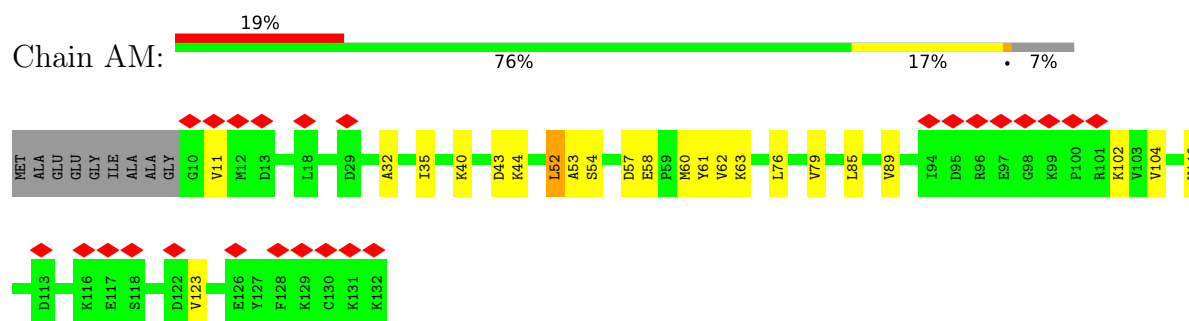
- Molecule 28: 40S ribosomal protein S10



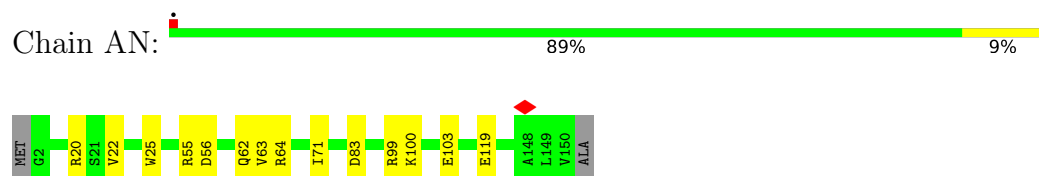
- Molecule 29: 40S ribosomal protein S11



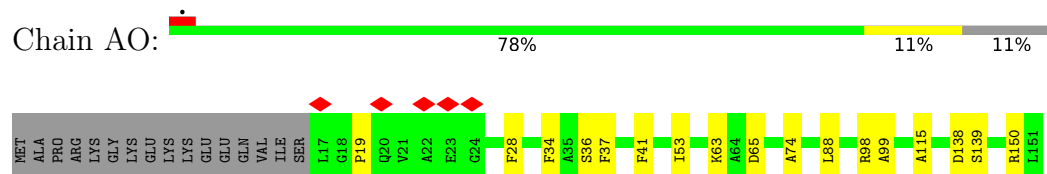
- Molecule 30: 40S ribosomal protein S12



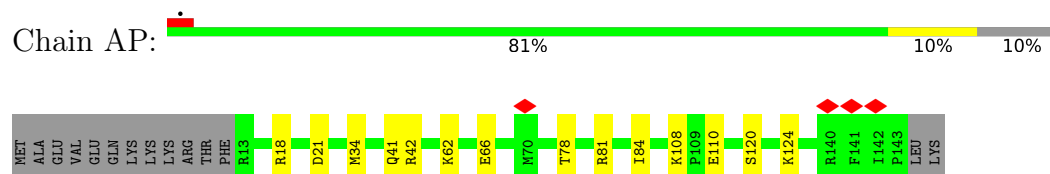
- Molecule 31: 40S ribosomal protein S13



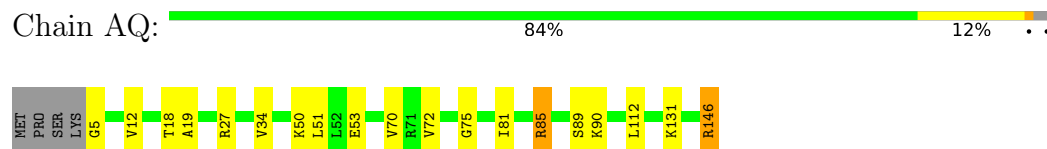
- Molecule 32: 40S ribosomal protein S14



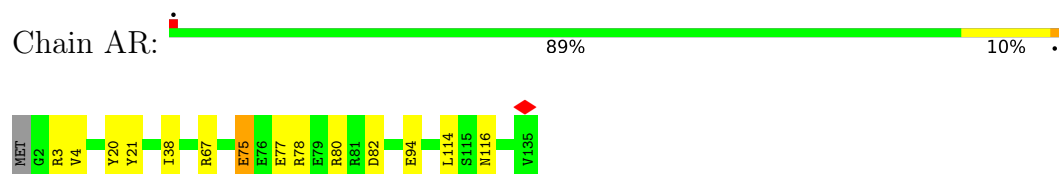
- Molecule 33: 40S ribosomal protein S15



- Molecule 34: 40S ribosomal protein S16

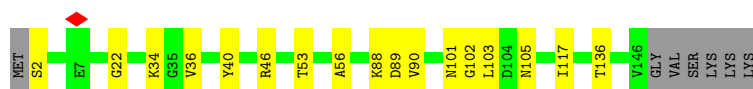


- Molecule 35: 40S ribosomal protein S17



- Molecule 36: Small ribosomal subunit protein uS13

Chain AS:  84% 11% 5%



- Molecule 37: Small ribosomal subunit protein eS19

Chain AT:  91% 8% .

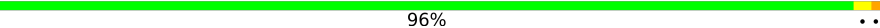


- Molecule 38: 40S ribosomal protein S20

Chain AU:  75% 10% 15%



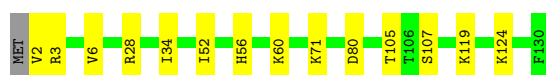
- Molecule 39: 40S ribosomal protein S21

Chain AV:  96% ..



- Molecule 40: 40S ribosomal protein S15a

Chain AW:  88% 11% .



- Molecule 41: 40S ribosomal protein S23

Chain AX:  91% 8% .

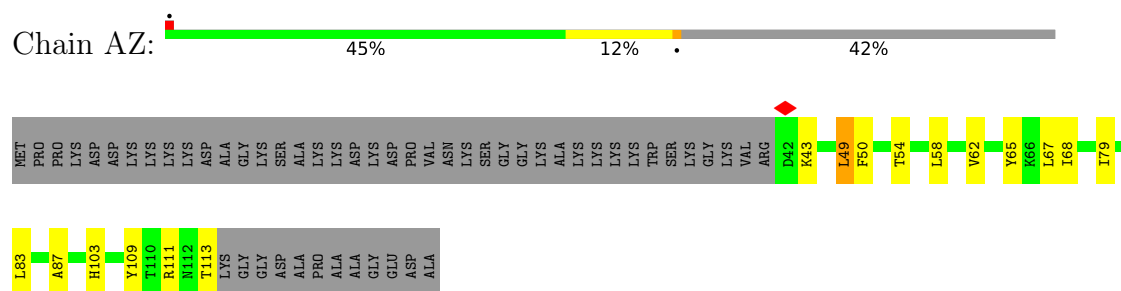


- Molecule 42: 40S ribosomal protein S24

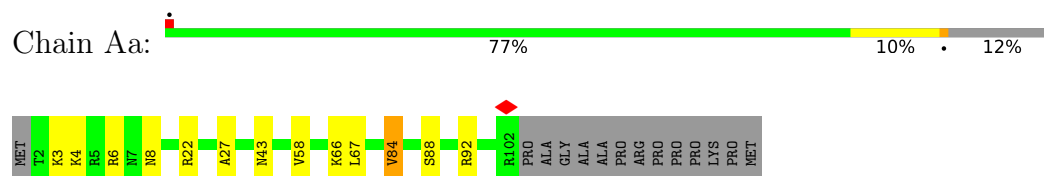
Chain AY:  77% 16% . 7%



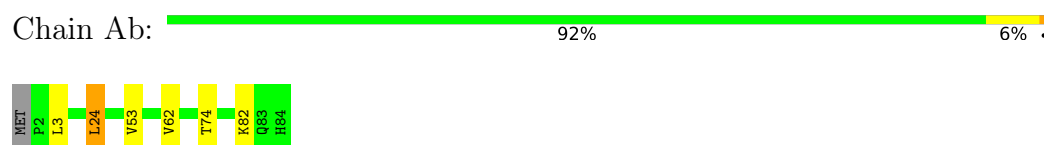
- Molecule 43: 40S ribosomal protein S25



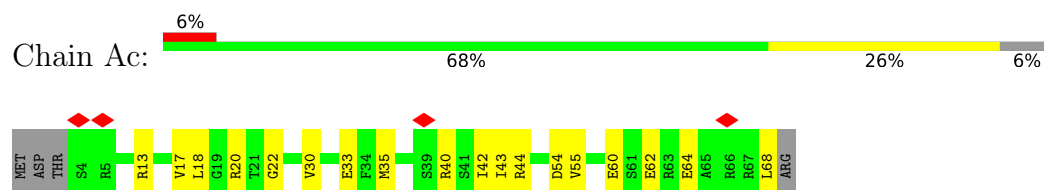
- Molecule 44: 40S ribosomal protein S26



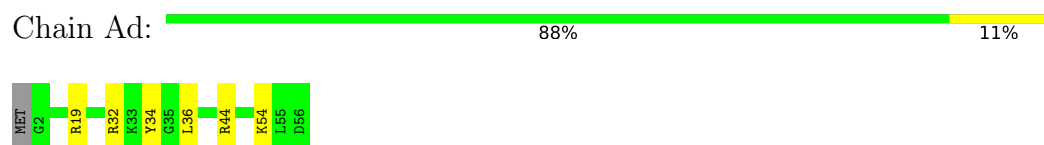
- Molecule 45: 40S ribosomal protein S27



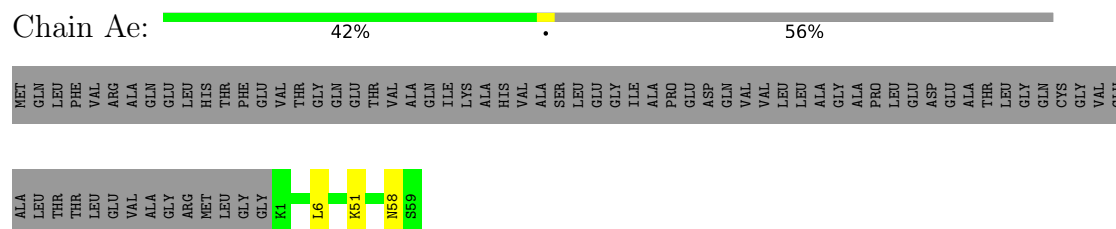
- Molecule 46: 40S ribosomal protein S28



- Molecule 47: 40S ribosomal protein S29



- Molecule 48: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein

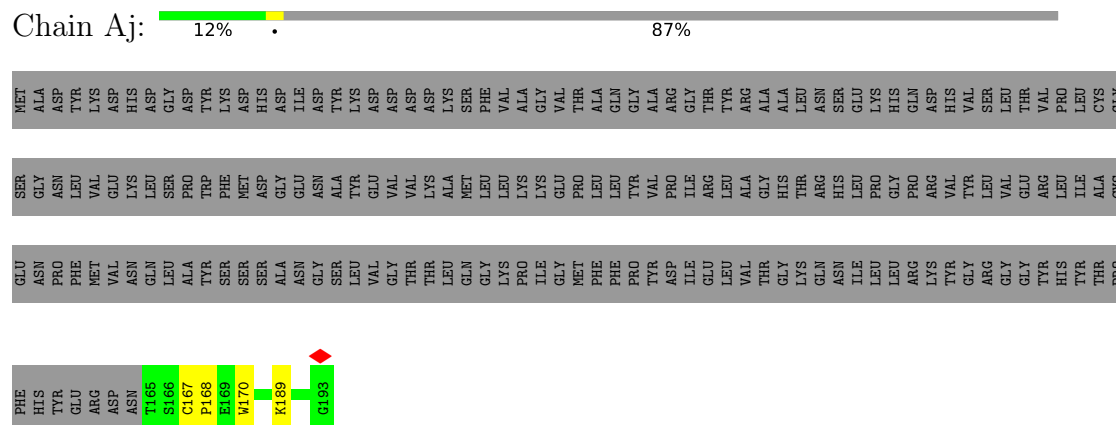


- Molecule 49: Ubiquitin-40S ribosomal protein S27a

- Molecule 50: Receptor of activated protein C kinase 1

- Molecule 51: 60S ribosomal protein L41

- Molecule 52: Host translation inhibitor nsp1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	218516	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.673	Depositor
Minimum map value	-0.615	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.15	Depositor
Map size ($\text{\AA}$)	596.4, 596.4, 596.4	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.065, 1.065, 1.065	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, 6MZ, 1MG, UNX, ZN, 1MA, MG, 2MG, A2M, 4AC, SAC, MA6, G7M, OMU, PSU, HY3, OMG, NMM, T6A, GTP, IAS, OMC, AME, B8N, H2U

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	I3	0.08	0/1785	0.24	0/2414
2	I4	0.06	0/2123	0.19	0/2885
3	I5	0.10	0/3187	0.29	0/4299
4	I6	0.07	0/2793	0.21	0/3770
5	I8	0.06	0/2645	0.18	0/3570
6	Io	0.08	0/628	0.27	0/846
7	Ip	0.12	0/808	0.34	1/1085 (0.1%)
8	Iq	0.10	0/845	0.24	0/1128
9	Ir	0.08	0/2400	0.25	0/3234
10	Is	0.08	0/1309	0.21	0/1757
11	It	0.07	0/3502	0.21	0/4739
12	Iu	0.07	0/4919	0.20	0/6647
13	Iv	0.06	0/3626	0.20	0/4902
14	Iw	0.24	0/1601	0.28	0/2492
15	Ix	0.06	0/3763	0.19	0/5089
16	Iy	0.15	0/5032	0.27	2/6800 (0.0%)
17	A2	0.18	1/40497 (0.0%)	0.18	0/63121
18	AA	0.12	0/1736	0.21	0/2359
19	AB	0.11	0/1841	0.20	0/2459
20	AC	0.12	0/1737	0.22	0/2346
21	AD	0.10	0/1780	0.20	0/2397
22	AE	0.12	0/2118	0.24	0/2849
23	AF	0.10	0/1539	0.22	0/2071
24	AG	0.08	0/1968	0.18	0/2619
25	AH	0.10	0/1538	0.23	0/2060
26	AI	0.10	0/1711	0.22	0/2282
27	AJ	0.11	0/1524	0.19	0/2035
28	AK	0.09	0/840	0.22	0/1133
29	AL	0.11	0/1250	0.20	0/1673
30	AM	0.07	0/963	0.23	0/1291
31	AN	0.11	0/1226	0.19	0/1649

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	AO	0.12	0/1014	0.22	0/1358
33	AP	0.09	0/1097	0.19	0/1467
34	AQ	0.12	0/1146	0.22	0/1534
35	AR	0.10	0/1097	0.20	0/1474
36	AS	0.09	0/1209	0.21	0/1620
37	AT	0.10	0/1130	0.18	0/1513
38	AU	0.11	0/813	0.25	0/1092
39	AV	0.12	0/635	0.21	0/850
40	AW	0.15	0/1051	0.24	0/1406
41	AX	0.12	0/1127	0.24	0/1501
42	AY	0.10	0/1031	0.19	0/1370
43	AZ	0.10	0/580	0.22	0/780
44	Aa	0.13	0/828	0.23	0/1109
45	Ab	0.11	0/664	0.21	0/891
46	Ac	0.11	0/514	0.22	0/688
47	Ad	0.12	0/469	0.23	0/623
48	Ae	0.10	0/473	0.21	0/623
49	Af	0.35	0/622	0.46	0/822
50	Ag	0.09	0/2497	0.24	0/3399
51	Ah	0.11	0/240	0.18	0/305
52	Aj	0.12	0/232	0.22	0/311
All	All	0.13	1/121703 (0.0%)	0.21	3/172737 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A2	668	A2M	O3'-P	5.03	1.61	1.56

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Ip	12	PRO	N-CA-CB	7.66	111.29	103.25
16	Iy	309	PRO	N-CA-CB	6.30	109.87	103.25
16	Iy	315	PRO	N-CA-CB	6.27	110.22	103.33

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	I3	1750	0	1717	55	0
2	I4	2087	0	2089	74	0
3	I5	3111	0	3085	90	0
4	I6	2751	0	2796	68	0
5	I8	2594	0	2571	71	0
6	Io	616	0	600	10	0
7	Ip	797	0	770	17	0
8	Iq	835	0	836	11	0
9	Ir	2368	0	2408	70	0
10	Is	1288	0	1329	35	0
11	It	3445	0	3603	64	0
12	Iu	4830	0	4902	90	0
13	Iv	3553	0	3537	53	0
14	Iw	1624	0	835	18	0
15	Ix	3680	0	3556	58	0
16	Iy	4949	0	4823	85	0
17	A2	38049	0	19284	283	0
18	AA	1708	0	1710	13	0
19	AB	1815	0	1908	17	0
20	AC	1698	0	1790	19	0
21	AD	1752	0	1848	18	0
22	AE	2076	0	2177	15	0
23	AF	1517	0	1569	16	0
24	AG	1945	0	2112	32	0
25	AH	1515	0	1611	20	0
26	AI	1682	0	1769	15	0
27	AJ	1499	0	1618	10	0
28	AK	816	0	841	6	0
29	AL	1229	0	1302	4	0
30	AM	953	0	990	15	0
31	AN	1202	0	1289	9	0
32	AO	1010	0	1033	11	0
33	AP	1075	0	1123	11	0
34	AQ	1128	0	1195	11	0
35	AR	1082	0	1137	11	0
36	AS	1200	0	1262	11	0
37	AT	1123	0	1152	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	AU	803	0	873	8	0
39	AV	639	0	638	5	0
40	AW	1034	0	1080	11	0
41	AX	1112	0	1182	4	0
42	AY	1014	0	1082	15	0
43	AZ	574	0	627	10	0
44	Aa	814	0	863	8	0
45	Ab	650	0	672	3	0
46	Ac	512	0	541	14	0
47	Ad	458	0	448	5	0
48	Ae	467	0	519	2	0
49	Af	610	0	634	22	0
50	Ag	2440	0	2396	39	0
51	Ah	239	0	289	4	0
52	Aj	227	0	220	3	0
53	Aa	1	0	0	0	0
53	Ad	1	0	0	0	0
53	Af	1	0	0	0	0
53	Is	1	0	0	0	0
54	It	32	0	12	3	0
55	A2	110	0	0	0	0
55	AG	1	0	0	0	0
55	AS	2	0	0	0	0
55	AT	1	0	0	0	0
55	AX	1	0	0	0	0
55	It	1	0	0	0	0
56	Iw	8	0	8	1	0
57	A2	122	0	0	0	0
57	AJ	1	0	0	0	0
57	AN	1	0	0	0	0
57	AO	2	0	0	0	0
57	Ad	1	0	0	0	0
57	Iw	2	0	0	0	0
58	It	2	0	0	0	0
All	All	118236	0	100261	1293	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 6.

All (1293) 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)
17:A2:1091:C:HO2'	40:AW:2:VAL:N	1.76	0.83
9:Ir:232:PRO:HB3	11:It:345:PRO:HB2	1.62	0.82
17:A2:512:A2M:HM'2	17:A2:513:G:H5'	1.67	0.77
17:A2:1480:A:H5'	34:AQ:131:LYS:HD3	1.66	0.77
5:I8:233:LEU:HB2	12:Iu:521:ASN:H	1.52	0.75
14:Iw:57:1MA:O2'	14:Iw:59:A:OP2	2.05	0.74
3:I5:438:GLU:HG3	3:I5:439:PRO:HD3	1.69	0.74
25:AH:93:VAL:HG11	25:AH:133:LEU:HD12	1.68	0.73
11:It:300:ILE:HB	11:It:312:LYS:HB2	1.70	0.73
1:I3:152:HIS:HB2	3:I5:507:SER:HA	1.71	0.73
17:A2:563:G:H1	17:A2:592:C:H5	1.37	0.72
4:I6:364:VAL:HG11	5:I8:343:MET:HB3	1.70	0.72
14:Iw:19:A:H61	14:Iw:56:G:H1'	1.54	0.72
15:Ix:329:ARG:HB3	15:Ix:332:LYS:HD2	1.71	0.72
11:It:349:ARG:NH2	14:Iw:72:A:OP1	2.22	0.72
9:Ir:132:GLN:HA	9:Ir:136:TRP:HB2	1.72	0.72
50:Ag:87:LEU:HB2	50:Ag:101:PHE:HB2	1.72	0.72
26:AI:141:ARG:HB2	26:AI:146:GLN:HG2	1.72	0.71
12:Iu:55:LEU:HD13	12:Iu:93:TYR:HB2	1.73	0.71
16:Iy:347:ARG:HH22	16:Iy:387:PRO:HB3	1.55	0.71
2:I4:308:LEU:HD13	4:I6:350:LEU:HD13	1.71	0.71
17:A2:228:C:O2'	17:A2:887:U:O2	2.08	0.71
3:I5:472:VAL:HB	3:I5:511:GLY:HA3	1.71	0.70
10:Is:219:PHE:HB3	10:Is:256:LEU:HB3	1.73	0.70
11:It:139:ASP:HB3	11:It:169:GLN:HE21	1.57	0.70
48:Ae:51:LYS:HD3	52:Aj:167:CYS:H	1.55	0.70
20:AC:117:ARG:H	20:AC:117:ARG:HH11	1.40	0.69
1:I3:18:ILE:O	3:I5:262:ARG:NH2	2.25	0.69
4:I6:312:VAL:HG11	4:I6:325:ILE:HD11	1.74	0.69
17:A2:436:OMG:HM22	17:A2:437:G:H5'	1.75	0.69
2:I4:99:LEU:HB3	5:I8:214:LEU:HD21	1.73	0.69
3:I5:376:THR:HG22	3:I5:398:MET:HE2	1.74	0.69
6:I0:309:ILE:HB	21:AD:89:GLU:HG2	1.73	0.69
17:A2:1376:A:OP2	35:AR:67:ARG:NH1	2.26	0.69
1:I3:91:GLN:HA	1:I3:94:GLN:HB3	1.75	0.68
9:Ir:163:LEU:O	9:Ir:173:ARG:NH1	2.26	0.68
14:Iw:17:G:N2	14:Iw:56:G:O2'	2.27	0.68
32:AO:34:PHE:HB3	32:AO:41:PHE:HB2	1.74	0.68
2:I4:97:VAL:HG21	5:I8:51:LYS:HB2	1.77	0.67
5:I8:66:VAL:HA	5:I8:119:TRP:HA	1.77	0.67
17:A2:925:G:H1	17:A2:1017:U:H3	1.40	0.67
46:Ac:44:ARG:NH2	46:Ac:60:GLU:O	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I5:486:PHE:HB3	3:I5:487:ARG:HE	1.59	0.67
12:Iu:165:ARG:O	12:Iu:166:ASN:ND2	2.27	0.67
17:A2:867:G:H1	25:AH:109:ARG:HH21	1.43	0.66
17:A2:928:G:H1	17:A2:1013:U:H3	1.43	0.66
17:A2:1842:4AC:O7	51:Ah:4:LYS:NZ	2.24	0.66
1:I3:165:LEU:HD23	1:I3:169:GLN:HG3	1.77	0.66
2:I4:336:MET:SD	13:Iv:409:LYS:NZ	2.68	0.66
17:A2:462:OMC:HM22	17:A2:463:C:H5'	1.78	0.66
17:A2:1153:C:OP2	40:AW:71:LYS:NZ	2.28	0.66
3:I5:424:VAL:HG22	3:I5:425:VAL:HG23	1.77	0.66
13:Iv:263:THR:O	13:Iv:270:ARG:NH2	2.29	0.66
15:Ix:266:ASP:HB2	15:Ix:507:LEU:HD11	1.78	0.66
9:Ir:24:VAL:HA	9:Ir:34:VAL:HG23	1.76	0.66
17:A2:1147:C:OP1	44:Aa:6:ARG:NH1	2.28	0.66
2:I4:97:VAL:HG22	5:I8:47:LEU:HB3	1.78	0.66
9:Ir:71:VAL:HG21	9:Ir:85:LEU:HD13	1.78	0.65
3:I5:485:GLU:HB3	3:I5:489:GLN:HB2	1.77	0.65
9:Ir:223:MET:HB3	9:Ir:241:THR:HB	1.78	0.65
13:Iv:95:PHE:HZ	13:Iv:157:LEU:HD11	1.59	0.65
17:A2:1521:C:OP2	36:AS:136:THR:OG1	2.14	0.65
15:Ix:318:TYR:O	15:Ix:322:ASN:ND2	2.28	0.65
15:Ix:271:ARG:NH1	15:Ix:501:LEU:O	2.30	0.65
17:A2:576:A2M:HM'2	17:A2:577:U:H5'	1.78	0.65
37:AT:76:THR:HG22	37:AT:94:ARG:HB3	1.78	0.65
9:Ir:196:GLU:HB2	9:Ir:270:ASN:HB3	1.79	0.65
12:Iu:407:VAL:HG11	12:Iu:435:THR:HG21	1.79	0.65
28:AK:91:PRO:HG2	28:AK:94:LEU:HD23	1.77	0.65
9:Ir:157:VAL:HG11	9:Ir:185:THR:HB	1.78	0.65
34:AQ:53:GLU:OE1	34:AQ:85:ARG:NH2	2.29	0.65
2:I4:323:PHE:HZ	5:I8:345:GLN:HA	1.62	0.65
17:A2:693:A:H2	17:A2:737:G:H22	1.44	0.65
17:A2:1485:U:OP1	21:AD:151:LYS:NZ	2.30	0.64
13:Iv:229:ARG:NH2	13:Iv:328:CYS:SG	2.70	0.64
20:AC:259:THR:HG21	39:AV:16:LYS:H	1.61	0.64
17:A2:1396:A:O2'	17:A2:1398:G:N7	2.29	0.64
3:I5:245:GLU:HB3	3:I5:436:HIS:HD1	1.62	0.64
15:Ix:423:THR:OG1	46:Ac:13:ARG:NH2	2.30	0.64
3:I5:360:ILE:O	3:I5:364:ASN:ND2	2.31	0.64
8:Iq:127:ASP:O	8:Iq:130:GLN:NE2	2.27	0.63
31:AN:55:ARG:NH1	31:AN:56:ASP:OD1	2.30	0.63
33:AP:62:LYS:NZ	33:AP:66:GLU:OE2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I4:138:PRO:HD3	5:I8:110:VAL:HG13	1.81	0.63
9:Ir:230:ILE:HD11	9:Ir:236:VAL:HG23	1.79	0.63
22:AE:100:ARG:NH2	22:AE:121:TYR:O	2.32	0.63
2:I4:338:THR:O	2:I4:342:ASN:ND2	2.30	0.63
17:A2:1776:G:H5'	24:AG:143:LYS:HG3	1.79	0.63
17:A2:387:C:OP2	26:AI:10:LYS:NZ	2.32	0.63
18:AA:184:ARG:HD2	18:AA:191:ARG:HG2	1.81	0.63
24:AG:64:LYS:HB2	24:AG:97:VAL:HG11	1.81	0.63
3:I5:323:TYR:HA	3:I5:326:MET:HB2	1.80	0.62
6:Io:262:PHE:O	6:Io:295:ARG:NH2	2.32	0.62
17:A2:1679:A:OP1	46:Ac:20:ARG:NH2	2.31	0.62
3:I5:235:VAL:O	3:I5:239:ASN:ND2	2.32	0.62
12:Iu:445:GLN:O	12:Iu:512:GLN:NE2	2.32	0.62
38:AU:33:GLU:OE2	38:AU:87:ARG:NH1	2.33	0.62
9:Ir:46:ILE:HG12	9:Ir:85:LEU:HB2	1.82	0.62
9:Ir:205:ILE:O	9:Ir:209:LYS:N	2.32	0.62
17:A2:752:G:N2	17:A2:792:C:O2	2.33	0.62
10:Is:325:ARG:NH2	17:A2:1059:G:OP1	2.33	0.62
17:A2:165:G:H2'	17:A2:166:A2M:H8	1.82	0.62
17:A2:1490:OMG:HM22	17:A2:1491:G:H5'	1.80	0.62
2:I4:335:LEU:HD13	3:I5:530:ILE:HG21	1.81	0.62
4:I6:208:ILE:HG12	4:I6:223:LEU:HD21	1.82	0.62
6:Io:266:SER:OG	6:Io:286:SER:OG	2.17	0.62
12:Iu:415:ARG:HE	12:Iu:428:VAL:HG11	1.63	0.62
12:Iu:436:ILE:HD11	12:Iu:462:VAL:HG21	1.82	0.62
6:Io:292:ASP:OD1	6:Io:295:ARG:NH2	2.32	0.62
6:Io:307:HIS:HB3	21:AD:66:ILE:HD13	1.83	0.61
17:A2:1030:A:H2'	17:A2:1031:A2M:H8	1.82	0.61
49:Af:82:LYS:HE3	49:Af:85:TYR:HE2	1.64	0.61
11:It:288:LEU:HB2	11:It:331:ALA:HB3	1.83	0.61
1:I3:97:ARG:HD2	1:I3:98:PRO:HA	1.82	0.61
4:I6:135:GLY:O	4:I6:138:GLN:NE2	2.34	0.61
4:I6:98:ARG:HB3	4:I6:101:LEU:HB3	1.83	0.61
17:A2:1354:G:N2	17:A2:1357:A:OP2	2.31	0.61
3:I5:243:GLN:HG2	3:I5:252:ASP:H	1.66	0.61
14:Iw:50:U:H2'	14:Iw:51:G:C8	2.34	0.61
17:A2:1767:C:O2	17:A2:1768:A:N6	2.33	0.61
4:I6:83:ILE:HD12	4:I6:109:LEU:HD21	1.81	0.61
17:A2:96:C:H1'	17:A2:474:G:H5'	1.83	0.61
12:Iu:485:ASP:OD1	16:Iy:801:SER:OG	2.18	0.61
5:I8:145:GLU:O	5:I8:168:ARG:NH2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A2:170:A:OP2	24:AG:140:ARG:NH1	2.34	0.60
22:AE:153:LEU:O	22:AE:174:LYS:NZ	2.33	0.60
17:A2:165:G:N2	17:A2:165:G:OP2	2.32	0.60
13:Iv:10:ILE:HG23	13:Iv:216:HIS:HD2	1.65	0.60
22:AE:46:ILE:HA	22:AE:50:ASN:HD22	1.66	0.60
26:AI:130:THR:OG1	26:AI:133:GLU:OE1	2.19	0.60
32:AO:98:ARG:NH1	32:AO:99:ALA:O	2.34	0.60
2:I4:350:LEU:HD23	3:I5:544:ILE:HD13	1.82	0.60
38:Au:20:ILE:HG12	38:Au:116:ILE:HG12	1.83	0.60
3:I5:418:PRO:HA	3:I5:422:SER:HB3	1.83	0.60
50:Ag:165:ILE:HG13	50:Ag:177:TRP:HB2	1.83	0.60
11:It:309:LEU:HD13	11:It:432:PRO:HD3	1.82	0.60
12:Iu:233:ARG:HB3	12:Iu:256:ILE:HG12	1.83	0.60
17:A2:1563:G:OP1	37:AT:121:ARG:NH1	2.34	0.60
2:I4:115:ARG:NH1	2:I4:141:GLU:OE2	2.35	0.59
16:Iy:247:GLY:N	16:Iy:250:THR:HG1	2.00	0.59
17:A2:1383:A2M:HM'2	17:A2:1384:C:H5'	1.83	0.59
42:AY:114:MET:O	42:AY:122:LYS:NZ	2.35	0.59
5:I8:137:GLN:NE2	5:I8:141:GLN:OE1	2.35	0.59
11:It:17:ARG:HA	11:It:38:ARG:HH21	1.67	0.59
33:AP:18:ARG:NH1	36:AS:88:LYS:O	2.35	0.59
50:Ag:166:VAL:HG12	50:Ag:176:VAL:HG22	1.85	0.59
9:Ir:199:CYS:HA	9:Ir:267:GLY:HA2	1.84	0.59
12:Iu:483:ARG:NH2	12:Iu:496:ASP:OD1	2.36	0.59
13:Iv:263:THR:O	13:Iv:265:LYS:N	2.34	0.59
17:A2:542:U:H2'	17:A2:543:C:O4'	2.03	0.59
37:AT:41:LYS:NZ	37:AT:83:GLN:OE1	2.36	0.59
12:Iu:533:ALA:HA	12:Iu:537:ILE:HB	1.83	0.59
30:AM:52:LEU:HB2	30:AM:76:LEU:HD11	1.83	0.59
40:AW:80:ASP:OD1	40:AW:124:LYS:NZ	2.36	0.59
12:Iu:564:GLU:HG3	12:Iu:567:ARG:HD2	1.85	0.59
9:Ir:278:VAL:HG13	9:Ir:279:THR:HG23	1.84	0.58
17:A2:317:C:OP2	24:AG:183:ARG:NH1	2.32	0.58
17:A2:1566:G:N7	37:AT:101:ARG:NH2	2.51	0.58
20:AC:83:LEU:O	39:AV:15:ARG:NH1	2.36	0.58
5:I8:68:LEU:HD13	5:I8:114:HIS:HA	1.85	0.58
8:Iq:83:ASP:N	8:Iq:83:ASP:OD1	2.34	0.58
5:I8:228:HIS:HB3	12:Iu:524:THR:HA	1.85	0.58
15:Ix:31:GLN:NE2	16:Iy:591:MET:O	2.36	0.58
17:A2:506:G:OP1	42:AY:108:LYS:NZ	2.33	0.58
2:I4:277:ALA:HA	4:I6:365:LYS:HE2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AB:3:VAL:HB	32:AO:63:LYS:HG2	1.85	0.58
50:Ag:120:ILE:HB	50:Ag:132:TRP:HB2	1.86	0.58
5:I8:208:SER:H	5:I8:211:ILE:HD12	1.68	0.58
11:It:69:PHE:HD1	11:It:71:ASN:H	1.51	0.58
12:Iu:310:LEU:HD23	12:Iu:315:MET:HG2	1.86	0.58
4:I6:249:LEU:HD13	4:I6:278:ARG:HG2	1.84	0.58
43:AZ:68:ILE:HB	43:AZ:109:TYR:HB2	1.85	0.58
2:I4:106:TYR:HA	2:I4:116:VAL:HG21	1.84	0.58
2:I4:339:TYR:HD2	13:Iv:409:LYS:HE3	1.68	0.58
10:Is:217:THR:HG21	10:Is:262:PHE:H	1.69	0.58
1:I3:174:MET:HB3	1:I3:179:TRP:HB2	1.86	0.58
50:Ag:275:ILE:HG22	50:Ag:278:SER:H	1.68	0.58
17:A2:984:C:HO2'	32:AO:139:SER:N	2.01	0.58
24:AG:10:THR:HG23	24:AG:12:CYS:H	1.69	0.58
50:Ag:159:ASN:ND2	50:Ag:162:ASN:OD1	2.37	0.58
13:Iv:393:MET:SD	13:Iv:393:MET:N	2.77	0.57
17:A2:601:OMG:HM22	17:A2:602:G:H5'	1.86	0.57
15:Ix:42:VAL:HG21	16:Iy:645:LEU:HD13	1.85	0.57
16:Iy:663:GLU:OE2	16:Iy:667:ARG:NH2	2.37	0.57
24:AG:10:THR:HA	24:AG:129:VAL:HG12	1.86	0.57
3:I5:432:HIS:CD2	3:I5:433:PRO:HD3	2.39	0.57
42:AY:55:ILE:HG13	42:AY:75:ILE:HG12	1.86	0.57
27:AJ:136:ARG:NH1	27:AJ:159:PHE:O	2.37	0.57
1:I3:15:LEU:HD22	1:I3:20:ARG:HA	1.87	0.57
8:Iq:62:ARG:NH2	17:A2:614:C:OP1	2.37	0.57
9:Ir:285:GLU:OE2	9:Ir:289:GLN:NE2	2.37	0.57
16:Iy:672:PRO:HD2	16:Iy:675:LEU:HD12	1.87	0.57
17:A2:532:C:H2'	17:A2:533:A:C8	2.39	0.57
11:It:164:SER:O	11:It:167:GLN:NE2	2.37	0.57
25:AH:9:VAL:HG12	25:AH:11:PRO:HD3	1.87	0.57
50:Ag:215:GLN:NE2	50:Ag:231:ASP:OD1	2.38	0.57
12:Iu:327:LEU:O	12:Iu:434:ASN:ND2	2.37	0.57
15:Ix:251:ILE:HG23	15:Ix:267:ILE:HD13	1.86	0.57
16:Iy:252:LEU:HD13	16:Iy:255:ARG:HH21	1.69	0.57
17:A2:1239:U:H5''	33:AP:124:LYS:HD3	1.87	0.57
9:Ir:231:ALA:HB3	9:Ir:234:ARG:HG2	1.86	0.57
17:A2:1679:A:H2'	23:AF:60:ARG:HD2	1.86	0.57
10:Is:263:GLN:OE1	10:Is:265:LYS:NZ	2.34	0.57
11:It:160:ALA:O	11:It:203:GLN:NE2	2.36	0.57
17:A2:1241:A:HO2'	17:A2:1266:C:HO2'	1.52	0.57
17:A2:1285:G:O6	30:AM:57:ASP:N	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AB:34:LYS:NZ	19:AB:95:ASN:OD1	2.32	0.57
5:I8:213:VAL:HG11	12:Iu:557:TYR:HB2	1.86	0.57
9:Ir:108:VAL:HG13	9:Ir:153:PHE:HE2	1.68	0.57
15:Ix:71:TYR:HD1	16:Iy:562:ASP:HB2	1.70	0.57
17:A2:893:U:H2'	17:A2:894:G:C8	2.38	0.57
17:A2:919:A:OP2	31:AN:64:ARG:NH1	2.36	0.57
17:A2:1763:G:H2'	17:A2:1764:G:H8	1.70	0.57
25:AH:57:ARG:NH2	25:AH:89:GLY:O	2.37	0.57
36:AS:101:ASN:O	36:AS:105:ASN:ND2	2.38	0.57
16:Iy:872:ARG:O	16:Iy:876:HIS:ND1	2.31	0.56
22:AE:115:THR:HG22	22:AE:117:GLU:H	1.70	0.56
25:AH:168:HIS:CD2	25:AH:169:LYS:HG3	2.40	0.56
4:I6:141:PRO:O	4:I6:146:GLN:NE2	2.38	0.56
5:I8:70:LEU:HD22	12:Iu:575:ILE:HG12	1.87	0.56
5:I8:160:GLY:HA3	5:I8:230:LEU:HA	1.87	0.56
12:Iu:348:ILE:HA	12:Iu:351:LYS:HE2	1.86	0.56
13:Iv:49:ASN:ND2	13:Iv:140:GLU:OE1	2.38	0.56
40:AW:6:VAL:HG12	40:AW:34:ILE:HD11	1.86	0.56
2:I4:247:ILE:HG12	5:I8:160:GLY:HA2	1.88	0.56
11:It:323:ALA:HB2	11:It:328:LEU:HD11	1.86	0.56
17:A2:1703:OMC:HM22	17:A2:1704:C:H5'	1.87	0.56
20:AC:196:ILE:HB	20:AC:223:TYR:HB2	1.88	0.56
25:AH:46:THR:HG23	25:AH:65:PRO:HD3	1.87	0.56
11:It:225:SER:HB3	11:It:230:TYR:HB2	1.88	0.56
24:AG:7:PHE:HD2	24:AG:10:THR:HG22	1.70	0.56
50:Ag:223:GLU:OE1	50:Ag:225:LYS:NZ	2.38	0.56
17:A2:468:A2M:HM'2	17:A2:469:A:H5'	1.87	0.56
17:A2:792:C:H2'	17:A2:793:G:H8	1.71	0.56
17:A2:792:C:H2'	17:A2:793:G:C8	2.41	0.56
17:A2:1550:G:H3'	17:A2:1579:A:H61	1.69	0.56
19:AB:5:LYS:NZ	32:AO:65:ASP:OD2	2.37	0.56
31:AN:99:ARG:NH2	31:AN:119:GLU:OE2	2.38	0.56
28:AK:80:ARG:NH2	28:AK:89:ILE:O	2.38	0.56
1:I3:87:CYS:HB2	3:I5:447:PHE:CD1	2.40	0.56
2:I4:102:ILE:HG21	2:I4:202:VAL:HG21	1.88	0.56
9:Ir:203:GLU:HB2	9:Ir:205:ILE:HG13	1.86	0.56
17:A2:1291:A:HO2'	49:Af:145:CYS:HG	1.52	0.56
3:I5:430:ASN:OD1	3:I5:436:HIS:NE2	2.38	0.56
17:A2:1759:G:H2'	17:A2:1760:G:H8	1.71	0.56
17:A2:847:A:O2'	22:AE:106:LYS:NZ	2.35	0.56
16:Iy:762:ASN:OD1	16:Iy:776:ARG:NH2	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A2:54:A:OP1	42:AY:111:LYS:NZ	2.33	0.55
18:AA:77:ILE:HG12	18:AA:99:ILE:HB	1.88	0.55
25:AH:51:ILE:HG21	25:AH:179:LYS:HG2	1.88	0.55
26:AI:3:ILE:O	26:AI:30:GLY:N	2.38	0.55
4:I6:212:LEU:O	4:I6:276:LYS:NZ	2.39	0.55
17:A2:1017:U:OP1	31:AN:62:GLN:NE2	2.39	0.55
50:Ag:283:PRO:O	50:Ag:285:GLN:NE2	2.39	0.55
4:I6:364:VAL:HG21	5:I8:343:MET:HA	1.87	0.55
17:A2:1601:A:OP1	43:AZ:43:LYS:NZ	2.39	0.55
49:Af:82:LYS:HE3	49:Af:85:TYR:CE2	2.42	0.55
2:I4:285:THR:HG21	12:Iu:542:ILE:HB	1.88	0.55
7:Ip:100:ILE:HA	16:Iy:249:GLN:HG2	1.89	0.55
11:It:405:MET:HB3	11:It:444:SER:HB2	1.89	0.55
14:Iw:60:C:H2'	14:Iw:61:C:C6	2.41	0.55
16:Iy:373:LYS:O	16:Iy:377:ASN:ND2	2.38	0.55
44:Aa:3:LYS:NZ	44:Aa:8:ASN:OD1	2.39	0.55
2:I4:156:MET:HA	2:I4:159:LEU:HD12	1.88	0.55
13:Iv:352:SER:HB2	13:Iv:355:MET:HG3	1.89	0.55
16:Iy:701:HIS:ND1	16:Iy:704:ASP:OD2	2.38	0.55
17:A2:1756:C:H2'	17:A2:1757:G:H8	1.71	0.55
27:AJ:110:LEU:HB2	27:AJ:147:PHE:HB3	1.88	0.55
2:I4:269:LEU:HD12	4:I6:371:LEU:HB3	1.89	0.55
16:Iy:422:GLU:HG2	16:Iy:443:CYS:HB2	1.89	0.55
17:A2:1310:U:H5''	49:Af:130:VAL:HG13	1.88	0.55
38:AU:54:VAL:HB	38:AU:88:LEU:HB2	1.89	0.55
41:AX:68:LYS:HB3	41:AX:91:LEU:HD22	1.88	0.55
16:Iy:504:LEU:HD22	16:Iy:564:ILE:HG23	1.88	0.55
49:Af:133:ALA:N	49:Af:140:TYR:O	2.38	0.55
50:Ag:159:ASN:HD21	50:Ag:161:SER:HB2	1.71	0.55
11:It:52:HIS:CE1	11:It:160:ALA:H	2.24	0.55
10:Is:209:VAL:HG21	10:Is:267:ILE:HG21	1.89	0.55
17:A2:1314:U:O2'	28:AK:8:ARG:NH1	2.40	0.55
18:AA:205:ARG:NH2	35:AR:82:ASP:OD2	2.33	0.55
2:I4:343:LEU:HD22	16:Iy:863:LEU:HD13	1.89	0.55
11:It:262:PHE:HB2	11:It:278:VAL:HB	1.88	0.55
15:Ix:305:SER:O	15:Ix:311:ASN:ND2	2.40	0.55
15:Ix:319:ILE:HG22	15:Ix:395:THR:HG21	1.88	0.55
16:Iy:865:SER:O	16:Iy:869:ASN:ND2	2.33	0.55
21:AD:62:LYS:HD2	28:AK:96:ARG:HH22	1.72	0.55
1:I3:116:ALA:HA	1:I3:120:ALA:HB3	1.89	0.54
2:I4:313:ASN:HB3	4:I6:336:HIS:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Ir:48:LEU:HD12	23:AF:134:VAL:HG11	1.89	0.54
10:Is:299:PHE:HB3	10:Is:308:ARG:HG2	1.88	0.54
15:Ix:294:THR:OG1	15:Ix:426:LYS:O	2.23	0.54
17:A2:1447:OMG:HM22	17:A2:1448:A:H5'	1.88	0.54
25:AH:83:LEU:HD23	25:AH:92:VAL:HG11	1.89	0.54
4:I6:324:LYS:HD3	12:Iu:448:GLN:HB2	1.88	0.54
15:Ix:479:GLN:NE2	23:AF:30:ILE:O	2.40	0.54
17:A2:965:U:OP1	19:AB:7:LYS:NZ	2.39	0.54
25:AH:100:ILE:HD13	25:AH:122:LEU:HD12	1.89	0.54
4:I6:223:LEU:HD12	4:I6:226:LEU:HD12	1.89	0.54
13:Iv:263:THR:C	13:Iv:265:LYS:H	2.15	0.54
17:A2:734:C:H5'	40:AW:119:LYS:HG2	1.89	0.54
21:AD:45:ARG:HH11	21:AD:85:GLU:HB2	1.72	0.54
50:Ag:107:ASP:OD2	50:Ag:125:ARG:NH1	2.38	0.54
15:Ix:334:ARG:HH22	15:Ix:351:ASN:HA	1.73	0.54
17:A2:1288:OMU:HM22	17:A2:1289:U:H5'	1.90	0.54
33:AP:81:ARG:NH1	33:AP:120:SER:OG	2.39	0.54
38:AU:78:ASP:OD2	47:Ad:44:ARG:NH1	2.40	0.54
17:A2:588:G:OP2	17:A2:588:G:N2	2.38	0.54
17:A2:920:A:O2'	17:A2:922:A:OP1	2.23	0.54
1:I3:86:LYS:HD2	3:I5:450:GLU:HB2	1.90	0.54
10:Is:214:THR:O	10:Is:261:ARG:NH2	2.40	0.54
15:Ix:507:LEU:HB2	15:Ix:522:LEU:HD11	1.89	0.54
17:A2:74:G:OP2	17:A2:74:G:N2	2.38	0.54
17:A2:1783:C:H5'	17:A2:1784:G:H8	1.72	0.54
7:Ip:105:ASP:OD1	7:Ip:105:ASP:N	2.41	0.54
17:A2:234:C:H2'	17:A2:235:A:C8	2.43	0.54
23:AF:128:ILE:HD13	23:AF:137:GLN:HB2	1.90	0.54
32:AO:28:PHE:HZ	44:Aa:58:VAL:HG21	1.70	0.54
12:Iu:343:ASP:OD1	16:Iy:707:ARG:NH1	2.41	0.54
50:Ag:275:ILE:HB	50:Ag:278:SER:HB3	1.90	0.54
3:I5:200:TYR:HB3	3:I5:205:ALA:HB2	1.90	0.54
3:I5:201:ARG:HA	3:I5:205:ALA:HB3	1.90	0.54
4:I6:293:SER:O	4:I6:296:THR:OG1	2.24	0.54
6:Io:260:ARG:NH1	6:Io:263:GLY:O	2.41	0.54
14:Iw:18:G:OP1	14:Iw:59:A:N6	2.28	0.54
10:Is:202:PHE:HE1	10:Is:287:PRO:HB3	1.73	0.54
12:Iu:155:GLU:OE2	12:Iu:158:ARG:NH2	2.32	0.54
12:Iu:398:PHE:HE1	12:Iu:446:ILE:HD11	1.73	0.54
16:Iy:825:MET:HE2	16:Iy:831:LEU:HB2	1.90	0.54
18:AA:184:ARG:HG2	18:AA:189:ILE:HG13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AG:159:ARG:NH2	24:AG:171:THR:O	2.32	0.54
46:Ac:17:VAL:HA	46:Ac:30:VAL:HG12	1.90	0.54
4:I6:338:THR:O	4:I6:340:ARG:NH2	2.41	0.53
11:It:321:LEU:HD13	11:It:331:ALA:HB2	1.90	0.53
17:A2:1805:G:H2'	17:A2:1806:A:C8	2.43	0.53
38:AU:56:MET:HB2	38:AU:86:LYS:HB3	1.90	0.53
3:I5:544:ILE:O	3:I5:548:HIS:ND1	2.39	0.53
13:Iv:313:ARG:HH21	13:Iv:361:ASN:HD21	1.56	0.53
12:Iu:109:GLN:OE1	12:Iu:138:GLN:NE2	2.41	0.53
15:Ix:53:LYS:O	15:Ix:57:ASN:ND2	2.41	0.53
16:Iy:284:ARG:O	16:Iy:288:ARG:N	2.36	0.53
17:A2:1114:U:H3	17:A2:1117:C:H5	1.56	0.53
44:Aa:22:ARG:NH1	44:Aa:27:ALA:O	2.41	0.53
1:I3:84:LEU:HD11	3:I5:326:MET:HG2	1.89	0.53
3:I5:343:ILE:HG22	3:I5:345:ARG:HG2	1.90	0.53
9:Ir:48:LEU:HD13	9:Ir:51:LEU:HD12	1.90	0.53
13:Iv:319:LEU:HD23	13:Iv:325:LEU:HD13	1.90	0.53
15:Ix:38:ARG:HB3	15:Ix:59:TYR:HB3	1.91	0.53
17:A2:1757:G:H1	17:A2:1775:U:H3	1.56	0.53
17:A2:1759:G:H2'	17:A2:1760:G:C8	2.44	0.53
17:A2:1808:U:H2'	17:A2:1809:A:C8	2.43	0.53
23:AF:71:ARG:NH2	23:AF:148:ASN:OD1	2.40	0.53
9:Ir:234:ARG:NH2	14:Iw:71:U:O2'	2.42	0.53
13:Iv:399:SER:O	13:Iv:403:GLN:N	2.31	0.53
16:Iy:288:ARG:O	16:Iy:292:GLU:N	2.37	0.53
16:Iy:834:SER:HB2	16:Iy:843:VAL:HB	1.89	0.53
23:AF:128:ILE:HG22	46:Ac:68:LEU:HD13	1.91	0.53
50:Ag:240:CYS:HG	50:Ag:291:TRP:CD1	2.27	0.53
1:I3:87:CYS:HB2	3:I5:447:PHE:HD1	1.74	0.53
3:I5:242:ARG:HD3	3:I5:427:ASN:HB3	1.90	0.53
4:I6:220:PHE:HB2	4:I6:245:VAL:HG22	1.91	0.53
13:Iv:67:PRO:HD2	13:Iv:70:LEU:HD12	1.91	0.53
17:A2:75:G:H21	17:A2:75:G:P	2.31	0.53
17:A2:1415:C:O2'	37:AT:132:ASP:OD2	2.25	0.53
30:AM:40:LYS:HG3	49:Af:129:GLY:HA3	1.89	0.53
50:Ag:237:ASN:ND2	50:Ag:286:CYS:O	2.32	0.53
15:Ix:315:GLU:OE1	15:Ix:454:ARG:NH2	2.40	0.53
36:AS:34:LYS:HG2	36:AS:103:LEU:HD23	1.89	0.53
1:I3:139:ARG:HH21	1:I3:165:LEU:HD13	1.73	0.53
16:Iy:300:GLU:C	16:Iy:302:GLU:H	2.16	0.53
16:Iy:325:THR:HB	16:Iy:328:VAL:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Iy:329:VAL:HG13	16:Iy:357:LEU:HD11	1.90	0.53
10:Is:229:LEU:HD23	10:Is:279:VAL:HG21	1.91	0.53
11:It:23:LEU:HD11	11:It:28:LEU:HD11	1.91	0.53
12:Iu:324:LEU:HD12	12:Iu:424:LEU:HD22	1.90	0.53
13:Iv:51:VAL:HG11	13:Iv:74:ARG:HB2	1.91	0.53
15:Ix:29:PRO:O	15:Ix:69:TYR:OH	2.22	0.53
15:Ix:197:GLY:HA3	15:Ix:357:ALA:HA	1.90	0.53
25:AH:8:ILE:HG22	25:AH:44:ASN:HA	1.91	0.53
12:Iu:129:LEU:HD13	12:Iu:140:ARG:HH12	1.74	0.52
15:Ix:222:ARG:HD3	15:Ix:354:ALA:HA	1.90	0.52
17:A2:1714:U:H2'	17:A2:1715:A:C8	2.43	0.52
1:I3:197:LYS:HG2	1:I3:199:LYS:HG3	1.91	0.52
5:I8:80:ASN:OD1	5:I8:81:CYS:N	2.41	0.52
17:A2:466:G:H1'	24:AG:59:GLN:HE21	1.73	0.52
22:AE:11:ARG:HA	22:AE:28:ALA:HB2	1.90	0.52
49:Af:107:LYS:HB2	49:Af:117:LEU:HD21	1.90	0.52
9:Ir:22:VAL:HG23	9:Ir:36:LEU:HA	1.91	0.52
13:Iv:19:VAL:HG12	13:Iv:23:LEU:HG	1.91	0.52
15:Ix:28:MET:SD	15:Ix:69:TYR:OH	2.68	0.52
2:I4:280:GLN:HG3	4:I6:358:LYS:HG2	1.91	0.52
3:I5:377:MET:HE1	13:Iv:379:ARG:HH12	1.74	0.52
17:A2:1726:G:H2'	17:A2:1727:G:H8	1.74	0.52
17:A2:1863:A:OP2	44:Aa:4:LYS:NZ	2.42	0.52
25:AH:60:ILE:HB	25:AH:92:VAL:HG22	1.92	0.52
2:I4:187:HIS:CE1	2:I4:218:SER:HG	2.25	0.52
9:Ir:72:VAL:HG11	9:Ir:89:ARG:HB2	1.92	0.52
11:It:89:TYR:HB3	11:It:124:PHE:HB3	1.90	0.52
12:Iu:12:LEU:HD11	12:Iu:49:PRO:HB2	1.91	0.52
17:A2:538:U:H2'	17:A2:539:C:C6	2.44	0.52
17:A2:1060:A:O2'	17:A2:1062:A:N7	2.40	0.52
17:A2:1775:U:H2'	17:A2:1776:G:H8	1.74	0.52
16:Iy:476:GLU:OE2	16:Iy:512:TYR:OH	2.28	0.52
17:A2:871:U:O2'	17:A2:873:G:OP1	2.26	0.52
50:Ag:238:ALA:H	50:Ag:251:ALA:HB3	1.74	0.52
9:Ir:131:PHE:HB3	9:Ir:136:TRP:CE2	2.43	0.52
17:A2:1614:A:OP2	33:AP:42:ARG:NH1	2.42	0.52
20:AC:60:TRP:O	20:AC:71:LYS:NZ	2.36	0.52
17:A2:532:C:H2'	17:A2:533:A:H8	1.73	0.52
3:I5:243:GLN:O	3:I5:247:TYR:N	2.39	0.52
11:It:105:CYS:HB3	11:It:109:THR:HG21	1.92	0.52
17:A2:1031:A2M:HM'2	17:A2:1032:C:H5'	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A2:1763:G:H2'	17:A2:1764:G:C8	2.44	0.52
20:AC:254:ASP:HB2	39:AV:1:AME:HT22	1.90	0.52
21:AD:16:ILE:HD11	47:Ad:36:LEU:HD23	1.92	0.52
3:I5:396:ASP:HB2	13:Iv:268:ARG:HH12	1.75	0.51
13:Iv:8:THR:O	13:Iv:12:HIS:ND1	2.43	0.51
14:Iw:29:G:OP1	17:A2:1524:G:O2'	2.28	0.51
17:A2:539:C:H2'	17:A2:540:U:O4'	2.10	0.51
17:A2:544:G:H2'	17:A2:545:A:C8	2.45	0.51
30:AM:44:LYS:HD3	49:Af:128:ALA:HB3	1.91	0.51
50:Ag:190:GLY:HA3	50:Ag:217:MET:HE1	1.92	0.51
3:I5:398:MET:HG3	13:Iv:379:ARG:HH22	1.75	0.51
15:Ix:396:LEU:HD21	15:Ix:432:LEU:HD21	1.92	0.51
17:A2:1391:OMC:HM22	17:A2:1392:U:H5'	1.92	0.51
30:AM:43:ASP:OD2	49:Af:106:TYR:OH	2.27	0.51
1:I3:88:MET:HG3	3:I5:291:ILE:HG23	1.92	0.51
9:Ir:285:GLU:HA	9:Ir:288:ARG:HD2	1.92	0.51
13:Iv:348:HIS:HE1	16:Iy:835:LEU:HD22	1.74	0.51
15:Ix:193:ILE:HD11	15:Ix:362:ARG:HB2	1.91	0.51
17:A2:582:U:H1'	42:AY:33:ALA:HB2	1.92	0.51
2:I4:187:HIS:NE2	2:I4:218:SER:OG	2.42	0.51
17:A2:1265:A:O2'	17:A2:1327:G:OP2	2.24	0.51
1:I3:161:MET:HE1	3:I5:494:LYS:HE2	1.92	0.51
12:Iu:297:HIS:HE1	12:Iu:370:LEU:HB3	1.75	0.51
17:A2:736:C:H2'	17:A2:737:G:C8	2.45	0.51
24:AG:159:ARG:HB3	24:AG:171:THR:HG22	1.92	0.51
2:I4:315:VAL:HG21	5:I8:348:GLN:HG2	1.92	0.51
2:I4:338:THR:HG23	5:I8:331:LYS:HG2	1.92	0.51
13:Iv:23:LEU:HD13	13:Iv:41:LYS:HG2	1.93	0.51
17:A2:67:C:C5	24:AG:162:LEU:HB3	2.45	0.51
17:A2:581:U:H4'	42:AY:66:GLY:HA2	1.91	0.51
22:AE:246:LEU:HB3	22:AE:250:GLU:HG3	1.91	0.51
3:I5:489:GLN:O	3:I5:493:PHE:N	2.41	0.51
15:Ix:505:LYS:HG2	15:Ix:522:LEU:HD12	1.93	0.51
45:Ab:62:VAL:O	45:Ab:74:THR:OG1	2.29	0.51
49:Af:138:ARG:HA	49:Af:149:CYS:HA	1.93	0.51
9:Ir:195:ILE:HD11	9:Ir:271:VAL:HG12	1.92	0.51
1:I3:36:GLN:HA	1:I3:41:ALA:HB3	1.93	0.51
1:I3:47:ASN:HD22	1:I3:69:ILE:HD13	1.76	0.51
4:I6:309:GLU:OE2	12:Iu:447:TYR:OH	2.26	0.51
12:Iu:568:ILE:HA	12:Iu:571:ARG:HB2	1.93	0.51
17:A2:1400:U:O4	17:A2:1401:A:N6	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Af:121:CYS:HA	49:Af:132:MET:HE3	1.92	0.51
3:I5:466:LEU:HD22	13:Iv:376:ARG:HD2	1.91	0.50
3:I5:526:ASP:O	3:I5:530:ILE:N	2.41	0.50
3:I5:533:THR:O	3:I5:537:ARG:N	2.37	0.50
7:Ip:27:THR:HG22	7:Ip:51:ALA:HB2	1.93	0.50
9:Ir:233:PRO:HG3	11:It:346:THR:HG23	1.93	0.50
11:It:127:VAL:HG12	11:It:128:ARG:HG3	1.93	0.50
17:A2:1786:U:H2'	17:A2:1787:G:C8	2.45	0.50
9:Ir:106:LYS:NZ	14:Iw:18:G:OP2	2.38	0.50
17:A2:1005:G:OP2	19:AB:162:ARG:NH1	2.43	0.50
17:A2:1725:U:H2'	17:A2:1726:G:C8	2.46	0.50
46:Ac:40:ARG:HH22	46:Ac:62:GLU:HA	1.77	0.50
5:I8:159:GLN:HE22	5:I8:238:HIS:CG	2.29	0.50
5:I8:261:ASN:HD22	16:Iy:869:ASN:HB3	1.75	0.50
9:Ir:185:THR:OG1	9:Ir:187:GLN:NE2	2.44	0.50
12:Iu:334:GLU:HG3	12:Iu:336:THR:HG23	1.94	0.50
13:Iv:12:HIS:O	15:Ix:10:GLN:NE2	2.28	0.50
49:Af:102:VAL:HA	49:Af:105:TYR:HD2	1.75	0.50
2:I4:184:VAL:HG13	2:I4:230:VAL:HG11	1.92	0.50
3:I5:490:LEU:HA	3:I5:493:PHE:HB2	1.92	0.50
16:Iy:275:GLU:O	16:Iy:279:LYS:N	2.39	0.50
17:A2:1116:C:H2'	17:A2:1117:C:C6	2.46	0.50
2:I4:110:ASN:HB3	12:Iu:572:ARG:HH22	1.75	0.50
8:Iq:133:ASP:HB3	10:Is:206:PRO:HG2	1.92	0.50
17:A2:234:C:H2'	17:A2:235:A:H8	1.76	0.50
17:A2:484:A2M:O5'	17:A2:484:A2M:H8	2.11	0.50
17:A2:1091:C:O2'	40:AW:2:VAL:N	2.43	0.50
26:AI:101:ILE:HD12	26:AI:190:LEU:HD11	1.94	0.50
42:AY:12:PHE:HZ	42:AY:21:LYS:HD3	1.76	0.50
50:Ag:268:ASP:OD1	50:Ag:269:GLU:N	2.43	0.50
9:Ir:50:GLU:HA	9:Ir:88:ARG:HD3	1.93	0.50
15:Ix:212:ARG:NH2	17:A2:1471:C:OP1	2.45	0.50
16:Iy:300:GLU:C	16:Iy:302:GLU:N	2.70	0.50
16:Iy:383:TYR:HB3	16:Iy:450:ARG:HE	1.77	0.50
17:A2:548:C:H2'	17:A2:549:C:C6	2.46	0.50
1:I3:11:VAL:HG21	1:I3:46:ALA:HB2	1.93	0.50
4:I6:195:ASP:OD1	4:I6:196:ASN:ND2	2.44	0.50
5:I8:36:VAL:H	5:I8:168:ARG:HH12	1.60	0.50
5:I8:44:LEU:HD11	5:I8:48:LYS:HE3	1.93	0.50
16:Iy:648:GLN:NE2	16:Iy:677:ILE:H	2.10	0.50
17:A2:1272:OMC:HM22	17:A2:1273:C:H5'	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AB:123:ALA:HB2	19:AB:165:ARG:HG3	1.94	0.50
1:I3:7:MET:HE2	1:I3:32:TYR:HD1	1.77	0.50
1:I3:11:VAL:HG23	1:I3:15:LEU:HD12	1.93	0.50
9:Ir:34:VAL:O	9:Ir:44:GLY:N	2.34	0.50
9:Ir:123:LYS:HE2	9:Ir:126:GLN:HB2	1.94	0.50
12:Iu:350:GLU:HA	12:Iu:353:ARG:HE	1.77	0.50
17:A2:1033:G:N1	17:A2:1080:A:O2'	2.37	0.50
24:AG:1:MET:HE1	24:AG:106:LEU:HB2	1.94	0.50
31:AN:25:TRP:CD2	45:Ab:82:LYS:HD3	2.47	0.50
43:AZ:54:THR:HG21	43:AZ:79:ILE:HD11	1.94	0.50
50:Ag:251:ALA:HB2	50:Ag:289:LEU:HD22	1.93	0.50
4:I6:213:LYS:HD3	4:I6:268:LEU:HA	1.94	0.50
15:Ix:296:ASN:OD1	15:Ix:296:ASN:N	2.44	0.50
17:A2:691:G:H2'	17:A2:692:G:C8	2.47	0.50
3:I5:380:MET:SD	3:I5:380:MET:N	2.75	0.49
13:Iv:255:ARG:HG3	13:Iv:292:ILE:HD12	1.92	0.49
17:A2:1786:U:H2'	17:A2:1787:G:H8	1.77	0.49
50:Ag:68:ASP:HB3	50:Ag:111:VAL:HG12	1.94	0.49
50:Ag:159:ASN:HD22	50:Ag:162:ASN:CG	2.20	0.49
10:Is:251:ASP:OD1	10:Is:252:GLY:N	2.45	0.49
10:Is:302:CYS:O	10:Is:306:HIS:N	2.42	0.49
12:Iu:394:LEU:HD23	12:Iu:403:LEU:HD11	1.93	0.49
13:Iv:402:GLN:HA	13:Iv:405:ILE:HD12	1.94	0.49
17:A2:706:U:H3	17:A2:724:A:H61	1.59	0.49
17:A2:1226:G:N1	17:A2:1639:G7M:OP2	2.31	0.49
2:I4:294:LEU:HD13	4:I6:347:TRP:HB2	1.94	0.49
2:I4:304:VAL:HG23	12:Iu:537:ILE:HD13	1.94	0.49
7:Ip:20:ASP:O	11:It:446:ARG:NH2	2.45	0.49
17:A2:1753:C:H2'	17:A2:1754:G:H8	1.77	0.49
3:I5:450:GLU:HG2	3:I5:454:GLN:HG3	1.93	0.49
5:I8:72:VAL:N	5:I8:75:ARG:O	2.43	0.49
5:I8:341:LEU:O	5:I8:345:GLN:N	2.43	0.49
40:AW:3:ARG:HD3	40:AW:6:VAL:HG22	1.92	0.49
2:I4:309:MET:HE2	4:I6:339:HIS:CE1	2.48	0.49
3:I5:307:ARG:NH1	3:I5:312:GLN:OE1	2.45	0.49
10:Is:283:THR:HG1	54:It:1000:GTP:HO3'	1.59	0.49
12:Iu:68:LYS:HD2	12:Iu:159:GLN:HG2	1.95	0.49
15:Ix:162:VAL:HG11	15:Ix:507:LEU:HD21	1.95	0.49
24:AG:57:ASP:HA	24:AG:106:LEU:HA	1.94	0.49
9:Ir:195:ILE:HG13	9:Ir:272:GLN:H	1.77	0.49
9:Ir:229:LEU:HD13	9:Ir:229:LEU:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:It:369:THR:HG21	11:It:465:ILE:HD12	1.94	0.49
12:Iu:12:LEU:HD21	12:Iu:50:ILE:HA	1.95	0.49
16:Iy:713:GLN:HE21	16:Iy:717:GLN:HE21	1.59	0.49
17:A2:1866:A:N6	44:Aa:84:VAL:HG22	2.28	0.49
25:AH:119:SER:HB2	25:AH:120:ARG:HH11	1.78	0.49
31:AN:63:VAL:HG21	31:AN:71:ILE:HD11	1.94	0.49
4:I6:196:ASN:HB2	4:I6:199:GLN:HE21	1.77	0.49
9:Ir:30:MET:SD	9:Ir:31:GLY:N	2.86	0.49
11:It:157:LEU:HD11	11:It:170:THR:HG23	1.93	0.49
3:I5:373:ILE:HG21	3:I5:412:LEU:HD13	1.95	0.49
17:A2:1531:A:H4'	17:A2:1605:G:H4'	1.95	0.49
17:A2:1764:G:C5	17:A2:1765:C:H1'	2.47	0.49
35:AR:21:TYR:CE1	35:AR:77:GLU:HG2	2.48	0.49
3:I5:449:ASP:OD1	3:I5:450:GLU:N	2.45	0.49
13:Iv:236:PHE:HD2	13:Iv:257:LEU:HD13	1.78	0.49
17:A2:438:G:OP2	17:A2:438:G:N2	2.42	0.49
17:A2:860:G:H21	40:AW:107:SER:HB2	1.78	0.49
2:I4:227:THR:HG22	4:I6:14:GLN:HG2	1.94	0.48
5:I8:67:LEU:HD11	5:I8:150:LEU:HB2	1.95	0.48
9:Ir:281:THR:OG1	9:Ir:284:THR:OG1	2.27	0.48
11:It:16:SER:O	11:It:38:ARG:NE	2.42	0.48
17:A2:533:A:H2'	17:A2:534:G:C8	2.47	0.48
22:AE:124:CYS:HB3	22:AE:141:THR:HB	1.95	0.48
26:AI:46:VAL:HG21	26:AI:56:ARG:HH11	1.78	0.48
2:I4:109:ARG:HB3	12:Iu:565:HIS:HE1	1.78	0.48
2:I4:156:MET:HE1	5:I8:103:MET:HE1	1.95	0.48
3:I5:507:SER:HB3	3:I5:511:GLY:H	1.76	0.48
4:I6:360:ASN:HB3	5:I8:346:ALA:HB1	1.94	0.48
11:It:294:ILE:HD12	11:It:358:LEU:HD11	1.95	0.48
17:A2:282:G:H2'	17:A2:283:G:C8	2.48	0.48
27:AJ:114:VAL:HG13	27:AJ:119:LEU:HB2	1.94	0.48
50:Ag:5:MET:HB2	50:Ag:270:LEU:HD21	1.94	0.48
2:I4:264:GLY:HA3	5:I8:204:VAL:HA	1.95	0.48
9:Ir:64:ARG:NE	9:Ir:67:ARG:HB2	2.28	0.48
12:Iu:450:ILE:HG22	12:Iu:493:PHE:HE1	1.79	0.48
16:Iy:272:LYS:O	16:Iy:276:ASP:N	2.40	0.48
17:A2:145:G:H2'	17:A2:146:G:C8	2.48	0.48
17:A2:549:C:H2'	17:A2:550:C:C6	2.48	0.48
20:AC:209:VAL:HB	20:AC:210:PRO:HD3	1.95	0.48
1:I3:149:THR:HG21	3:I5:498:LYS:HG2	1.94	0.48
4:I6:80:GLU:HG2	4:I6:119:VAL:HG11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Ip:36:GLN:HE22	10:Is:319:GLN:HA	1.79	0.48
15:Ix:508:ILE:HG12	15:Ix:519:VAL:HG22	1.94	0.48
17:A2:377:G:H5'	26:AI:98:LYS:HB3	1.94	0.48
17:A2:1155:U:OP1	20:AC:185:THR:OG1	2.24	0.48
17:A2:1725:U:H2'	17:A2:1726:G:H8	1.79	0.48
17:A2:1808:U:H2'	17:A2:1809:A:H8	1.79	0.48
21:AD:106:ARG:HG3	21:AD:175:VAL:HG22	1.95	0.48
30:AM:58:GLU:HG3	30:AM:61:TYR:H	1.77	0.48
1:I3:68:GLN:HE22	1:I3:127:LEU:HB3	1.78	0.48
4:I6:110:PHE:HE1	4:I6:120:ARG:HB3	1.78	0.48
9:Ir:131:PHE:HB3	9:Ir:136:TRP:CD2	2.49	0.48
17:A2:1779:G:H2'	17:A2:1780:G:C8	2.47	0.48
42:AY:102:THR:HG23	42:AY:107:ARG:HH11	1.78	0.48
12:Iu:485:ASP:OD1	12:Iu:487:THR:OG1	2.30	0.48
19:AB:30:TRP:CD2	32:AO:19:PRO:HG3	2.48	0.48
26:AI:11:ARG:O	29:AL:136:LYS:NZ	2.33	0.48
30:AM:60:MET:HG3	49:Af:103:LEU:HD22	1.96	0.48
2:I4:265:LEU:HD11	5:I8:202:PRO:HB3	1.96	0.48
11:It:187:ILE:HB	11:It:221:ILE:HG12	1.96	0.48
16:Iy:644:GLU:HG3	16:Iy:651:LEU:HG	1.95	0.48
17:A2:186:C:H2'	17:A2:187:G:C8	2.49	0.48
19:AB:38:MET:HE2	19:AB:182:LYS:HA	1.96	0.48
1:I3:83:THR:HA	1:I3:86:LYS:HE3	1.95	0.48
1:I3:97:ARG:NH1	1:I3:101:GLN:OE1	2.44	0.48
9:Ir:126:GLN:O	9:Ir:130:LEU:N	2.41	0.48
9:Ir:220:THR:OG1	9:Ir:223:MET:O	2.30	0.48
10:Is:187:MET:HE2	10:Is:195:VAL:HA	1.95	0.48
16:Iy:281:LYS:O	16:Iy:285:LYS:N	2.37	0.48
17:A2:453:C:O2'	24:AG:92:ARG:O	2.23	0.48
17:A2:1836:G:OP1	17:A2:1839:U:H4'	2.13	0.48
1:I3:74:LEU:HD12	1:I3:106:GLY:HA2	1.95	0.48
1:I3:179:TRP:HB3	1:I3:187:ILE:HD11	1.96	0.48
3:I5:243:GLN:HA	3:I5:246:VAL:HG12	1.94	0.48
4:I6:148:ARG:HH12	12:Iu:538:LYS:HZ3	1.62	0.48
6:I0:244:THR:HB	21:AD:90:LYS:HD3	1.94	0.48
13:Iv:118:ALA:HA	13:Iv:123:PHE:H	1.79	0.48
17:A2:1759:G:H1	17:A2:1773:C:H42	1.61	0.48
18:AA:135:THR:O	18:AA:138:SER:OG	2.30	0.48
21:AD:226:GLN:NE2	50:Ag:224:GLY:O	2.46	0.48
36:AS:36:VAL:HG13	36:AS:40:TYR:HD2	1.78	0.48
2:I4:314:GLN:HB3	12:Iu:526:MET:SD	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I6:97:GLU:HB3	4:I6:98:ARG:HD2	1.96	0.48
17:A2:240:G:H1	17:A2:278:C:H42	1.61	0.48
17:A2:1232:PSU:H2'	17:A2:1233:G:C8	2.49	0.48
17:A2:1841:C:H2'	17:A2:1842:4AC:H6	1.95	0.48
1:I3:146:VAL:HA	1:I3:149:THR:HG22	1.94	0.47
3:I5:379:PRO:HG3	3:I5:391:ARG:HH12	1.79	0.47
5:I8:233:LEU:HB2	12:Iu:521:ASN:N	2.25	0.47
12:Iu:214:GLN:HB2	12:Iu:217:ALA:HB2	1.94	0.47
15:Ix:33:PHE:HB2	16:Iy:590:LEU:HG	1.96	0.47
44:Aa:43:ASN:OD1	44:Aa:66:LYS:NZ	2.46	0.47
4:I6:158:THR:HG23	4:I6:161:LYS:HE2	1.95	0.47
4:I6:323:CYS:HB3	4:I6:334:VAL:HG12	1.96	0.47
5:I8:113:ASP:CG	12:Iu:575:ILE:HD12	2.39	0.47
7:Ip:54:TYR:HA	16:Iy:257:LEU:HA	1.96	0.47
17:A2:547:G:H21	17:A2:549:C:H5'	1.78	0.47
17:A2:641:A:O2'	17:A2:645:C:OP1	2.28	0.47
17:A2:1328:OMG:HM22	17:A2:1329:U:H5'	1.96	0.47
3:I5:187:ILE:HD11	3:I5:242:ARG:HD2	1.96	0.47
9:Ir:259:LYS:HE2	9:Ir:269:PHE:CG	2.49	0.47
11:It:254:PRO:HA	11:It:286:GLY:HA3	1.97	0.47
15:Ix:345:GLU:H	15:Ix:348:MET:HE2	1.78	0.47
17:A2:835:C:H4'	17:A2:836:G:C4	2.49	0.47
17:A2:1124:C:H5''	19:AB:150:ILE:HG12	1.96	0.47
17:A2:1434:C:H5	17:A2:1437:C:H42	1.61	0.47
10:Is:253:ASN:O	10:Is:253:ASN:ND2	2.40	0.47
11:It:137:GLY:HA2	11:It:173:HIS:HE1	1.79	0.47
15:Ix:447:LEU:N	15:Ix:471:PHE:O	2.35	0.47
16:Iy:566:THR:HA	16:Iy:569:ILE:HD12	1.96	0.47
17:A2:67:C:C4	24:AG:164:LYS:HB2	2.49	0.47
17:A2:1606:G:N2	17:A2:1632:G:H1'	2.29	0.47
24:AG:120:ASP:HB2	24:AG:125:THR:HB	1.96	0.47
2:I4:269:LEU:HD22	2:I4:269:LEU:H	1.79	0.47
5:I8:208:SER:HB3	5:I8:211:ILE:HG13	1.97	0.47
6:Io:255:LEU:HB3	6:Io:285:ILE:HD11	1.97	0.47
10:Is:283:THR:O	10:Is:285:ARG:NH1	2.47	0.47
11:It:46:THR:HG22	11:It:156:LEU:HD12	1.95	0.47
11:It:264:VAL:HA	14:Iw:74:C:H1'	1.97	0.47
11:It:445:ARG:HB2	11:It:454:ILE:HD13	1.96	0.47
17:A2:809:A:H2'	17:A2:810:A:O4'	2.14	0.47
27:AJ:93:LYS:HB2	27:AJ:96:TYR:CD2	2.50	0.47
3:I5:402:GLN:NE2	3:I5:462:SER:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Ix:289:LEU:HD13	15:Ix:435:TRP:HZ2	1.79	0.47
17:A2:1753:C:H2'	17:A2:1754:G:C8	2.49	0.47
1:I3:207:PHE:O	1:I3:211:SER:N	2.47	0.47
5:I8:70:LEU:HB2	12:Iu:575:ILE:HG12	1.97	0.47
9:Ir:232:PRO:HG2	11:It:349:ARG:HB2	1.97	0.47
20:AC:159:LYS:HA	20:AC:162:ILE:HG13	1.97	0.47
33:AP:34:MET:HB3	33:AP:42:ARG:HG3	1.96	0.47
36:AS:22:GLY:HA2	36:AS:56:ALA:HB3	1.97	0.47
2:I4:124:VAL:HG23	2:I4:170:LEU:HD22	1.97	0.47
9:Ir:78:LYS:H	9:Ir:78:LYS:HD2	1.80	0.47
13:Iv:6:LEU:HD13	13:Iv:252:HIS:HB2	1.96	0.47
16:Iy:576:HIS:HA	16:Iy:581:ARG:HE	1.80	0.47
17:A2:75:G:O2'	24:AG:159:ARG:HD2	2.15	0.47
2:I4:304:VAL:HG22	2:I4:308:LEU:HB2	1.97	0.47
10:Is:229:LEU:HG	10:Is:279:VAL:HG11	1.96	0.47
12:Iu:289:ALA:HA	12:Iu:292:HIS:HB3	1.96	0.47
15:Ix:430:TYR:CZ	15:Ix:434:ARG:HD2	2.50	0.47
16:Iy:695:ILE:HD11	16:Iy:741:SER:HB3	1.97	0.47
17:A2:71:G:O6	24:AG:170:ARG:NH1	2.47	0.47
17:A2:1758:G:H2'	17:A2:1759:G:C8	2.49	0.47
17:A2:1781:A:H2'	17:A2:1782:G:C8	2.49	0.47
2:I4:334:LEU:HB3	5:I8:334:THR:HG23	1.97	0.47
2:I4:339:TYR:CD2	13:Iv:409:LYS:HE3	2.49	0.47
5:I8:134:LEU:HD22	5:I8:318:LEU:HD21	1.97	0.47
9:Ir:177:ILE:HA	9:Ir:180:ILE:HG22	1.97	0.47
10:Is:194:MET:HE1	10:Is:199:LYS:HE3	1.97	0.47
46:Ac:13:ARG:HB2	46:Ac:35:MET:HE2	1.97	0.47
4:I6:226:LEU:O	4:I6:230:LYS:N	2.37	0.46
11:It:49:HIS:HB3	11:It:52:HIS:CE1	2.50	0.46
12:Iu:48:GLU:HB3	12:Iu:49:PRO:HD3	1.97	0.46
12:Iu:384:VAL:HG12	12:Iu:386:GLU:H	1.80	0.46
16:Iy:426:GLU:OE2	16:Iy:441:ARG:NH1	2.48	0.46
22:AE:100:ARG:HG2	22:AE:102:ILE:HG12	1.97	0.46
50:Ag:233:GLY:HA3	50:Ag:252:THR:HG21	1.97	0.46
1:I3:17:GLY:O	3:I5:262:ARG:NH1	2.48	0.46
2:I4:213:ILE:H	5:I8:221:LYS:NZ	2.14	0.46
3:I5:548:HIS:NE2	5:I8:193:THR:HG21	2.31	0.46
4:I6:339:HIS:HD2	4:I6:346:GLN:HE21	1.63	0.46
15:Ix:391:ILE:HG22	15:Ix:446:TYR:HB2	1.96	0.46
16:Iy:545:ALA:HB2	16:Iy:581:ARG:HH22	1.80	0.46
21:AD:32:ASP:OD2	21:AD:65:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AF:49:LEU:HD12	34:AQ:50:LYS:HG2	1.97	0.46
25:AH:144:ILE:HB	40:AW:52:ILE:HB	1.97	0.46
4:I6:263:ILE:O	4:I6:268:LEU:HB2	2.15	0.46
8:Iq:72:ASN:HD22	10:Is:263:GLN:HE22	1.63	0.46
15:Ix:190:PRO:HB3	15:Ix:363:TRP:CE2	2.50	0.46
16:Iy:451:MET:HE3	16:Iy:479:VAL:HG13	1.96	0.46
17:A2:1662:U:O4	17:A2:1663:A:N6	2.44	0.46
17:A2:1810:U:H2'	17:A2:1811:C:C6	2.51	0.46
1:I3:20:ARG:NH2	3:I5:287:TYR:OH	2.48	0.46
13:Iv:16:ARG:HG2	13:Iv:44:LEU:HD22	1.96	0.46
17:A2:753:C:H2'	17:A2:754:G:H8	1.80	0.46
17:A2:1013:U:OP1	17:A2:1129:G:O2'	2.33	0.46
17:A2:1756:C:H2'	17:A2:1757:G:C8	2.49	0.46
19:AB:129:THR:OG1	19:AB:131:ASP:OD1	2.30	0.46
2:I4:306:ARG:NH2	4:I6:219:LEU:HB3	2.31	0.46
2:I4:328:ASN:HB3	3:I5:523:ILE:HD12	1.98	0.46
5:I8:254:SER:HA	16:Iy:866:LEU:HD21	1.98	0.46
43:AZ:50:PHE:HE2	43:AZ:87:ALA:HB2	1.80	0.46
5:I8:45:VAL:HG21	5:I8:78:ILE:HG22	1.98	0.46
15:Ix:456:HIS:CD2	50:Ag:275:ILE:HG23	2.51	0.46
17:A2:127:C:O2	22:AE:134:LYS:NZ	2.49	0.46
17:A2:799:OMU:H6	25:AH:109:ARG:HD3	1.98	0.46
17:A2:1083:A:N7	17:A2:1841:C:O2'	2.47	0.46
17:A2:1285:G:O3'	49:Af:99:LYS:NZ	2.49	0.46
17:A2:1726:G:H2'	17:A2:1727:G:C8	2.51	0.46
17:A2:1762:C:H2'	17:A2:1763:G:C8	2.50	0.46
3:I5:284:LEU:O	3:I5:288:TYR:N	2.48	0.46
17:A2:730:C:H2'	17:A2:731:G:C8	2.51	0.46
19:AB:146:ARG:HB2	19:AB:149:GLN:HB2	1.98	0.46
21:AD:117:ARG:HH21	52:Aj:168:PRO:HD2	1.81	0.46
2:I4:108:ARG:HH22	5:I8:79:THR:HB	1.80	0.46
5:I8:36:VAL:H	5:I8:168:ARG:NH1	2.13	0.46
11:It:54:LYS:NZ	54:It:1000:GTP:O1G	2.37	0.46
17:A2:1037:G:H4'	17:A2:1845:A:H4'	1.98	0.46
17:A2:1707:U:O2	17:A2:1849:G:N2	2.47	0.46
17:A2:1838:U:O2	32:AO:150:ARG:NH1	2.43	0.46
32:AO:53:ILE:HG23	32:AO:88:LEU:HD12	1.96	0.46
50:Ag:20:GLN:HB3	50:Ag:69:VAL:HG12	1.97	0.46
4:I6:183:LYS:HA	4:I6:186:VAL:HG22	1.97	0.46
4:I6:323:CYS:HA	4:I6:334:VAL:HA	1.98	0.46
9:Ir:246:GLU:OE1	9:Ir:246:GLU:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:It:31:LEU:HD21	11:It:245:VAL:HG21	1.98	0.46
13:Iv:348:HIS:HB2	13:Iv:351:ILE:HG12	1.97	0.46
17:A2:3:C:O2	27:AJ:18:ARG:NH2	2.40	0.46
21:AD:75:LYS:NZ	28:AK:34:GLU:OE2	2.49	0.46
22:AE:107:GLY:HA2	22:AE:189:LEU:HG	1.97	0.46
36:AS:46:ARG:HG2	37:AT:35:ASP:HB2	1.98	0.46
40:AW:28:ARG:HB3	40:AW:60:LYS:HG2	1.98	0.46
3:I5:490:LEU:HD22	3:I5:494:LYS:NZ	2.30	0.46
5:I8:46:VAL:O	5:I8:50:ILE:HG13	2.16	0.46
8:Iq:84:TYR:HB2	41:AX:54:LYS:HB2	1.98	0.46
12:Iu:519:ILE:HD12	12:Iu:520:ARG:HG3	1.98	0.46
13:Iv:144:TYR:HB2	13:Iv:179:MET:HE2	1.98	0.46
17:A2:472:C:H4'	17:A2:474:G:OP1	2.16	0.46
19:AB:41:ILE:HD11	19:AB:76:ASN:HB2	1.98	0.46
5:I8:234:ALA:HB2	12:Iu:520:ARG:HB3	1.98	0.45
12:Iu:286:SER:HA	16:Iy:728:GLY:HA2	1.97	0.45
17:A2:1482:C:OP1	47:Ad:54:LYS:NZ	2.39	0.45
29:AL:125:ILE:HB	29:AL:146:THR:HG23	1.98	0.45
36:AS:102:GLY:HA2	36:AS:105:ASN:HD21	1.80	0.45
47:Ad:19:ARG:HD2	47:Ad:32:ARG:HD3	1.98	0.45
4:I6:339:HIS:HB2	4:I6:342:PHE:CE2	2.51	0.45
9:Ir:4:LEU:HD22	9:Ir:124:ASP:HB3	1.97	0.45
12:Iu:387:VAL:HG12	12:Iu:410:VAL:HG13	1.98	0.45
17:A2:812:A:H5''	22:AE:16:LYS:HD2	1.99	0.45
17:A2:1846:G:O6	51:Ah:8:LYS:NZ	2.48	0.45
34:AQ:51:LEU:HD13	34:AQ:81:ILE:HG23	1.97	0.45
50:Ag:163:PRO:HB2	50:Ag:179:LEU:HB3	1.97	0.45
3:I5:281:HIS:ND1	3:I5:311:CYS:HB3	2.31	0.45
5:I8:71:VAL:HG22	5:I8:76:LEU:HD13	1.98	0.45
5:I8:129:VAL:O	5:I8:322:GLN:NE2	2.40	0.45
7:Ip:40:GLY:HA2	10:Is:261:ARG:NH1	2.31	0.45
9:Ir:131:PHE:O	9:Ir:136:TRP:N	2.30	0.45
10:Is:227:LYS:HE3	10:Is:227:LYS:HB3	1.79	0.45
14:Iw:47:5MC:H2'	14:Iw:58:A:H1'	1.98	0.45
17:A2:476:A:N3	17:A2:488:U:O2'	2.43	0.45
17:A2:969:U:OP1	17:A2:970:G:O2'	2.25	0.45
17:A2:1775:U:H2'	17:A2:1776:G:C8	2.50	0.45
4:I6:240:LEU:HD21	4:I6:255:PHE:CG	2.51	0.45
5:I8:239:LEU:HB2	5:I8:333:PHE:HE2	1.80	0.45
13:Iv:162:ASP:OD1	13:Iv:163:ARG:N	2.49	0.45
16:Iy:278:ALA:O	16:Iy:282:HIS:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:AL:3:ASP:OD1	29:AL:3:ASP:N	2.49	0.45
4:I6:53:LEU:HD13	4:I6:60:VAL:HG13	1.97	0.45
5:I8:40:GLN:NE2	5:I8:75:ARG:HD3	2.32	0.45
7:Ip:30:TYR:HD1	7:Ip:107:GLN:HA	1.80	0.45
11:It:349:ARG:HH11	11:It:350:ALA:HB2	1.82	0.45
12:Iu:539:PRO:HG2	12:Iu:542:ILE:HG22	1.99	0.45
15:Ix:76:ASP:OD1	15:Ix:76:ASP:N	2.42	0.45
17:A2:190:G:H1'	17:A2:209:A:H61	1.81	0.45
18:AA:103:PHE:CG	18:AA:133:PRO:HG3	2.51	0.45
25:AH:7:LYS:O	25:AH:10:LYS:NZ	2.47	0.45
3:I5:383:ASP:HB2	3:I5:388:LEU:HD13	1.98	0.45
3:I5:521:PHE:HB3	3:I5:524:ASP:HB3	1.98	0.45
12:Iu:157:TYR:OH	12:Iu:180:GLN:NE2	2.50	0.45
14:Iw:19:A:C6	14:Iw:57:1MA:H5'	2.51	0.45
16:Iy:505:LEU:O	16:Iy:509:HIS:ND1	2.49	0.45
17:A2:235:A:H2'	17:A2:236:A:C8	2.51	0.45
17:A2:1549:U:OP1	47:Ad:34:TYR:OH	2.33	0.45
24:AG:58:LYS:HE3	24:AG:105:ASN:HA	1.98	0.45
50:Ag:87:LEU:HD21	50:Ag:122:SER:HB3	1.98	0.45
1:I3:48:LEU:HD22	3:I5:294:LEU:HD12	1.99	0.45
1:I3:75:THR:HB	1:I3:137:SER:HB2	1.99	0.45
2:I4:287:LEU:HG	4:I6:354:LEU:HB3	1.99	0.45
3:I5:535:VAL:O	3:I5:539:TYR:N	2.44	0.45
5:I8:170:THR:HG22	5:I8:172:LYS:H	1.81	0.45
7:Ip:27:THR:HG21	7:Ip:31:ILE:HD11	1.98	0.45
12:Iu:153:LEU:O	12:Iu:156:SER:OG	2.35	0.45
13:Iv:255:ARG:HH22	13:Iv:318:VAL:HG12	1.82	0.45
16:Iy:644:GLU:HG2	16:Iy:650:LEU:HA	1.99	0.45
16:Iy:863:LEU:HD23	16:Iy:866:LEU:HD12	1.99	0.45
34:AQ:85:ARG:H	34:AQ:85:ARG:HG3	1.58	0.45
1:I3:125:MET:HG3	1:I3:127:LEU:H	1.82	0.45
5:I8:187:LEU:HD21	5:I8:317:LEU:HD11	1.97	0.45
5:I8:234:ALA:HA	12:Iu:520:ARG:HD2	1.99	0.45
13:Iv:91:ILE:HD11	13:Iv:127:TYR:HD1	1.82	0.45
15:Ix:253:ALA:HB1	15:Ix:434:ARG:HA	1.98	0.45
16:Iy:778:MET:HE3	16:Iy:778:MET:HB3	1.90	0.45
17:A2:166:A2M:HM'2	17:A2:167:G:O4'	2.17	0.45
17:A2:906:U:H2'	17:A2:907:G:H8	1.81	0.45
17:A2:1142:G:N2	17:A2:1145:A:OP2	2.41	0.45
42:AY:76:TYR:OH	42:AY:86:GLU:OE1	2.30	0.45
43:AZ:49:LEU:HD12	43:AZ:49:LEU:HA	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:AA:33:GLN:HB3	18:AA:154:LEU:HD12	1.98	0.45
26:AI:141:ARG:HD3	26:AI:145:ILE:HG22	1.98	0.45
31:AN:20:ARG:HH21	40:AW:56:HIS:HB3	1.81	0.45
50:Ag:157:SER:HB3	50:Ag:164:ILE:HB	1.98	0.45
3:I5:275:VAL:HG22	3:I5:279:ARG:HG2	1.98	0.45
4:I6:321:VAL:HG12	4:I6:337:SER:HA	1.98	0.45
5:I8:209:HIS:HD2	12:Iu:564:GLU:HB2	1.82	0.45
17:A2:656:G:H5'	17:A2:662:G:N2	2.32	0.45
31:AN:100:LYS:O	31:AN:103:GLU:HG2	2.17	0.45
42:AY:8:ARG:HB3	42:AY:26:ASP:HB2	1.98	0.45
3:I5:460:ILE:HA	3:I5:496:LYS:HG2	1.99	0.44
5:I8:197:MET:HE1	5:I8:318:LEU:HD23	1.99	0.44
11:It:91:LEU:HG	11:It:93:ASP:H	1.82	0.44
15:Ix:33:PHE:HD2	16:Iy:590:LEU:HD23	1.82	0.44
17:A2:929:G:H2'	17:A2:930:C:O4'	2.17	0.44
17:A2:1143:A:H5'	20:AC:190:SER:HB3	1.99	0.44
3:I5:232:HIS:HA	3:I5:235:VAL:HG22	2.00	0.44
7:Ip:61:LYS:NZ	17:A2:1849:G:OP1	2.42	0.44
11:It:355:GLY:HA3	11:It:411:LEU:HD13	1.99	0.44
13:Iv:371:ILE:O	13:Iv:375:ILE:HG13	2.18	0.44
15:Ix:344:VAL:HG21	15:Ix:353:ILE:HD13	1.98	0.44
17:A2:324:C:H4'	17:A2:325:C:C5	2.52	0.44
24:AG:234:LEU:HA	24:AG:237:LEU:HD12	1.97	0.44
9:Ir:196:GLU:HG2	9:Ir:233:PRO:HB2	1.98	0.44
11:It:314:ILE:HD13	11:It:347:LEU:HD13	1.99	0.44
12:Iu:125:GLU:HB2	16:Iy:473:LEU:HD23	1.99	0.44
15:Ix:39:LEU:HA	16:Iy:595:GLN:HE22	1.83	0.44
15:Ix:285:ASP:OD2	15:Ix:310:ARG:NH1	2.50	0.44
17:A2:1404:U:OP1	38:AU:21:ARG:NH2	2.48	0.44
17:A2:1447:OMG:OP1	38:AU:87:ARG:NH2	2.50	0.44
17:A2:1729:U:O2'	17:A2:1730:U:H5'	2.17	0.44
33:AP:108:LYS:HB2	36:AS:117:ILE:HD11	2.00	0.44
34:AQ:34:VAL:HG22	34:AQ:70:VAL:HB	1.99	0.44
50:Ag:101:PHE:CE2	50:Ag:136:GLY:HA2	2.53	0.44
1:I3:214:MET:HE3	5:I8:335:ALA:HB1	1.99	0.44
14:Iw:32:C:OP2	34:AQ:146:ARG:NH2	2.50	0.44
17:A2:535:G:H2'	17:A2:536:A:C8	2.51	0.44
17:A2:559:G:O2'	17:A2:560:A:H5''	2.18	0.44
17:A2:641:A:OP1	27:AJ:40:LYS:NZ	2.43	0.44
17:A2:752:G:H2'	17:A2:753:C:O4'	2.17	0.44
17:A2:1285:G:H5'	30:AM:35:ILE:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A2:1398:G:H4'	50:Ag:88:ARG:HH22	1.82	0.44
25:AH:69:LEU:HD22	25:AH:96:ALA:HB2	2.00	0.44
43:AZ:79:ILE:HG23	43:AZ:83:LEU:HD23	1.98	0.44
43:AZ:111:ARG:HG3	43:AZ:113:THR:HG23	1.99	0.44
49:Af:139:HIS:HB2	49:Af:148:TYR:HB2	2.00	0.44
1:I3:48:LEU:HD21	3:I5:292:LYS:O	2.17	0.44
1:I3:139:ARG:HA	1:I3:142:ILE:HG22	1.98	0.44
11:It:189:GLN:HB3	11:It:223:PRO:HA	1.99	0.44
13:Iv:384:ILE:HG12	13:Iv:391:VAL:HG13	1.99	0.44
17:A2:886:A:N6	17:A2:900:C:H42	2.16	0.44
20:AC:259:THR:HG21	39:AV:15:ARG:HA	1.99	0.44
34:AQ:89:SER:HB3	34:AQ:112:LEU:HD13	1.98	0.44
50:Ag:3:GLU:HG3	50:Ag:314:ILE:HA	2.00	0.44
2:I4:251:LEU:HD23	5:I8:162:LEU:HD23	2.00	0.44
7:Ip:45:THR:OG1	7:Ip:87:GLY:O	2.31	0.44
9:Ir:78:LYS:HE2	9:Ir:78:LYS:HB3	1.85	0.44
12:Iu:487:THR:HG22	16:Iy:841:THR:HG21	1.99	0.44
12:Iu:542:ILE:HG13	12:Iu:546:LYS:HG2	1.99	0.44
13:Iv:348:HIS:ND1	16:Iy:835:LEU:O	2.28	0.44
17:A2:1283:C:H42	30:AM:102:LYS:HE2	1.83	0.44
17:A2:1617:G:N1	17:A2:1620:A:OP2	2.51	0.44
44:Aa:88:SER:O	44:Aa:92:ARG:HG3	2.17	0.44
4:I6:239:ASP:OD1	4:I6:240:LEU:N	2.50	0.44
11:It:260:ARG:HH21	56:Iw:101:MET:HE2	1.81	0.44
15:Ix:44:ASP:OD2	16:Iy:641:ARG:NH2	2.50	0.44
17:A2:692:G:H2'	17:A2:693:A:C8	2.53	0.44
17:A2:907:G:H2'	17:A2:908:A:C8	2.52	0.44
17:A2:1292:C:HO2'	49:Af:147:THR:HG1	1.57	0.44
21:AD:40:ARG:NH2	21:AD:47:GLU:OE1	2.50	0.44
29:AL:76:VAL:HG12	29:AL:125:ILE:HD13	1.99	0.44
33:AP:21:ASP:OD1	33:AP:21:ASP:N	2.51	0.44
4:I6:358:LYS:HE3	4:I6:358:LYS:HB3	1.78	0.44
9:Ir:196:GLU:HA	9:Ir:234:ARG:HA	1.98	0.44
13:Iv:263:THR:OG1	13:Iv:264:ASN:N	2.51	0.44
15:Ix:423:THR:HG1	46:Ac:13:ARG:HH22	1.64	0.44
17:A2:1101:U:H2'	17:A2:1102:G:C8	2.53	0.44
17:A2:1284:A:C2	30:AM:104:VAL:HG11	2.53	0.44
21:AD:137:VAL:HG22	21:AD:151:LYS:HG3	1.99	0.44
3:I5:288:TYR:OH	3:I5:318:TYR:O	2.19	0.44
5:I8:129:VAL:HB	5:I8:322:GLN:HG2	1.98	0.44
10:Is:204:MET:SD	10:Is:229:LEU:HD11	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:It:45:GLY:O	11:It:156:LEU:N	2.44	0.44
12:Iu:522:GLN:O	12:Iu:526:MET:HG2	2.18	0.44
17:A2:28:U:H2'	17:A2:29:G:H8	1.82	0.44
17:A2:65:C:C6	24:AG:174:PRO:HB3	2.52	0.44
17:A2:520:A:O2'	17:A2:825:A:N3	2.46	0.44
18:AA:80:ARG:NH1	18:AA:165:ASN:O	2.42	0.44
18:AA:106:GLY:N	18:AA:136:GLU:OE2	2.33	0.44
23:AF:80:GLY:HA2	23:AF:83:ASN:OD1	2.18	0.44
30:AM:54:SER:N	30:AM:79:VAL:O	2.32	0.44
49:Af:89:LYS:HG2	49:Af:90:LYS:H	1.83	0.44
2:I4:308:LEU:HD22	4:I6:350:LEU:HD22	1.99	0.43
2:I4:349:ALA:HB1	3:I5:544:ILE:HG12	2.00	0.43
3:I5:420:PHE:HB3	3:I5:447:PHE:CD2	2.53	0.43
5:I8:265:ARG:HA	16:Iy:876:HIS:CD2	2.53	0.43
11:It:169:GLN:N	11:It:169:GLN:OE1	2.50	0.43
16:Iy:602:ASP:HB2	16:Iy:605:VAL:HG23	2.00	0.43
17:A2:166:A2M:HM'1	24:AG:11:GLY:HA2	1.99	0.43
17:A2:537:C:H2'	17:A2:538:U:C6	2.53	0.43
17:A2:874:G:H2'	17:A2:875:A:C8	2.53	0.43
17:A2:1803:U:H2'	17:A2:1804:OMU:O4'	2.18	0.43
3:I5:308:VAL:HB	3:I5:311:CYS:HB2	2.00	0.43
3:I5:361:ASN:HA	3:I5:364:ASN:HD21	1.84	0.43
4:I6:148:ARG:HH12	12:Iu:538:LYS:NZ	2.15	0.43
4:I6:324:LYS:HA	12:Iu:446:ILE:O	2.19	0.43
12:Iu:202:ARG:NE	12:Iu:255:ASP:OD2	2.51	0.43
15:Ix:472:LYS:HB2	15:Ix:475:GLU:HG3	1.99	0.43
16:Iy:324:ILE:HB	16:Iy:364:ASN:ND2	2.33	0.43
25:AH:9:VAL:HG23	25:AH:24:SER:HB3	1.99	0.43
1:I3:90:ASP:HB3	3:I5:442:GLN:HG2	1.99	0.43
9:Ir:64:ARG:HE	9:Ir:67:ARG:NE	2.16	0.43
9:Ir:292:ARG:HA	9:Ir:295:ARG:HD2	2.01	0.43
13:Iv:355:MET:HE2	16:Iy:838:PRO:HG2	2.01	0.43
15:Ix:200:GLU:HG2	15:Ix:334:ARG:HG2	1.99	0.43
16:Iy:249:GLN:HA	16:Iy:252:LEU:HG	1.99	0.43
17:A2:656:G:O2'	20:AC:227:ARG:NH1	2.51	0.43
30:AM:32:ALA:HB3	30:AM:110:VAL:HB	1.99	0.43
3:I5:197:PHE:HB3	3:I5:201:ARG:NH1	2.34	0.43
4:I6:77:ASP:OD1	4:I6:77:ASP:N	2.52	0.43
4:I6:256:TYR:HA	4:I6:263:ILE:HD12	1.98	0.43
7:Ip:67:PHE:CE1	7:Ip:92:ASN:HB3	2.53	0.43
15:Ix:39:LEU:O	16:Iy:595:GLN:NE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Iy:614:VAL:HG13	16:Iy:682:LEU:HD13	2.01	0.43
16:Iy:837:GLN:HB3	16:Iy:838:PRO:HD3	2.01	0.43
17:A2:695:C:H2'	17:A2:696:G:C8	2.53	0.43
19:AB:47:THR:OG1	19:AB:65:ARG:NH1	2.51	0.43
25:AH:69:LEU:O	25:AH:73:GLN:HG2	2.18	0.43
50:Ag:125:ARG:HG2	50:Ag:150:TRP:CG	2.53	0.43
2:I4:133:ASN:OD1	2:I4:134:CYS:N	2.51	0.43
5:I8:233:LEU:HD12	12:Iu:522:GLN:H	1.83	0.43
6:Io:251:ARG:H	6:Io:254:ASP:HB2	1.84	0.43
12:Iu:571:ARG:O	12:Iu:575:ILE:HG13	2.17	0.43
17:A2:1454:A:H5''	35:AR:3:ARG:HD2	2.00	0.43
23:AF:40:ALA:HB1	23:AF:45:TYR:CG	2.54	0.43
25:AH:86:LYS:HG3	25:AH:87:PHE:HD1	1.83	0.43
50:Ag:11:LEU:HB2	50:Ag:307:VAL:HB	1.99	0.43
50:Ag:191:HIS:CG	50:Ag:195:LEU:HD21	2.54	0.43
3:I5:460:ILE:HG12	3:I5:496:LYS:HA	2.01	0.43
7:Ip:36:GLN:HE22	10:Is:320:ALA:H	1.64	0.43
9:Ir:28:ALA:HB3	9:Ir:30:MET:HE3	2.00	0.43
12:Iu:421:GLU:HB3	12:Iu:424:LEU:HG	2.01	0.43
15:Ix:54:ARG:HA	15:Ix:57:ASN:HD21	1.83	0.43
15:Ix:246:PHE:HE2	15:Ix:372:ILE:HD12	1.82	0.43
17:A2:681:PSU:H4'	41:AX:9:THR:HG22	2.01	0.43
26:AI:89:GLU:OE2	26:AI:92:ARG:NH2	2.36	0.43
31:AN:83:ASP:OD1	31:AN:83:ASP:N	2.51	0.43
7:Ip:46:THR:HG21	10:Is:318:PHE:HD2	1.83	0.43
13:Iv:45:LEU:HD13	13:Iv:54:ALA:HA	2.00	0.43
16:Iy:300:GLU:O	16:Iy:302:GLU:N	2.52	0.43
17:A2:65:C:C2	24:AG:133:LEU:HD22	2.54	0.43
17:A2:145:G:O6	24:AG:178:ARG:NH2	2.52	0.43
17:A2:151:C:OP1	42:AY:120:THR:OG1	2.34	0.43
17:A2:645:C:H2'	17:A2:646:G:H8	1.84	0.43
17:A2:796:G:H2'	17:A2:797:OMC:O4'	2.19	0.43
23:AF:91:ARG:HD2	43:AZ:103:HIS:CE1	2.53	0.43
33:AP:110:GLU:HB2	36:AS:117:ILE:HD13	2.00	0.43
7:Ip:44:LEU:HD21	7:Ip:84:GLN:NE2	2.34	0.43
9:Ir:212:LEU:HD22	11:It:271:VAL:HG22	2.01	0.43
11:It:283:ILE:HB	11:It:333:PRO:HA	2.01	0.43
12:Iu:339:ALA:HB1	12:Iu:345:ASP:HA	2.01	0.43
15:Ix:216:PRO:HA	15:Ix:464:VAL:HG12	1.99	0.43
15:Ix:362:ARG:NH2	15:Ix:370:ASP:OD2	2.52	0.43
17:A2:1097:G:H4'	18:AA:32:PHE:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:AS:89:ASP:OD1	36:AS:90:VAL:N	2.51	0.43
1:I3:49:ALA:HA	3:I5:292:LYS:NZ	2.34	0.43
1:I3:150:TYR:HD1	1:I3:150:TYR:HA	1.71	0.43
2:I4:267:SER:HB3	2:I4:270:GLN:NE2	2.33	0.43
2:I4:301:ASP:O	2:I4:304:VAL:HG12	2.19	0.43
5:I8:226:ASP:HB3	5:I8:228:HIS:CD2	2.53	0.43
12:Iu:11:ALA:HB2	12:Iu:34:VAL:HG21	2.01	0.43
13:Iv:192:LEU:HD23	13:Iv:214:LEU:HD12	2.00	0.43
17:A2:239:C:H2'	17:A2:240:G:C8	2.53	0.43
30:AM:53:ALA:HB2	30:AM:85:LEU:HD13	1.99	0.43
2:I4:294:LEU:HD11	4:I6:344:LYS:HG2	2.01	0.43
12:Iu:380:LEU:HB3	12:Iu:388:LYS:HE3	2.00	0.43
17:A2:1733:U:H2'	17:A2:1734:G:O4'	2.19	0.43
20:AC:167:ARG:HG2	20:AC:219:ILE:HD13	2.01	0.43
2:I4:252:ILE:HG23	5:I8:207:ASN:HD21	1.84	0.42
9:Ir:209:LYS:HA	9:Ir:212:LEU:HG	2.01	0.42
16:Iy:603:PRO:N	16:Iy:604:PRO:HD2	2.34	0.42
17:A2:285:U:H2'	17:A2:286:U:C6	2.54	0.42
17:A2:493:A:H1'	17:A2:574:A:H5'	2.01	0.42
17:A2:868:G:OP2	17:A2:868:G:N2	2.39	0.42
23:AF:143:PRO:HG2	46:Ac:54:ASP:HB3	2.00	0.42
23:AF:168:THR:HB	23:AF:171:GLU:HG3	2.00	0.42
2:I4:107:GLU:HB3	12:Iu:568:ILE:HG13	2.00	0.42
2:I4:287:LEU:HD11	4:I6:355:ASN:HA	2.00	0.42
2:I4:313:ASN:HB3	4:I6:336:HIS:CB	2.49	0.42
8:Iq:62:ARG:HG2	8:Iq:64:LYS:H	1.84	0.42
13:Iv:5:ASP:OD2	13:Iv:32:TYR:OH	2.30	0.42
13:Iv:23:LEU:HB3	13:Iv:41:LYS:HE2	2.01	0.42
16:Iy:464:PRO:HB3	16:Iy:673:PHE:CG	2.54	0.42
20:AC:65:LYS:HB2	20:AC:266:TYR:HE1	1.84	0.42
22:AE:153:LEU:HG	24:AG:216:ARG:HE	1.84	0.42
42:AY:45:ALA:HB1	42:AY:50:THR:O	2.19	0.42
50:Ag:207:CYS:SG	50:Ag:219:TRP:HB2	2.59	0.42
1:I3:18:ILE:HD13	3:I5:263:HIS:CG	2.54	0.42
2:I4:311:LEU:HB2	12:Iu:529:VAL:HG11	2.00	0.42
5:I8:342:PHE:HA	5:I8:345:GLN:HB3	2.01	0.42
10:Is:275:ILE:HG23	10:Is:279:VAL:HB	2.00	0.42
11:It:52:HIS:NE2	11:It:163:GLU:OE1	2.42	0.42
12:Iu:167:ASN:HB3	12:Iu:170:VAL:HG22	2.01	0.42
12:Iu:259:LEU:HD23	12:Iu:262:LEU:HD12	1.99	0.42
17:A2:562:U:H2'	17:A2:563:G:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AF:42:LYS:HD3	23:AF:42:LYS:HA	1.78	0.42
3:I5:452:GLN:O	3:I5:456:GLN:HG2	2.19	0.42
5:I8:176:VAL:HG21	5:I8:192:ILE:HD11	2.01	0.42
7:Ip:56:LYS:HE2	7:Ip:83:ILE:HG13	2.01	0.42
8:Iq:129:ILE:HG23	10:Is:202:PHE:HD2	1.83	0.42
16:Iy:285:LYS:O	16:Iy:289:LEU:N	2.42	0.42
16:Iy:736:HIS:CE1	16:Iy:761:MET:HE3	2.54	0.42
17:A2:1310:U:OP2	49:Af:105:TYR:OH	2.25	0.42
22:AE:174:LYS:O	22:AE:179:ASN:ND2	2.52	0.42
23:AF:73:THR:O	23:AF:89:THR:HG21	2.19	0.42
42:AY:108:LYS:O	42:AY:112:ASN:ND2	2.41	0.42
4:I6:79:GLN:O	4:I6:83:ILE:HG12	2.18	0.42
5:I8:268:SER:HB3	16:Iy:876:HIS:HD2	1.84	0.42
9:Ir:163:LEU:HA	9:Ir:166:LEU:HD13	2.01	0.42
10:Is:280:THR:HG23	10:Is:285:ARG:HA	2.01	0.42
14:Iw:22:C:H2'	14:Iw:23:G:C8	2.54	0.42
17:A2:1445:PSU:O2	17:A2:1446:A:N6	2.52	0.42
17:A2:1770:G:H2'	17:A2:1771:G:C8	2.55	0.42
21:AD:142:LEU:HD23	21:AD:182:LEU:HD11	2.02	0.42
26:AI:205:ARG:HA	26:AI:205:ARG:HD2	1.85	0.42
43:AZ:58:LEU:HD12	43:AZ:62:VAL:HG21	2.02	0.42
46:Ac:18:LEU:HD11	46:Ac:43:ILE:HD12	2.01	0.42
2:I4:302:ASN:HB3	4:I6:221:ASP:HB3	2.01	0.42
3:I5:424:VAL:HG13	3:I5:425:VAL:H	1.85	0.42
4:I6:345:GLN:HE21	4:I6:346:GLN:HE22	1.66	0.42
10:Is:210:VAL:HG22	10:Is:218:SER:OG	2.19	0.42
16:Iy:695:ILE:HG23	16:Iy:745:LYS:HE2	2.01	0.42
23:AF:125:SER:OG	23:AF:136:ARG:HB3	2.19	0.42
25:AH:163:GLN:O	25:AH:167:GLU:HB2	2.20	0.42
49:Af:83:LYS:HD3	49:Af:84:SER:H	1.84	0.42
1:I3:77:LEU:HB3	1:I3:141:PHE:CD1	2.54	0.42
1:I3:118:TRP:CH2	1:I3:139:ARG:HG3	2.55	0.42
1:I3:125:MET:HE3	1:I3:127:LEU:HG	2.01	0.42
2:I4:252:ILE:HG23	5:I8:207:ASN:ND2	2.35	0.42
4:I6:42:LEU:HD21	4:I6:70:LEU:HD12	2.02	0.42
8:Iq:66:ARG:HB2	8:Iq:66:ARG:HH11	1.85	0.42
10:Is:199:LYS:HD3	10:Is:286:SER:HA	2.01	0.42
12:Iu:206:SER:OG	12:Iu:210:ARG:NH2	2.52	0.42
13:Iv:215:ILE:HG23	13:Iv:236:PHE:CZ	2.55	0.42
16:Iy:577:ALA:HB2	16:Iy:616:LEU:HD23	2.01	0.42
16:Iy:758:ASN:O	16:Iy:762:ASN:N	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A2:115:U:H2'	17:A2:116:OMU:C6	2.50	0.42
17:A2:1844:U:OP1	51:Ah:11:ARG:NH2	2.43	0.42
32:AO:74:ALA:HB1	32:AO:115:ALA:HB2	2.02	0.42
9:Ir:259:LYS:O	9:Ir:263:GLU:HB2	2.20	0.42
17:A2:322:C:H2'	17:A2:323:C:C6	2.54	0.42
17:A2:539:C:H42	17:A2:544:G:H1	1.68	0.42
17:A2:606:G:O2'	48:Ae:58:ASN:OD1	2.27	0.42
17:A2:655:A:H4'	17:A2:656:G:H3'	2.02	0.42
17:A2:1289:U:H2'	17:A2:1290:G:C8	2.54	0.42
17:A2:1320:G:H2'	17:A2:1321:G:O4'	2.19	0.42
17:A2:1565:C:OP2	37:AT:101:ARG:NH1	2.50	0.42
17:A2:1804:OMU:HM22	17:A2:1805:G:O4'	2.20	0.42
32:AO:36:SER:OG	32:AO:37:PHE:N	2.52	0.42
42:AY:18:LEU:O	42:AY:85:ASN:ND2	2.52	0.42
50:Ag:65:PHE:C	50:Ag:82:SER:HG	2.26	0.42
1:I3:181:ALA:HA	1:I3:187:ILE:HD12	2.02	0.42
2:I4:290:ALA:HA	2:I4:293:VAL:HG12	2.01	0.42
3:I5:533:THR:HA	3:I5:536:ALA:HB3	2.02	0.42
11:It:171:SER:HA	11:It:210:PHE:HZ	1.85	0.42
16:Iy:270:ALA:O	16:Iy:274:ARG:N	2.45	0.42
17:A2:220:U:H2'	17:A2:221:A:C8	2.55	0.42
24:AG:48:TYR:OH	24:AG:119:LYS:O	2.31	0.42
35:AR:75:GLU:OE2	35:AR:78:ARG:NH2	2.38	0.42
2:I4:292:ASP:HB3	2:I4:297:LYS:HB2	2.02	0.42
2:I4:339:TYR:CE1	3:I5:533:THR:HB	2.55	0.42
3:I5:405:ASP:O	3:I5:408:VAL:HG22	2.20	0.42
4:I6:45:ILE:O	4:I6:49:CYS:N	2.44	0.42
17:A2:220:U:H2'	17:A2:221:A:H8	1.84	0.42
17:A2:879:C:H2'	17:A2:880:G:C8	2.55	0.42
17:A2:1499:U:H4'	21:AD:176:LEU:HD13	2.02	0.42
34:AQ:19:ALA:HB2	34:AQ:75:GLY:HA3	2.01	0.42
41:AX:86:PRO:O	41:AX:87:ASN:HB2	2.20	0.42
2:I4:306:ARG:H	2:I4:306:ARG:HD2	1.84	0.41
3:I5:329:TYR:HB3	3:I5:371:LEU:HD21	2.01	0.41
5:I8:110:VAL:HB	5:I8:112:ILE:HG13	2.01	0.41
7:Ip:40:GLY:HA2	10:Is:261:ARG:HH11	1.85	0.41
9:Ir:88:ARG:HG3	9:Ir:89:ARG:HD2	2.02	0.41
11:It:263:ASP:O	11:It:265:ASN:N	2.53	0.41
13:Iv:38:LEU:HD22	13:Iv:57:VAL:HG13	2.02	0.41
13:Iv:344:PHE:HD2	13:Iv:351:ILE:HD13	1.85	0.41
17:A2:75:G:H2'	17:A2:76:U:H4'	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A2:835:C:C4	42:AY:8:ARG:HD2	2.55	0.41
17:A2:1848:U:O4	51:Ah:12:ARG:NH1	2.44	0.41
19:AB:33:VAL:HA	19:AB:96:CYS:HB2	2.02	0.41
30:AM:63:LYS:NZ	49:Af:112:GLY:HA2	2.34	0.41
1:I3:26:LEU:O	1:I3:30:GLU:N	2.53	0.41
3:I5:265:LEU:HD13	3:I5:279:ARG:HB3	2.02	0.41
3:I5:376:THR:HG21	3:I5:461:ARG:HG2	2.02	0.41
11:It:447:VAL:N	11:It:450:HIS:O	2.45	0.41
17:A2:195:C:H2'	17:A2:196:C:C6	2.55	0.41
17:A2:210:PSU:H2'	17:A2:211:G:C8	2.55	0.41
19:AB:83:LYS:HE3	19:AB:83:LYS:HB2	1.85	0.41
24:AG:136:LYS:NZ	24:AG:175:LYS:O	2.45	0.41
50:Ag:72:SER:OG	50:Ag:74:ASP:OD1	2.33	0.41
9:Ir:192:ARG:HH12	14:Iw:4:A:H5'	1.84	0.41
11:It:47:ILE:HD13	11:It:173:HIS:HB3	2.01	0.41
16:Iy:354:LEU:HB3	16:Iy:378:ILE:HG12	2.01	0.41
24:AG:162:LEU:HD21	24:AG:172:LYS:HE2	2.02	0.41
24:AG:201:LYS:NZ	24:AG:202:ASN:OD1	2.43	0.41
50:Ag:270:LEU:HD13	50:Ag:310:TRP:CD2	2.56	0.41
1:I3:21:TYR:HB2	3:I5:262:ARG:NH2	2.34	0.41
1:I3:69:ILE:HA	1:I3:72:LYS:HG2	2.02	0.41
9:Ir:124:ASP:OD1	9:Ir:124:ASP:N	2.53	0.41
11:It:12:GLN:HE22	11:It:326:ASN:HA	1.85	0.41
11:It:203:GLN:O	11:It:207:ILE:HG13	2.21	0.41
12:Iu:108:SER:O	12:Iu:112:VAL:HG23	2.20	0.41
17:A2:92:A:C6	17:A2:446:G:C6	3.08	0.41
17:A2:206:G:H2'	17:A2:207:G:C8	2.55	0.41
17:A2:727:G:H2'	17:A2:728:C:C6	2.55	0.41
17:A2:1536:G:H2'	17:A2:1537:A:C8	2.55	0.41
24:AG:7:PHE:CE2	24:AG:9:ALA:HB3	2.54	0.41
26:AI:4:SER:OG	26:AI:6:ASP:OD2	2.26	0.41
1:I3:77:LEU:HD23	1:I3:141:PHE:CZ	2.56	0.41
2:I4:312:VAL:HG21	4:I6:349:GLN:OE1	2.19	0.41
3:I5:541:ASP:HB2	3:I5:545:ARG:HE	1.86	0.41
10:Is:224:ASP:OD1	10:Is:224:ASP:N	2.52	0.41
11:It:193:ASP:OD1	11:It:193:ASP:N	2.54	0.41
12:Iu:206:SER:O	12:Iu:210:ARG:HG3	2.20	0.41
17:A2:49:C:H2'	17:A2:472:C:H41	1.85	0.41
17:A2:448:A:H5''	26:AI:25:ARG:HA	2.02	0.41
17:A2:1292:C:O2'	49:Af:147:THR:OG1	2.29	0.41
17:A2:1337:4AC:H2'	17:A2:1338:G:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A2:1729:U:H2'	17:A2:1730:U:C6	2.54	0.41
17:A2:1761:U:H2'	17:A2:1762:C:C6	2.56	0.41
27:AJ:87:LEU:HD23	27:AJ:87:LEU:HA	1.92	0.41
35:AR:67:ARG:HE	35:AR:67:ARG:HB3	1.64	0.41
3:I5:197:PHE:HB3	3:I5:201:ARG:HH12	1.85	0.41
8:Iq:29:LYS:HB2	8:Iq:35:TYR:CE2	2.56	0.41
8:Iq:45:GLY:O	8:Iq:61:ILE:HG22	2.19	0.41
9:Ir:214:ALA:HB1	9:Ir:258:ILE:HG12	2.03	0.41
17:A2:436:OMG:OP2	17:A2:471:G:O2'	2.35	0.41
17:A2:640:A:H2'	17:A2:641:A:C8	2.55	0.41
17:A2:1291:A:N3	49:Af:140:TYR:OH	2.44	0.41
17:A2:1441:U:O4'	17:A2:1442:OMU:H5	2.19	0.41
18:AA:12:GLU:HG3	35:AR:114:LEU:HD22	2.01	0.41
24:AG:227:GLN:HA	24:AG:230:LYS:HD2	2.02	0.41
30:AM:85:LEU:O	30:AM:89:VAL:HG23	2.20	0.41
35:AR:20:TYR:CD1	35:AR:38:ILE:HD12	2.56	0.41
2:I4:93:ARG:HD2	2:I4:130:GLU:HG2	2.03	0.41
9:Ir:208:VAL:O	9:Ir:212:LEU:HG	2.20	0.41
10:Is:294:ASP:OD1	10:Is:308:ARG:NH2	2.54	0.41
11:It:45:GLY:HA3	11:It:152:MET:SD	2.61	0.41
11:It:327:ASP:OD1	11:It:327:ASP:N	2.51	0.41
13:Iv:244:ASN:HD21	15:Ix:63:PHE:HE1	1.68	0.41
15:Ix:229:THR:HG23	15:Ix:235:ILE:HD13	2.03	0.41
16:Iy:652:LEU:O	16:Iy:656:GLN:HG3	2.20	0.41
17:A2:320:G:H2'	17:A2:321:C:C6	2.56	0.41
17:A2:704:G:H1	17:A2:726:C:H42	1.68	0.41
17:A2:874:G:H2'	17:A2:875:A:H8	1.84	0.41
18:AA:198:MET:HE2	18:AA:200:ASP:HB2	2.01	0.41
20:AC:194:ARG:HD3	20:AC:196:ILE:HD11	2.02	0.41
27:AJ:106:LEU:HA	27:AJ:106:LEU:HD12	1.87	0.41
34:AQ:5:GLY:O	34:AQ:27:ARG:NH1	2.54	0.41
45:Ab:24:LEU:HD23	45:Ab:24:LEU:HA	1.81	0.41
4:I6:241:LEU:O	4:I6:245:VAL:HG23	2.20	0.41
9:Ir:64:ARG:HE	9:Ir:67:ARG:HE	1.68	0.41
9:Ir:77:ASP:OD1	9:Ir:77:ASP:N	2.54	0.41
9:Ir:228:ASN:HB3	11:It:268:GLY:HA2	2.01	0.41
10:Is:190:LYS:HD2	11:It:230:TYR:CZ	2.55	0.41
11:It:139:ASP:OD1	11:It:139:ASP:N	2.54	0.41
11:It:227:GLN:HB2	54:It:1000:GTP:C6	2.55	0.41
17:A2:230:A:H2'	17:A2:231:A:C8	2.56	0.41
17:A2:1763:G:C2	17:A2:1770:G:C2	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:AJ:131:ARG:HA	27:AJ:131:ARG:HD2	1.87	0.41
35:AR:77:GLU:OE2	35:AR:80:ARG:NH1	2.54	0.41
38:AU:32:LEU:HD21	38:AU:87:ARG:HG2	2.03	0.41
43:AZ:65:TYR:C	43:AZ:67:LEU:H	2.29	0.41
1:I3:190:CYS:SG	1:I3:191:SER:N	2.94	0.41
2:I4:163:VAL:HG11	5:I8:83:PRO:HB2	2.02	0.41
3:I5:291:ILE:HD11	3:I5:325:MET:HE1	2.01	0.41
3:I5:344:GLN:NE2	3:I5:354:THR:OG1	2.54	0.41
3:I5:460:ILE:CG2	3:I5:502:TRP:HE1	2.33	0.41
3:I5:490:LEU:O	3:I5:494:LYS:HG2	2.20	0.41
4:I6:12:GLU:HA	4:I6:38:LEU:HB3	2.03	0.41
5:I8:40:GLN:O	5:I8:78:ILE:N	2.45	0.41
5:I8:169:LEU:HD11	5:I8:173:LEU:HD22	2.02	0.41
6:Io:245:ASN:HB2	21:AD:90:LYS:HG2	2.02	0.41
11:It:31:LEU:HA	11:It:36:ILE:HD11	2.02	0.41
12:Iu:14:ARG:NH1	19:AB:77:ASP:OD2	2.34	0.41
12:Iu:39:LYS:HG3	12:Iu:40:HIS:CD2	2.56	0.41
12:Iu:80:GLN:HB3	12:Iu:169:ARG:NH1	2.36	0.41
13:Iv:379:ARG:HD3	13:Iv:379:ARG:HA	1.87	0.41
14:Iw:22:C:H2'	14:Iw:23:G:H8	1.85	0.41
17:A2:71:G:H2'	17:A2:72:C:O4'	2.21	0.41
17:A2:207:G:H2'	17:A2:208:G:O4'	2.21	0.41
17:A2:1098:C:H2'	17:A2:1099:G:C8	2.56	0.41
17:A2:1298:G:H4'	33:AP:78:THR:HA	2.01	0.41
17:A2:1730:U:H2'	17:A2:1731:A:C8	2.56	0.41
20:AC:252:THR:OG1	20:AC:254:ASP:OD1	2.32	0.41
33:AP:41:GLN:HG3	33:AP:84:ILE:HD13	2.02	0.41
46:Ac:42:ILE:HB	46:Ac:64:GLU:HG3	2.03	0.41
1:I3:177:TYR:HB2	1:I3:179:TRP:HE1	1.86	0.41
2:I4:146:VAL:HG21	2:I4:182:HIS:HB3	2.03	0.41
2:I4:282:ALA:O	2:I4:286:VAL:HG23	2.20	0.41
16:Iy:487:GLN:OE1	16:Iy:506:ARG:NH1	2.53	0.41
20:AC:257:LYS:O	39:AV:16:LYS:NZ	2.47	0.41
26:AI:21:TYR:CZ	26:AI:22:HIS:HD2	2.38	0.41
27:AJ:134:HIS:ND1	27:AJ:163:SER:OG	2.37	0.41
34:AQ:12:VAL:HG11	34:AQ:90:LYS:HB3	2.03	0.41
1:I3:177:TYR:HB2	1:I3:179:TRP:NE1	2.35	0.40
4:I6:143:GLU:HG2	4:I6:146:GLN:HG2	2.04	0.40
9:Ir:23:ASN:HB2	9:Ir:37:LEU:HD23	2.03	0.40
9:Ir:132:GLN:HB3	9:Ir:136:TRP:HE3	1.86	0.40
12:Iu:252:ALA:O	12:Iu:256:ILE:HG13	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Iu:441:GLN:HE22	12:Iu:506:PRO:HB2	1.85	0.40
13:Iv:426:LEU:HD21	16:Iy:874:PHE:HE1	1.86	0.40
15:Ix:3:LYS:HE3	15:Ix:3:LYS:HB3	1.83	0.40
16:Iy:543:ASP:HB2	16:Iy:546:VAL:HG23	2.03	0.40
17:A2:1512:C:H2'	17:A2:1513:C:C6	2.56	0.40
17:A2:1778:C:H2'	17:A2:1779:G:C8	2.55	0.40
1:I3:205:ILE:HG13	1:I3:209:SER:OG	2.21	0.40
2:I4:285:THR:HG23	12:Iu:541:HIS:HB3	2.04	0.40
3:I5:541:ASP:OD1	3:I5:542:PHE:N	2.55	0.40
4:I6:312:VAL:O	4:I6:316:VAL:HG23	2.20	0.40
12:Iu:25:GLN:NE2	12:Iu:29:ASP:OD1	2.54	0.40
12:Iu:202:ARG:HA	12:Iu:233:ARG:HH22	1.86	0.40
12:Iu:400:PRO:HG3	12:Iu:446:ILE:HD12	2.04	0.40
13:Iv:342:GLU:OE2	13:Iv:346:ARG:NH2	2.54	0.40
15:Ix:183:ARG:NH1	15:Ix:486:ASN:HD22	2.19	0.40
16:Iy:554:TYR:CZ	16:Iy:558:LYS:HG3	2.56	0.40
22:AE:140:VAL:HG22	22:AE:146:THR:HG22	2.03	0.40
35:AR:94:GLU:O	35:AR:116:ASN:ND2	2.38	0.40
1:I3:73:ALA:HA	1:I3:76:ASN:HB2	2.02	0.40
2:I4:302:ASN:HB2	4:I6:222:HIS:NE2	2.37	0.40
4:I6:179:ASP:OD1	4:I6:179:ASP:N	2.55	0.40
4:I6:243:ILE:HG23	4:I6:247:ALA:HB3	2.04	0.40
9:Ir:241:THR:OG1	9:Ir:243:GLU:OE2	2.39	0.40
16:Iy:705:ALA:N	16:Iy:861:GLU:OE1	2.52	0.40
17:A2:530:U:H2'	17:A2:531:A:C8	2.57	0.40
17:A2:729:C:H2'	17:A2:730:C:C6	2.56	0.40
17:A2:885:U:H3	17:A2:901:G:H1	1.68	0.40
17:A2:1144:A:H8	17:A2:1144:A:OP2	2.04	0.40
17:A2:1466:G:H5'	35:AR:4:VAL:HG22	2.02	0.40
26:AI:105:ASP:OD1	26:AI:106:SER:N	2.54	0.40
46:Ac:22:GLY:HA2	46:Ac:68:LEU:HD12	2.03	0.40
52:Aj:170:TRP:CE2	52:Aj:189:LYS:HD3	2.56	0.40
9:Ir:144:ARG:CZ	9:Ir:147:TYR:HB3	2.52	0.40
9:Ir:196:GLU:HG3	9:Ir:234:ARG:HB3	2.02	0.40
9:Ir:208:VAL:O	9:Ir:212:LEU:N	2.51	0.40
10:Is:275:ILE:HA	10:Is:279:VAL:HG23	2.03	0.40
11:It:349:ARG:NH1	11:It:350:ALA:HB2	2.35	0.40
11:It:370:GLU:HB2	11:It:463:VAL:HB	2.03	0.40
12:Iu:68:LYS:HB2	12:Iu:159:GLN:CD	2.47	0.40
12:Iu:296:LEU:HD13	12:Iu:321:ARG:HG2	2.03	0.40
14:Iw:51:G:H1	14:Iw:61:C:H42	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A2:67:C:C5	24:AG:164:LYS:HB2	2.56	0.40
17:A2:1241:A:O2'	17:A2:1266:C:O2'	2.27	0.40
18:AA:180:ARG:O	18:AA:184:ARG:HG3	2.21	0.40
20:AC:116:THR:HG22	20:AC:117:ARG:HD2	2.02	0.40
21:AD:52:ALA:O	21:AD:90:LYS:HA	2.21	0.40
23:AF:34:SER:HA	46:Ac:55:VAL:HB	2.03	0.40
37:AT:65:TYR:HE2	37:AT:128:GLN:HG3	1.87	0.40
1:I3:204:LYS:HD2	2:I4:324:GLU:OE2	2.22	0.40
2:I4:104:ASP:OD1	2:I4:108:ARG:NH2	2.54	0.40
5:I8:105:ARG:O	5:I8:109:HIS:ND1	2.50	0.40
11:It:65:HIS:NE2	11:It:67:VAL:HB	2.37	0.40
12:Iu:399:ASN:HD21	12:Iu:402:LYS:HD2	1.87	0.40
15:Ix:426:LYS:HZ2	46:Ac:33:GLU:CD	2.30	0.40
16:Iy:268:LYS:O	16:Iy:272:LYS:N	2.42	0.40
16:Iy:424:ILE:HD13	16:Iy:439:ARG:HB3	2.03	0.40
17:A2:160:U:O2'	17:A2:161:U:H3'	2.22	0.40
17:A2:794:A:H2'	17:A2:795:A:C8	2.56	0.40
19:AB:168:MET:HG2	19:AB:197:ILE:HG21	2.04	0.40
20:AC:78:LEU:HD12	20:AC:81:ILE:HD12	2.03	0.40
28:AK:80:ARG:HH22	28:AK:90:VAL:HG12	1.86	0.40
50:Ag:292:SER:OG	50:Ag:297:THR:OG1	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I3	215/218 (99%)	205 (95%)	10 (5%)	0	100	100
2	I4	266/357 (74%)	261 (98%)	5 (2%)	0	100	100
3	I5	370/564 (66%)	340 (92%)	30 (8%)	0	100	100
4	I6	339/374 (91%)	326 (96%)	12 (4%)	1 (0%)	36	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	I8	316/352 (90%)	308 (98%)	8 (2%)	0	100	100
6	Io	75/320 (23%)	71 (95%)	4 (5%)	0	100	100
7	Ip	103/113 (91%)	99 (96%)	3 (3%)	1 (1%)	12	20
8	Iq	99/144 (69%)	97 (98%)	2 (2%)	0	100	100
9	Ir	291/315 (92%)	278 (96%)	12 (4%)	1 (0%)	36	52
10	Is	157/333 (47%)	151 (96%)	6 (4%)	0	100	100
11	It	447/472 (95%)	443 (99%)	4 (1%)	0	100	100
12	Iu	585/1382 (42%)	570 (97%)	15 (3%)	0	100	100
13	Iv	428/445 (96%)	424 (99%)	2 (0%)	2 (0%)	24	39
15	Ix	451/548 (82%)	443 (98%)	8 (2%)	0	100	100
16	Iy	631/913 (69%)	617 (98%)	13 (2%)	1 (0%)	43	60
18	AA	214/295 (72%)	210 (98%)	4 (2%)	0	100	100
19	AB	220/264 (83%)	216 (98%)	4 (2%)	0	100	100
20	AC	217/293 (74%)	215 (99%)	2 (1%)	0	100	100
21	AD	223/243 (92%)	223 (100%)	0	0	100	100
22	AE	260/263 (99%)	253 (97%)	7 (3%)	0	100	100
23	AF	190/204 (93%)	182 (96%)	8 (4%)	0	100	100
24	AG	238/249 (96%)	238 (100%)	0	0	100	100
25	AH	186/194 (96%)	183 (98%)	3 (2%)	0	100	100
26	AI	203/208 (98%)	200 (98%)	3 (2%)	0	100	100
27	AJ	178/194 (92%)	176 (99%)	2 (1%)	0	100	100
28	AK	95/165 (58%)	93 (98%)	2 (2%)	0	100	100
29	AL	149/158 (94%)	148 (99%)	1 (1%)	0	100	100
30	AM	121/132 (92%)	114 (94%)	7 (6%)	0	100	100
31	AN	147/151 (97%)	146 (99%)	1 (1%)	0	100	100
32	AO	131/151 (87%)	130 (99%)	1 (1%)	0	100	100
33	AP	129/145 (89%)	128 (99%)	1 (1%)	0	100	100
34	AQ	140/146 (96%)	138 (99%)	2 (1%)	0	100	100
35	AR	132/135 (98%)	132 (100%)	0	0	100	100
36	AS	143/152 (94%)	139 (97%)	4 (3%)	0	100	100
37	AT	141/145 (97%)	139 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	AU	99/119 (83%)	97 (98%)	2 (2%)	0	100	100
39	AV	81/83 (98%)	81 (100%)	0	0	100	100
40	AW	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
41	AX	140/143 (98%)	138 (99%)	2 (1%)	0	100	100
42	AY	122/133 (92%)	122 (100%)	0	0	100	100
43	AZ	70/125 (56%)	68 (97%)	2 (3%)	0	100	100
44	Aa	99/115 (86%)	99 (100%)	0	0	100	100
45	Ab	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
46	Ac	63/69 (91%)	63 (100%)	0	0	100	100
47	Ad	53/56 (95%)	53 (100%)	0	0	100	100
48	Ae	57/133 (43%)	56 (98%)	1 (2%)	0	100	100
49	Af	72/156 (46%)	66 (92%)	5 (7%)	1 (1%)	9	14
50	Ag	312/317 (98%)	298 (96%)	14 (4%)	0	100	100
51	Ah	23/25 (92%)	23 (100%)	0	0	100	100
52	Aj	27/216 (12%)	27 (100%)	0	0	100	100
All	All	9656/12641 (76%)	9431 (98%)	218 (2%)	7 (0%)	49	66

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	Ip	12	PRO
9	Ir	202	TYR
13	Iv	265	LYS
13	Iv	264	ASN
16	Iy	301	TRP
4	I6	97	GLU
49	Af	88	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I3	192/193 (100%)	184 (96%)	8 (4%)	26	45
2	I4	237/289 (82%)	227 (96%)	10 (4%)	26	45
3	I5	342/515 (66%)	324 (95%)	18 (5%)	20	35
4	I6	308/335 (92%)	299 (97%)	9 (3%)	37	58
5	I8	290/310 (94%)	281 (97%)	9 (3%)	35	56
6	Io	64/277 (23%)	59 (92%)	5 (8%)	11	20
7	Ip	77/96 (80%)	74 (96%)	3 (4%)	28	48
8	Iq	88/123 (72%)	81 (92%)	7 (8%)	11	19
9	Ir	264/280 (94%)	247 (94%)	17 (6%)	16	28
10	Is	144/304 (47%)	136 (94%)	8 (6%)	19	32
11	It	384/397 (97%)	377 (98%)	7 (2%)	51	72
12	Iu	540/1259 (43%)	528 (98%)	12 (2%)	45	67
13	Iv	394/406 (97%)	391 (99%)	3 (1%)	73	85
15	Ix	406/494 (82%)	401 (99%)	5 (1%)	63	79
16	Iy	516/811 (64%)	509 (99%)	7 (1%)	59	76
18	AA	179/242 (74%)	176 (98%)	3 (2%)	53	73
19	AB	203/231 (88%)	202 (100%)	1 (0%)	81	91
20	AC	185/225 (82%)	183 (99%)	2 (1%)	65	80
21	AD	189/202 (94%)	187 (99%)	2 (1%)	65	80
22	AE	224/225 (100%)	221 (99%)	3 (1%)	61	77
23	AF	162/170 (95%)	162 (100%)	0	100	100
24	AG	209/218 (96%)	208 (100%)	1 (0%)	81	91
25	AH	168/174 (97%)	168 (100%)	0	100	100
26	AI	178/180 (99%)	178 (100%)	0	100	100
27	AJ	160/168 (95%)	158 (99%)	2 (1%)	61	77
28	AK	88/136 (65%)	87 (99%)	1 (1%)	65	80
29	AL	135/142 (95%)	133 (98%)	2 (2%)	57	75
30	AM	104/108 (96%)	100 (96%)	4 (4%)	29	49
31	AN	130/131 (99%)	129 (99%)	1 (1%)	73	85
32	AO	104/118 (88%)	104 (100%)	0	100	100
33	AP	117/130 (90%)	117 (100%)	0	100	100
34	AQ	117/121 (97%)	113 (97%)	4 (3%)	32	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	AR	121/122 (99%)	120 (99%)	1 (1%)	73	85
36	AS	125/131 (95%)	124 (99%)	1 (1%)	73	85
37	AT	113/114 (99%)	112 (99%)	1 (1%)	70	82
38	AU	93/107 (87%)	92 (99%)	1 (1%)	65	80
39	AV	66/66 (100%)	66 (100%)	0	100	100
40	AW	112/113 (99%)	111 (99%)	1 (1%)	70	82
41	AX	114/114 (100%)	110 (96%)	4 (4%)	32	52
42	AY	108/115 (94%)	107 (99%)	1 (1%)	70	82
43	AZ	64/103 (62%)	63 (98%)	1 (2%)	55	74
44	Aa	88/98 (90%)	86 (98%)	2 (2%)	44	66
45	Ab	75/76 (99%)	72 (96%)	3 (4%)	28	47
46	Ac	58/62 (94%)	58 (100%)	0	100	100
47	Ad	48/49 (98%)	48 (100%)	0	100	100
48	Ae	48/104 (46%)	47 (98%)	1 (2%)	47	69
49	Af	67/140 (48%)	66 (98%)	1 (2%)	57	75
50	Ag	272/275 (99%)	263 (97%)	9 (3%)	33	55
51	Ah	24/24 (100%)	24 (100%)	0	100	100
52	Aj	24/182 (13%)	24 (100%)	0	100	100
All	All	8518/11005 (77%)	8337 (98%)	181 (2%)	46	69

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I3	74	LEU
1	I3	76	ASN
1	I3	94	GLN
1	I3	111	THR
1	I3	150	TYR
1	I3	187	ILE
1	I3	202	VAL
1	I3	213	ILE
2	I4	103	VAL
2	I4	226	ARG
2	I4	263	ILE
2	I4	269	LEU
2	I4	308	LEU

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Mol	Chain	Res	Type
2	I4	311	LEU
2	I4	315	VAL
2	I4	318	ILE
2	I4	327	LEU
2	I4	348	ILE
3	I5	347	LYS
3	I5	380	MET
3	I5	382	ILE
3	I5	390	LEU
3	I5	401	MET
3	I5	424	VAL
3	I5	428	TYR
3	I5	432	HIS
3	I5	446	VAL
3	I5	479	LEU
3	I5	487	ARG
3	I5	488	ILE
3	I5	490	LEU
3	I5	491	LEU
3	I5	499	ASN
3	I5	501	VAL
3	I5	519	VAL
3	I5	523	ILE
4	I6	64	MET
4	I6	79	GLN
4	I6	137	ILE
4	I6	164	LEU
4	I6	193	THR
4	I6	328	THR
4	I6	340	ARG
4	I6	361	LEU
4	I6	368	LEU
5	I8	60	THR
5	I8	84	PHE
5	I8	88	THR
5	I8	110	VAL
5	I8	113	ASP
5	I8	114	HIS
5	I8	115	LEU
5	I8	164	LEU
5	I8	253	MET
6	Io	243	VAL

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Mol	Chain	Res	Type
6	Io	258	LEU
6	Io	270	LEU
6	Io	276	THR
6	Io	312	VAL
7	Ip	105	ASP
7	Ip	110	VAL
7	Ip	113	PHE
8	Iq	26	LEU
8	Iq	27	VAL
8	Iq	76	ILE
8	Iq	81	LEU
8	Iq	83	ASP
8	Iq	133	ASP
8	Iq	134	ILE
9	Ir	4	LEU
9	Ir	37	LEU
9	Ir	45	MET
9	Ir	48	LEU
9	Ir	72	VAL
9	Ir	78	LYS
9	Ir	104	LYS
9	Ir	134	THR
9	Ir	170	GLU
9	Ir	205	ILE
9	Ir	208	VAL
9	Ir	229	LEU
9	Ir	230	ILE
9	Ir	236	VAL
9	Ir	240	THR
9	Ir	243	GLU
9	Ir	278	VAL
10	Is	179	LEU
10	Is	210	VAL
10	Is	224	ASP
10	Is	226	CYS
10	Is	253	ASN
10	Is	279	VAL
10	Is	291	LEU
10	Is	295	THR
11	It	192	ILE
11	It	195	VAL
11	It	230	TYR

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Mol	Chain	Res	Type
11	It	271	VAL
11	It	274	LEU
11	It	336	LEU
11	It	347	LEU
12	Iu	180	GLN
12	Iu	187	GLN
12	Iu	272	MET
12	Iu	310	LEU
12	Iu	311	THR
12	Iu	341	LEU
12	Iu	359	LEU
12	Iu	382	TYR
12	Iu	401	LEU
12	Iu	542	ILE
12	Iu	552	LEU
12	Iu	569	LEU
13	Iv	192	LEU
13	Iv	290	ASP
13	Iv	322	ASP
15	Ix	8	VAL
15	Ix	35	LYS
15	Ix	55	TYR
15	Ix	83	VAL
15	Ix	296	ASN
16	Iy	519	HIS
16	Iy	600	HIS
16	Iy	727	LEU
16	Iy	745	LYS
16	Iy	798	VAL
16	Iy	847	THR
16	Iy	873	VAL
18	AA	34	MET
18	AA	38	ILE
18	AA	111	GLN
19	AB	228	LEU
20	AC	116	THR
20	AC	117	ARG
21	AD	3	VAL
21	AD	182	LEU
22	AE	46	ILE
22	AE	48	LEU
22	AE	220	THR

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Mol	Chain	Res	Type
24	AG	69	THR
27	AJ	29	LEU
27	AJ	106	LEU
28	AK	72	THR
29	AL	69	ARG
29	AL	146	THR
30	AM	11	VAL
30	AM	52	LEU
30	AM	62	VAL
30	AM	123	VAL
31	AN	22	VAL
34	AQ	18	THR
34	AQ	72	VAL
34	AQ	85	ARG
34	AQ	146	ARG
35	AR	75	GLU
36	AS	53	THR
37	AT	85	ASN
38	AU	68	THR
40	AW	105	THR
41	AX	72	VAL
41	AX	81	ILE
41	AX	105	PHE
41	AX	125	VAL
42	AY	50	THR
43	AZ	49	LEU
44	Aa	67	LEU
44	Aa	84	VAL
45	Ab	3	LEU
45	Ab	24	LEU
45	Ab	53	VAL
48	Ae	6	LEU
49	Af	126	CYS
50	Ag	64	HIS
50	Ag	76	GLN
50	Ag	113	PHE
50	Ag	162	ASN
50	Ag	182	CYS
50	Ag	266	ILE
50	Ag	298	LEU
50	Ag	303	THR
50	Ag	309	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (134) such sidechains are listed below:

Mol	Chain	Res	Type
1	I3	6	GLN
1	I3	47	ASN
1	I3	62	GLN
1	I3	68	GLN
1	I3	91	GLN
1	I3	94	GLN
1	I3	218	GLN
2	I4	139	HIS
2	I4	208	ASN
2	I4	270	GLN
2	I4	271	GLN
2	I4	302	ASN
3	I5	195	GLN
3	I5	199	GLN
3	I5	225	HIS
3	I5	243	GLN
3	I5	344	GLN
3	I5	364	ASN
3	I5	489	GLN
3	I5	499	ASN
4	I6	79	GLN
4	I6	205	HIS
4	I6	238	HIS
4	I6	339	HIS
4	I6	345	GLN
4	I6	359	GLN
4	I6	360	ASN
4	I6	366	ASN
5	I8	159	GLN
5	I8	191	ASN
5	I8	207	ASN
5	I8	209	HIS
5	I8	238	HIS
5	I8	242	ASN
5	I8	329	ASN
5	I8	345	GLN
7	Ip	36	GLN
7	Ip	84	GLN
7	Ip	86	GLN
8	Iq	33	GLN
8	Iq	72	ASN

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Mol	Chain	Res	Type
8	Iq	96	ASN
9	Ir	10	GLN
9	Ir	114	HIS
9	Ir	187	GLN
9	Ir	228	ASN
10	Is	232	GLN
10	Is	292	GLN
11	It	12	GLN
12	Iu	25	GLN
12	Iu	44	GLN
12	Iu	73	GLN
12	Iu	122	GLN
12	Iu	180	GLN
12	Iu	212	HIS
12	Iu	219	ASN
12	Iu	226	GLN
12	Iu	312	GLN
12	Iu	441	GLN
12	Iu	442	GLN
12	Iu	477	HIS
12	Iu	522	GLN
13	Iv	216	HIS
13	Iv	244	ASN
13	Iv	361	ASN
15	Ix	31	GLN
15	Ix	57	ASN
15	Ix	311	ASN
15	Ix	320	ASN
15	Ix	321	HIS
15	Ix	336	ASN
15	Ix	403	HIS
15	Ix	456	HIS
15	Ix	486	ASN
15	Ix	513	ASN
16	Iy	415	ASN
16	Iy	461	ASN
16	Iy	534	GLN
16	Iy	595	GLN
16	Iy	597	ASN
16	Iy	630	HIS
16	Iy	648	GLN
16	Iy	717	GLN

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Mol	Chain	Res	Type
16	Iy	753	HIS
16	Iy	840	GLN
16	Iy	845	HIS
16	Iy	858	GLN
18	AA	169	HIS
19	AB	40	ASN
19	AB	158	HIS
20	AC	136	HIS
20	AC	172	ASN
21	AD	4	GLN
22	AE	17	HIS
22	AE	50	ASN
22	AE	67	GLN
22	AE	161	GLN
22	AE	179	ASN
22	AE	188	ASN
22	AE	201	HIS
23	AF	36	GLN
23	AF	83	ASN
23	AF	95	HIS
23	AF	137	GLN
23	AF	203	ASN
25	AH	76	GLN
26	AI	7	ASN
26	AI	165	GLN
29	AL	94	HIS
29	AL	100	ASN
29	AL	112	HIS
30	AM	19	GLN
30	AM	75	ASN
31	AN	105	ASN
32	AO	32	HIS
32	AO	103	ASN
33	AP	32	GLN
36	AS	105	ASN
39	AV	2	GLN
39	AV	49	GLN
40	AW	70	ASN
40	AW	90	GLN
41	AX	16	HIS
41	AX	92	ASN
42	AY	63	HIS

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Mol	Chain	Res	Type
44	Aa	25	ASN
45	Ab	9	HIS
45	Ab	49	HIS
47	Ad	3	HIS
49	Af	111	ASN
50	Ag	20	GLN
50	Ag	26	GLN
50	Ag	159	ASN
50	Ag	226	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	Iw	74/75 (98%)	14 (18%)	0
17	A2	1774/1869 (94%)	231 (13%)	0
All	All	1848/1944 (95%)	245 (13%)	0

All (245) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	Iw	9	1MG
14	Iw	16	C
14	Iw	17	G
14	Iw	18	G
14	Iw	19	A
14	Iw	47	5MC
14	Iw	48	G
14	Iw	52	G
14	Iw	53	A
14	Iw	57	1MA
14	Iw	58	A
14	Iw	60	C
14	Iw	74	C
14	Iw	75	A
17	A2	4	C
17	A2	33	G
17	A2	41	G
17	A2	43	U
17	A2	44	U
17	A2	46	A
17	A2	56	G

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Mol	Chain	Res	Type
17	A2	64	A
17	A2	67	C
17	A2	68	A
17	A2	75	G
17	A2	76	U
17	A2	79	A
17	A2	103	A
17	A2	113	G
17	A2	114	G
17	A2	115	U
17	A2	126	G
17	A2	130	G
17	A2	143	U
17	A2	155	G
17	A2	163	U
17	A2	168	C
17	A2	184	G
17	A2	204	G
17	A2	226	A
17	A2	228	C
17	A2	229	A
17	A2	230	A
17	A2	231	A
17	A2	232	A
17	A2	234	C
17	A2	235	A
17	A2	236	A
17	A2	238	C
17	A2	281	C
17	A2	295	C
17	A2	312	G
17	A2	319	C
17	A2	320	G
17	A2	325	C
17	A2	328	U
17	A2	335	G
17	A2	347	G
17	A2	362	C
17	A2	364	A
17	A2	369	C
17	A2	370	G
17	A2	385	G

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Mol	Chain	Res	Type
17	A2	386	C
17	A2	409	C
17	A2	421	G
17	A2	448	A
17	A2	449	A
17	A2	450	C
17	A2	464	A
17	A2	471	G
17	A2	472	C
17	A2	474	G
17	A2	482	G
17	A2	487	U
17	A2	492	C
17	A2	512	A2M
17	A2	525	A
17	A2	534	G
17	A2	537	C
17	A2	546	G
17	A2	547	G
17	A2	548	C
17	A2	549	C
17	A2	555	A
17	A2	559	G
17	A2	564	A
17	A2	568	C
17	A2	583	A
17	A2	588	G
17	A2	591	U
17	A2	607	U
17	A2	608	C
17	A2	614	C
17	A2	615	C
17	A2	626	G
17	A2	629	A
17	A2	643	A
17	A2	644	OMG
17	A2	655	A
17	A2	660	C
17	A2	664	A
17	A2	668	A2M
17	A2	669	A
17	A2	671	A

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Mol	Chain	Res	Type
17	A2	672	A
17	A2	673	G
17	A2	688	U
17	A2	738	C
17	A2	746	C
17	A2	748	C
17	A2	749	U
17	A2	788	G
17	A2	790	C
17	A2	798	G
17	A2	799	OMU
17	A2	811	A
17	A2	821	G
17	A2	822	PSU
17	A2	830	A
17	A2	831	G
17	A2	836	G
17	A2	837	A
17	A2	839	C
17	A2	840	C
17	A2	841	G
17	A2	847	A
17	A2	870	A
17	A2	872	A
17	A2	885	U
17	A2	891	G
17	A2	903	A
17	A2	913	A
17	A2	920	A
17	A2	922	A
17	A2	933	G
17	A2	943	U
17	A2	971	G
17	A2	985	G
17	A2	990	A
17	A2	992	A
17	A2	999	G
17	A2	1017	U
17	A2	1023	A
17	A2	1061	U
17	A2	1062	A
17	A2	1083	A

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Mol	Chain	Res	Type
17	A2	1085	C
17	A2	1114	U
17	A2	1115	U
17	A2	1116	C
17	A2	1120	U
17	A2	1121	G
17	A2	1130	G
17	A2	1138	C
17	A2	1144	A
17	A2	1153	C
17	A2	1154	U
17	A2	1171	G
17	A2	1195	A
17	A2	1207	G
17	A2	1215	C
17	A2	1217	A
17	A2	1224	G
17	A2	1227	G
17	A2	1242	U
17	A2	1243	U
17	A2	1251	A
17	A2	1253	A
17	A2	1256	G
17	A2	1257	G
17	A2	1259	A
17	A2	1274	G
17	A2	1275	G
17	A2	1302	G
17	A2	1303	C
17	A2	1308	U
17	A2	1342	U
17	A2	1343	U
17	A2	1348	G
17	A2	1358	U
17	A2	1371	U
17	A2	1372	U
17	A2	1378	A
17	A2	1382	A
17	A2	1405	A
17	A2	1406	G
17	A2	1419	C
17	A2	1420	G

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Mol	Chain	Res	Type
17	A2	1421	A
17	A2	1423	C
17	A2	1433	C
17	A2	1435	C
17	A2	1438	A
17	A2	1454	A
17	A2	1463	U
17	A2	1466	G
17	A2	1480	A
17	A2	1489	A
17	A2	1490	OMG
17	A2	1494	U
17	A2	1497	G
17	A2	1508	A
17	A2	1509	U
17	A2	1521	C
17	A2	1533	A
17	A2	1553	C
17	A2	1560	U
17	A2	1570	G
17	A2	1578	U
17	A2	1580	A
17	A2	1585	U
17	A2	1588	A
17	A2	1599	U
17	A2	1601	A
17	A2	1621	U
17	A2	1623	A
17	A2	1637	A
17	A2	1654	G
17	A2	1665	G
17	A2	1671	G
17	A2	1675	A
17	A2	1695	A
17	A2	1698	C
17	A2	1699	A
17	A2	1710	C
17	A2	1721	U
17	A2	1730	U
17	A2	1783	C
17	A2	1784	G
17	A2	1800	A

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Mol	Chain	Res	Type
17	A2	1822	A
17	A2	1829	G
17	A2	1831	A
17	A2	1835	A
17	A2	1836	G
17	A2	1838	U
17	A2	1849	G
17	A2	1851	MA6
17	A2	1861	G
17	A2	1862	G
17	A2	1863	A
17	A2	1864	U
17	A2	1865	C
17	A2	1869	A

There are no RNA pucker outliers to report.

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

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
41	HY3	AX	62	41	6,8,9	2.17	1 (16%)	5,10,12	1.13	1 (20%)
17	PSU	A2	651	17	18,21,22	1.37	2 (11%)	22,30,33	1.92	3 (13%)
17	PSU	A2	1445	17	18,21,22	1.36	2 (11%)	22,30,33	1.92	4 (18%)
18	SAC	AA	2	18	7,8,9	0.52	0	8,9,11	0.86	1 (12%)
17	PSU	A2	1046	17	18,21,22	1.37	2 (11%)	22,30,33	1.89	3 (13%)
17	OMU	A2	799	17	19,22,23	1.21	3 (15%)	26,31,34	1.68	4 (15%)
17	PSU	A2	966	17	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
17	PSU	A2	1692	17	18,21,22	1.37	2 (11%)	22,30,33	1.90	3 (13%)
17	B8N	A2	1248	17	24,29,30	1.28	3 (12%)	29,42,45	1.28	3 (10%)
36	SAC	AS	2	36	7,8,9	0.53	0	8,9,11	0.91	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	OMC	A2	174	17,55	19,22,23	0.82	0	26,31,34	0.79	0
17	PSU	A2	218	17	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
17	PSU	A2	1081	17	18,21,22	1.39	3 (16%)	22,30,33	1.86	3 (13%)
17	A2M	A2	590	17	22,25,26	1.46	4 (18%)	31,36,39	2.16	7 (22%)
17	PSU	A2	1238	17	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
14	T6A	Iw	36	14	31,34,35	1.39	6 (19%)	44,49,52	1.87	9 (20%)
17	OMC	A2	517	17	19,22,23	0.81	0	26,31,34	0.83	0
17	A2M	A2	576	17	22,25,26	1.46	4 (18%)	31,36,39	2.14	10 (32%)
14	5MC	Iw	47	14	18,22,23	0.61	0	26,32,35	0.82	1 (3%)
17	OMU	A2	1288	17	19,22,23	1.21	3 (15%)	26,31,34	1.70	4 (15%)
17	PSU	A2	609	17	18,21,22	1.37	2 (11%)	22,30,33	1.91	3 (13%)
17	PSU	A2	34	17	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
17	OMC	A2	1272	17	19,22,23	0.83	0	26,31,34	0.90	1 (3%)
17	PSU	A2	1136	17	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
17	A2M	A2	1383	17	22,25,26	1.45	4 (18%)	31,36,39	2.15	9 (29%)
17	OMC	A2	462	17	19,22,23	0.82	0	26,31,34	0.82	0
17	PSU	A2	406	17	18,21,22	1.35	2 (11%)	22,30,33	1.92	3 (13%)
17	OMG	A2	1490	17,55	23,26,27	1.21	3 (13%)	33,38,41	1.93	6 (18%)
17	G7M	A2	1639	17,14	23,26,27	3.06	9 (39%)	35,39,42	3.31	13 (37%)
17	OMU	A2	116	17	19,22,23	1.19	3 (15%)	26,31,34	1.69	4 (15%)
17	PSU	A2	1232	17	18,21,22	1.37	2 (11%)	22,30,33	1.93	4 (18%)
17	OMG	A2	509	17,55	23,26,27	1.22	3 (13%)	33,38,41	1.94	6 (18%)
17	A2M	A2	27	17,55	22,25,26	1.45	4 (18%)	31,36,39	2.13	9 (29%)
17	OMG	A2	1447	17	23,26,27	1.21	3 (13%)	33,38,41	1.93	6 (18%)
14	G7M	Iw	45	14	23,26,27	3.10	9 (39%)	35,39,42	3.37	14 (40%)
17	OMU	A2	428	17	19,22,23	1.20	3 (15%)	26,31,34	1.72	5 (19%)
37	NMM	AT	67	37	9,11,12	1.63	1 (11%)	6,12,14	3.45	2 (33%)
14	2MG	Iw	25	14	23,26,27	1.25	4 (17%)	32,38,41	2.18	7 (21%)
17	A2M	A2	1678	17	22,25,26	1.44	4 (18%)	31,36,39	2.15	10 (32%)
17	MA6	A2	1850	17	23,26,27	2.28	5 (21%)	34,38,41	3.70	13 (38%)
17	PSU	A2	296	17	18,21,22	1.37	2 (11%)	22,30,33	1.92	3 (13%)
17	OMU	A2	1804	17	19,22,23	1.21	2 (10%)	26,31,34	1.71	4 (15%)
32	IAS	AO	138	32	6,7,8	0.96	0	6,8,10	1.33	1 (16%)
17	PSU	A2	93	17	18,21,22	1.37	2 (11%)	22,30,33	1.90	3 (13%)
17	OMU	A2	121	17	19,22,23	1.22	3 (15%)	26,31,34	1.73	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	PSU	A2	210	17	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
17	PSU	A2	801	17	18,21,22	1.35	2 (11%)	22,30,33	1.93	4 (18%)
17	4AC	A2	1842	17	21,24,25	1.10	2 (9%)	29,34,37	1.17	2 (6%)
17	OMU	A2	627	17	19,22,23	1.18	2 (10%)	26,31,34	1.72	5 (19%)
14	H2U	Iw	46	14	18,21,22	1.00	2 (11%)	21,30,33	1.72	1 (4%)
17	4AC	A2	1337	17	21,24,25	1.09	2 (9%)	29,34,37	1.00	2 (6%)
17	A2M	A2	166	17	22,25,26	1.46	4 (18%)	31,36,39	2.17	10 (32%)
17	PSU	A2	814	17	18,21,22	1.36	2 (11%)	22,30,33	1.93	3 (13%)
17	OMC	A2	1391	17	19,22,23	0.82	0	26,31,34	0.82	0
14	1MA	Iw	57	14	21,25,26	1.41	4 (19%)	31,37,40	1.78	4 (12%)
17	OMG	A2	683	17	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
17	OMU	A2	172	17	19,22,23	1.19	2 (10%)	26,31,34	1.73	5 (19%)
17	PSU	A2	105	17	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
17	PSU	A2	572	17	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
17	OMG	A2	1328	17	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
17	PSU	A2	822	17	18,21,22	1.36	2 (11%)	22,30,33	1.91	4 (18%)
17	PSU	A2	686	17	18,21,22	1.36	2 (11%)	22,30,33	1.93	3 (13%)
17	A2M	A2	484	17	22,25,26	1.51	4 (18%)	31,36,39	2.11	8 (25%)
17	PSU	A2	1056	17	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
17	A2M	A2	512	17	22,25,26	1.44	4 (18%)	31,36,39	2.17	10 (32%)
17	OMG	A2	436	17	23,26,27	1.21	3 (13%)	33,38,41	1.97	6 (18%)
17	PSU	A2	119	17	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
17	MA6	A2	1851	17	23,26,27	2.26	5 (21%)	34,38,41	3.65	13 (38%)
17	OMU	A2	354	17	19,22,23	1.25	3 (15%)	26,31,34	1.75	4 (15%)
17	PSU	A2	1643	17,55	18,21,22	1.36	2 (11%)	22,30,33	1.92	3 (13%)
17	PSU	A2	1045	17	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
17	OMG	A2	601	17	23,26,27	1.21	3 (13%)	33,38,41	1.93	6 (18%)
17	OMG	A2	644	17	23,26,27	1.20	3 (13%)	33,38,41	1.96	6 (18%)
17	OMU	A2	1442	17,55	19,22,23	1.22	3 (15%)	26,31,34	1.71	4 (15%)
14	2MG	Iw	10	14	23,26,27	1.26	4 (17%)	32,38,41	2.18	6 (18%)
17	PSU	A2	1004	17	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
39	AME	AV	1	39	9,10,11	0.47	0	9,11,13	0.87	1 (11%)
17	PSU	A2	1177	17	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
17	OMC	A2	797	17	19,22,23	0.81	0	26,31,34	0.84	0
17	PSU	A2	1244	17	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	PSU	A2	866	17	18,21,22	1.36	2 (11%)	22,30,33	1.92	3 (13%)
17	PSU	A2	863	17	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
17	PSU	A2	36	17	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
17	PSU	A2	1347	17	18,21,22	1.34	2 (11%)	22,30,33	1.95	4 (18%)
17	PSU	A2	815	17	18,21,22	1.36	3 (16%)	22,30,33	1.92	3 (13%)
17	PSU	A2	1367	17	18,21,22	1.35	2 (11%)	22,30,33	1.92	4 (18%)
17	PSU	A2	681	17	18,21,22	1.37	3 (16%)	22,30,33	1.90	3 (13%)
17	6MZ	A2	1832	17,55	22,25,26	1.41	4 (18%)	30,36,39	2.13	9 (30%)
17	PSU	A2	109	17	18,21,22	1.37	2 (11%)	22,30,33	1.91	3 (13%)
17	A2M	A2	1031	17	22,25,26	1.45	4 (18%)	31,36,39	2.12	10 (32%)
17	OMU	A2	1326	17,55	19,22,23	1.19	3 (15%)	26,31,34	1.72	5 (19%)
17	OMC	A2	1703	17	19,22,23	0.81	0	26,31,34	0.83	1 (3%)
17	PSU	A2	1625	17	18,21,22	1.39	2 (11%)	22,30,33	1.88	3 (13%)
17	A2M	A2	99	17,55	22,25,26	1.50	4 (18%)	31,36,39	2.17	9 (29%)
17	PSU	A2	1174	17	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
17	A2M	A2	668	17,55	22,25,26	1.43	4 (18%)	31,36,39	2.06	9 (29%)
17	A2M	A2	468	17	22,25,26	1.46	4 (18%)	31,36,39	2.12	10 (32%)
17	PSU	A2	649	17	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
14	1MG	Iw	9	14	22,26,27	1.12	2 (9%)	33,39,42	1.73	5 (15%)
17	A2M	A2	159	17	22,25,26	1.45	4 (18%)	31,36,39	2.18	10 (32%)

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
41	HY3	AX	62	41	-	0/1/12/14	0/1/1/1
17	PSU	A2	651	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	1445	17	-	0/7/25/26	0/2/2/2
18	SAC	AA	2	18	-	2/7/8/10	-
17	PSU	A2	1046	17	-	0/7/25/26	0/2/2/2
17	OMU	A2	799	17	-	3/9/27/28	0/2/2/2
17	PSU	A2	966	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	1692	17	-	0/7/25/26	0/2/2/2
17	B8N	A2	1248	17	-	4/16/34/35	0/2/2/2
36	SAC	AS	2	36	-	0/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	OMC	A2	174	17,55	-	0/9/27/28	0/2/2/2
17	PSU	A2	218	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	1081	17	-	0/7/25/26	0/2/2/2
17	A2M	A2	590	17	-	3/9/27/28	0/3/3/3
17	PSU	A2	1238	17	-	0/7/25/26	0/2/2/2
14	T6A	Iw	36	14	-	4/23/41/42	0/3/3/3
17	OMC	A2	517	17	-	0/9/27/28	0/2/2/2
17	A2M	A2	576	17	-	2/9/27/28	0/3/3/3
14	5MC	Iw	47	14	-	3/7/25/26	0/2/2/2
17	OMU	A2	1288	17	-	1/9/27/28	0/2/2/2
17	PSU	A2	609	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	34	17	-	0/7/25/26	0/2/2/2
17	OMC	A2	1272	17	-	0/9/27/28	0/2/2/2
17	PSU	A2	1136	17	-	0/7/25/26	0/2/2/2
17	A2M	A2	1383	17	-	0/9/27/28	0/3/3/3
17	OMC	A2	462	17	-	0/9/27/28	0/2/2/2
17	PSU	A2	406	17	-	0/7/25/26	0/2/2/2
17	OMG	A2	1490	17,55	-	0/9/27/28	0/3/3/3
17	G7M	A2	1639	17,14	-	0/7/25/26	0/3/3/3
17	OMU	A2	116	17	-	1/9/27/28	0/2/2/2
17	PSU	A2	1232	17	-	0/7/25/26	0/2/2/2
17	OMG	A2	509	17,55	-	1/9/27/28	0/3/3/3
17	A2M	A2	27	17,55	-	0/9/27/28	0/3/3/3
17	OMG	A2	1447	17	-	2/9/27/28	0/3/3/3
14	G7M	Iw	45	14	-	0/7/25/26	0/3/3/3
17	OMU	A2	428	17	-	4/9/27/28	0/2/2/2
37	NMM	AT	67	37	-	1/9/11/13	-
14	2MG	Iw	25	14	-	0/9/27/28	0/3/3/3
17	A2M	A2	1678	17	-	0/9/27/28	0/3/3/3
17	MA6	A2	1850	17	-	0/11/29/30	0/3/3/3
17	PSU	A2	296	17	-	0/7/25/26	0/2/2/2
17	OMU	A2	1804	17	-	0/9/27/28	0/2/2/2
32	IAS	AO	138	32	-	2/7/7/8	-
17	PSU	A2	93	17	-	0/7/25/26	0/2/2/2
17	OMU	A2	121	17	-	0/9/27/28	0/2/2/2
17	PSU	A2	210	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	801	17	-	0/7/25/26	0/2/2/2
17	4AC	A2	1842	17	-	4/11/29/30	0/2/2/2
17	OMU	A2	627	17	-	1/9/27/28	0/2/2/2
14	H2U	Iw	46	14	-	1/7/38/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	4AC	A2	1337	17	-	2/11/29/30	0/2/2/2
17	A2M	A2	166	17	-	0/9/27/28	0/3/3/3
17	PSU	A2	814	17	-	0/7/25/26	0/2/2/2
17	OMC	A2	1391	17	-	0/9/27/28	0/2/2/2
14	1MA	Iw	57	14	-	0/7/25/26	0/3/3/3
17	OMG	A2	683	17	-	3/9/27/28	0/3/3/3
17	OMU	A2	172	17	-	0/9/27/28	0/2/2/2
17	PSU	A2	105	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	572	17	-	0/7/25/26	0/2/2/2
17	OMG	A2	1328	17	-	1/9/27/28	0/3/3/3
17	PSU	A2	822	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	686	17	-	0/7/25/26	0/2/2/2
17	A2M	A2	484	17	-	0/9/27/28	0/3/3/3
17	PSU	A2	1056	17	-	0/7/25/26	0/2/2/2
17	A2M	A2	512	17	-	3/9/27/28	0/3/3/3
17	OMG	A2	436	17	-	1/9/27/28	0/3/3/3
17	PSU	A2	119	17	-	0/7/25/26	0/2/2/2
17	MA6	A2	1851	17	-	2/11/29/30	0/3/3/3
17	OMU	A2	354	17	-	1/9/27/28	0/2/2/2
17	PSU	A2	1643	17,55	-	0/7/25/26	0/2/2/2
17	PSU	A2	1045	17	-	0/7/25/26	0/2/2/2
17	OMG	A2	601	17	-	0/9/27/28	0/3/3/3
17	OMG	A2	644	17	-	4/9/27/28	0/3/3/3
17	OMU	A2	1442	17,55	-	1/9/27/28	0/2/2/2
14	2MG	Iw	10	14	-	0/9/27/28	0/3/3/3
17	PSU	A2	1004	17	-	0/7/25/26	0/2/2/2
39	AME	AV	1	39	-	2/9/10/12	-
17	PSU	A2	1177	17	-	0/7/25/26	0/2/2/2
17	OMC	A2	797	17	-	1/9/27/28	0/2/2/2
17	PSU	A2	1244	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	866	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	863	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	36	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	1347	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	815	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	1367	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	681	17	-	0/7/25/26	0/2/2/2
17	6MZ	A2	1832	17,55	-	0/9/27/28	0/3/3/3
17	PSU	A2	109	17	-	0/7/25/26	0/2/2/2
17	A2M	A2	1031	17	-	1/9/27/28	0/3/3/3
17	OMU	A2	1326	17,55	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	OMC	A2	1703	17	-	1/9/27/28	0/2/2/2
17	PSU	A2	1625	17	-	2/7/25/26	0/2/2/2
17	A2M	A2	99	17,55	-	2/9/27/28	0/3/3/3
17	PSU	A2	1174	17	-	0/7/25/26	0/2/2/2
17	A2M	A2	668	17,55	-	3/9/27/28	0/3/3/3
17	A2M	A2	468	17	-	1/9/27/28	0/3/3/3
17	PSU	A2	649	17	-	0/7/25/26	0/2/2/2
14	1MG	Iw	9	14	-	3/7/25/26	0/3/3/3
17	A2M	A2	159	17	-	1/9/27/28	0/3/3/3

All (252) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	Iw	45	G7M	C4-N9	7.78	1.58	1.38
17	A2	1639	G7M	C4-N9	7.69	1.58	1.38
17	A2	1639	G7M	O6-C6	7.57	1.38	1.23
14	Iw	45	G7M	O6-C6	7.54	1.37	1.23
17	A2	1850	MA6	C5-N7	6.75	1.51	1.39
17	A2	1851	MA6	C5-N7	6.73	1.51	1.39
14	Iw	45	G7M	C5-C4	6.14	1.53	1.38
17	A2	1639	G7M	C5-C4	6.05	1.53	1.38
17	A2	1850	MA6	C8-N9	-5.56	1.27	1.37
17	A2	1851	MA6	C8-N9	-5.50	1.27	1.37
41	AX	62	HY3	C3-CA	-4.98	1.50	1.55
17	A2	484	A2M	C5-C4	4.58	1.47	1.39
17	A2	590	A2M	C5-C4	4.52	1.47	1.39
17	A2	99	A2M	C5-C4	4.49	1.47	1.39
14	Iw	45	G7M	C2-N2	4.47	1.44	1.34
37	AT	67	NMM	CZ-NH2	4.42	1.45	1.34
17	A2	1639	G7M	C2-N2	4.42	1.44	1.34
17	A2	468	A2M	C5-C4	4.42	1.47	1.39
17	A2	159	A2M	C5-C4	4.41	1.47	1.39
14	Iw	36	T6A	C5-C4	4.41	1.47	1.39
17	A2	576	A2M	C5-C4	4.41	1.47	1.39
17	A2	166	A2M	C5-C4	4.37	1.47	1.39
17	A2	1832	6MZ	C5-C4	4.35	1.47	1.39
17	A2	27	A2M	C5-C4	4.33	1.47	1.39
17	A2	1383	A2M	C5-C4	4.32	1.47	1.39
17	A2	512	A2M	C5-C4	4.31	1.47	1.39
17	A2	1678	A2M	C5-C4	4.31	1.47	1.39
17	A2	1031	A2M	C5-C4	4.27	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A2	668	A2M	C5-C4	4.25	1.46	1.39
14	Iw	45	G7M	C2-N1	3.82	1.47	1.37
17	A2	1850	MA6	C4-N9	-3.80	1.29	1.37
17	A2	1639	G7M	C2-N1	3.80	1.47	1.37
17	A2	1851	MA6	C4-N9	-3.70	1.29	1.37
14	Iw	45	G7M	C2-N3	3.42	1.41	1.33
14	Iw	57	1MA	C5-C4	3.26	1.47	1.38
14	Iw	57	1MA	C6-N6	3.26	1.36	1.28
14	Iw	9	1MG	C5-C4	3.24	1.47	1.38
17	A2	1851	MA6	C5-C4	3.24	1.45	1.39
17	A2	1639	G7M	C2-N3	3.18	1.40	1.33
17	A2	1850	MA6	C5-C4	3.16	1.44	1.39
17	A2	296	PSU	C6-C5	3.16	1.39	1.35
17	A2	1248	B8N	C4-N3	-3.15	1.34	1.40
17	A2	210	PSU	C6-C5	3.14	1.39	1.35
17	A2	866	PSU	C6-C5	3.12	1.39	1.35
17	A2	1625	PSU	C6-C5	3.07	1.38	1.35
17	A2	93	PSU	C6-C5	3.06	1.38	1.35
14	Iw	10	2MG	C5-C4	3.06	1.47	1.38
17	A2	609	PSU	C6-C5	3.05	1.38	1.35
17	A2	218	PSU	C6-C5	3.04	1.38	1.35
17	A2	1328	OMG	C5-C4	3.03	1.47	1.38
17	A2	1447	OMG	C5-C4	3.03	1.47	1.38
17	A2	509	OMG	C5-C4	3.02	1.47	1.38
17	A2	966	PSU	C6-C5	3.02	1.38	1.35
17	A2	105	PSU	C6-C5	3.02	1.38	1.35
17	A2	1238	PSU	C6-C5	3.02	1.38	1.35
17	A2	1174	PSU	C6-C5	3.01	1.38	1.35
17	A2	1232	PSU	C6-C5	3.01	1.38	1.35
17	A2	1445	PSU	C6-C5	3.00	1.38	1.35
17	A2	1842	4AC	C4-N4	-2.99	1.35	1.39
17	A2	1244	PSU	C6-C5	2.99	1.38	1.35
14	Iw	25	2MG	C5-C4	2.99	1.47	1.38
17	A2	814	PSU	C6-C5	2.99	1.38	1.35
17	A2	815	PSU	C6-C5	2.98	1.38	1.35
17	A2	1490	OMG	C5-C4	2.98	1.47	1.38
17	A2	1004	PSU	C6-C5	2.97	1.38	1.35
17	A2	601	OMG	C5-C4	2.97	1.47	1.38
17	A2	34	PSU	C6-C5	2.97	1.38	1.35
17	A2	1177	PSU	C6-C5	2.97	1.38	1.35
17	A2	436	OMG	C5-C4	2.96	1.47	1.38
17	A2	644	OMG	C5-C4	2.96	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A2	1337	4AC	C4-N4	-2.96	1.35	1.39
17	A2	119	PSU	C6-C5	2.96	1.38	1.35
17	A2	109	PSU	C6-C5	2.96	1.38	1.35
17	A2	1850	MA6	C6-N6	2.96	1.45	1.36
17	A2	649	PSU	C6-C5	2.95	1.38	1.35
17	A2	1643	PSU	C6-C5	2.95	1.38	1.35
17	A2	1692	PSU	C6-C5	2.95	1.38	1.35
17	A2	651	PSU	C6-C5	2.95	1.38	1.35
17	A2	1081	PSU	C6-C5	2.95	1.38	1.35
17	A2	1046	PSU	C6-C5	2.95	1.38	1.35
17	A2	863	PSU	C6-C5	2.94	1.38	1.35
17	A2	1851	MA6	C6-N6	2.94	1.45	1.36
17	A2	683	OMG	C5-C4	2.94	1.46	1.38
17	A2	686	PSU	C6-C5	2.93	1.38	1.35
17	A2	1136	PSU	C6-C5	2.93	1.38	1.35
17	A2	406	PSU	C6-C5	2.93	1.38	1.35
17	A2	801	PSU	C6-C5	2.92	1.38	1.35
17	A2	1367	PSU	C6-C5	2.92	1.38	1.35
17	A2	572	PSU	C6-C5	2.92	1.38	1.35
17	A2	36	PSU	C6-C5	2.91	1.38	1.35
17	A2	1056	PSU	C6-C5	2.91	1.38	1.35
17	A2	822	PSU	C6-C5	2.89	1.38	1.35
17	A2	1045	PSU	C6-C5	2.88	1.38	1.35
17	A2	681	PSU	C6-C5	2.86	1.38	1.35
17	A2	109	PSU	C4-N3	-2.85	1.33	1.38
17	A2	1347	PSU	C4-N3	-2.85	1.33	1.38
17	A2	1248	B8N	C6-C5	2.85	1.39	1.34
17	A2	651	PSU	C4-N3	-2.85	1.33	1.38
17	A2	686	PSU	C4-N3	-2.84	1.33	1.38
17	A2	801	PSU	C4-N3	-2.84	1.33	1.38
17	A2	1347	PSU	C6-C5	2.83	1.38	1.35
17	A2	681	PSU	C4-N3	-2.82	1.33	1.38
17	A2	1367	PSU	C4-N3	-2.82	1.33	1.38
17	A2	1232	PSU	C4-N3	-2.81	1.33	1.38
17	A2	1081	PSU	C4-N3	-2.81	1.33	1.38
17	A2	1136	PSU	C4-N3	-2.81	1.33	1.38
17	A2	1692	PSU	C4-N3	-2.80	1.33	1.38
17	A2	1625	PSU	C4-N3	-2.79	1.33	1.38
17	A2	609	PSU	C4-N3	-2.79	1.33	1.38
17	A2	406	PSU	C4-N3	-2.78	1.33	1.38
17	A2	863	PSU	C4-N3	-2.78	1.33	1.38
17	A2	34	PSU	C4-N3	-2.78	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A2	649	PSU	C4-N3	-2.78	1.33	1.38
17	A2	1045	PSU	C4-N3	-2.77	1.33	1.38
17	A2	1174	PSU	C4-N3	-2.77	1.33	1.38
17	A2	572	PSU	C4-N3	-2.77	1.33	1.38
17	A2	1004	PSU	C4-N3	-2.77	1.33	1.38
17	A2	93	PSU	C4-N3	-2.77	1.33	1.38
17	A2	1177	PSU	C4-N3	-2.76	1.33	1.38
17	A2	814	PSU	C4-N3	-2.76	1.33	1.38
17	A2	105	PSU	C4-N3	-2.76	1.33	1.38
17	A2	815	PSU	C4-N3	-2.76	1.33	1.38
17	A2	119	PSU	C4-N3	-2.76	1.33	1.38
17	A2	1643	PSU	C4-N3	-2.76	1.33	1.38
17	A2	296	PSU	C4-N3	-2.75	1.33	1.38
17	A2	36	PSU	C4-N3	-2.75	1.33	1.38
17	A2	1445	PSU	C4-N3	-2.75	1.33	1.38
17	A2	1046	PSU	C4-N3	-2.75	1.33	1.38
17	A2	866	PSU	C4-N3	-2.74	1.33	1.38
17	A2	966	PSU	C4-N3	-2.73	1.33	1.38
17	A2	1244	PSU	C4-N3	-2.73	1.33	1.38
17	A2	484	A2M	C5-C6	2.73	1.48	1.41
17	A2	1238	PSU	C4-N3	-2.73	1.33	1.38
17	A2	218	PSU	C4-N3	-2.72	1.33	1.38
17	A2	1056	PSU	C4-N3	-2.69	1.33	1.38
17	A2	509	OMG	C6-N1	-2.67	1.33	1.38
17	A2	210	PSU	C4-N3	-2.67	1.33	1.38
17	A2	99	A2M	C5-C6	2.67	1.48	1.41
17	A2	822	PSU	C4-N3	-2.67	1.33	1.38
17	A2	166	A2M	C5-C6	2.66	1.48	1.41
17	A2	354	OMU	C4-N3	-2.65	1.33	1.38
17	A2	601	OMG	C6-N1	-2.65	1.33	1.38
17	A2	159	A2M	C5-C6	2.64	1.48	1.41
17	A2	468	A2M	C5-C6	2.64	1.48	1.41
17	A2	1678	A2M	C5-C6	2.63	1.48	1.41
17	A2	1490	OMG	C6-N1	-2.62	1.34	1.38
17	A2	590	A2M	C5-C6	2.62	1.48	1.41
17	A2	644	OMG	C6-N1	-2.61	1.34	1.38
17	A2	27	A2M	C5-C6	2.61	1.48	1.41
17	A2	1447	OMG	C6-N1	-2.60	1.34	1.38
17	A2	121	OMU	C4-N3	-2.60	1.33	1.38
17	A2	1383	A2M	C5-C6	2.59	1.48	1.41
17	A2	512	A2M	C5-C6	2.59	1.48	1.41
17	A2	683	OMG	C6-N1	-2.59	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A2	576	A2M	C5-C6	2.58	1.48	1.41
17	A2	436	OMG	C6-N1	-2.58	1.34	1.38
17	A2	1031	A2M	C5-C6	2.58	1.48	1.41
17	A2	1442	OMU	C4-N3	-2.58	1.33	1.38
17	A2	668	A2M	C5-C6	2.57	1.48	1.41
17	A2	1248	B8N	C2-N3	-2.56	1.34	1.38
17	A2	428	OMU	C4-N3	-2.54	1.34	1.38
14	Iw	10	2MG	C6-N1	-2.54	1.34	1.38
17	A2	1804	OMU	C4-N3	-2.54	1.34	1.38
17	A2	1328	OMG	C6-N1	-2.53	1.34	1.38
17	A2	172	OMU	C4-N3	-2.53	1.34	1.38
14	Iw	46	H2U	C2-N3	-2.52	1.33	1.38
17	A2	116	OMU	C4-N3	-2.50	1.34	1.38
14	Iw	36	T6A	C5-C6	2.50	1.48	1.41
17	A2	1326	OMU	C4-N3	-2.50	1.34	1.38
17	A2	627	OMU	C4-N3	-2.49	1.34	1.38
17	A2	1288	OMU	C4-N3	-2.49	1.34	1.38
17	A2	799	OMU	C4-N3	-2.49	1.34	1.38
14	Iw	25	2MG	C6-N1	-2.48	1.34	1.38
17	A2	1832	6MZ	C5-N7	-2.48	1.34	1.39
17	A2	166	A2M	C8-N7	2.41	1.36	1.31
14	Iw	57	1MA	C2-N3	2.40	1.35	1.30
17	A2	159	A2M	C8-N7	2.39	1.36	1.31
17	A2	484	A2M	C5-N7	-2.39	1.34	1.39
17	A2	468	A2M	C8-N7	2.35	1.36	1.31
17	A2	99	A2M	C8-N7	2.35	1.36	1.31
17	A2	509	OMG	C5-N7	-2.33	1.34	1.39
17	A2	354	OMU	C2-N3	-2.33	1.33	1.38
17	A2	590	A2M	C5-N7	-2.33	1.34	1.39
17	A2	512	A2M	C8-N7	2.33	1.36	1.31
17	A2	576	A2M	C8-N7	2.32	1.36	1.31
17	A2	99	A2M	C5-N7	-2.32	1.34	1.39
17	A2	590	A2M	C8-N7	2.31	1.36	1.31
17	A2	121	OMU	C2-N3	-2.31	1.33	1.38
14	Iw	36	T6A	C6-N6	-2.31	1.35	1.39
17	A2	1031	A2M	C5-N7	-2.30	1.34	1.39
14	Iw	36	T6A	C8-N7	2.30	1.35	1.31
17	A2	1678	A2M	C8-N7	2.29	1.35	1.31
17	A2	1442	OMU	C2-N3	-2.29	1.33	1.38
17	A2	1383	A2M	C5-N7	-2.28	1.34	1.39
17	A2	668	A2M	C8-N7	2.28	1.35	1.31
17	A2	27	A2M	C5-N7	-2.28	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A2	576	A2M	C5-N7	-2.27	1.34	1.39
14	Iw	45	G7M	C5-N7	2.26	1.41	1.39
17	A2	484	A2M	C8-N7	2.26	1.35	1.31
17	A2	1031	A2M	C8-N7	2.26	1.35	1.31
17	A2	1326	OMU	C2-N3	-2.26	1.33	1.38
17	A2	668	A2M	C5-N7	-2.26	1.34	1.39
17	A2	1447	OMG	C5-N7	-2.26	1.34	1.39
17	A2	27	A2M	C8-N7	2.26	1.35	1.31
17	A2	166	A2M	C5-N7	-2.25	1.34	1.39
17	A2	172	OMU	C2-N3	-2.25	1.33	1.38
17	A2	1832	6MZ	C5-C6	2.25	1.47	1.41
17	A2	428	OMU	C2-N3	-2.25	1.34	1.38
17	A2	468	A2M	C5-N7	-2.25	1.34	1.39
17	A2	1328	OMG	C5-N7	-2.25	1.34	1.39
17	A2	601	OMG	C5-N7	-2.24	1.34	1.39
14	Iw	46	H2U	C4-N3	-2.24	1.33	1.37
17	A2	1383	A2M	C8-N7	2.24	1.35	1.31
17	A2	1678	A2M	C5-N7	-2.24	1.34	1.39
17	A2	1842	4AC	C7-N4	-2.24	1.33	1.37
17	A2	1490	OMG	C5-N7	-2.24	1.34	1.39
17	A2	644	OMG	C5-N7	-2.23	1.34	1.39
17	A2	436	OMG	C5-N7	-2.23	1.34	1.39
17	A2	512	A2M	C5-N7	-2.23	1.34	1.39
14	Iw	45	G7M	C4-N3	2.22	1.39	1.34
17	A2	683	OMG	C5-N7	-2.21	1.34	1.39
17	A2	159	A2M	C5-N7	-2.20	1.34	1.39
17	A2	116	OMU	C2-N3	-2.19	1.34	1.38
14	Iw	36	T6A	C5-N7	-2.19	1.34	1.39
14	Iw	25	2MG	C5-N7	-2.17	1.34	1.39
14	Iw	10	2MG	C2-N3	2.17	1.36	1.31
14	Iw	10	2MG	C5-N7	-2.17	1.34	1.39
14	Iw	9	1MG	C5-N7	-2.16	1.34	1.39
14	Iw	57	1MA	C5-N7	-2.16	1.34	1.39
17	A2	1804	OMU	C2-N3	-2.16	1.34	1.38
17	A2	627	OMU	C2-N3	-2.15	1.34	1.38
17	A2	1639	G7M	C5-N7	2.14	1.41	1.39
17	A2	1288	OMU	C2-N3	-2.12	1.34	1.38
17	A2	1337	4AC	C7-N4	-2.11	1.33	1.37
17	A2	1081	PSU	C2-N3	-2.10	1.33	1.37
14	Iw	25	2MG	C2-N3	2.10	1.35	1.31
17	A2	354	OMU	C5-C4	-2.10	1.39	1.43
17	A2	116	OMU	C5-C4	-2.09	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A2	799	OMU	C2-N3	-2.09	1.34	1.38
17	A2	1639	G7M	C4-N3	2.08	1.39	1.34
14	Iw	45	G7M	C6-N1	2.08	1.42	1.38
17	A2	1832	6MZ	C8-N7	2.08	1.35	1.31
17	A2	121	OMU	C5-C4	-2.07	1.39	1.43
17	A2	1442	OMU	C5-C4	-2.05	1.39	1.43
17	A2	428	OMU	C5-C4	-2.04	1.39	1.43
17	A2	1639	G7M	C6-N1	2.04	1.42	1.38
17	A2	1288	OMU	C2-N1	2.03	1.41	1.38
17	A2	799	OMU	C5-C4	-2.03	1.39	1.43
17	A2	815	PSU	C2-N3	-2.01	1.34	1.37
14	Iw	36	T6A	C10-N6	-2.01	1.33	1.37
17	A2	681	PSU	C2-N3	-2.01	1.34	1.37
17	A2	1326	OMU	C5-C4	-2.00	1.39	1.43

All (455) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A2	1850	MA6	C4-N9-C8	14.67	121.63	105.73
17	A2	1851	MA6	C4-N9-C8	14.38	121.31	105.73
14	Iw	45	G7M	C8-N7-C5	11.50	122.17	107.78
17	A2	1639	G7M	C8-N7-C5	11.41	122.04	107.78
37	AT	67	NMM	NE-CZ-NH2	-7.19	112.89	119.48
14	Iw	10	2MG	C2-N3-C4	7.15	120.91	112.04
14	Iw	25	2MG	C2-N3-C4	7.13	120.88	112.04
14	Iw	46	H2U	C4-N3-C2	-6.91	120.06	125.79
17	A2	1850	MA6	N3-C4-N9	6.82	138.32	127.08
17	A2	590	A2M	C5-C4-N3	-6.82	117.85	126.75
14	Iw	45	G7M	N9-C4-N3	6.79	139.56	125.94
17	A2	1851	MA6	N3-C4-N9	6.71	138.14	127.08
17	A2	484	A2M	C5-C4-N3	-6.53	118.22	126.75
17	A2	1639	G7M	N9-C4-N3	6.51	139.00	125.94
17	A2	1639	G7M	C6-C5-N7	6.50	140.10	132.25
17	A2	1832	6MZ	C5-C4-N3	-6.48	118.30	126.75
14	Iw	45	G7M	C6-C5-N7	6.45	140.04	132.25
17	A2	166	A2M	C5-C4-N3	-6.31	118.52	126.75
17	A2	99	A2M	C5-C4-N3	-6.30	118.53	126.75
17	A2	27	A2M	C5-C4-N3	-6.28	118.56	126.75
17	A2	512	A2M	C5-C4-N3	-6.24	118.60	126.75
17	A2	1031	A2M	C5-C4-N3	-6.19	118.67	126.75
14	Iw	36	T6A	C5-C4-N3	-6.18	118.68	126.75
17	A2	1347	PSU	N1-C2-N3	6.18	122.13	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A2	509	OMG	C5-C4-N3	-6.15	118.48	128.46
17	A2	159	A2M	C5-C4-N3	-6.15	118.73	126.75
17	A2	1232	PSU	N1-C2-N3	6.14	122.09	115.13
17	A2	651	PSU	N1-C2-N3	6.14	122.09	115.13
17	A2	1678	A2M	C5-C4-N3	-6.14	118.74	126.75
17	A2	1383	A2M	C5-C4-N3	-6.14	118.75	126.75
17	A2	601	OMG	C5-C4-N3	-6.14	118.51	128.46
17	A2	468	A2M	C5-C4-N3	-6.13	118.75	126.75
17	A2	644	OMG	C5-C4-N3	-6.12	118.53	128.46
17	A2	814	PSU	N1-C2-N3	6.12	122.06	115.13
17	A2	1447	OMG	C5-C4-N3	-6.11	118.55	128.46
17	A2	1328	OMG	C5-C4-N3	-6.10	118.56	128.46
17	A2	436	OMG	C5-C4-N3	-6.09	118.58	128.46
17	A2	406	PSU	N1-C2-N3	6.09	122.03	115.13
17	A2	686	PSU	N1-C2-N3	6.08	122.02	115.13
17	A2	1490	OMG	C5-C4-N3	-6.08	118.59	128.46
17	A2	866	PSU	N1-C2-N3	6.07	122.01	115.13
17	A2	1643	PSU	N1-C2-N3	6.07	122.01	115.13
17	A2	683	OMG	C5-C4-N3	-6.07	118.62	128.46
17	A2	1238	PSU	N1-C2-N3	6.07	122.00	115.13
17	A2	1445	PSU	N1-C2-N3	6.07	122.00	115.13
17	A2	815	PSU	N1-C2-N3	6.06	122.00	115.13
17	A2	1367	PSU	N1-C2-N3	6.06	122.00	115.13
17	A2	609	PSU	N1-C2-N3	6.05	121.99	115.13
17	A2	576	A2M	C5-C4-N3	-6.05	118.85	126.75
17	A2	296	PSU	N1-C2-N3	6.05	121.99	115.13
17	A2	34	PSU	N1-C2-N3	6.05	121.98	115.13
17	A2	105	PSU	N1-C2-N3	6.05	121.98	115.13
17	A2	681	PSU	N1-C2-N3	6.04	121.98	115.13
14	Iw	10	2MG	C5-C4-N3	-6.04	118.66	128.46
17	A2	1625	PSU	N1-C2-N3	6.04	121.97	115.13
17	A2	801	PSU	N1-C2-N3	6.04	121.97	115.13
17	A2	109	PSU	N1-C2-N3	6.03	121.97	115.13
17	A2	822	PSU	N1-C2-N3	6.03	121.96	115.13
17	A2	966	PSU	N1-C2-N3	6.03	121.96	115.13
17	A2	1004	PSU	N1-C2-N3	6.02	121.95	115.13
17	A2	1639	G7M	CN7-N7-C5	-6.02	119.29	126.77
17	A2	1046	PSU	N1-C2-N3	6.01	121.94	115.13
17	A2	218	PSU	N1-C2-N3	6.01	121.94	115.13
17	A2	1136	PSU	N1-C2-N3	6.01	121.94	115.13
17	A2	1692	PSU	N1-C2-N3	6.01	121.94	115.13
17	A2	1045	PSU	N1-C2-N3	6.01	121.94	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A2	668	A2M	C5-C4-N3	-6.00	118.92	126.75
17	A2	649	PSU	N1-C2-N3	5.99	121.92	115.13
17	A2	93	PSU	N1-C2-N3	5.99	121.92	115.13
17	A2	36	PSU	N1-C2-N3	5.99	121.92	115.13
17	A2	1056	PSU	N1-C2-N3	5.99	121.92	115.13
17	A2	1174	PSU	N1-C2-N3	5.99	121.91	115.13
17	A2	1244	PSU	N1-C2-N3	5.97	121.89	115.13
17	A2	119	PSU	N1-C2-N3	5.96	121.89	115.13
17	A2	1177	PSU	N1-C2-N3	5.96	121.88	115.13
17	A2	863	PSU	N1-C2-N3	5.96	121.88	115.13
14	Iw	25	2MG	C5-C4-N3	-5.95	118.81	128.46
17	A2	210	PSU	N1-C2-N3	5.95	121.87	115.13
17	A2	572	PSU	N1-C2-N3	5.93	121.85	115.13
17	A2	1851	MA6	C4-C5-N7	-5.90	103.43	110.62
17	A2	1850	MA6	N9-C8-N7	-5.85	105.92	113.91
17	A2	1081	PSU	N1-C2-N3	5.83	121.74	115.13
17	A2	1850	MA6	C4-C5-N7	-5.83	103.52	110.62
17	A2	1851	MA6	C5-C4-N3	-5.80	119.19	126.75
17	A2	1850	MA6	C5-C4-N3	-5.78	119.22	126.75
17	A2	1851	MA6	N9-C8-N7	-5.73	106.07	113.91
14	Iw	45	G7M	CN7-N7-C5	-5.69	119.70	126.77
14	Iw	57	1MA	C5-C4-N3	-5.64	118.84	127.26
17	A2	590	A2M	N3-C4-N9	5.40	135.99	127.08
17	A2	1832	6MZ	N3-C4-N9	5.38	135.94	127.08
14	Iw	9	1MG	C5-C4-N3	-5.31	119.85	128.46
17	A2	484	A2M	N3-C4-N9	5.06	135.42	127.08
14	Iw	45	G7M	C2-N3-C4	4.94	121.10	112.30
17	A2	436	OMG	C2-N3-C4	4.92	121.07	112.30
17	A2	644	OMG	C2-N3-C4	4.91	121.06	112.30
17	A2	683	OMG	C2-N3-C4	4.90	121.03	112.30
17	A2	1328	OMG	C2-N3-C4	4.88	120.99	112.30
14	Iw	36	T6A	N3-C4-N9	4.88	135.12	127.08
17	A2	1490	OMG	C2-N3-C4	4.87	120.98	112.30
17	A2	27	A2M	N3-C4-N9	4.87	135.10	127.08
17	A2	512	A2M	N3-C4-N9	4.85	135.08	127.08
17	A2	166	A2M	N3-C4-N9	4.85	135.07	127.08
17	A2	601	OMG	C2-N3-C4	4.84	120.92	112.30
17	A2	1447	OMG	C2-N3-C4	4.83	120.90	112.30
17	A2	509	OMG	C2-N3-C4	4.83	120.90	112.30
17	A2	1678	A2M	N3-C4-N9	4.82	135.03	127.08
17	A2	1031	A2M	N3-C4-N9	4.81	135.01	127.08
17	A2	1383	A2M	N3-C4-N9	4.79	134.97	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A2	159	A2M	N3-C4-N9	4.77	134.95	127.08
17	A2	1639	G7M	C2-N3-C4	4.75	120.77	112.30
17	A2	99	A2M	N3-C4-N9	4.75	134.90	127.08
17	A2	576	A2M	N3-C4-N9	4.74	134.90	127.08
17	A2	468	A2M	N3-C4-N9	4.74	134.89	127.08
14	Iw	57	1MA	C2-N3-C4	4.73	121.70	112.41
17	A2	668	A2M	N3-C4-N9	4.70	134.82	127.08
17	A2	509	OMG	N9-C4-N3	4.62	135.22	125.94
17	A2	172	OMU	C4-N3-C2	-4.60	120.51	126.58
17	A2	436	OMG	N9-C4-N3	4.59	135.16	125.94
17	A2	1326	OMU	C4-N3-C2	-4.58	120.54	126.58
17	A2	644	OMG	N9-C4-N3	4.58	135.13	125.94
14	Iw	10	2MG	N9-C4-N3	4.58	135.13	125.94
17	A2	428	OMU	C4-N3-C2	-4.57	120.55	126.58
17	A2	1328	OMG	N9-C4-N3	4.57	135.11	125.94
17	A2	354	OMU	C4-N3-C2	-4.57	120.56	126.58
17	A2	1490	OMG	N9-C4-N3	4.53	135.04	125.94
17	A2	121	OMU	C4-N3-C2	-4.53	120.60	126.58
17	A2	601	OMG	N9-C4-N3	4.52	135.02	125.94
17	A2	1447	OMG	N9-C4-N3	4.52	135.02	125.94
17	A2	683	OMG	N9-C4-N3	4.51	135.00	125.94
14	Iw	45	G7M	C5-C4-N3	-4.51	119.50	128.15
17	A2	1442	OMU	C4-N3-C2	-4.48	120.67	126.58
17	A2	1804	OMU	C4-N3-C2	-4.48	120.67	126.58
17	A2	627	OMU	C4-N3-C2	-4.47	120.68	126.58
17	A2	1288	OMU	C4-N3-C2	-4.43	120.74	126.58
17	A2	799	OMU	C4-N3-C2	-4.42	120.75	126.58
14	Iw	9	1MG	C2-N3-C4	4.42	121.91	111.98
17	A2	116	OMU	C4-N3-C2	-4.36	120.82	126.58
14	Iw	25	2MG	N9-C4-N3	4.34	134.66	125.94
14	Iw	45	G7M	CN7-N7-C8	-4.34	118.14	124.84
17	A2	1639	G7M	C5-C4-N3	-4.30	119.90	128.15
17	A2	1850	MA6	N1-C2-N3	-4.27	121.92	128.60
17	A2	121	OMU	N3-C2-N1	4.24	120.52	114.89
17	A2	354	OMU	N3-C2-N1	4.20	120.46	114.89
17	A2	1442	OMU	N3-C2-N1	4.14	120.39	114.89
17	A2	1804	OMU	N3-C2-N1	4.14	120.38	114.89
17	A2	590	A2M	C2-N3-C4	4.13	121.50	111.75
37	AT	67	NMM	NE-CZ-NH1	4.10	127.95	120.26
17	A2	1850	MA6	C2-N1-C6	4.10	121.44	111.75
17	A2	801	PSU	C4-N3-C2	-4.10	120.43	126.34
17	A2	172	OMU	N3-C2-N1	4.09	120.33	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A2	1326	OMU	N3-C2-N1	4.09	120.32	114.89
17	A2	1288	OMU	N3-C2-N1	4.08	120.31	114.89
17	A2	428	OMU	N3-C2-N1	4.08	120.30	114.89
17	A2	1347	PSU	C4-N3-C2	-4.07	120.48	126.34
17	A2	686	PSU	C4-N3-C2	-4.07	120.48	126.34
17	A2	116	OMU	N3-C2-N1	4.06	120.27	114.89
17	A2	799	OMU	N3-C2-N1	4.05	120.26	114.89
17	A2	1232	PSU	C4-N3-C2	-4.04	120.52	126.34
17	A2	1842	4AC	N4-C4-N3	4.04	120.63	113.85
17	A2	815	PSU	C4-N3-C2	-4.04	120.52	126.34
17	A2	1851	MA6	N1-C2-N3	-4.04	122.29	128.60
14	Iw	9	1MG	N9-C4-N3	4.03	134.04	125.94
17	A2	1851	MA6	C2-N1-C6	4.03	121.28	111.75
17	A2	814	PSU	C4-N3-C2	-4.03	120.54	126.34
17	A2	1445	PSU	C4-N3-C2	-4.03	120.54	126.34
17	A2	1367	PSU	C4-N3-C2	-4.01	120.56	126.34
17	A2	1639	G7M	CN7-N7-C8	-4.00	118.67	124.84
17	A2	105	PSU	C4-N3-C2	-4.00	120.58	126.34
17	A2	1056	PSU	C4-N3-C2	-3.99	120.59	126.34
17	A2	109	PSU	C4-N3-C2	-3.98	120.60	126.34
17	A2	1177	PSU	C4-N3-C2	-3.98	120.60	126.34
17	A2	651	PSU	C4-N3-C2	-3.98	120.61	126.34
17	A2	296	PSU	C4-N3-C2	-3.98	120.61	126.34
17	A2	406	PSU	C4-N3-C2	-3.98	120.61	126.34
17	A2	1136	PSU	C4-N3-C2	-3.97	120.62	126.34
17	A2	1045	PSU	C4-N3-C2	-3.97	120.62	126.34
17	A2	866	PSU	C4-N3-C2	-3.97	120.62	126.34
17	A2	1643	PSU	C4-N3-C2	-3.97	120.62	126.34
17	A2	627	OMU	N3-C2-N1	3.97	120.16	114.89
17	A2	93	PSU	C4-N3-C2	-3.96	120.63	126.34
17	A2	572	PSU	C4-N3-C2	-3.96	120.63	126.34
17	A2	966	PSU	C4-N3-C2	-3.96	120.64	126.34
17	A2	166	A2M	C2-N3-C4	3.96	121.10	111.75
17	A2	218	PSU	C4-N3-C2	-3.96	120.64	126.34
17	A2	681	PSU	C4-N3-C2	-3.96	120.64	126.34
17	A2	649	PSU	C4-N3-C2	-3.95	120.64	126.34
17	A2	1692	PSU	C4-N3-C2	-3.95	120.64	126.34
17	A2	34	PSU	C4-N3-C2	-3.95	120.65	126.34
17	A2	1004	PSU	C4-N3-C2	-3.95	120.65	126.34
17	A2	36	PSU	C4-N3-C2	-3.94	120.66	126.34
17	A2	210	PSU	C4-N3-C2	-3.94	120.67	126.34
17	A2	1174	PSU	C4-N3-C2	-3.94	120.67	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A2	99	A2M	C2'-C1'-N9	-3.93	106.91	113.53
17	A2	609	PSU	C4-N3-C2	-3.92	120.69	126.34
17	A2	1238	PSU	C4-N3-C2	-3.91	120.71	126.34
17	A2	27	A2M	C2-N3-C4	3.91	120.98	111.75
17	A2	119	PSU	C4-N3-C2	-3.91	120.71	126.34
17	A2	159	A2M	C2'-C1'-N9	-3.89	106.97	113.53
17	A2	863	PSU	C4-N3-C2	-3.89	120.74	126.34
17	A2	1031	A2M	C2-N3-C4	3.88	120.92	111.75
17	A2	1678	A2M	C2-N3-C4	3.88	120.92	111.75
17	A2	1046	PSU	C4-N3-C2	-3.88	120.75	126.34
17	A2	1244	PSU	C4-N3-C2	-3.88	120.75	126.34
17	A2	512	A2M	C2-N3-C4	3.88	120.92	111.75
14	Iw	45	G7M	C5-C6-N1	3.87	119.87	111.79
17	A2	822	PSU	C4-N3-C2	-3.86	120.78	126.34
17	A2	484	A2M	C2-N3-C4	3.85	120.85	111.75
17	A2	159	A2M	C2-N3-C4	3.85	120.85	111.75
17	A2	1383	A2M	C2-N3-C4	3.84	120.82	111.75
17	A2	1625	PSU	C4-N3-C2	-3.84	120.81	126.34
17	A2	468	A2M	C2-N3-C4	3.84	120.82	111.75
17	A2	99	A2M	C2-N3-C4	3.83	120.79	111.75
14	Iw	36	T6A	C2-N3-C4	3.82	120.77	111.75
17	A2	512	A2M	C2'-C1'-N9	-3.80	107.13	113.53
17	A2	1639	G7M	C5-C6-N1	3.79	119.71	111.79
17	A2	668	A2M	C2-N3-C4	3.79	120.71	111.75
17	A2	576	A2M	C2-N3-C4	3.78	120.69	111.75
17	A2	1832	6MZ	C2-N3-C4	3.78	120.68	111.75
14	Iw	45	G7M	N9-C8-N7	-3.78	102.87	112.21
17	A2	1639	G7M	N9-C8-N7	-3.77	102.88	112.21
17	A2	1081	PSU	C4-N3-C2	-3.74	120.95	126.34
17	A2	428	OMU	C5-C4-N3	3.66	120.32	114.84
17	A2	172	OMU	C5-C4-N3	3.65	120.31	114.84
17	A2	354	OMU	C5-C4-N3	3.64	120.29	114.84
17	A2	1326	OMU	C5-C4-N3	3.64	120.28	114.84
17	A2	822	PSU	O2-C2-N1	-3.63	118.79	122.79
17	A2	627	OMU	C5-C4-N3	3.63	120.27	114.84
14	Iw	45	G7M	C4-C5-N7	-3.62	101.75	107.67
17	A2	1056	PSU	O2-C2-N1	-3.61	118.81	122.79
17	A2	1850	MA6	C1'-N9-C8	-3.60	119.00	127.14
17	A2	1639	G7M	C4-C5-N7	-3.56	101.84	107.67
17	A2	1804	OMU	C5-C4-N3	3.56	120.17	114.84
17	A2	1643	PSU	O2-C2-N1	-3.56	118.88	122.79
17	A2	121	OMU	C5-C4-N3	3.55	120.16	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A2	1442	OMU	C5-C4-N3	3.55	120.16	114.84
17	A2	1288	OMU	C5-C4-N3	3.55	120.15	114.84
17	A2	116	OMU	C5-C4-N3	3.55	120.15	114.84
17	A2	799	OMU	C5-C4-N3	3.54	120.14	114.84
17	A2	1850	MA6	C2-N3-C4	3.53	120.09	111.75
14	Iw	57	1MA	N9-C4-N3	3.53	135.17	126.94
14	Iw	45	G7M	O6-C6-C5	-3.53	120.11	128.06
17	A2	296	PSU	O2-C2-N1	-3.51	118.93	122.79
17	A2	814	PSU	O2-C2-N1	-3.50	118.93	122.79
17	A2	1347	PSU	O2-C2-N1	-3.50	118.93	122.79
17	A2	1850	MA6	C6-C5-N7	3.50	139.16	133.28
17	A2	1445	PSU	O2-C2-N1	-3.50	118.94	122.79
17	A2	1851	MA6	C6-C5-N7	3.49	139.15	133.28
17	A2	609	PSU	O2-C2-N1	-3.49	118.95	122.79
17	A2	1851	MA6	C1'-N9-C8	-3.48	119.28	127.14
17	A2	105	PSU	O2-C2-N1	-3.46	118.98	122.79
17	A2	1238	PSU	O2-C2-N1	-3.46	118.98	122.79
17	A2	576	A2M	C2'-C1'-N9	-3.46	107.70	113.53
17	A2	863	PSU	O2-C2-N1	-3.46	118.98	122.79
17	A2	1004	PSU	O2-C2-N1	-3.45	118.99	122.79
17	A2	1046	PSU	O2-C2-N1	-3.45	118.99	122.79
17	A2	1692	PSU	O2-C2-N1	-3.45	118.99	122.79
17	A2	1174	PSU	O2-C2-N1	-3.44	119.00	122.79
17	A2	93	PSU	O2-C2-N1	-3.44	119.00	122.79
17	A2	1367	PSU	O2-C2-N1	-3.44	119.00	122.79
17	A2	99	A2M	C4-C5-N7	-3.44	106.43	110.62
17	A2	1851	MA6	C2-N3-C4	3.43	119.85	111.75
17	A2	866	PSU	O2-C2-N1	-3.42	119.02	122.79
17	A2	686	PSU	O2-C2-N1	-3.42	119.02	122.79
17	A2	218	PSU	O2-C2-N1	-3.42	119.02	122.79
17	A2	649	PSU	O2-C2-N1	-3.41	119.03	122.79
17	A2	1248	B8N	C4-N3-C2	-3.41	121.15	125.46
17	A2	406	PSU	O2-C2-N1	-3.40	119.05	122.79
17	A2	1045	PSU	O2-C2-N1	-3.40	119.05	122.79
17	A2	1232	PSU	O2-C2-N1	-3.39	119.06	122.79
17	A2	36	PSU	O2-C2-N1	-3.38	119.07	122.79
17	A2	681	PSU	O2-C2-N1	-3.37	119.08	122.79
17	A2	34	PSU	O2-C2-N1	-3.36	119.09	122.79
17	A2	210	PSU	O2-C2-N1	-3.36	119.09	122.79
14	Iw	25	2MG	C6-C5-N7	3.36	136.50	130.25
17	A2	651	PSU	O2-C2-N1	-3.36	119.09	122.79
17	A2	1244	PSU	O2-C2-N1	-3.36	119.09	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A2	109	PSU	O2-C2-N1	-3.35	119.10	122.79
17	A2	1625	PSU	O2-C2-N1	-3.35	119.11	122.79
17	A2	801	PSU	O2-C2-N1	-3.34	119.11	122.79
17	A2	966	PSU	O2-C2-N1	-3.34	119.12	122.79
17	A2	119	PSU	O2-C2-N1	-3.33	119.12	122.79
17	A2	1639	G7M	O6-C6-C5	-3.33	120.54	128.06
17	A2	159	A2M	C4-C5-N7	-3.32	106.58	110.62
17	A2	815	PSU	O2-C2-N1	-3.32	119.14	122.79
17	A2	27	A2M	C4-C5-N7	-3.32	106.58	110.62
17	A2	484	A2M	C4-C5-N7	-3.30	106.60	110.62
17	A2	166	A2M	C4-C5-N7	-3.30	106.60	110.62
17	A2	166	A2M	C2'-C1'-N9	-3.29	107.99	113.53
17	A2	468	A2M	C4-C5-N7	-3.29	106.61	110.62
17	A2	1031	A2M	C4-C5-N7	-3.28	106.62	110.62
17	A2	572	PSU	O2-C2-N1	-3.28	119.18	122.79
14	Iw	36	T6A	N6-C10-N11	3.27	118.33	113.76
17	A2	512	A2M	C4-C5-N7	-3.27	106.63	110.62
17	A2	1177	PSU	O2-C2-N1	-3.27	119.19	122.79
17	A2	576	A2M	C4-C5-N7	-3.27	106.64	110.62
17	A2	1383	A2M	C2'-C1'-N9	-3.26	108.05	113.53
17	A2	1136	PSU	O2-C2-N1	-3.25	119.21	122.79
17	A2	1383	A2M	C4-C5-N7	-3.25	106.66	110.62
17	A2	1678	A2M	C4-C5-N7	-3.25	106.67	110.62
17	A2	1678	A2M	C2'-C1'-N9	-3.23	108.09	113.53
17	A2	1081	PSU	O2-C2-N1	-3.21	119.26	122.79
17	A2	436	OMG	C6-C5-N7	3.20	136.21	130.25
17	A2	668	A2M	C4-C5-N7	-3.20	106.72	110.62
17	A2	1678	A2M	N3-C2-N1	-3.19	123.61	128.60
17	A2	166	A2M	N3-C2-N1	-3.19	123.61	128.60
17	A2	683	OMG	C6-C5-N7	3.19	136.18	130.25
14	Iw	36	T6A	C6-C5-N7	3.19	135.84	132.39
17	A2	1031	A2M	N3-C2-N1	-3.19	123.62	128.60
17	A2	590	A2M	N3-C2-N1	-3.18	123.62	128.60
14	Iw	36	T6A	C4-C5-N7	-3.18	106.74	110.62
17	A2	601	OMG	C6-C5-N7	3.16	136.12	130.25
17	A2	644	OMG	C6-C5-N7	3.15	136.12	130.25
17	A2	1447	OMG	C6-C5-N7	3.15	136.11	130.25
17	A2	159	A2M	N3-C2-N1	-3.14	123.69	128.60
17	A2	1490	OMG	C6-C5-N7	3.14	136.09	130.25
17	A2	468	A2M	N3-C2-N1	-3.14	123.69	128.60
17	A2	1328	OMG	C6-C5-N7	3.14	136.08	130.25
17	A2	428	OMU	O4-C4-C5	-3.13	119.65	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A2	1383	A2M	N3-C2-N1	-3.13	123.71	128.60
14	Iw	10	2MG	C6-C5-N7	3.13	136.07	130.25
17	A2	27	A2M	N3-C2-N1	-3.13	123.71	128.60
17	A2	512	A2M	N3-C2-N1	-3.11	123.74	128.60
17	A2	668	A2M	N3-C2-N1	-3.10	123.75	128.60
17	A2	590	A2M	C4-C5-N7	-3.10	106.84	110.62
17	A2	627	OMU	O4-C4-C5	-3.10	119.71	125.16
14	Iw	36	T6A	N3-C2-N1	-3.10	123.76	128.60
17	A2	576	A2M	N3-C2-N1	-3.09	123.76	128.60
17	A2	1248	B8N	N3-C2-N1	3.09	121.12	116.76
17	A2	509	OMG	C6-C5-N7	3.06	135.93	130.25
17	A2	1850	MA6	C4-N9-C1'	-3.04	119.36	126.59
17	A2	1326	OMU	O4-C4-C5	-3.02	119.84	125.16
17	A2	116	OMU	O4-C4-C5	-3.02	119.85	125.16
17	A2	1851	MA6	C4-N9-C1'	-3.02	119.41	126.59
17	A2	172	OMU	O4-C4-C5	-2.99	119.89	125.16
17	A2	1639	G7M	C2-N1-C6	-2.99	119.65	125.10
17	A2	1442	OMU	O4-C4-C5	-2.98	119.93	125.16
17	A2	121	OMU	O4-C4-C5	-2.97	119.94	125.16
17	A2	354	OMU	O4-C4-C5	-2.96	119.95	125.16
14	Iw	45	G7M	C2-N1-C6	-2.96	119.70	125.10
17	A2	1804	OMU	O4-C4-C5	-2.96	119.96	125.16
17	A2	799	OMU	O4-C4-C5	-2.96	119.96	125.16
17	A2	1288	OMU	O4-C4-C5	-2.96	119.96	125.16
17	A2	99	A2M	N3-C2-N1	-2.94	124.01	128.60
17	A2	27	A2M	C2'-C1'-N9	-2.93	108.59	113.53
17	A2	1337	4AC	N4-C4-N3	2.92	118.75	113.85
17	A2	1832	6MZ	N1-C2-N3	-2.87	124.11	128.60
17	A2	1850	MA6	C5-C4-N9	-2.85	102.47	105.78
17	A2	484	A2M	N3-C2-N1	-2.84	124.17	128.60
17	A2	159	A2M	C5-N7-C8	2.81	107.50	103.51
17	A2	468	A2M	C2'-C1'-N9	-2.81	108.81	113.53
17	A2	166	A2M	C5-N7-C8	2.80	107.48	103.51
17	A2	576	A2M	C5-N7-C8	2.79	107.47	103.51
17	A2	27	A2M	C5-N7-C8	2.77	107.45	103.51
17	A2	468	A2M	C5-N7-C8	2.76	107.44	103.51
17	A2	1832	6MZ	C4-C5-N7	-2.76	107.26	110.62
17	A2	1678	A2M	C5-N7-C8	2.75	107.42	103.51
17	A2	512	A2M	C5-N7-C8	2.75	107.42	103.51
17	A2	99	A2M	C5-N7-C8	2.75	107.41	103.51
17	A2	1031	A2M	C5-N7-C8	2.74	107.40	103.51
14	Iw	25	2MG	C4-C5-N7	-2.72	106.41	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A2	1383	A2M	C5-N7-C8	2.72	107.37	103.51
17	A2	668	A2M	C4-N9-C8	2.71	108.66	105.73
17	A2	590	A2M	C5-N7-C8	2.69	107.33	103.51
17	A2	576	A2M	C4-N9-C8	2.69	108.64	105.73
17	A2	668	A2M	C5-N7-C8	2.68	107.31	103.51
17	A2	1851	MA6	C5-C4-N9	-2.68	102.67	105.78
17	A2	1031	A2M	C2'-C1'-N9	-2.67	109.03	113.53
14	Iw	36	T6A	C5-N7-C8	2.67	107.30	103.51
17	A2	1678	A2M	C4-N9-C8	2.67	108.62	105.73
14	Iw	9	1MG	C6-C5-N7	2.67	135.38	129.35
14	Iw	9	1MG	C4-C5-N7	-2.65	106.53	110.72
17	A2	159	A2M	C4-N9-C8	2.65	108.59	105.73
17	A2	1447	OMG	C4-C5-N7	-2.62	106.57	110.72
14	Iw	36	T6A	C4-N9-C8	2.61	108.56	105.73
17	A2	601	OMG	C4-C5-N7	-2.61	106.59	110.72
17	A2	484	A2M	C5-N7-C8	2.60	107.20	103.51
17	A2	683	OMG	C4-C5-N7	-2.59	106.63	110.72
17	A2	436	OMG	C4-C5-N7	-2.58	106.64	110.72
17	A2	1031	A2M	C4-N9-C8	2.58	108.52	105.73
17	A2	644	OMG	C4-C5-N7	-2.58	106.64	110.72
17	A2	1490	OMG	C4-C5-N7	-2.57	106.65	110.72
17	A2	512	A2M	C4-N9-C8	2.56	108.51	105.73
17	A2	1328	OMG	C4-C5-N7	-2.56	106.66	110.72
32	AO	138	IAS	OD1-CG-CB	-2.56	117.96	125.43
17	A2	1383	A2M	C4-N9-C8	2.56	108.50	105.73
17	A2	509	OMG	C4-C5-N7	-2.55	106.68	110.72
17	A2	468	A2M	C4-N9-C8	2.54	108.48	105.73
14	Iw	10	2MG	C4-C5-N7	-2.53	106.71	110.72
39	AV	1	AME	O-C-CA	-2.52	118.18	124.78
17	A2	1337	4AC	C6-C5-C4	2.51	120.04	116.96
17	A2	27	A2M	C4-N9-C8	2.51	108.45	105.73
14	Iw	57	1MA	C4-C5-N7	-2.50	106.77	110.72
17	A2	1832	6MZ	C4-N9-C8	2.49	108.43	105.73
17	A2	166	A2M	C4-N9-C8	2.47	108.41	105.73
17	A2	1842	4AC	C6-C5-C4	2.46	119.97	116.96
17	A2	1832	6MZ	C5-N7-C8	2.44	106.97	103.51
36	AS	2	SAC	O-C-CA	-2.43	118.41	124.78
17	A2	99	A2M	C4-N9-C8	2.39	108.31	105.73
18	AA	2	SAC	O-C-CA	-2.34	118.64	124.78
17	A2	484	A2M	C4-N9-C8	2.27	108.19	105.73
14	Iw	45	G7M	C5-C4-N9	-2.26	100.93	105.89
17	A2	1272	OMC	O2-C2-N3	-2.25	118.68	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A2	590	A2M	C4-N9-C8	2.24	108.16	105.73
17	A2	1832	6MZ	C6-C5-N7	2.24	134.81	132.39
17	A2	172	OMU	O2-C2-N1	-2.24	119.81	122.79
17	A2	159	A2M	C6-C5-N7	2.22	136.16	132.02
17	A2	627	OMU	O2-C2-N1	-2.22	119.83	122.79
17	A2	1678	A2M	C6-C5-N7	2.22	136.15	132.02
17	A2	484	A2M	C2'-C1'-N9	-2.22	109.80	113.53
17	A2	468	A2M	C6-C5-N7	2.21	136.14	132.02
17	A2	1383	A2M	C6-C5-N7	2.21	136.13	132.02
41	AX	62	HY3	O-C-CA	-2.20	118.70	124.83
14	Iw	10	2MG	O6-C6-C5	-2.20	120.77	126.60
17	A2	27	A2M	C6-C5-N7	2.19	136.11	132.02
17	A2	1639	G7M	C5-C4-N9	-2.19	101.09	105.89
17	A2	166	A2M	C6-C5-N7	2.19	136.10	132.02
17	A2	99	A2M	C6-C5-N7	2.19	136.10	132.02
17	A2	576	A2M	C6-C5-N7	2.19	136.10	132.02
17	A2	668	A2M	C6-C5-N7	2.18	136.09	132.02
17	A2	1326	OMU	O2-C2-N1	-2.18	119.89	122.79
17	A2	1031	A2M	C6-C5-N7	2.18	136.09	132.02
17	A2	436	OMG	O6-C6-C5	-2.18	120.81	126.60
14	Iw	47	5MC	C1'-N1-C6	-2.18	117.50	121.12
17	A2	644	OMG	O6-C6-C5	-2.18	120.83	126.60
17	A2	428	OMU	O2-C2-N1	-2.17	119.90	122.79
17	A2	1447	OMG	O6-C6-C5	-2.15	120.91	126.60
17	A2	121	OMU	O2-C2-N1	-2.14	119.94	122.79
17	A2	512	A2M	C6-C5-N7	2.14	136.01	132.02
17	A2	1328	OMG	O6-C6-C5	-2.14	120.93	126.60
17	A2	1832	6MZ	C9-N6-C6	-2.14	121.03	122.87
17	A2	509	OMG	O6-C6-C5	-2.14	120.94	126.60
17	A2	576	A2M	N9-C8-N7	-2.13	111.00	113.91
17	A2	159	A2M	N9-C8-N7	-2.12	111.01	113.91
17	A2	1851	MA6	C5-N7-C8	2.12	106.52	103.51
17	A2	1248	B8N	C5-C4-N3	2.12	120.09	116.17
17	A2	801	PSU	C5-C6-N1	-2.12	118.94	122.11
17	A2	1490	OMG	O6-C6-C5	-2.11	121.01	126.60
17	A2	822	PSU	O4'-C1'-C2'	2.11	108.11	105.14
17	A2	668	A2M	N9-C8-N7	-2.10	111.05	113.91
17	A2	601	OMG	O6-C6-C5	-2.09	121.05	126.60
17	A2	683	OMG	O6-C6-C5	-2.09	121.06	126.60
17	A2	1678	A2M	N9-C8-N7	-2.08	111.06	113.91
14	Iw	25	2MG	O6-C6-C5	-2.08	121.08	126.60
17	A2	1850	MA6	C5-N7-C8	2.08	106.46	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A2	1703	OMC	O2-C2-N3	-2.07	118.96	122.33
17	A2	166	A2M	N9-C8-N7	-2.06	111.10	113.91
17	A2	468	A2M	N9-C8-N7	-2.05	111.11	113.91
17	A2	1347	PSU	C5-C6-N1	-2.04	119.04	122.11
17	A2	1445	PSU	C5-C6-N1	-2.04	119.05	122.11
17	A2	512	A2M	N9-C8-N7	-2.04	111.12	113.91
17	A2	1031	A2M	N9-C8-N7	-2.03	111.14	113.91
14	Iw	45	G7M	C8-N9-C4	2.03	112.28	107.16
14	Iw	25	2MG	C2-N1-C6	-2.02	122.16	124.48
17	A2	1367	PSU	C5-C6-N1	-2.02	119.08	122.11
17	A2	1232	PSU	C5-C6-N1	-2.01	119.09	122.11

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
37	AT	67	NMM	O-C-CA-CB
14	Iw	9	1MG	O4'-C4'-C5'-O5'
14	Iw	36	T6A	O10-C10-N6-C6
14	Iw	36	T6A	N11-C10-N6-C6
14	Iw	36	T6A	N6-C10-N11-C12
17	A2	512	A2M	O4'-C4'-C5'-O5'
17	A2	627	OMU	C1'-C2'-O2'-CM2
17	A2	644	OMG	O4'-C4'-C5'-O5'
17	A2	644	OMG	C3'-C4'-C5'-O5'
17	A2	799	OMU	C3'-C4'-C5'-O5'
17	A2	1248	B8N	N34-C33-C34-O35
17	A2	1337	4AC	O7-C7-N4-C4
17	A2	1337	4AC	CM7-C7-N4-C4
17	A2	1447	OMG	C3'-C4'-C5'-O5'
17	A2	1842	4AC	N3-C4-N4-C7
17	A2	1842	4AC	C5-C4-N4-C7
14	Iw	36	T6A	O10-C10-N11-C12
17	A2	428	OMU	C2'-C1'-N1-C6
17	A2	512	A2M	C3'-C4'-C5'-O5'
17	A2	668	A2M	O4'-C4'-C5'-O5'
17	A2	668	A2M	C3'-C4'-C5'-O5'
17	A2	1625	PSU	C3'-C4'-C5'-O5'
39	AV	1	AME	CT2-CT1-N-CA
39	AV	1	AME	OT-CT1-N-CA
14	Iw	9	1MG	C3'-C4'-C5'-O5'
17	A2	99	A2M	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
17	A2	1625	PSU	O4'-C4'-C5'-O5'
17	A2	1248	B8N	N34-C33-C34-O36
17	A2	428	OMU	C2'-C1'-N1-C2
17	A2	799	OMU	C4'-C5'-O5'-P
14	Iw	47	5MC	C3'-C4'-C5'-O5'
17	A2	576	A2M	C3'-C4'-C5'-O5'
17	A2	799	OMU	O4'-C4'-C5'-O5'
14	Iw	47	5MC	O4'-C4'-C5'-O5'
17	A2	1447	OMG	O4'-C4'-C5'-O5'
17	A2	576	A2M	O4'-C4'-C5'-O5'
17	A2	683	OMG	O4'-C4'-C5'-O5'
17	A2	1842	4AC	O7-C7-N4-C4
17	A2	1248	B8N	C32-C33-C34-O36
17	A2	428	OMU	O4'-C1'-N1-C6
17	A2	644	OMG	C4'-C5'-O5'-P
17	A2	590	A2M	C2'-C1'-N9-C4
18	AA	2	SAC	C-CA-N-C1A
18	AA	2	SAC	CB-CA-N-C1A
17	A2	1248	B8N	C32-C33-C34-O35
17	A2	428	OMU	O4'-C1'-N1-C2
17	A2	354	OMU	C3'-C2'-O2'-CM2
17	A2	436	OMG	C3'-C2'-O2'-CM2
17	A2	797	OMC	C3'-C2'-O2'-CM2
17	A2	1288	OMU	C3'-C2'-O2'-CM2
17	A2	1328	OMG	C3'-C2'-O2'-CM2
17	A2	1442	OMU	C3'-C2'-O2'-CM2
14	Iw	47	5MC	C4'-C5'-O5'-P
17	A2	509	OMG	O4'-C4'-C5'-O5'
17	A2	590	A2M	C2'-C1'-N9-C8
17	A2	683	OMG	C3'-C2'-O2'-CM2
17	A2	1031	A2M	C3'-C2'-O2'-CM'
17	A2	1851	MA6	C4'-C5'-O5'-P
17	A2	116	OMU	C3'-C2'-O2'-CM2
17	A2	644	OMG	C3'-C2'-O2'-CM2
32	AO	138	IAS	O-C-CA-N
14	Iw	9	1MG	C2'-C1'-N9-C8
17	A2	1851	MA6	C3'-C4'-C5'-O5'
17	A2	1842	4AC	CM7-C7-N4-C4
17	A2	590	A2M	O4'-C1'-N9-C8
17	A2	99	A2M	C3'-C4'-C5'-O5'
17	A2	683	OMG	C3'-C4'-C5'-O5'
17	A2	468	A2M	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
14	Iw	46	H2U	O4'-C1'-N1-C6
17	A2	1703	OMC	O4'-C4'-C5'-O5'
32	AO	138	IAS	CA-CB-CG-OD1
17	A2	512	A2M	C3'-C2'-O2'-CM'
17	A2	159	A2M	O4'-C4'-C5'-O5'
17	A2	668	A2M	C2'-C1'-N9-C8

There are no ring outliers.

32 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A2	1445	PSU	1	0
17	A2	799	OMU	1	0
17	A2	576	A2M	1	0
14	Iw	47	5MC	1	0
17	A2	1288	OMU	1	0
17	A2	1272	OMC	1	0
17	A2	1383	A2M	1	0
17	A2	462	OMC	1	0
17	A2	1490	OMG	1	0
17	A2	1639	G7M	1	0
17	A2	116	OMU	1	0
17	A2	1232	PSU	1	0
17	A2	1447	OMG	2	0
17	A2	1804	OMU	2	0
17	A2	210	PSU	1	0
17	A2	1842	4AC	2	0
17	A2	1337	4AC	1	0
17	A2	166	A2M	3	0
17	A2	1391	OMC	1	0
14	Iw	57	1MA	2	0
17	A2	1328	OMG	1	0
17	A2	484	A2M	1	0
17	A2	512	A2M	1	0
17	A2	436	OMG	2	0
17	A2	601	OMG	1	0
17	A2	1442	OMU	1	0
39	AV	1	AME	1	0
17	A2	797	OMC	1	0
17	A2	681	PSU	1	0
17	A2	1031	A2M	2	0
17	A2	1703	OMC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A2	468	A2M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 251 ligands modelled in this entry, 120 are monoatomic and 129 are unknown - 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	$\# Z > 2$
56	MET	Iw	101	14	6,7,8	0.48	0	2,7,9	0.24	0
54	GTP	It	1000	55	30,34,34	0.52	0	46,54,54	0.60	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
56	MET	Iw	101	14	-	0/5/6/8	-
54	GTP	It	1000	55	-	0/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	Iw	101	MET	1	0
54	It	1000	GTP	3	0

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.

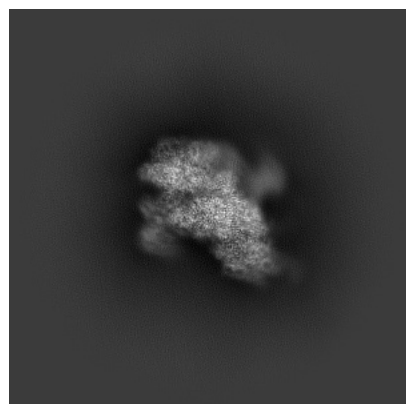
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17805. These allow visual inspection of the internal detail of the map and identification of artifacts.

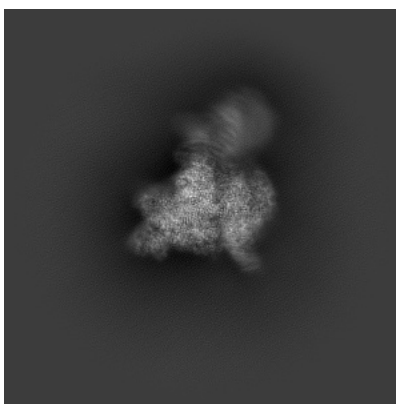
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

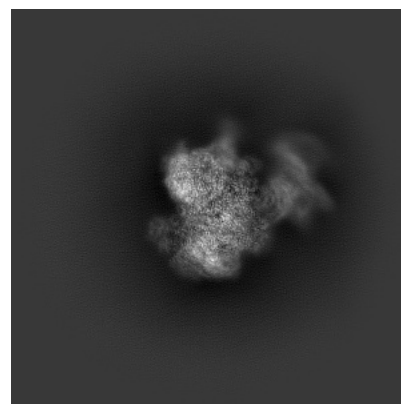
6.1.1 Primary map



X

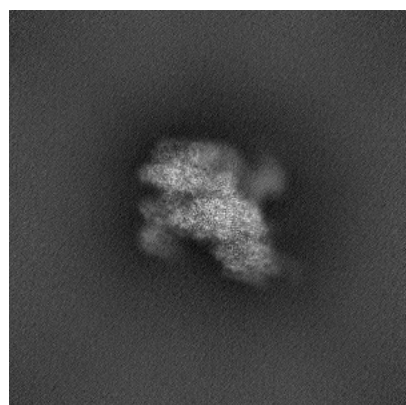


Y

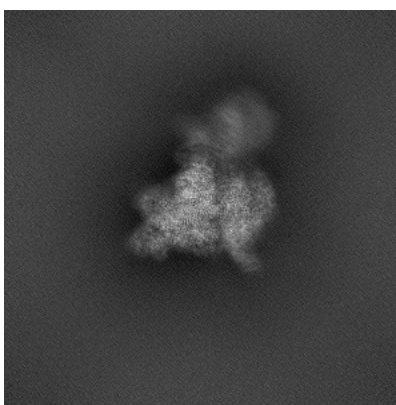


Z

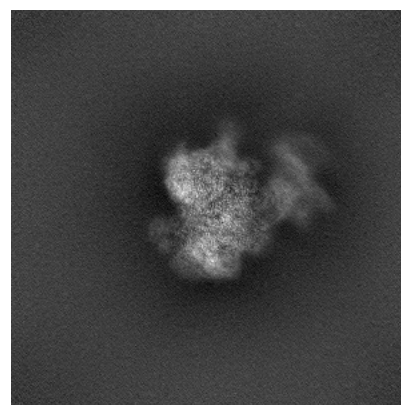
6.1.2 Raw map



X



Y

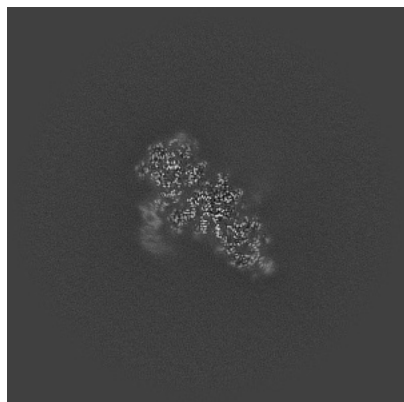


Z

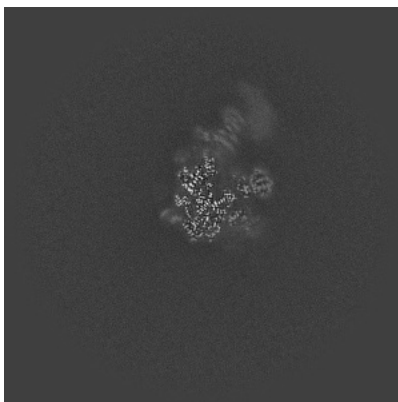
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

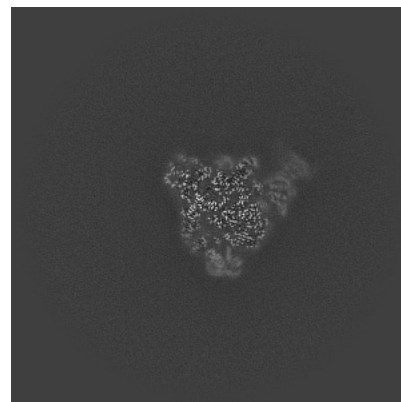
6.2.1 Primary map



X Index: 280



Y Index: 280

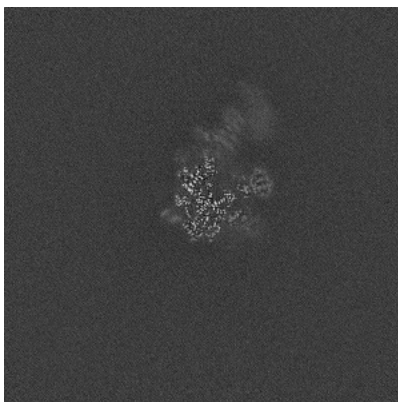


Z Index: 280

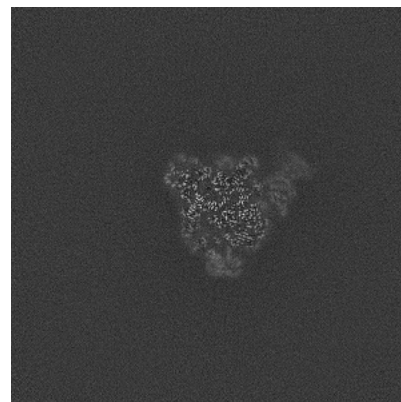
6.2.2 Raw map



X Index: 280



Y Index: 280

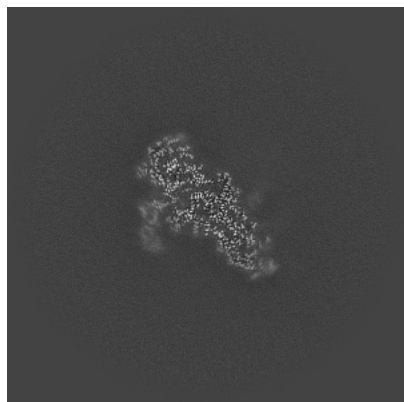


Z Index: 280

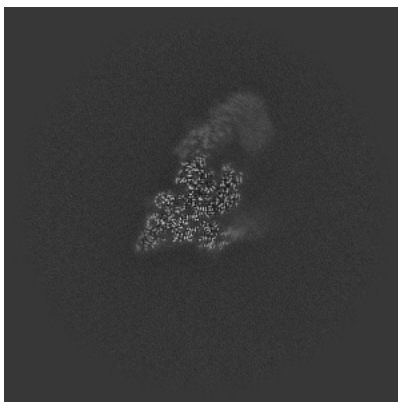
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

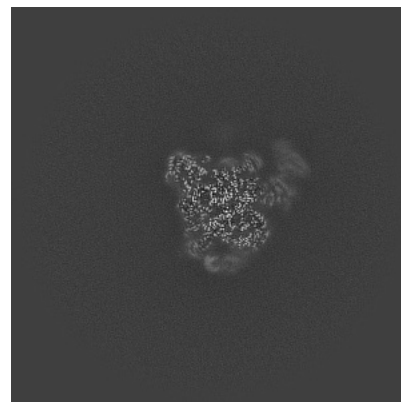
6.3.1 Primary map



X Index: 284

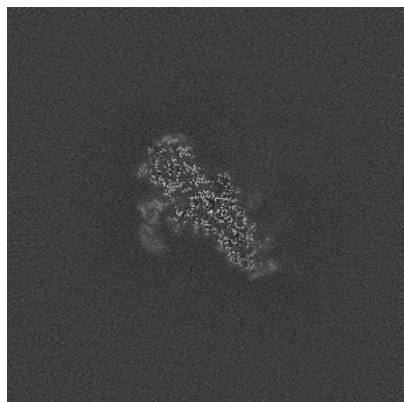


Y Index: 308

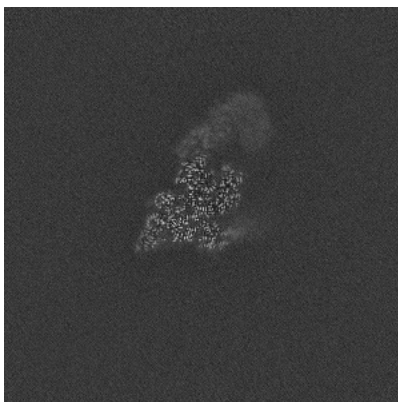


Z Index: 268

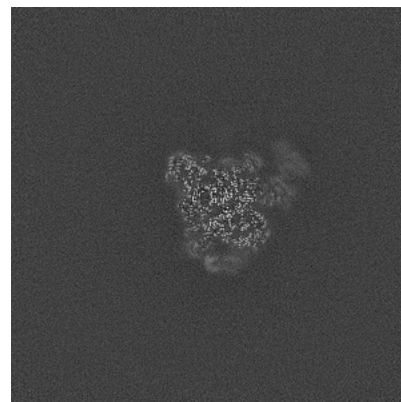
6.3.2 Raw map



X Index: 285



Y Index: 308

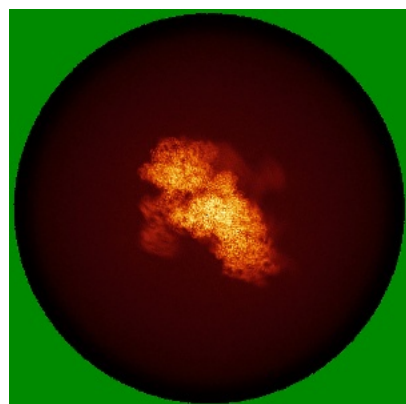


Z Index: 268

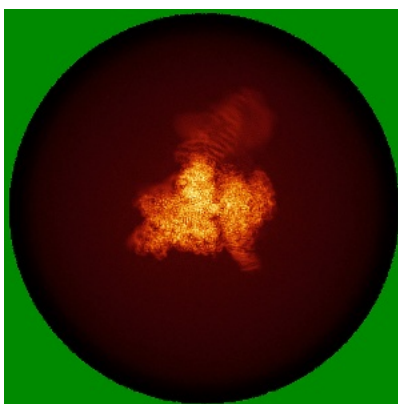
The images above show the largest variance slices of the map in three orthogonal directions.

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

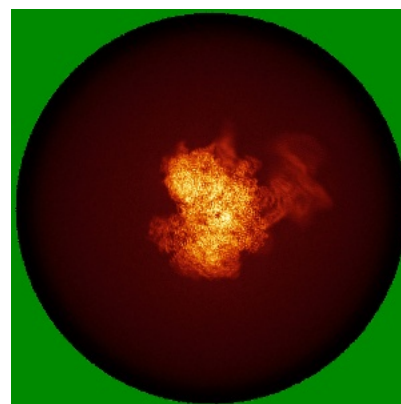
6.4.1 Primary map



X

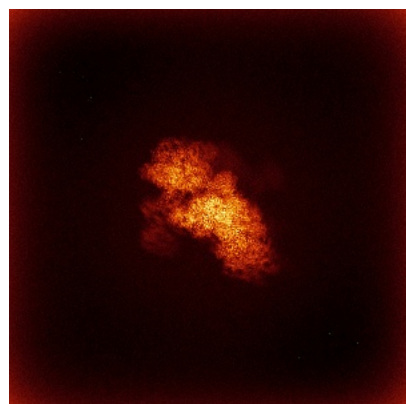


Y

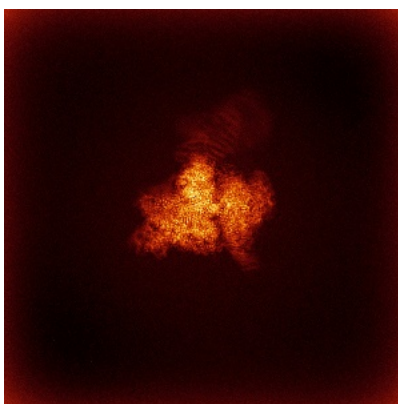


Z

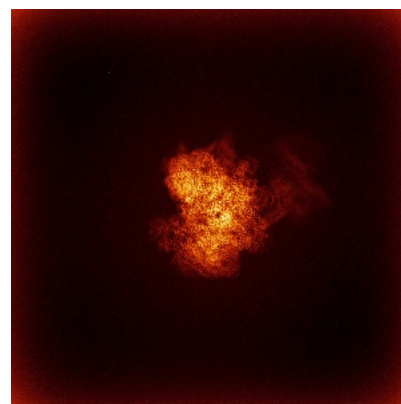
6.4.2 Raw map



X



Y

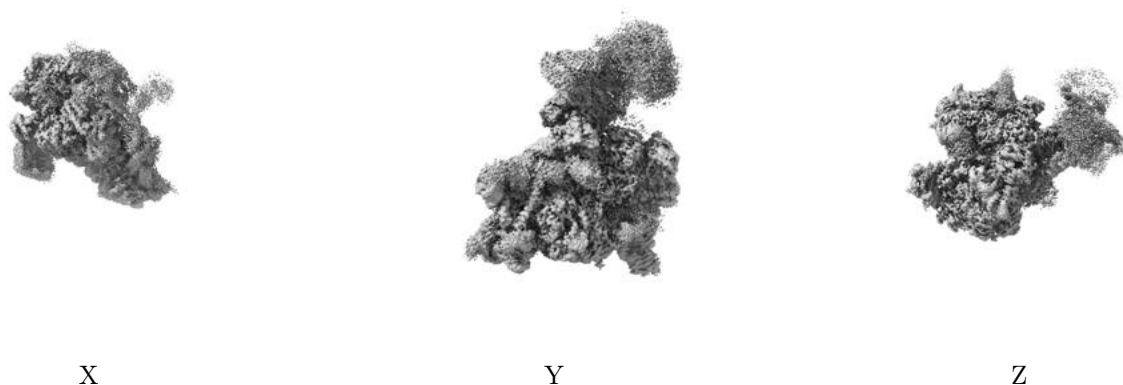


Z

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

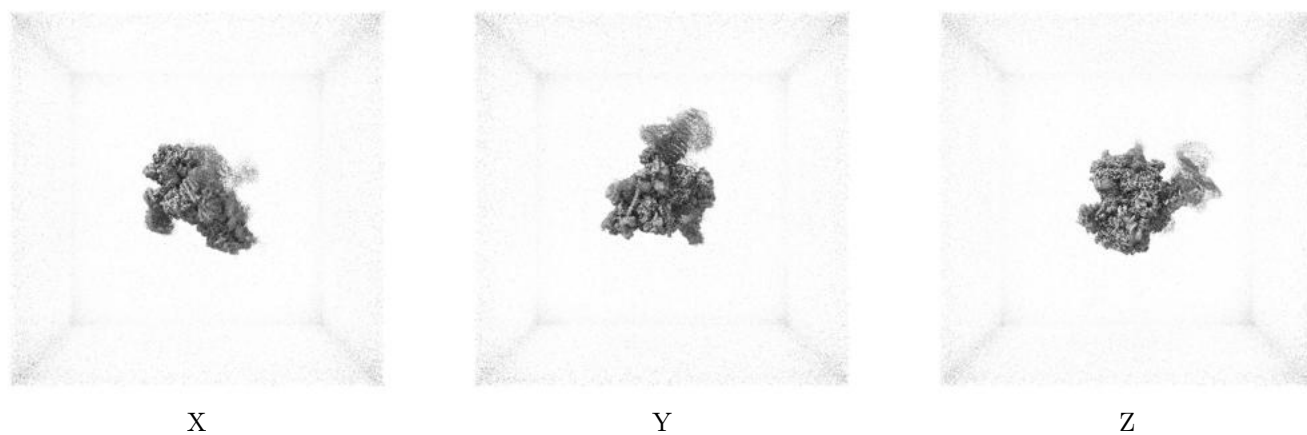
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

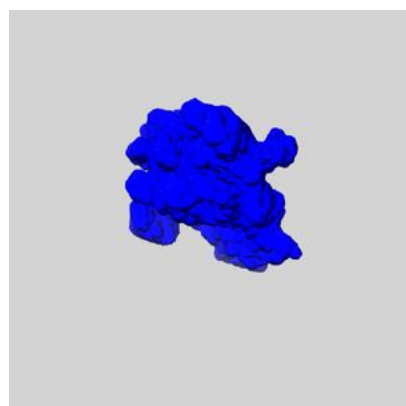
6.6 Mask visualisation [i](#)

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

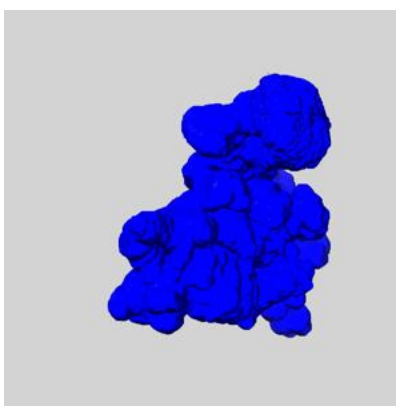
A mask typically either:

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

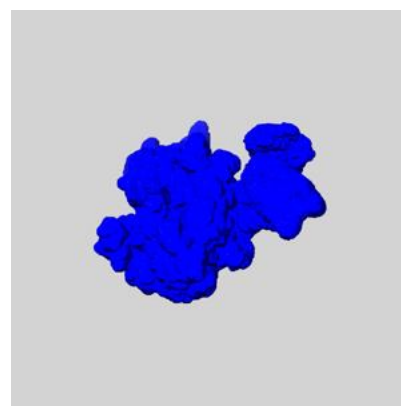
6.6.1 emd_17805_msk_1.map [i](#)



X

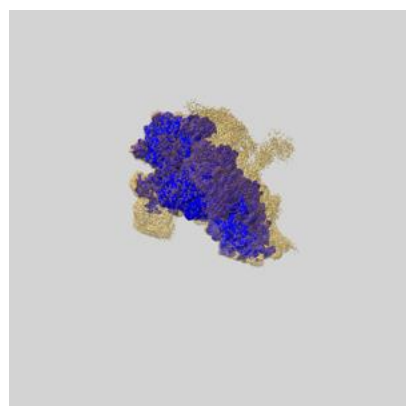


Y

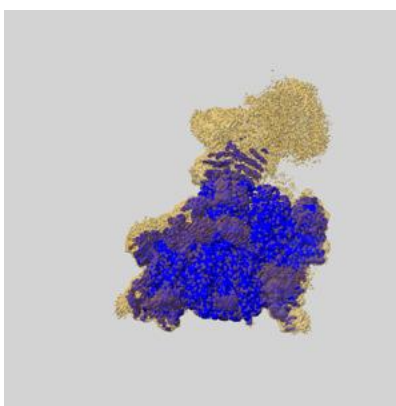


Z

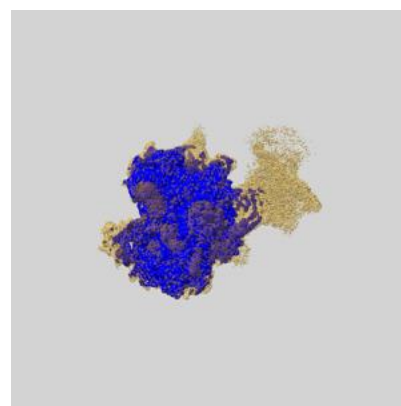
6.6.2 emd_17805_msk_2.map [i](#)



X



Y

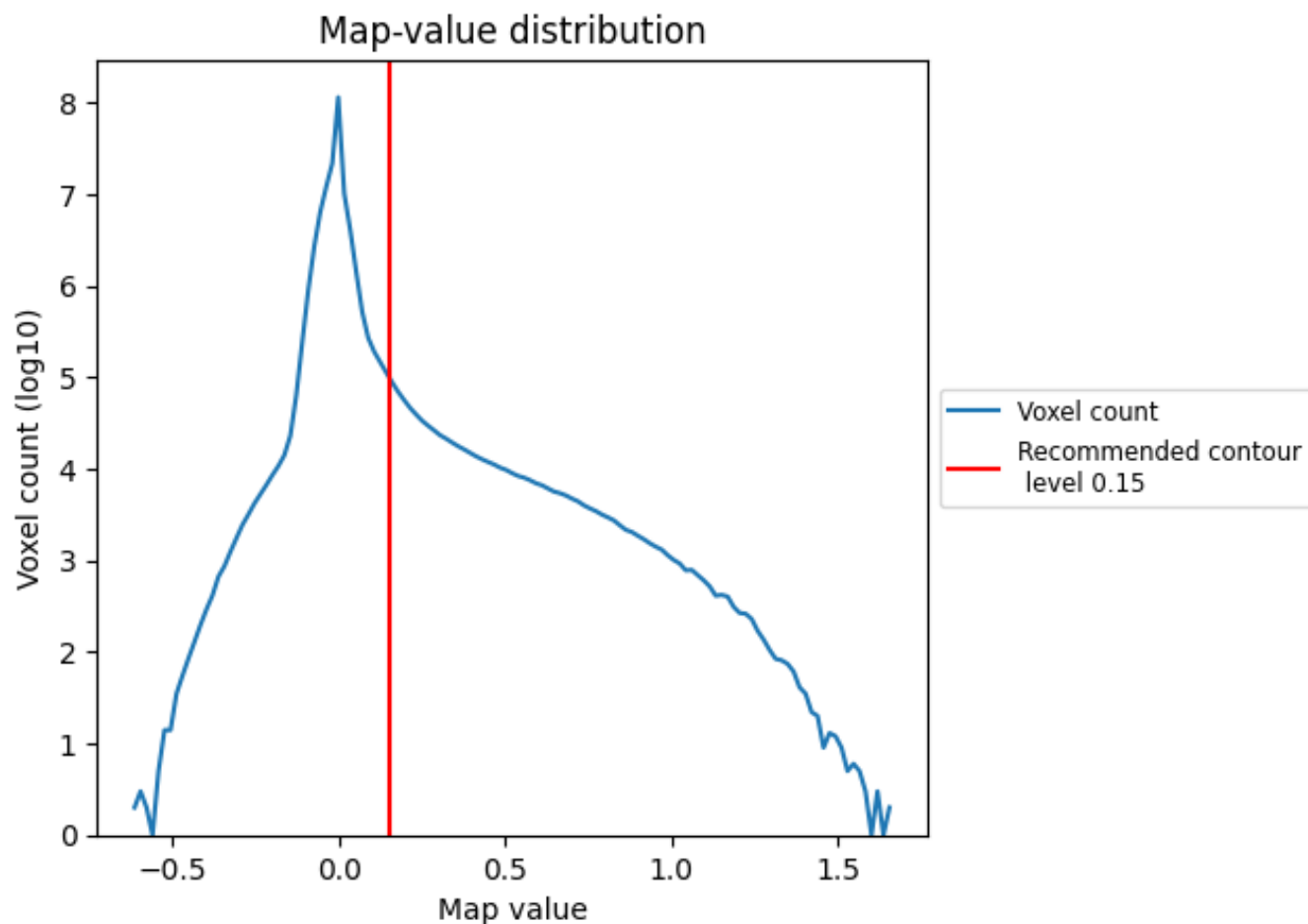


Z

7 Map analysis [i](#)

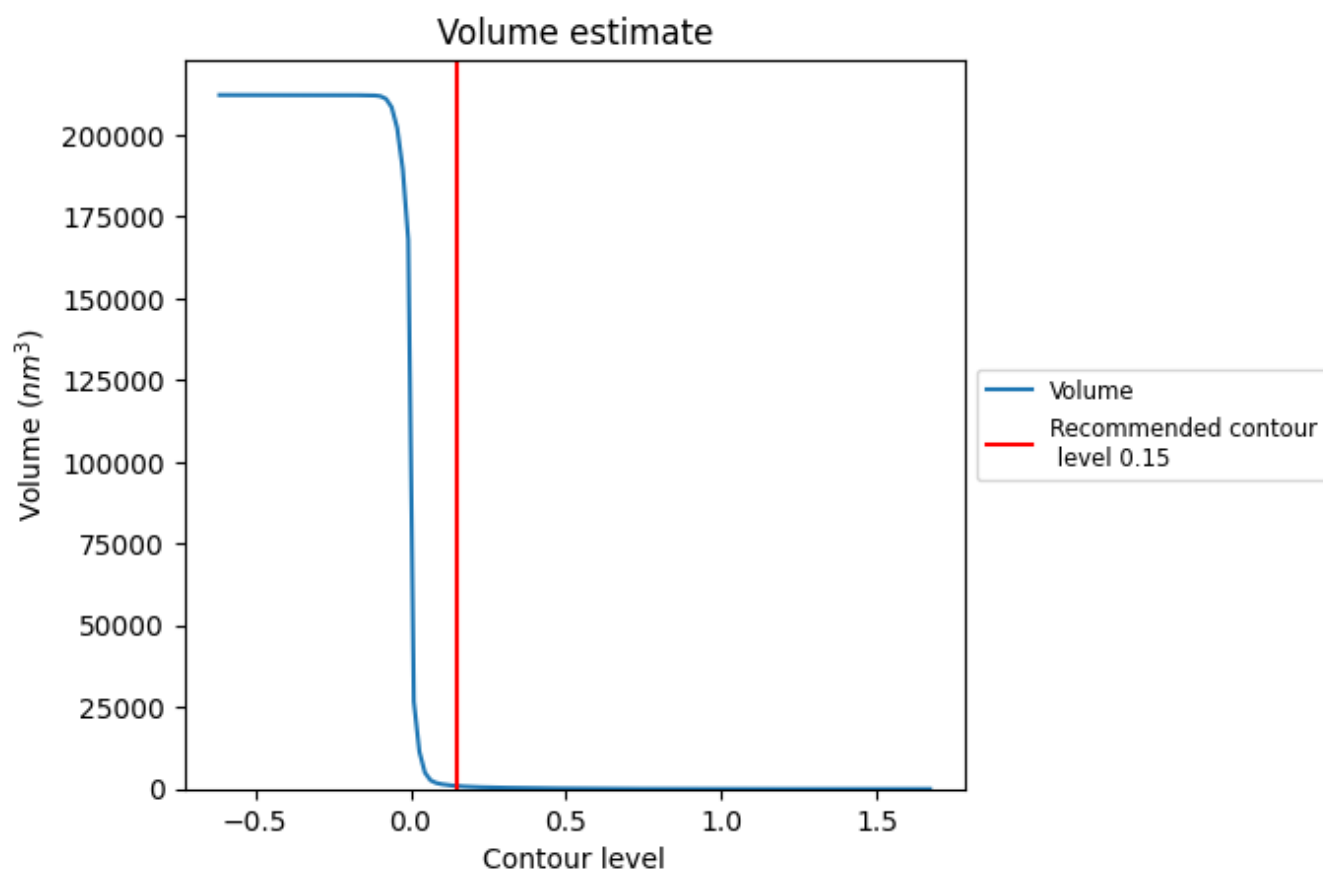
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

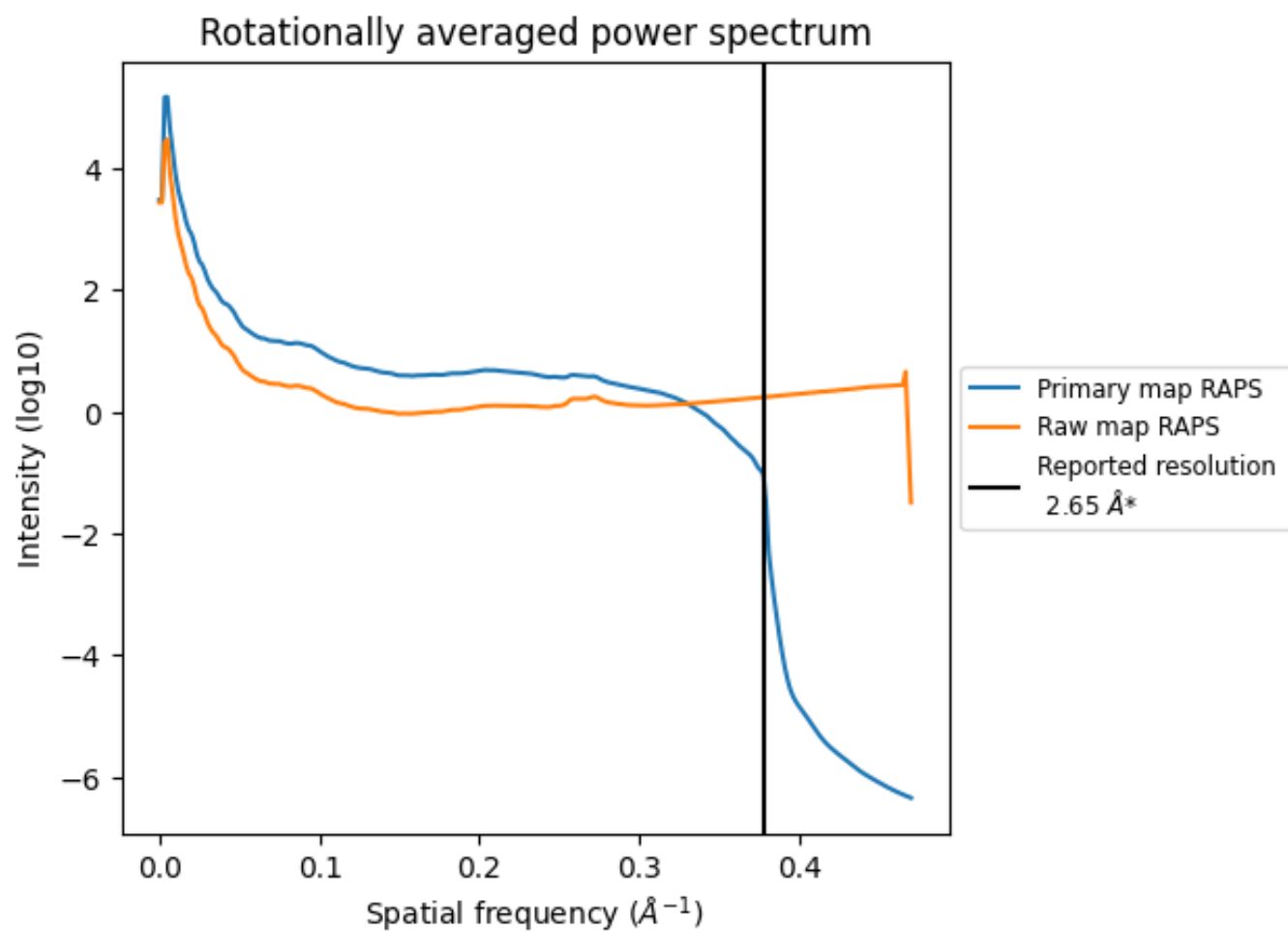
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 907 nm^3 ; this corresponds to an approximate mass of 819 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

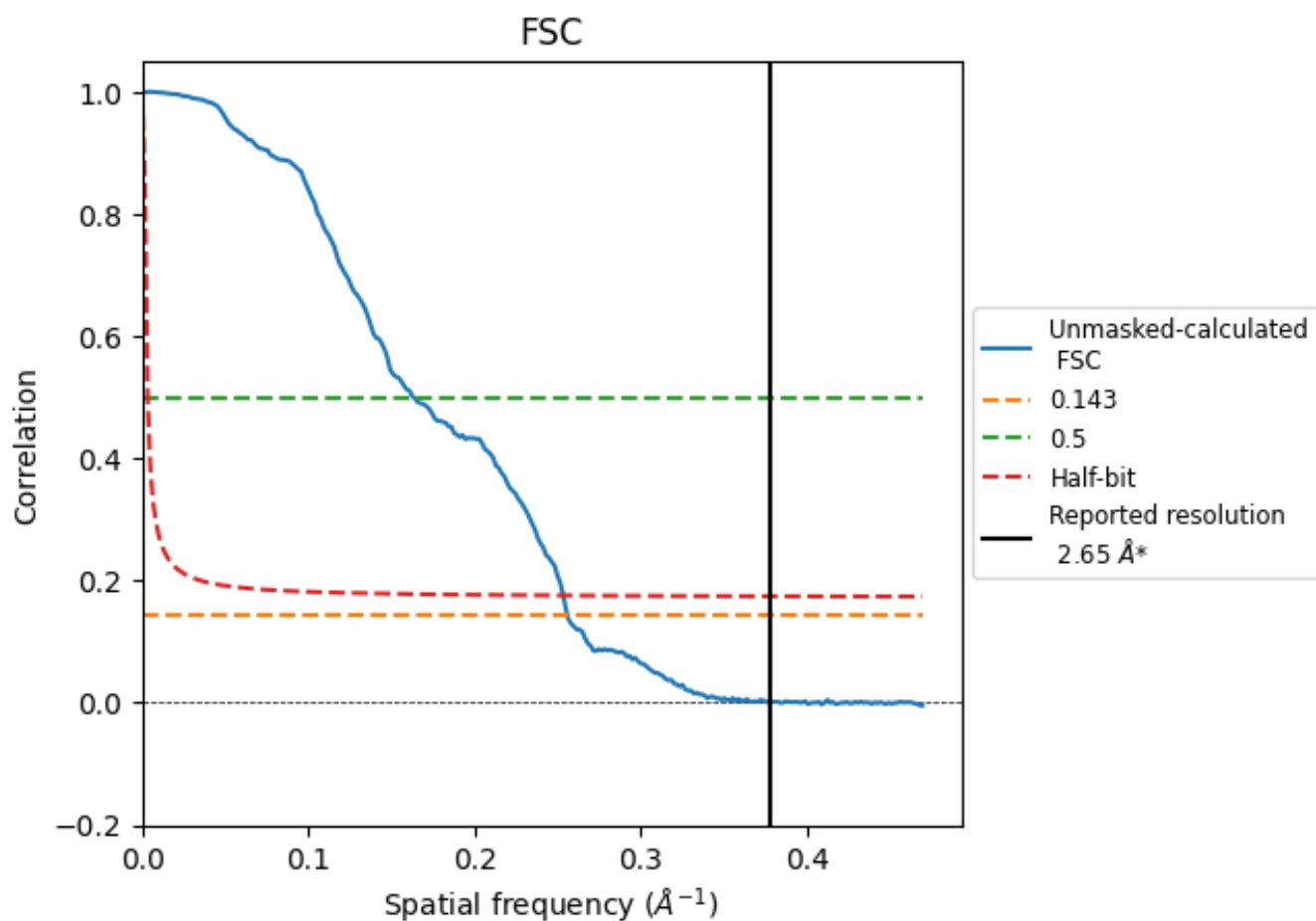


*Reported resolution corresponds to spatial frequency of $0.377 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.377 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

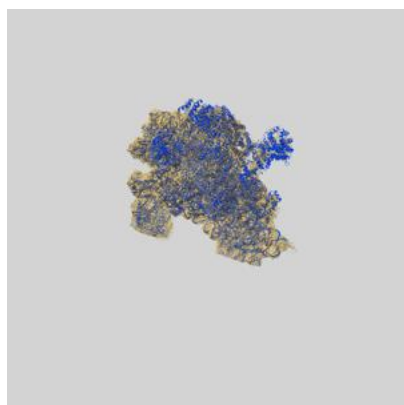
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.65	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.91	6.12	3.95

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.91 differs from the reported value 2.65 by more than 10 %

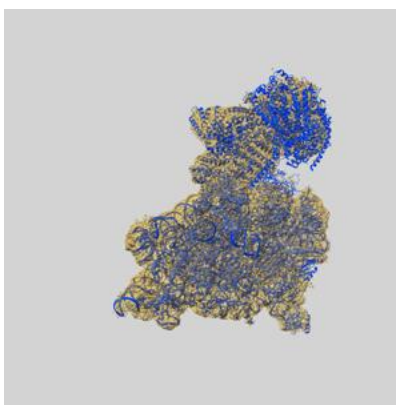
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17805 and PDB model 8PPL. Per-residue inclusion information can be found in section [3](#) on page [16](#).

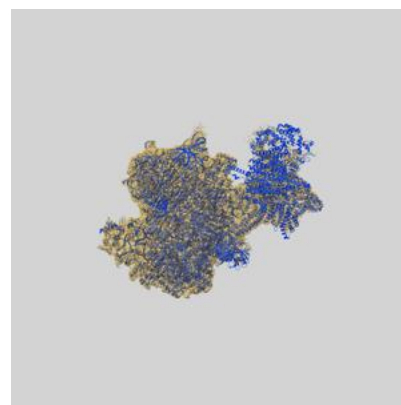
9.1 Map-model overlay [i](#)



X



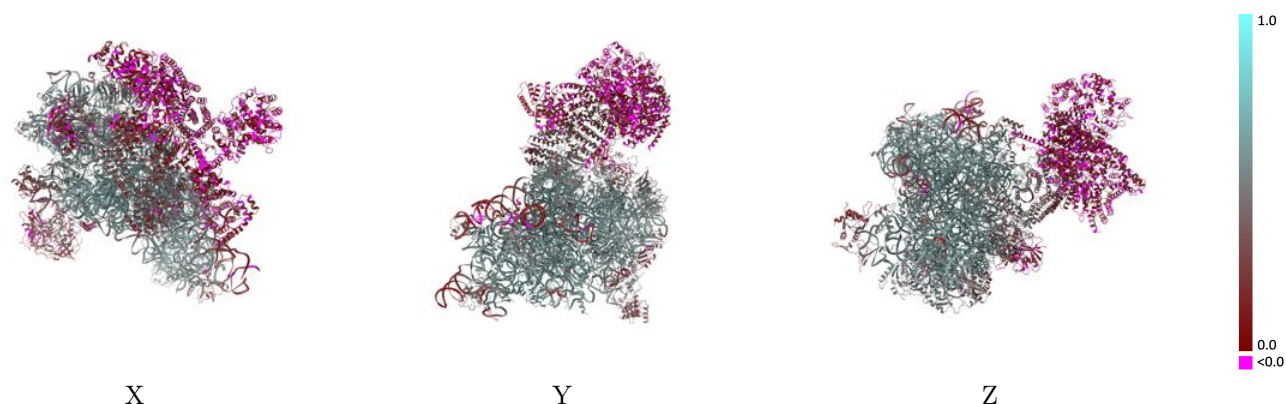
Y



Z

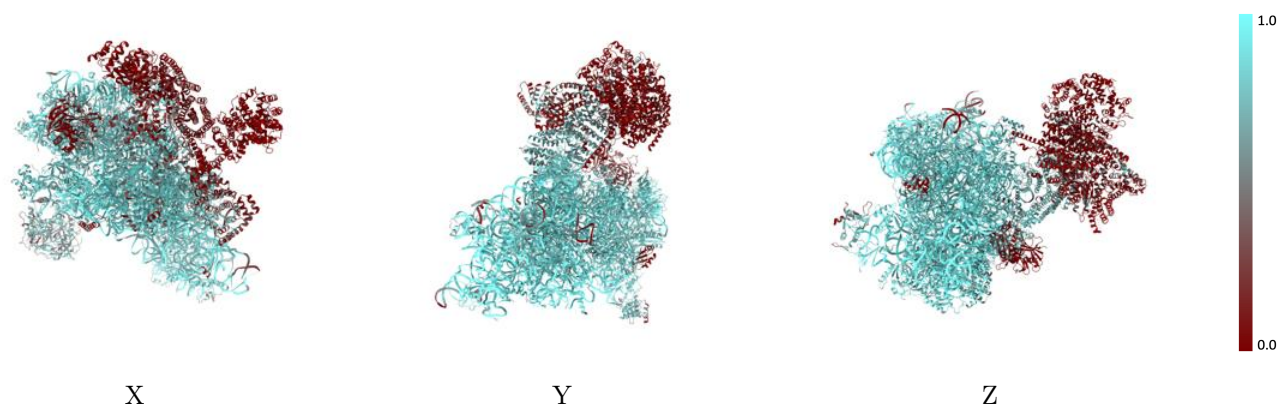
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



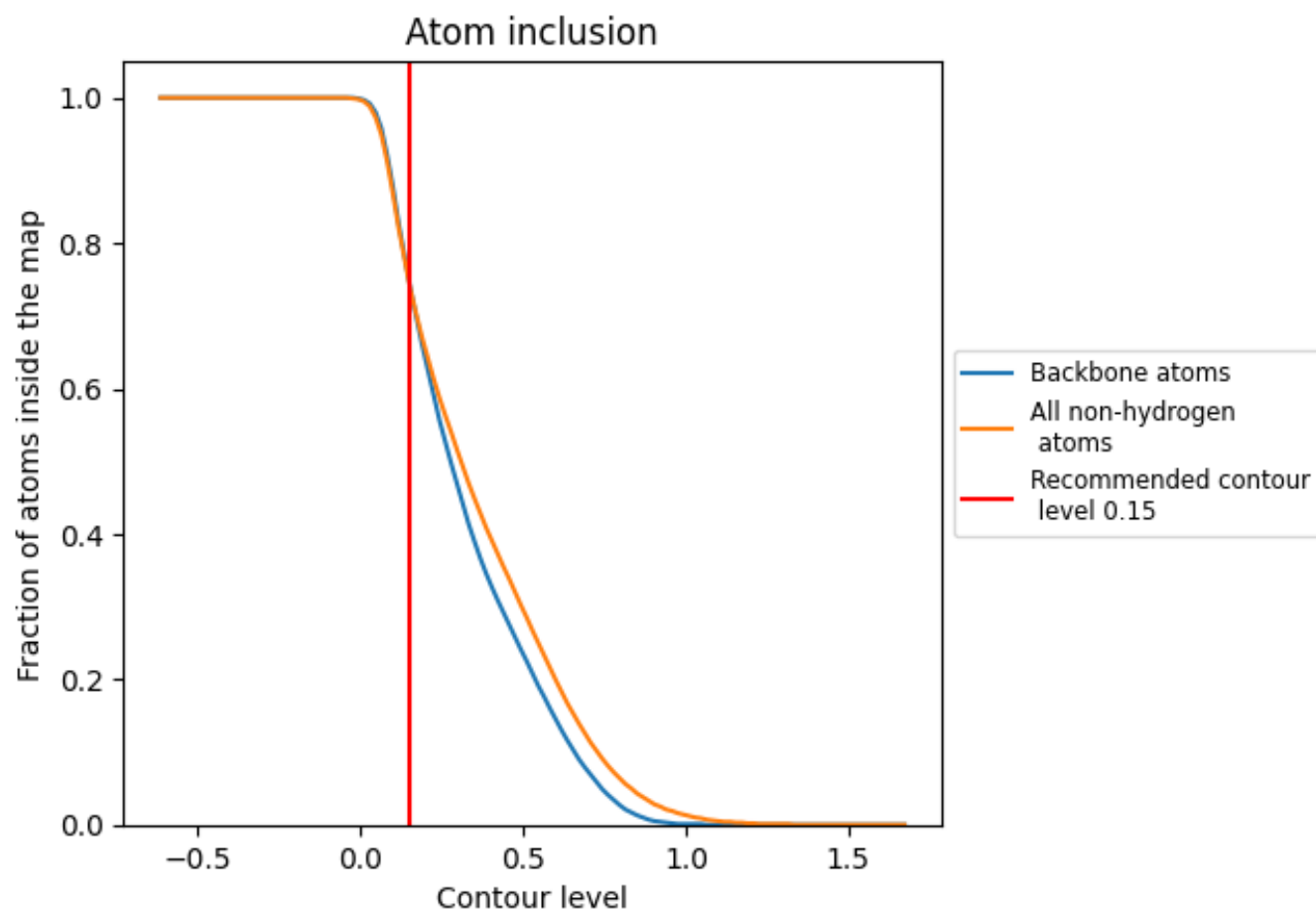
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7430	 0.4270
A2	 0.9630	 0.5460
AA	 0.9230	 0.5740
AB	 0.9150	 0.5600
AC	 0.9640	 0.6080
AD	 0.9120	 0.5440
AE	 0.9600	 0.5900
AF	 0.9290	 0.5620
AG	 0.8860	 0.4830
AH	 0.8370	 0.4640
AI	 0.9140	 0.5340
AJ	 0.9470	 0.5870
AK	 0.9110	 0.5070
AL	 0.9080	 0.5640
AM	 0.6040	 0.2490
AN	 0.9470	 0.5800
AO	 0.9260	 0.5730
AP	 0.8760	 0.5200
AQ	 0.9620	 0.5850
AR	 0.9020	 0.5520
AS	 0.9170	 0.5350
AT	 0.9310	 0.5730
AU	 0.8890	 0.5310
AV	 0.9380	 0.5870
AW	 0.9770	 0.6210
AX	 0.9600	 0.6050
AY	 0.9480	 0.5710
AZ	 0.8720	 0.5110
Aa	 0.9460	 0.5900
Ab	 0.9170	 0.5590
Ac	 0.8310	 0.5210
Ad	 0.9550	 0.5900
Ae	 0.9110	 0.5580
Af	 0.7220	 0.3300
Ag	 0.8790	 0.4820



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Chain	Atom inclusion	Q-score
Ah	 0.8300	 0.5380
Aj	 0.9070	 0.5640
I3	 0.0100	 0.0450
I4	 0.0660	 0.0650
I5	 0.0280	 0.0790
I6	 0.1460	 0.1010
I8	 0.0440	 0.0650
Io	 0.1820	 0.2490
Ip	 0.8560	 0.5060
Iq	 0.8010	 0.5260
Ir	 0.6910	 0.2930
Is	 0.8090	 0.4270
It	 0.6150	 0.1920
Iu	 0.5100	 0.2280
Iv	 0.2250	 0.1000
Iw	 0.9840	 0.4350
Ix	 0.1410	 0.2120
Iy	 0.5820	 0.2770