



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:32 PM GMT

PDB ID : 4KJC
Title : Control of ribosomal subunit rotation by elongation factor G
Authors : Pulk, A.; Cate, J.H.D.
Deposited on : 2013-05-03
Resolution : 2.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

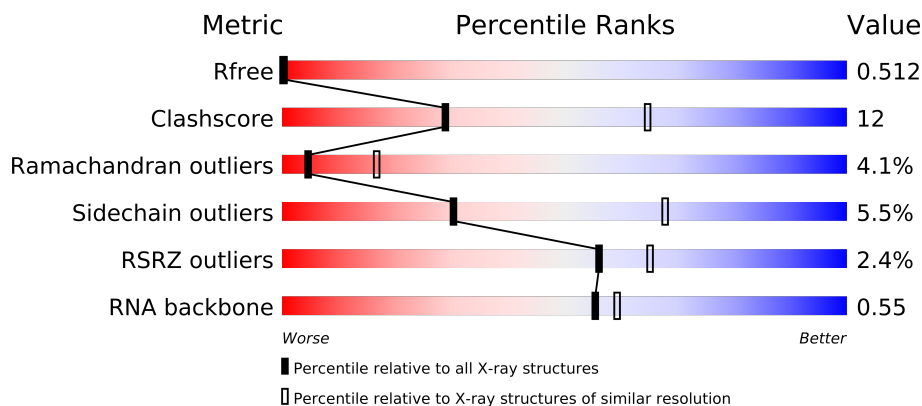
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.90 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.












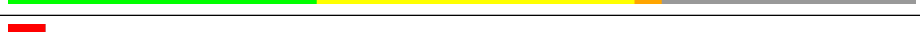

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)
RNA backbone	1838	1055 (3.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1542	
2	B	241	
3	C	233	
4	D	206	
5	E	167	
6	F	135	
7	G	179	
8	H	130	
9	I	130	
10	J	103	
11	K	129	

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Mol	Chain	Length	Quality of chain
12	L	124	
13	M	118	
14	N	101	
15	O	89	
16	P	82	
17	Q	84	
18	R	75	
19	S	92	
20	T	87	
21	U	71	
22	V	704	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
23	MG	A	1601	-	X
23	MG	A	1604	-	X
23	MG	A	1605	-	X
23	MG	A	1609	-	X
23	MG	A	1613	-	X
23	MG	A	1621	-	X
23	MG	A	1633	-	X
23	MG	A	1634	-	X
23	MG	T	101	-	X

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 57042 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1533	Total	C	N	O	P	0	0	0
			32895	14671	6036	10655	1533			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	55	Total	C	N	O	0	0	0
			455	288	86	81			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	U	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			

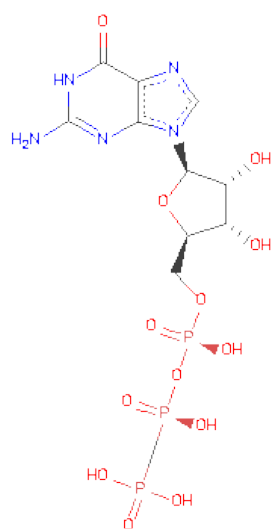
- Molecule 22 is a protein called elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	689	Total	C	N	O	S	0	0	0
			5319	3345	919	1030	25			

- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	40	Total	Mg	0	0
			40	40		
23	T	1	Total	Mg	0	0
			1	1		
23	C	1	Total	Mg	0	0
			1	1		
23	V	1	Total	Mg	0	0
			1	1		
23	E	1	Total	Mg	0	0
			1	1		

- Molecule 24 is PHOSPHOMETHYLPHOSPHONICACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	V	1	Total	C	N	O	P	0	0
			32	11	5	13	3		

- Molecule 25 is water.

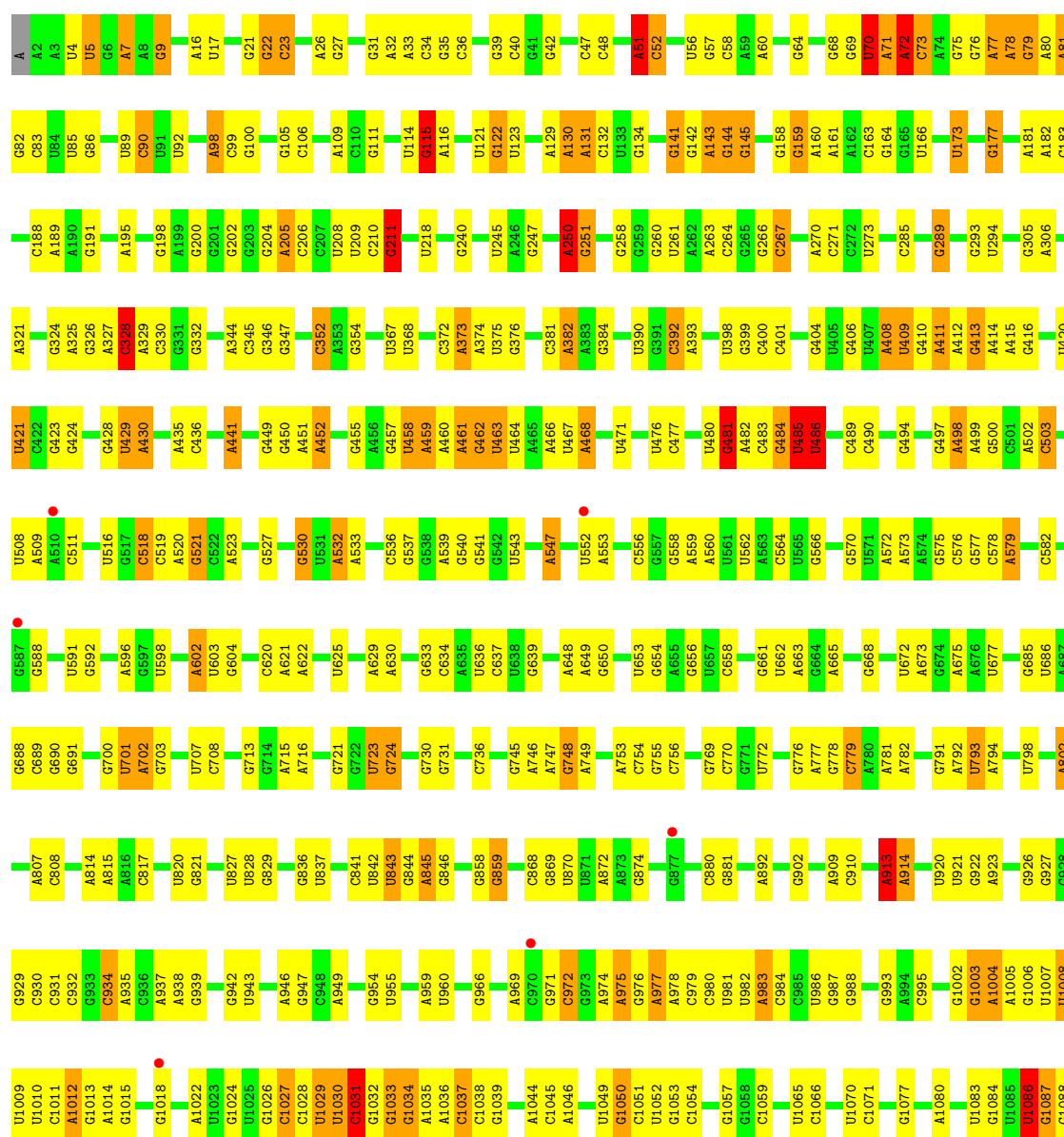
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	198	Total	O	0	0
			198	198		
25	D	1	Total	O	0	0
			1	1		
25	E	2	Total	O	0	0
			2	2		
25	N	5	Total	O	0	0
			5	5		
25	T	1	Total	O	0	0
			1	1		
25	U	1	Total	O	0	0
			1	1		
25	V	1	Total	O	0	0
			1	1		

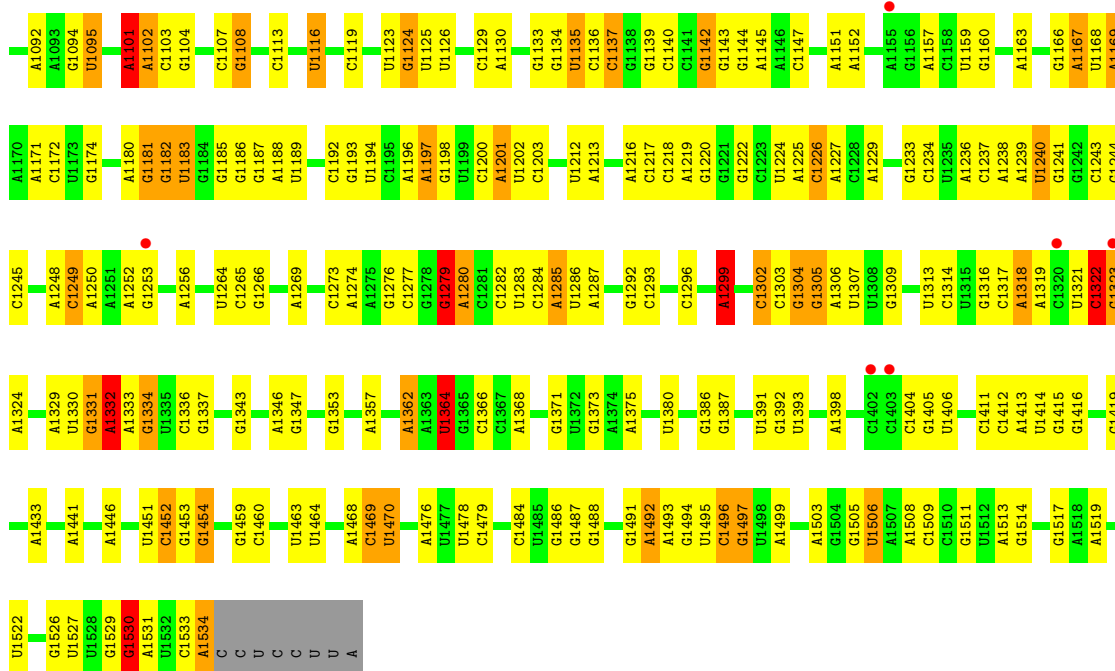
3 Residue-property plots

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

• Molecule 1: 16S rRNA

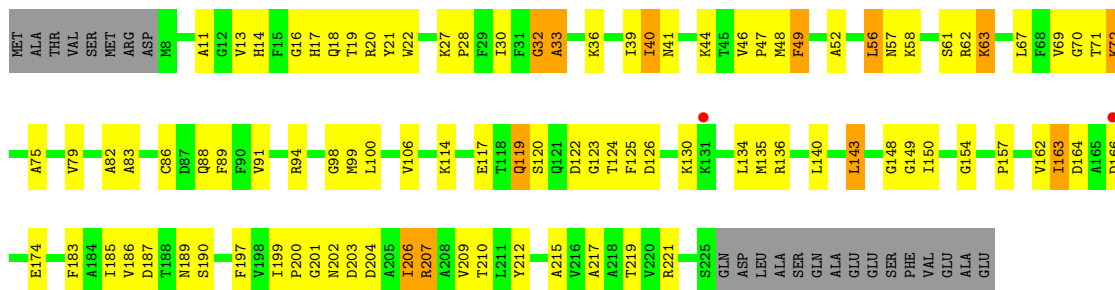
Chain A: 





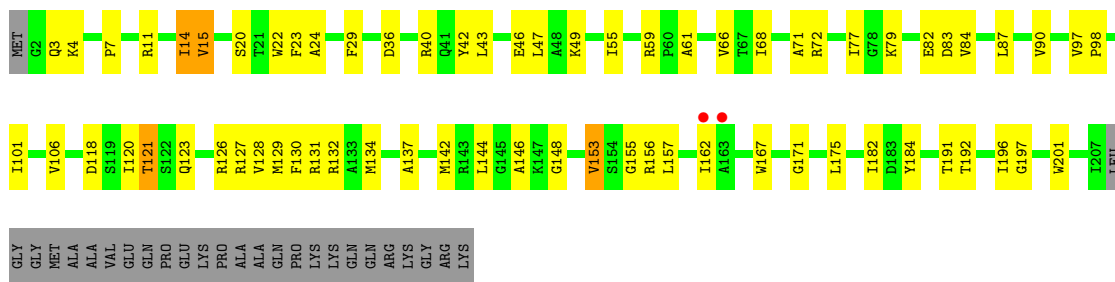
• Molecule 2: 30S ribosomal protein S2

Chain B:



• Molecule 3: 30S ribosomal protein S3

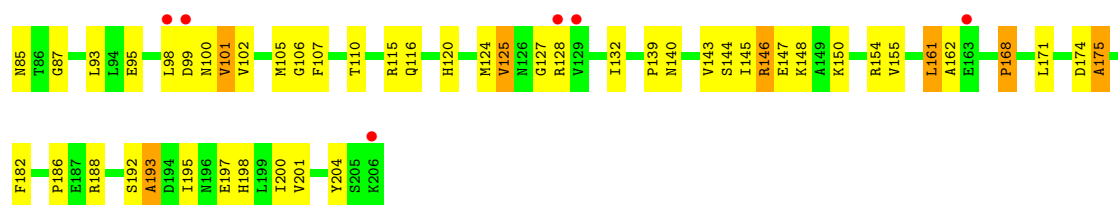
Chain C:



• Molecule 4: 30S ribosomal protein S4

Chain D:





• Molecule 5: 30S ribosomal protein S5

Chain E:

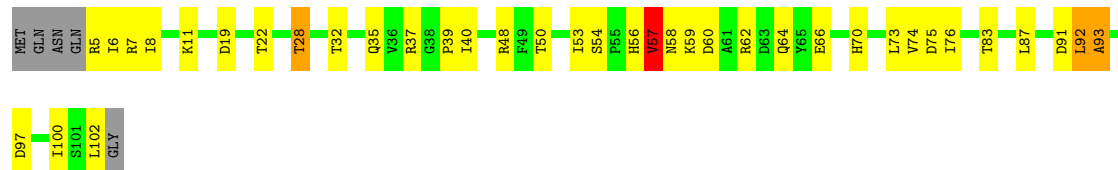
• Molecule 6: 30S ribosomal protein S6

Chain F:



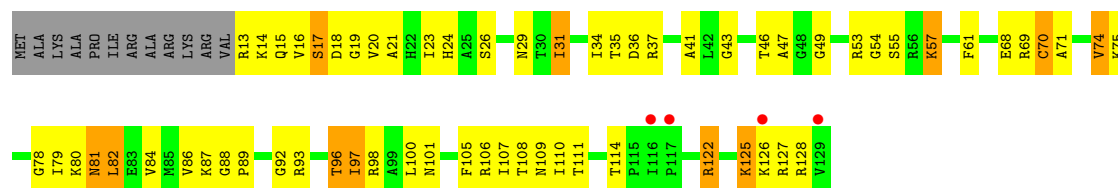
• Molecule 10: 30S ribosomal protein S10

Chain J:



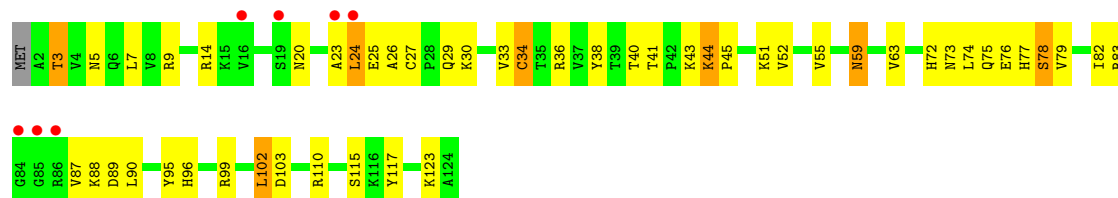
• Molecule 11: 30S ribosomal protein S11

Chain K:



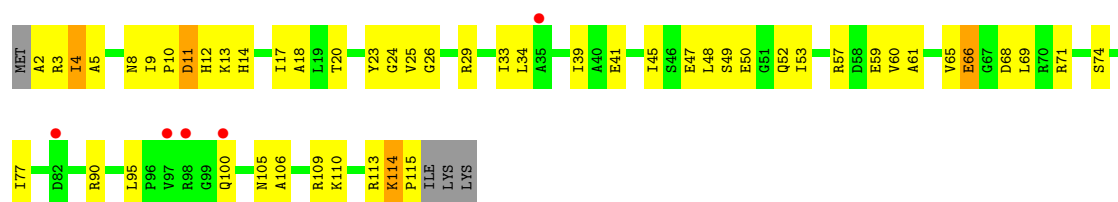
• Molecule 12: 30S ribosomal protein S12

Chain L:



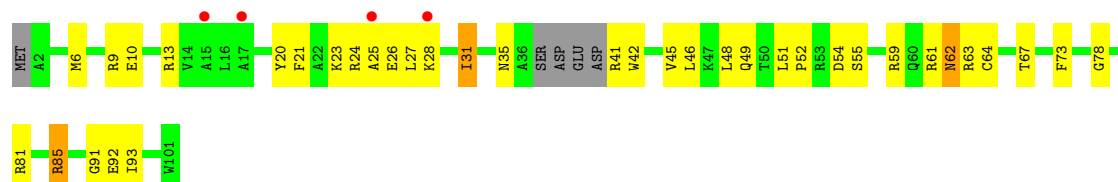
• Molecule 13: 30S ribosomal protein S13

Chain M:



• Molecule 14: 30S ribosomal protein S14

Chain N:



- Molecule 15: 30S ribosomal protein S15

Chain O:



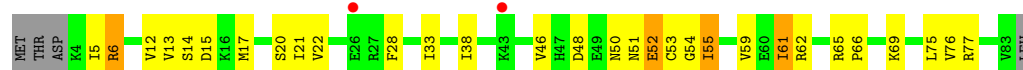
- Molecule 16: 30S ribosomal protein S16

Chain P:



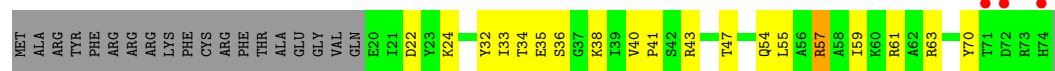
- Molecule 17: 30S ribosomal protein S17

Chain Q:



- Molecule 18: 30S ribosomal protein S18

Chain R:



- Molecule 19: 30S ribosomal protein S19

Chain S:



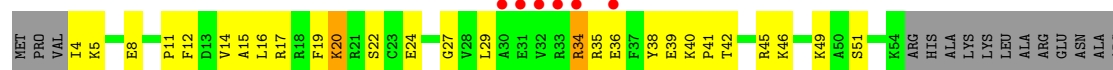
- Molecule 20: 30S ribosomal protein S20

Chain T:

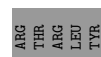


- Molecule 21: 30S ribosomal protein S21

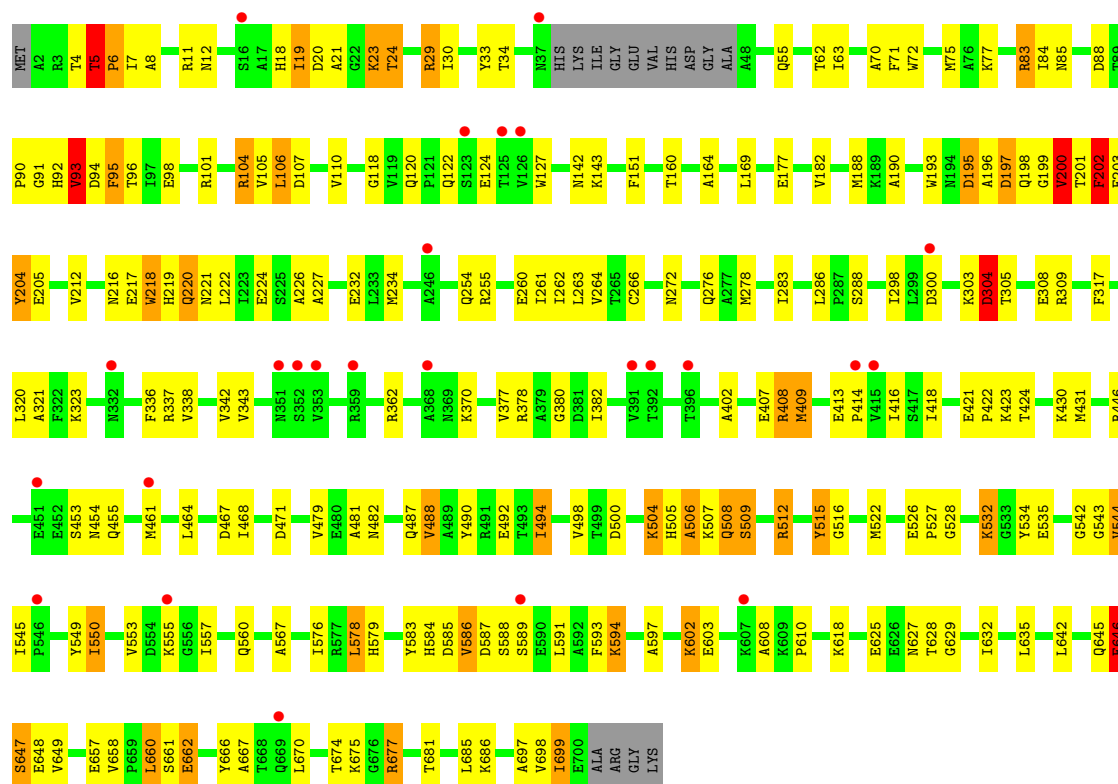
Chain U:



- Molecule 22: elongation factor G



Chain V:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	361.14Å 360.51Å 429.73Å 90.00° 103.22° 90.00°	Depositor
Resolution (Å)	70.00 – 2.90 69.13 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (70.00-2.90) 77.4 (69.13-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.81Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.215 , 0.267 0.503 , 0.512	Depositor DCC
R_{free} test set	3890 reflections (0.43%)	DCC
Wilson B-factor (Å ²)	54.5	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 330.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	1 of 2019725 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.41	EDS
Total number of atoms	57042	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.58 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.8072e-03.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	A	0.64	0/36834	1.13	101/57462 (0.2%)
2	B	0.52	0/1735	0.72	0/2338
3	C	0.48	0/1651	0.67	0/2225
4	D	0.52	0/1665	0.73	0/2227
5	E	0.52	0/1118	0.76	0/1504
6	F	0.58	0/835	0.72	0/1128
7	G	0.51	0/1195	0.73	0/1602
8	H	0.45	0/989	0.66	0/1326
9	I	0.56	0/1034	0.76	1/1375 (0.1%)
10	J	0.54	0/796	0.77	0/1077
11	K	0.71	0/893	0.92	2/1205 (0.2%)
12	L	0.50	0/969	0.78	0/1300
13	M	0.60	0/892	0.83	0/1193
14	N	0.48	0/785	0.67	0/1043
15	O	0.50	0/722	0.68	0/964
16	P	0.51	0/659	0.67	0/884
17	Q	0.51	0/657	0.75	0/881
18	R	0.53	0/462	0.77	1/621 (0.2%)
19	S	0.66	0/652	0.79	0/877
20	T	0.49	0/671	0.72	0/888
21	U	0.78	0/430	0.82	0/570
22	V	0.50	0/5418	0.70	1/7329 (0.0%)
All	All	0.60	0/61062	1.01	106/90019 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	L	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
22	V	0	3
All	All	0	4

There are no bond length outliers.

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	U	C2-N1-C1'	9.96	129.65	117.70
1	A	1087	G	C6-C5-N7	-8.31	125.42	130.40
1	A	481	G	C5-C6-O6	-8.14	123.71	128.60
1	A	1087	G	N7-C8-N9	7.84	117.02	113.10
1	A	1086	U	N3-C2-O2	-7.79	116.75	122.20
1	A	51	A	P-O3'-C3'	7.67	128.91	119.70
1	A	5	U	C6-N1-C1'	-7.44	110.79	121.20
1	A	1087	G	C4-N9-C1'	7.34	136.04	126.50
1	A	1101	A	P-O3'-C3'	7.27	128.43	119.70
1	A	1299	A	N1-C6-N6	7.24	122.95	118.60
1	A	1279	G	C8-N9-C4	-7.17	103.53	106.40
1	A	1454	G	O5'-P-OP1	-7.17	99.25	105.70
1	A	481	G	N9-C4-C5	-7.10	102.56	105.40
1	A	481	G	N3-C4-N9	7.06	130.24	126.00
1	A	913	A	P-O3'-C3'	6.93	128.01	119.70
1	A	1362	A	O4'-C1'-N9	6.87	113.69	108.20
1	A	1087	G	C8-N9-C4	-6.84	103.67	106.40
1	A	602	A	N1-C6-N6	6.81	122.69	118.60
1	A	250	A	P-O3'-C3'	6.74	127.79	119.70
1	A	503	C	C6-N1-C2	-6.72	117.61	120.30
1	A	1496	C	C6-N1-C2	-6.62	117.65	120.30
1	A	27	G	C8-N9-C4	-6.57	103.77	106.40
1	A	1299	A	C5-C6-N6	-6.55	118.46	123.70
1	A	485	U	N3-C2-O2	-6.41	117.71	122.20
1	A	1031	C	C6-N1-C2	-6.41	117.73	120.30
1	A	947	G	N1-C6-O6	6.35	123.71	119.90
1	A	1307	U	C5-C6-N1	6.34	125.87	122.70
1	A	1304	G	C8-N9-C4	-6.32	103.87	106.40
9	I	57	MET	CG-SD-CE	6.27	110.23	100.20
1	A	1012	A	C8-N9-C4	-6.16	103.34	105.80
1	A	1334	G	N3-C4-N9	6.09	129.65	126.00
1	A	206	C	C6-N1-C2	-6.07	117.87	120.30
1	A	578	C	N1-C2-O2	-6.03	115.28	118.90
1	A	5	U	C5-C4-O4	-6.01	122.29	125.90
1	A	485	U	N1-C2-O2	5.99	126.99	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	122	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	A	328	C	N1-C2-O2	5.98	122.49	118.90
1	A	1087	G	C4-C5-C6	5.97	122.38	118.80
22	V	93	VAL	N-CA-C	-5.96	94.92	111.00
1	A	639	G	C8-N9-C4	-5.92	104.03	106.40
1	A	1086	U	C6-N1-C2	-5.90	117.46	121.00
1	A	1279	G	N7-C8-N9	5.84	116.02	113.10
1	A	798	U	N3-C2-O2	5.83	126.28	122.20
1	A	1086	U	N1-C2-O2	5.83	126.88	122.80
1	A	1116	U	O5'-P-OP2	-5.83	100.46	105.70
1	A	115	G	C8-N9-C4	-5.82	104.07	106.40
1	A	1087	G	C8-N9-C1'	-5.70	119.59	127.00
1	A	1137	C	C6-N1-C2	-5.69	118.02	120.30
1	A	1452	C	P-O3'-C3'	5.69	126.53	119.70
1	A	409	U	O5'-P-OP2	-5.68	100.58	105.70
1	A	1322	C	N1-C2-O2	5.68	122.31	118.90
1	A	1187	G	O5'-P-OP1	-5.67	100.59	105.70
1	A	1322	C	C2-N1-C1'	5.67	125.03	118.80
1	A	22	G	N1-C6-O6	5.65	123.29	119.90
1	A	1527	U	O5'-P-OP2	-5.65	100.61	105.70
1	A	211	G	C2-N3-C4	5.58	114.69	111.90
1	A	5	U	C5-C6-N1	5.57	125.49	122.70
1	A	779	C	N3-C2-O2	-5.57	118.00	121.90
1	A	5	U	O4'-C1'-N1	-5.56	103.75	108.20
1	A	1362	A	N1-C6-N6	-5.56	115.27	118.60
1	A	115	G	P-O3'-C3'	5.54	126.35	119.70
1	A	305	G	C8-N9-C4	-5.54	104.19	106.40
1	A	1362	A	C6-C5-N7	5.51	136.15	132.30
1	A	779	C	N1-C2-O2	5.50	122.20	118.90
1	A	1530	G	C4-N9-C1'	-5.48	119.37	126.50
1	A	328	C	N3-C2-O2	-5.47	118.07	121.90
1	A	70	U	C2-N1-C1'	5.46	124.26	117.70
1	A	1086	U	C2-N1-C1'	5.46	124.25	117.70
1	A	1362	A	C4-N9-C1'	-5.46	116.48	126.30
1	A	1201	A	P-O3'-C3'	5.45	126.24	119.70
1	A	1031	C	O5'-P-OP1	-5.43	100.81	105.70
1	A	1511	G	N1-C6-O6	5.38	123.13	119.90
1	A	177	G	C8-N9-C4	-5.35	104.26	106.40
1	A	582	C	N3-C2-O2	5.33	125.63	121.90
1	A	1101	A	N1-C6-N6	5.31	121.79	118.60
1	A	145	G	C5-C6-N1	-5.31	108.85	111.50
1	A	23	C	N1-C2-O2	5.30	122.08	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	57	ARG	CB-CG-CD	-5.30	97.83	111.60
1	A	972	C	C6-N1-C2	5.29	122.42	120.30
1	A	1012	A	N7-C8-N9	5.28	116.44	113.80
1	A	1334	G	N3-C4-C5	-5.27	125.97	128.60
1	A	1484	C	N1-C2-O2	-5.25	115.75	118.90
1	A	382	A	O5'-P-OP2	-5.24	100.98	105.70
1	A	481	G	C4-C5-N7	5.21	112.89	110.80
1	A	115	G	N3-C4-C5	-5.20	126.00	128.60
1	A	1364	U	N1-C2-O2	5.19	126.43	122.80
1	A	776	G	N3-C4-C5	5.18	131.19	128.60
1	A	70	U	C5-C6-N1	5.17	125.29	122.70
1	A	1087	G	N1-C6-O6	5.17	123.00	119.90
1	A	1332	A	O4'-C1'-N9	5.17	112.33	108.20
1	A	1486	G	C6-C5-N7	-5.15	127.31	130.40
11	K	49	GLY	N-CA-C	5.14	125.96	113.10
1	A	1364	U	C2-N1-C1'	5.14	123.86	117.70
1	A	1304	G	N7-C8-N9	5.13	115.67	113.10
1	A	772	U	O5'-P-OP1	5.13	116.85	110.70
1	A	541	G	N3-C4-C5	5.12	131.16	128.60
1	A	530	G	N7-C8-N9	5.09	115.65	113.10
1	A	486	U	N3-C2-O2	-5.09	118.64	122.20
1	A	1285	A	O4'-C1'-N9	5.08	112.27	108.20
1	A	1362	A	C8-N9-C1'	5.08	136.84	127.70
1	A	72	A	C8-N9-C4	-5.06	103.78	105.80
1	A	779	C	C6-N1-C2	-5.04	118.28	120.30
1	A	1332	A	N9-C1'-C2'	5.03	120.54	114.00
1	A	1087	G	N1-C2-N3	5.03	126.92	123.90
1	A	947	G	C5-C6-O6	-5.02	125.59	128.60
1	A	1322	C	N3-C2-O2	-5.02	118.39	121.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	23	ALA	Peptide
22	V	218	TRP	Peptide
22	V	304	ASP	Peptide
22	V	588	SER	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32895	0	16553	425	0
2	B	1704	0	1732	72	0
3	C	1624	0	1696	48	0
4	D	1643	0	1707	72	0
5	E	1105	0	1148	37	0
6	F	817	0	808	25	0
7	G	1181	0	1238	33	0
8	H	979	0	1031	28	0
9	I	1022	0	1070	59	0
10	J	786	0	828	34	0
11	K	877	0	887	75	0
12	L	955	0	1016	39	0
13	M	883	0	941	52	0
14	N	774	0	824	29	0
15	O	714	0	734	21	0
16	P	649	0	666	19	0
17	Q	648	0	691	21	0
18	R	455	0	478	15	0
19	S	637	0	665	20	0
20	T	665	0	714	19	0
21	U	425	0	449	36	0
22	V	5319	0	5227	128	0
23	A	40	0	0	0	0
23	C	1	0	0	0	0
23	E	1	0	0	0	0
23	T	1	0	0	0	0
23	V	1	0	0	0	0
24	V	32	0	14	1	0
25	A	198	0	0	33	0
25	D	1	0	0	0	0
25	E	2	0	0	0	0
25	N	5	0	0	0	0
25	T	1	0	0	0	0
25	U	1	0	0	0	0
25	V	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	57042	0	41117	1188	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (1188) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:V:55:GLN:NE2	22:V:471:ASP:OD2	2.01	0.94
11:K:127:ARG:O	21:U:34:ARG:NH1	2.08	0.86
1:A:946:A:HO2'	1:A:1333:A:HO2'	1.10	0.86
1:A:770:C:N4	25:A:1755:HOH:O	2.09	0.86
2:B:57:ASN:ND2	2:B:219:THR:O	2.11	0.84
22:V:526:GLU:O	22:V:528:GLY:N	2.09	0.83
1:A:1116:U:O2'	9:I:110:GLN:NE2	2.12	0.82
11:K:18:ASP:O	11:K:37:ARG:NE	2.13	0.82
11:K:108:THR:O	11:K:109:ASN:ND2	2.12	0.81
1:A:1366:C:O2'	10:J:62:ARG:NH2	2.14	0.81
1:A:1003:G:O6	1:A:1036:A:N6	2.14	0.80
22:V:93:VAL:O	22:V:95:PHE:N	2.14	0.80
1:A:937:A:OP2	25:A:1773:HOH:O	2.00	0.80
14:N:91:GLY:O	14:N:93:ILE:N	2.15	0.78
1:A:1095:U:OP2	25:A:1863:HOH:O	2.01	0.78
22:V:422:PRO:O	22:V:424:THR:N	2.17	0.78
1:A:460:A:N6	1:A:471:U:O4	2.15	0.78
3:C:49:LYS:O	3:C:72:ARG:NH2	2.17	0.78
22:V:62:THR:O	25:V:901:HOH:O	2.01	0.78
12:L:75:GLN:O	12:L:77:HIS:N	2.18	0.77
1:A:1134:G:N2	1:A:1140:C:N3	2.31	0.77
11:K:81:ASN:ND2	11:K:108:THR:OG1	2.17	0.77
7:G:113:ASP:OD2	7:G:122:ASN:ND2	2.18	0.76
1:A:723:U:O2'	1:A:724:G:OP1	2.03	0.76
1:A:1304:G:O2'	1:A:1333:A:N6	2.18	0.76
1:A:1266:G:N2	1:A:1269:A:OP2	2.19	0.76
1:A:537:G:OP2	25:A:1895:HOH:O	2.04	0.76
1:A:980:C:OP2	25:A:1833:HOH:O	2.04	0.75
1:A:1050:G:O2'	22:V:542:GLY:O	2.02	0.75
1:A:1433:A:OP2	25:A:1838:HOH:O	2.05	0.74
1:A:1416:G:N7	25:A:1794:HOH:O	2.21	0.74
2:B:14:HIS:ND1	2:B:14:HIS:O	2.20	0.74
1:A:978:A:OP2	1:A:1362:A:N6	2.20	0.73
1:A:1220:G:OP1	19:S:37:ARG:NE	2.22	0.73
22:V:219:HIS:O	22:V:222:LEU:N	2.21	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1180:A:OP2	9:I:99:ARG:NH2	2.22	0.73
1:A:1108:G:O6	25:A:1863:HOH:O	2.06	0.73
1:A:1194:U:H5'	5:E:27:GLY:HA2	1.72	0.72
1:A:521:G:OP2	12:L:51:LYS:NZ	2.23	0.72
1:A:195:A:OP2	25:A:1877:HOH:O	2.07	0.72
4:D:25:VAL:HG23	4:D:26:ARG:H	1.56	0.71
1:A:782:A:OP1	25:A:1813:HOH:O	2.07	0.71
14:N:27:LEU:O	14:N:31:ILE:N	2.24	0.71
22:V:508:GLN:O	22:V:508:GLN:NE2	2.24	0.71
1:A:404:G:O2'	1:A:498:A:N1	2.21	0.71
1:A:404:G:O6	4:D:2:ALA:N	2.24	0.71
7:G:126:ASP:O	7:G:130:ASN:N	2.24	0.70
1:A:858:G:N7	25:A:1820:HOH:O	2.24	0.70
1:A:1296:C:O3'	1:A:1302:C:N4	2.25	0.70
11:K:114:THR:OG1	21:U:24:GLU:OE1	2.09	0.70
1:A:937:A:OP2	25:A:1775:HOH:O	2.09	0.70
1:A:490:C:OP1	4:D:146:ARG:NH2	2.24	0.70
22:V:509:SER:OG	22:V:512:ARG:O	2.10	0.70
13:M:23:TYR:N	13:M:66:GLU:OE2	2.24	0.70
19:S:35:SER:HG	19:S:38:SER:HG	1.36	0.70
20:T:3:ASN:O	20:T:5:LYS:N	2.21	0.70
1:A:1027:C:O2'	1:A:1034:G:N2	2.24	0.70
14:N:64:CYS:SG	14:N:67:THR:OG1	2.50	0.69
1:A:808:C:OP2	15:O:48:LYS:NZ	2.19	0.69
9:I:92:GLU:O	9:I:96:SER:OG	2.09	0.69
11:K:16:VAL:O	11:K:37:ARG:NH2	2.26	0.69
1:A:1222:G:O6	25:A:1833:HOH:O	2.09	0.68
1:A:401:C:O2'	1:A:621:A:O2'	2.02	0.68
1:A:1198:G:OP2	25:A:1832:HOH:O	2.12	0.68
11:K:88:GLY:H	11:K:114:THR:HG22	1.58	0.68
22:V:92:HIS:O	22:V:122:GLN:NE2	2.26	0.67
1:A:181:A:N7	25:A:1879:HOH:O	2.26	0.67
1:A:1522:U:OP1	11:K:128:ARG:NH2	2.28	0.67
1:A:1166:G:N1	1:A:1169:A:OP2	2.28	0.67
5:E:70:ASN:O	5:E:70:ASN:ND2	2.27	0.66
1:A:579:A:O2'	15:O:54:ARG:NH1	2.27	0.66
1:A:71:A:O2'	1:A:72:A:O4'	2.12	0.66
8:H:9:ASP:OD1	8:H:13:ARG:NH1	2.29	0.66
14:N:54:ASP:OD1	14:N:59:ARG:NH1	2.28	0.66
1:A:769:G:H4'	1:A:1513:A:H4'	1.77	0.66
1:A:1508:A:OP1	25:A:1801:HOH:O	2.13	0.66
1:A:7:A:N3	25:A:1839:HOH:O	2.28	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:352:C:OP2	25:A:1893:HOH:O	2.14	0.66
1:A:1468:A:H2'	1:A:1469:C:H5'	1.77	0.65
1:A:1505:G:OP1	25:A:1801:HOH:O	2.12	0.65
11:K:125:LYS:O	21:U:34:ARG:NH2	2.29	0.65
1:A:922:G:H4'	5:E:25:VAL:HA	1.79	0.65
12:L:34:CYS:HA	12:L:55:VAL:HA	1.79	0.65
1:A:1033:G:H2'	1:A:1034:G:H5'	1.78	0.65
4:D:30:THR:HG22	4:D:31:LYS:H	1.60	0.65
22:V:512:ARG:HD3	22:V:589:SER:HB3	1.79	0.65
14:N:49:GLN:OE1	14:N:49:GLN:N	2.29	0.64
1:A:814:A:OP2	25:A:1756:HOH:O	2.15	0.64
1:A:1101:A:H4'	1:A:1102:A:O5'	1.98	0.64
21:U:41:PRO:O	21:U:45:ARG:N	2.26	0.64
22:V:8:ALA:O	22:V:288:SER:OG	2.14	0.64
10:J:8:ILE:HG12	10:J:100:ILE:HG12	1.78	0.64
1:A:1152:A:OP1	10:J:70:HIS:ND1	2.30	0.64
1:A:516:U:O2'	1:A:519:C:N3	2.29	0.64
1:A:143:A:H5'	1:A:144:G:H5'	1.79	0.63
13:M:3:ARG:HD2	13:M:9:ILE:HG22	1.81	0.63
13:M:33:ILE:HA	13:M:59:GLU:HG2	1.80	0.63
16:P:46:LYS:HG3	16:P:47:GLU:H	1.64	0.63
3:C:71:ALA:HA	3:C:106:VAL:HG22	1.81	0.63
5:E:111:MET:HB2	5:E:140:THR:HG21	1.80	0.63
5:E:82:GLN:HG2	5:E:150:PRO:HD3	1.81	0.63
1:A:416:G:OP2	25:A:1717:HOH:O	2.16	0.62
1:A:202:G:HO2'	1:A:468:A:H8	1.45	0.62
9:I:57:MET:N	9:I:57:MET:SD	2.73	0.62
22:V:203:GLU:O	22:V:205:GLU:N	2.33	0.62
5:E:41:ASP:OD1	5:E:42:GLY:N	2.33	0.62
1:A:1010:U:H2'	1:A:1011:C:C6	2.35	0.62
11:K:125:LYS:O	21:U:34:ARG:NE	2.33	0.62
5:E:111:MET:CB	5:E:140:THR:HG21	2.30	0.62
1:A:1239:A:N6	1:A:1299:A:H61	1.98	0.62
1:A:1239:A:H61	1:A:1299:A:H61	1.47	0.62
1:A:1329:A:OP1	13:M:26:GLY:N	2.32	0.62
11:K:111:THR:HG22	21:U:5:LYS:HB2	1.81	0.62
1:A:1306:A:H1'	1:A:1332:A:C4	2.36	0.61
1:A:73:C:H5'	1:A:73:C:H6	1.66	0.61
1:A:1277:C:HO2'	1:A:1279:G:H8	1.49	0.61
2:B:20:ARG:O	2:B:22:TRP:N	2.33	0.61
5:E:104:GLY:CA	5:E:122:ASN:HA	2.31	0.61
10:J:73:LEU:O	10:J:75:ASP:N	2.34	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:R:54:GLN:HA	18:R:57:ARG:HD3	1.81	0.61
10:J:37:ARG:CZ	10:J:76:ILE:HA	2.31	0.60
1:A:324:G:N7	25:A:1843:HOH:O	2.31	0.60
14:N:61:ARG:O	14:N:62:ASN:HB2	2.01	0.60
8:H:5:ASP:OD2	8:H:77:ARG:NH1	2.34	0.60
22:V:632:ILE:HD12	22:V:642:LEU:HD22	1.83	0.60
22:V:560:GLN:N	22:V:560:GLN:OE1	2.32	0.60
11:K:26:SER:OG	11:K:29:ASN:O	2.18	0.60
1:A:1304:G:OP2	25:A:1791:HOH:O	2.16	0.60
1:A:1147:C:O2	9:I:18:ARG:NH1	2.34	0.60
2:B:32:GLY:HA3	2:B:39:ILE:H	1.65	0.60
17:Q:12:VAL:O	17:Q:14:SER:N	2.32	0.60
1:A:677:U:H3	1:A:713:G:H22	1.50	0.60
1:A:1513:A:H2'	1:A:1514:G:C8	2.37	0.59
13:M:57:ARG:HA	13:M:60:VAL:HG12	1.84	0.59
15:O:46:HIS:C	15:O:48:LYS:H	2.06	0.59
1:A:1306:A:N3	1:A:1332:A:H1'	2.18	0.59
1:A:461:A:H2'	1:A:462:G:H5'	1.85	0.59
4:D:13:ARG:NH1	4:D:37:ALA:O	2.35	0.59
4:D:116:GLN:O	4:D:120:HIS:ND1	2.35	0.59
1:A:747:A:C6	1:A:748:G:C5	2.91	0.59
4:D:15:GLU:OE2	4:D:56:ARG:NH2	2.35	0.59
1:A:1203:C:OP1	25:A:1777:HOH:O	2.17	0.59
16:P:43:ALA:O	16:P:46:LYS:HG2	2.03	0.59
1:A:489:C:H5''	4:D:128:ARG:HH22	1.66	0.59
1:A:1391:U:H2'	1:A:1392:G:C8	2.37	0.59
7:G:126:ASP:O	7:G:130:ASN:HA	2.02	0.59
1:A:1468:A:C2'	1:A:1469:C:H5'	2.33	0.59
5:E:111:MET:HE1	5:E:125:ALA:HB1	1.85	0.59
1:A:1495:U:H2'	1:A:1496:C:O2	2.03	0.59
1:A:401:C:OP2	4:D:70:ARG:NH1	2.35	0.59
1:A:547:A:OP1	25:A:1730:HOH:O	2.17	0.59
4:D:188:ARG:NE	4:D:197:GLU:OE2	2.36	0.59
8:H:3:MET:HE1	8:H:6:PRO:HA	1.84	0.59
3:C:40:ARG:NH1	3:C:55:ILE:O	2.36	0.59
22:V:697:ALA:O	22:V:699:ILE:N	2.36	0.58
1:A:35:G:O2'	12:L:115:SER:O	2.16	0.58
3:C:79:LYS:N	3:C:82:GLU:OE1	2.34	0.58
17:Q:17:MET:SD	17:Q:20:SER:OG	2.50	0.58
20:T:82:GLN:HA	20:T:85:LYS:HB2	1.83	0.58
7:G:106:GLU:HA	7:G:109:ARG:HE	1.68	0.58
16:P:46:LYS:HG3	16:P:47:GLU:N	2.19	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:V:453:SER:O	22:V:455:GLN:N	2.36	0.58
1:A:1116:U:H4'	9:I:110:GLN:HE22	1.69	0.58
11:K:34:ILE:CD1	11:K:70:CYS:HB2	2.33	0.58
9:I:45:ARG:HG3	9:I:46:MET:SD	2.44	0.58
1:A:1229:A:OP2	13:M:113:ARG:NH1	2.37	0.58
1:A:131:A:H2'	1:A:132:C:C6	2.39	0.58
22:V:23:LYS:O	22:V:24:THR:OG1	2.22	0.58
3:C:42:TYR:CE2	3:C:90:VAL:HG21	2.39	0.58
7:G:57:SER:OG	7:G:58:GLU:N	2.30	0.58
8:H:106:THR:HG21	8:H:121:LEU:HD13	1.84	0.58
4:D:72:PHE:CZ	4:D:200:ILE:HD11	2.40	0.57
1:A:629:A:H2'	1:A:630:A:O4'	2.04	0.57
2:B:82:ALA:O	2:B:88:GLN:NE2	2.38	0.57
13:M:14:HIS:O	13:M:18:ALA:N	2.34	0.57
9:I:25:ASN:HB2	9:I:27:LYS:HE3	1.85	0.57
1:A:844:G:H2'	1:A:845:A:H5''	1.87	0.57
11:K:55:SER:HA	11:K:57:LYS:HE3	1.85	0.57
1:A:844:G:C3'	1:A:845:A:H5''	2.34	0.57
22:V:591:LEU:O	22:V:594:LYS:N	2.37	0.57
1:A:523:A:H61	12:L:89:ASP:HB2	1.70	0.57
10:J:5:ARG:HG3	10:J:6:ILE:HG13	1.85	0.57
11:K:75:LYS:O	11:K:78:GLY:N	2.37	0.56
6:F:38:ARG:HB3	6:F:63:ASN:HB2	1.87	0.56
2:B:114:LYS:HA	2:B:117:GLU:HG2	1.87	0.56
11:K:34:ILE:HD11	11:K:70:CYS:HB2	1.86	0.56
1:A:518:C:H2'	1:A:530:G:C8	2.40	0.56
3:C:142:MET:HE1	3:C:171:GLY:HA3	1.86	0.56
11:K:125:LYS:O	21:U:34:ARG:CZ	2.54	0.56
11:K:15:GLN:NE2	11:K:78:GLY:O	2.38	0.56
9:I:52:LEU:HA	9:I:57:MET:HG3	1.86	0.56
11:K:107:ILE:HG23	21:U:12:PHE:HE2	1.70	0.56
13:M:114:LYS:CB	13:M:115:PRO:HD3	2.36	0.56
1:A:51:A:H4'	1:A:52:C:O5'	2.05	0.56
22:V:195:ASP:OD1	22:V:196:ALA:N	2.38	0.56
17:Q:50:ASN:O	17:Q:52:GLU:N	2.38	0.56
13:M:20:THR:HA	13:M:25:VAL:HG23	1.87	0.56
1:A:1244:G:H2'	1:A:1245:C:C6	2.40	0.56
22:V:309:ARG:NH2	22:V:402:ALA:O	2.38	0.56
11:K:74:VAL:HG23	11:K:79:ILE:HD12	1.86	0.56
10:J:91:ASP:OD1	10:J:92:LEU:N	2.34	0.56
11:K:81:ASN:CB	11:K:106:ARG:O	2.54	0.56
4:D:58:LYS:NZ	4:D:69:GLU:OE2	2.38	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:V:586:VAL:HG22	22:V:587:ASP:N	2.21	0.56
1:A:769:G:O6	25:A:1755:HOH:O	2.17	0.56
22:V:190:ALA:N	22:V:205:GLU:O	2.38	0.56
11:K:14:LYS:O	11:K:15:GLN:HB3	2.06	0.56
11:K:74:VAL:CG2	11:K:79:ILE:HD12	2.36	0.56
11:K:21:ALA:CB	11:K:82:LEU:HD13	2.36	0.56
1:A:1243:C:OP1	25:A:1793:HOH:O	2.18	0.56
7:G:15:ASP:HB3	7:G:20:SER:H	1.71	0.56
6:F:3:HIS:H	6:F:92:THR:HG23	1.70	0.56
1:A:1313:U:H3	1:A:1324:A:H61	1.53	0.55
1:A:1003:G:N2	1:A:1005:A:H5'	2.21	0.55
1:A:411:A:OP1	4:D:26:ARG:NH2	2.39	0.55
12:L:24:LEU:O	12:L:26:ALA:N	2.39	0.55
1:A:1192:C:OP2	3:C:4:LYS:NZ	2.32	0.55
3:C:42:TYR:CZ	3:C:90:VAL:HG21	2.42	0.55
4:D:99:ASP:OD1	4:D:100:ASN:N	2.39	0.55
1:A:1030:U:H4'	1:A:1031:C:OP1	2.06	0.55
14:N:21:PHE:HA	14:N:25:ALA:HB3	1.88	0.55
1:A:483:C:O2	16:P:13:LYS:NZ	2.39	0.55
22:V:11:ARG:HE	22:V:283:ILE:HA	1.72	0.55
11:K:87:LYS:HA	11:K:114:THR:HG22	1.89	0.55
13:M:11:ASP:OD1	13:M:12:HIS:N	2.37	0.55
17:Q:21:ILE:HG23	17:Q:46:VAL:HB	1.87	0.55
11:K:19:GLY:HA2	11:K:37:ARG:HG3	1.89	0.55
4:D:145:ILE:CD1	4:D:155:VAL:HG21	2.37	0.55
5:E:45:ARG:HA	5:E:72:ILE:O	2.06	0.55
12:L:72:HIS:ND1	12:L:73:ASN:O	2.39	0.55
2:B:40:ILE:HG21	2:B:201:GLY:HA2	1.88	0.55
1:A:1491:G:H5'	1:A:1492:A:OP1	2.06	0.55
5:E:104:GLY:HA2	5:E:122:ASN:HA	1.88	0.55
11:K:80:LYS:O	11:K:106:ARG:N	2.34	0.55
12:L:44:LYS:CB	12:L:45:PRO:HD3	2.37	0.55
13:M:74:SER:HA	13:M:77:ILE:HD12	1.89	0.55
6:F:91:ARG:HG3	6:F:92:THR:H	1.71	0.54
4:D:58:LYS:HG3	4:D:59:GLN:N	2.22	0.54
13:M:66:GLU:O	13:M:69:LEU:N	2.40	0.54
1:A:1368:A:OP1	9:I:113:ARG:NH2	2.39	0.54
18:R:34:THR:OG1	18:R:35:GLU:N	2.40	0.54
1:A:9:G:H5'	5:E:108:GLY:HA3	1.89	0.54
1:A:1126:U:N3	1:A:1280:A:OP1	2.39	0.54
1:A:392:C:OP1	16:P:8:ARG:NH2	2.40	0.54
11:K:70:CYS:SG	11:K:71:ALA:N	2.81	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1123:U:H4'	10:J:39:PRO:HD2	1.88	0.54
1:A:1478:U:H2'	1:A:1479:C:C6	2.43	0.54
18:R:32:TYR:CD2	18:R:55:LEU:HD21	2.43	0.54
22:V:127:TRP:HH2	22:V:262:ILE:HD13	1.72	0.54
1:A:409:U:H5''	4:D:25:VAL:CG2	2.38	0.54
5:E:81:LEU:CD2	5:E:123:VAL:HG12	2.37	0.54
4:D:72:PHE:CE2	4:D:200:ILE:HD11	2.42	0.54
22:V:221:ASN:HA	22:V:224:GLU:HB3	1.90	0.54
6:F:51:ILE:HG21	6:F:85:ILE:HD12	1.90	0.54
1:A:204:G:H3'	1:A:205:A:H5''	1.90	0.54
11:K:53:ARG:NH2	11:K:54:GLY:O	2.41	0.54
1:A:1053:G:N7	1:A:1200:C:H5''	2.23	0.54
1:A:451:A:H4'	1:A:452:A:O5'	2.08	0.54
22:V:646:GLU:O	22:V:647:SER:HB2	2.08	0.54
3:C:7:PRO:HG2	3:C:184:TYR:CG	2.43	0.54
1:A:954:G:H2'	1:A:955:U:C6	2.42	0.54
10:J:35:GLN:CG	10:J:37:ARG:HE	2.21	0.54
9:I:10:GLY:HA2	9:I:81:HIS:CD2	2.43	0.54
1:A:1077:G:N2	1:A:1080:A:OP2	2.38	0.54
1:A:211:G:N3	1:A:211:G:H3'	2.23	0.54
1:A:859:G:OP2	1:A:869:G:N1	2.38	0.53
1:A:1011:C:H2'	1:A:1012:A:H5'	1.90	0.53
9:I:44:ALA:HA	9:I:47:VAL:HG13	1.90	0.53
2:B:67:LEU:HD21	2:B:91:VAL:HG23	1.88	0.53
22:V:585:ASP:O	22:V:586:VAL:HB	2.09	0.53
2:B:46:VAL:HB	2:B:47:PRO:HD3	1.89	0.53
2:B:20:ARG:HA	2:B:20:ARG:HH11	1.72	0.53
4:D:3:ARG:CZ	4:D:115:ARG:NE	2.71	0.53
1:A:129:A:H1'	1:A:130:A:C8	2.43	0.53
1:A:1496:C:C5	1:A:1497:G:C5	2.96	0.53
4:D:105:MET:SD	4:D:143:VAL:CG1	2.96	0.53
11:K:57:LYS:HD2	11:K:57:LYS:H	1.74	0.53
1:A:975:A:H8	1:A:1357:A:HO2'	1.55	0.53
6:F:18:VAL:HG11	6:F:58:HIS:CD2	2.43	0.53
3:C:36:ASP:OD1	3:C:59:ARG:NH1	2.32	0.53
10:J:6:ILE:O	10:J:76:ILE:HB	2.09	0.53
22:V:535:GLU:O	22:V:576:ILE:N	2.37	0.53
15:O:87:LEU:C	15:O:89:ARG:H	2.12	0.53
22:V:124:GLU:OE2	22:V:677:ARG:NH1	2.42	0.53
11:K:98:ARG:NH2	21:U:15:ALA:HB3	2.24	0.53
14:N:10:GLU:OE2	14:N:61:ARG:N	2.42	0.53
2:B:163:ILE:HG23	2:B:164:ASP:H	1.73	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:19:THR:O	2:B:20:ARG:NH1	2.41	0.53
4:D:73:ARG:O	4:D:76:TYR:N	2.41	0.53
9:I:21:ILE:CD1	9:I:86:ALA:HB3	2.39	0.53
2:B:71:THR:O	2:B:72:LYS:HG2	2.09	0.53
1:A:1279:G:H2'	1:A:1279:G:N3	2.23	0.53
1:A:995:C:N3	1:A:1046:A:O2'	2.40	0.53
2:B:209:VAL:HG23	2:B:210:THR:H	1.74	0.53
3:C:11:ARG:NH2	3:C:182:ILE:HG13	2.23	0.52
5:E:24:THR:HA	5:E:29:ARG:HA	1.90	0.52
1:A:981:U:O4	25:A:1833:HOH:O	2.19	0.52
10:J:37:ARG:NH2	10:J:76:ILE:HG23	2.23	0.52
22:V:494:ILE:HA	22:V:610:PRO:HA	1.90	0.52
1:A:373:A:H1'	1:A:481:G:H1'	1.91	0.52
4:D:29:ASP:O	4:D:31:LYS:NZ	2.26	0.52
1:A:1505:G:H4'	1:A:1506:U:H5''	1.91	0.52
1:A:70:U:HO2'	1:A:71:A:H8	1.58	0.52
1:A:202:G:O2'	1:A:468:A:H2'	2.10	0.52
13:M:74:SER:HA	13:M:77:ILE:HB	1.92	0.52
22:V:4:THR:CG2	22:V:378:ARG:HG3	2.39	0.52
1:A:21:G:H2'	1:A:22:G:C8	2.44	0.52
17:Q:48:ASP:HB2	17:Q:75:LEU:HD23	1.92	0.52
13:M:29:ARG:NH2	13:M:60:VAL:HA	2.24	0.52
16:P:10:GLY:HA3	16:P:15:PRO:HA	1.91	0.52
1:A:1323:G:H2'	1:A:1324:A:C8	2.44	0.52
1:A:553:A:O2'	12:L:26:ALA:O	2.28	0.52
22:V:492:GLU:OE1	22:V:567:ALA:N	2.38	0.52
10:J:28:THR:O	10:J:32:THR:HG22	2.10	0.52
6:F:20:GLY:O	6:F:23:GLU:HB3	2.09	0.52
8:H:106:THR:HG21	8:H:121:LEU:HD22	1.92	0.52
14:N:48:LEU:O	14:N:51:LEU:HG	2.10	0.52
10:J:35:GLN:HG3	10:J:37:ARG:NE	2.25	0.52
2:B:126:ASP:HB3	2:B:130:LYS:HE3	1.92	0.52
1:A:250:A:H4'	1:A:251:G:O5'	2.10	0.52
10:J:37:ARG:HD2	10:J:75:ASP:O	2.10	0.51
1:A:1306:A:H1'	1:A:1332:A:N9	2.25	0.51
11:K:68:GLU:O	11:K:70:CYS:N	2.32	0.51
2:B:83:ALA:O	2:B:88:GLN:HG3	2.10	0.51
12:L:44:LYS:HB3	12:L:45:PRO:HD3	1.92	0.51
1:A:98:A:H2'	1:A:99:C:C6	2.45	0.51
1:A:404:G:N7	4:D:2:ALA:HB3	2.25	0.51
1:A:374:A:H5''	1:A:452:A:C2	2.46	0.51
22:V:414:PRO:HA	22:V:461:MET:SD	2.50	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:K:24:HIS:HB3	11:K:31:ILE:HG12	1.91	0.51
14:N:41:ARG:HG2	14:N:42:TRP:N	2.26	0.51
1:A:1323:G:O6	19:S:4:SER:OG	2.19	0.51
5:E:106:ILE:HD11	5:E:124:LEU:CD2	2.40	0.51
11:K:98:ARG:CZ	21:U:15:ALA:HB3	2.41	0.51
4:D:193:ALA:HB3	4:D:195:ILE:HG23	1.93	0.51
8:H:10:MET:HE2	8:H:33:LYS:HG2	1.92	0.51
1:A:1386:G:H2'	1:A:1387:G:H8	1.75	0.51
2:B:70:GLY:HA2	2:B:163:ILE:HG22	1.93	0.51
18:R:41:PRO:HB2	18:R:43:ARG:HG2	1.91	0.51
11:K:15:GLN:OE1	11:K:78:GLY:HA3	2.10	0.51
1:A:1003:G:N2	1:A:1037:C:O2	2.43	0.51
1:A:461:A:H3'	1:A:461:A:N3	2.26	0.51
9:I:55:VAL:O	9:I:94:LEU:CD2	2.59	0.51
22:V:488:VAL:HB	22:V:490:TYR:CE2	2.46	0.51
9:I:95:ARG:HA	9:I:98:LEU:HB3	1.93	0.51
12:L:44:LYS:CB	12:L:45:PRO:CD	2.89	0.51
10:J:50:THR:HG21	10:J:64:GLN:HE21	1.76	0.51
18:R:36:SER:HB3	21:U:4:ILE:HG12	1.92	0.51
1:A:1330:U:H5''	13:M:23:TYR:CZ	2.45	0.50
1:A:1007:U:H2'	1:A:1008:U:H5'	1.94	0.50
1:A:1083:U:H5''	1:A:1086:U:C5	2.46	0.50
1:A:844:G:C2'	1:A:845:A:H5''	2.41	0.50
14:N:51:LEU:HB3	14:N:52:PRO:CD	2.41	0.50
19:S:51:VAL:HG22	19:S:71:LEU:HD21	1.92	0.50
7:G:107:ALA:HB2	7:G:133:THR:HG23	1.92	0.50
13:M:106:ALA:HB3	13:M:110:LYS:HD2	1.93	0.50
22:V:85:ASN:HD22	22:V:382:ILE:HG13	1.76	0.50
1:A:71:A:N6	1:A:100:G:C8	2.80	0.50
11:K:53:ARG:HH12	11:K:57:LYS:HB3	1.76	0.50
13:M:114:LYS:HB2	13:M:115:PRO:HD3	1.93	0.50
9:I:21:ILE:CD1	9:I:87:LEU:HD12	2.42	0.50
1:A:1296:C:H4'	1:A:1302:C:N3	2.27	0.50
17:Q:17:MET:HB3	17:Q:20:SER:HB3	1.92	0.50
11:K:55:SER:HA	11:K:57:LYS:CE	2.42	0.50
9:I:21:ILE:HG12	9:I:63:LEU:CD1	2.42	0.50
1:A:502:A:H2'	1:A:503:C:O4'	2.11	0.50
1:A:778:G:C6	1:A:779:C:N3	2.80	0.50
22:V:164:ALA:HB1	22:V:262:ILE:HD11	1.94	0.50
3:C:127:ARG:O	3:C:127:ARG:HG3	2.11	0.50
2:B:69:VAL:HG23	2:B:162:VAL:HB	1.93	0.50
2:B:67:LEU:HD22	2:B:69:VAL:HG13	1.94	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1032:G:C2	1:A:1033:G:H1'	2.47	0.50
1:A:409:U:H2'	1:A:410:G:O4'	2.12	0.50
3:C:71:ALA:HA	3:C:106:VAL:CG2	2.42	0.50
10:J:54:SER:O	14:N:81:ARG:NH1	2.43	0.50
1:A:1218:C:H2'	1:A:1219:A:C8	2.47	0.50
1:A:463:U:H5'	1:A:464:U:OP2	2.12	0.50
20:T:47:ALA:HB1	20:T:83:ILE:HG22	1.93	0.50
4:D:95:GLU:HG2	4:D:186:PRO:HG3	1.93	0.50
1:A:144:G:H2'	1:A:145:G:O4'	2.12	0.49
11:K:98:ARG:NH1	21:U:15:ALA:HB3	2.27	0.49
1:A:158:G:H2'	1:A:159:G:H5'	1.94	0.49
3:C:97:VAL:HB	3:C:98:PRO:HD2	1.94	0.49
8:H:29:SER:HB3	8:H:57:PRO:HB2	1.94	0.49
2:B:20:ARG:NH2	2:B:36:LYS:HD2	2.27	0.49
2:B:30:ILE:HG23	2:B:32:GLY:H	1.77	0.49
1:A:746:A:C6	1:A:747:A:N6	2.80	0.49
1:A:1413:A:C2	1:A:1488:G:C2	3.00	0.49
2:B:49:PHE:CD1	2:B:49:PHE:C	2.84	0.49
3:C:106:VAL:HG23	3:C:106:VAL:O	2.13	0.49
1:A:393:A:OP2	16:P:12:LYS:HD2	2.12	0.49
1:A:934:C:OP1	25:A:1766:HOH:O	2.20	0.49
9:I:11:ARG:HB2	9:I:15:SER:O	2.12	0.49
5:E:95:PHE:CZ	5:E:97:GLN:HG2	2.48	0.49
4:D:48:LEU:HD21	4:D:53:VAL:N	2.27	0.49
4:D:62:ARG:HH21	4:D:68:LEU:HA	1.78	0.49
6:F:66:ALA:HB1	6:F:67:PRO:HD2	1.92	0.49
1:A:1007:U:H2'	1:A:1008:U:C5'	2.43	0.49
4:D:107:PHE:HD2	4:D:145:ILE:HD11	1.77	0.49
2:B:49:PHE:HB2	2:B:212:TYR:OH	2.13	0.49
22:V:635:LEU:HD12	22:V:658:VAL:HG11	1.93	0.49
1:A:1181:G:C2	1:A:1182:G:N2	2.81	0.49
5:E:74:VAL:HG12	5:E:76:LEU:HD12	1.94	0.49
15:O:9:ALA:HA	15:O:12:VAL:HG12	1.94	0.49
1:A:537:G:H5''	12:L:110:ARG:NH1	2.28	0.49
7:G:133:THR:HA	7:G:136:LYS:HB3	1.95	0.49
9:I:7:TYR:CG	9:I:8:GLY:N	2.81	0.49
2:B:134:LEU:C	2:B:136:ARG:H	2.16	0.49
21:U:42:THR:O	21:U:46:LYS:N	2.45	0.49
1:A:1144:G:N1	1:A:1145:A:C2	2.81	0.49
13:M:8:ASN:OD1	13:M:9:ILE:N	2.43	0.49
5:E:41:ASP:OD1	5:E:43:ASN:N	2.38	0.49
10:J:6:ILE:HG23	10:J:100:ILE:HG21	1.94	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:L:43:LYS:HG2	12:L:44:LYS:HG3	1.95	0.49
21:U:4:ILE:N	21:U:19:PHE:CE1	2.81	0.49
3:C:77:ILE:HA	3:C:84:VAL:HG23	1.94	0.49
3:C:23:PHE:CD1	3:C:24:ALA:N	2.81	0.49
1:A:1237:C:O2	1:A:1334:G:O2'	2.30	0.48
11:K:93:ARG:HH22	21:U:20:LYS:CD	2.26	0.48
4:D:37:ALA:HA	4:D:42:GLY:HA3	1.95	0.48
7:G:145:ALA:O	7:G:147:ALA:N	2.47	0.48
16:P:4:ILE:HG13	16:P:21:VAL:CG1	2.43	0.48
22:V:261:ILE:HD11	22:V:263:LEU:CD2	2.43	0.48
10:J:32:THR:HG23	10:J:83:THR:OG1	2.13	0.48
5:E:97:GLN:HB2	5:E:124:LEU:HB2	1.94	0.48
11:K:96:THR:HG22	11:K:97:ILE:N	2.28	0.48
1:A:756:C:HO2'	8:H:2:SER:N	2.11	0.48
1:A:922:G:H2'	1:A:923:A:C8	2.49	0.48
5:E:80:THR:OG1	5:E:81:LEU:N	2.46	0.48
1:A:413:G:N2	1:A:428:G:H1'	2.28	0.48
18:R:22:ASP:OD1	18:R:24:LYS:HE3	2.13	0.48
2:B:11:ALA:HB1	2:B:14:HIS:CD2	2.48	0.48
1:A:1264:U:H2'	1:A:1265:C:C6	2.48	0.48
22:V:550:ILE:HA	22:V:553:VAL:HG12	1.95	0.48
1:A:484:G:H4'	1:A:485:U:O5'	2.12	0.48
5:E:154:ALA:O	5:E:158:GLY:N	2.46	0.48
6:F:55:HIS:ND1	6:F:55:HIS:N	2.60	0.48
1:A:134:G:H1'	1:A:325:A:C5	2.49	0.48
1:A:872:A:C8	1:A:874:G:C8	3.01	0.48
1:A:1330:U:O4	1:A:1331:G:N1	2.47	0.48
1:A:1304:G:H2'	1:A:1332:A:N1	2.28	0.48
9:I:41:ARG:CA	9:I:45:ARG:HD3	2.43	0.48
17:Q:46:VAL:HG21	17:Q:61:ILE:HD13	1.95	0.48
19:S:49:ILE:HD13	19:S:71:LEU:HD21	1.95	0.48
1:A:881:G:P	12:L:9:ARG:HH22	2.37	0.48
9:I:112:GLU:OE2	9:I:115:LYS:NZ	2.35	0.48
1:A:836:G:C6	1:A:837:U:N3	2.82	0.48
22:V:255:ARG:CG	22:V:260:GLU:HB2	2.44	0.48
11:K:109:ASN:ND2	21:U:8:GLU:HB2	2.29	0.48
7:G:126:ASP:O	7:G:130:ASN:CA	2.61	0.48
1:A:60:A:O2'	20:T:5:LYS:HD2	2.13	0.48
2:B:27:LYS:N	2:B:28:PRO:CD	2.77	0.48
1:A:1004:A:H5'	1:A:1024:G:N2	2.28	0.48
22:V:625:GLU:HA	22:V:628:THR:HG23	1.95	0.48
1:A:656:G:H4'	15:O:62:GLN:HE22	1.78	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:M:4:ILE:HB	13:M:57:ARG:NH2	2.28	0.48
7:G:106:GLU:HA	7:G:109:ARG:NE	2.28	0.48
22:V:200:VAL:HG23	22:V:201:THR:HG23	1.96	0.48
1:A:685:G:C2	1:A:686:U:C4	3.02	0.48
1:A:1283:U:H2'	1:A:1284:C:C6	2.49	0.48
9:I:21:ILE:HG12	9:I:63:LEU:HD12	1.96	0.48
1:A:977:A:N6	1:A:1224:U:O5'	2.46	0.48
1:A:461:A:C2'	1:A:462:G:H5'	2.43	0.48
4:D:26:ARG:NH1	4:D:31:LYS:HE3	2.28	0.48
1:A:1011:C:H2'	1:A:1012:A:C5'	2.44	0.48
2:B:20:ARG:HA	2:B:20:ARG:NH1	2.29	0.48
6:F:3:HIS:HB2	6:F:92:THR:HG23	1.96	0.48
1:A:656:G:H4'	15:O:62:GLN:NE2	2.29	0.48
9:I:129:LYS:HG3	9:I:130:ARG:H	1.78	0.48
1:A:1309:G:C6	1:A:1329:A:C2	3.02	0.47
1:A:736:C:OP1	18:R:61:ARG:NE	2.47	0.47
12:L:87:VAL:O	12:L:89:ASP:N	2.47	0.47
6:F:22:ILE:O	6:F:26:THR:OG1	2.21	0.47
4:D:61:VAL:HA	4:D:64:ILE:HD12	1.96	0.47
1:A:715:A:H2'	1:A:716:A:C8	2.49	0.47
11:K:84:VAL:N	11:K:109:ASN:O	2.47	0.47
14:N:35:ASN:HB2	14:N:41:ARG:HD3	1.96	0.47
5:E:80:THR:HB	5:E:122:ASN:ND2	2.30	0.47
19:S:51:VAL:CG2	19:S:71:LEU:HD21	2.43	0.47
6:F:17:GLN:O	6:F:21:MET:N	2.46	0.47
12:L:38:TYR:HB2	12:L:52:VAL:HG23	1.95	0.47
22:V:221:ASN:HA	22:V:224:GLU:CB	2.45	0.47
4:D:3:ARG:NH2	4:D:115:ARG:HE	2.12	0.47
13:M:106:ALA:HB3	13:M:110:LYS:CD	2.44	0.47
1:A:701:U:H5''	1:A:703:G:O4'	2.14	0.47
1:A:880:C:OP1	12:L:5:ASN:ND2	2.45	0.47
16:P:63:GLN:N	16:P:63:GLN:OE1	2.47	0.47
20:T:28:MET:HE1	20:T:67:ILE:CD1	2.44	0.47
8:H:78:VAL:HG11	8:H:125:ILE:HD11	1.95	0.47
9:I:41:ARG:HA	9:I:45:ARG:HD3	1.97	0.47
3:C:42:TYR:CZ	3:C:46:GLU:HG3	2.50	0.47
9:I:11:ARG:H	9:I:81:HIS:HD2	1.61	0.47
2:B:67:LEU:HD12	2:B:157:PRO:CG	2.44	0.47
22:V:169:LEU:HB2	22:V:263:LEU:HB3	1.96	0.47
20:T:62:ALA:HA	20:T:67:ILE:HG22	1.96	0.47
1:A:399:G:H2'	1:A:400:C:C6	2.49	0.47
7:G:130:ASN:HB2	7:G:135:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1197:A:OP1	25:A:1832:HOH:O	2.20	0.47
1:A:748:G:C6	1:A:749:A:C5	3.03	0.47
22:V:217:GLU:O	22:V:220:GLN:N	2.48	0.47
2:B:187:ASP:OD2	2:B:202:ASN:HA	2.14	0.47
1:A:685:G:N1	1:A:686:U:O4	2.47	0.47
1:A:1142:G:C2	1:A:1143:G:H1'	2.50	0.47
12:L:63:VAL:HG21	12:L:95:TYR:HE1	1.79	0.47
1:A:690:G:H2'	1:A:691:G:O4'	2.14	0.47
9:I:57:MET:HG2	9:I:58:VAL:H	1.80	0.47
13:M:11:ASP:OD1	13:M:45:ILE:HD13	2.14	0.47
22:V:557:ILE:HG21	22:V:576:ILE:CD1	2.45	0.47
9:I:83:ILE:O	9:I:87:LEU:HD13	2.14	0.47
1:A:791:G:C6	1:A:792:A:N7	2.82	0.47
22:V:430:LYS:HG2	22:V:479:VAL:CG2	2.45	0.47
20:T:6:SER:C	20:T:8:LYS:H	2.17	0.47
1:A:1513:A:H2'	1:A:1514:G:H8	1.80	0.47
1:A:982:U:H4'	1:A:983:A:O5'	2.14	0.47
1:A:747:A:C6	1:A:748:G:C6	3.03	0.47
1:A:51:A:N7	1:A:114:U:O2'	2.47	0.47
22:V:494:ILE:H	22:V:494:ILE:HD13	1.79	0.47
22:V:382:ILE:O	22:V:382:ILE:HD12	2.15	0.47
13:M:95:LEU:C	13:M:109:ARG:HG2	2.34	0.47
1:A:668:G:HO2'	15:O:46:HIS:HD1	1.62	0.47
1:A:451:A:C2	1:A:480:U:C4	3.02	0.47
9:I:44:ALA:O	9:I:47:VAL:HG22	2.14	0.47
13:M:34:LEU:HD22	13:M:39:ILE:HB	1.96	0.47
11:K:46:THR:OG1	11:K:47:ALA:N	2.40	0.47
1:A:1113:C:H4'	3:C:14:ILE:HG21	1.97	0.47
22:V:544:VAL:HG12	22:V:545:ILE:N	2.29	0.47
12:L:24:LEU:HG	12:L:25:GLU:N	2.30	0.47
1:A:1107:C:C4	1:A:1108:G:C8	3.03	0.46
4:D:124:MET:HG3	4:D:144:SER:OG	2.15	0.46
1:A:60:A:OP1	1:A:111:G:N2	2.37	0.46
21:U:40:LYS:N	21:U:41:PRO:CD	2.79	0.46
10:J:7:ARG:HG3	10:J:75:ASP:HA	1.97	0.46
1:A:420:U:C2'	1:A:421:U:H5''	2.45	0.46
21:U:34:ARG:HG3	21:U:35:ARG:H	1.80	0.46
5:E:81:LEU:HB3	5:E:147:MET:HE2	1.97	0.46
1:A:368:U:C6	22:V:362:ARG:HD3	2.50	0.46
1:A:260:G:H2'	1:A:261:U:C6	2.49	0.46
2:B:183:PHE:CE2	2:B:197:PHE:CD2	3.03	0.46
1:A:1044:A:C5	1:A:1045:C:H1'	2.50	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
19:S:36:ARG:HB3	19:S:72:GLY:CA	2.45	0.46
2:B:67:LEU:HD12	2:B:157:PRO:HG2	1.97	0.46
1:A:328:C:O2	1:A:328:C:C2'	2.63	0.46
1:A:1276:G:N3	1:A:1282:C:O2'	2.45	0.46
1:A:1092:A:H5''	7:G:4:ARG:NH2	2.31	0.46
11:K:126:LYS:HE3	11:K:127:ARG:HH21	1.81	0.46
1:A:1005:A:H2'	1:A:1006:G:O4'	2.16	0.46
12:L:87:VAL:C	12:L:89:ASP:H	2.19	0.46
1:A:1533:C:H3'	1:A:1534:A:C5'	2.46	0.46
9:I:12:ARG:HH11	9:I:13:LYS:HB2	1.80	0.46
12:L:79:VAL:HG12	12:L:102:LEU:HD23	1.97	0.46
13:M:68:ASP:HA	13:M:71:ARG:HD3	1.97	0.46
1:A:843:U:O4	1:A:844:G:N2	2.49	0.46
1:A:22:G:C6	1:A:23:C:C4	3.04	0.46
14:N:51:LEU:HB3	14:N:52:PRO:HD2	1.98	0.46
1:A:1182:G:H4'	1:A:1183:U:C5'	2.46	0.46
1:A:398:U:H2'	1:A:399:G:C8	2.50	0.46
22:V:298:ILE:HG23	22:V:304:ASP:HA	1.97	0.46
1:A:539:A:H2'	1:A:540:G:C8	2.50	0.46
11:K:80:LYS:O	11:K:105:PHE:HA	2.15	0.46
19:S:36:ARG:HE	19:S:72:GLY:HA2	1.81	0.46
1:A:7:A:H1'	25:A:1839:HOH:O	2.15	0.46
5:E:114:VAL:HG11	5:E:137:VAL:HG23	1.97	0.46
22:V:586:VAL:HG13	22:V:587:ASP:H	1.80	0.46
1:A:972:C:P	10:J:59:LYS:HD3	2.55	0.46
5:E:46:VAL:HG22	5:E:118:ALA:HA	1.97	0.46
1:A:289:G:OP2	25:A:1888:HOH:O	2.20	0.46
14:N:41:ARG:NH1	14:N:45:VAL:HG21	2.31	0.46
15:O:45:GLU:O	15:O:46:HIS:HB2	2.15	0.46
1:A:747:A:N6	1:A:748:G:O6	2.49	0.46
8:H:106:THR:CG2	8:H:121:LEU:HD13	2.45	0.46
2:B:117:GLU:HA	2:B:120:SER:HB2	1.96	0.46
12:L:59:ASN:H	12:L:59:ASN:HD22	1.64	0.46
2:B:16:GLY:HA3	2:B:40:ILE:HG23	1.98	0.46
3:C:7:PRO:CG	3:C:184:TYR:CG	2.99	0.46
4:D:76:TYR:HE2	4:D:201:VAL:HG13	1.80	0.46
22:V:177:GLU:N	22:V:177:GLU:OE1	2.45	0.46
4:D:31:LYS:HD3	4:D:31:LYS:N	2.31	0.46
14:N:31:ILE:HG23	14:N:45:VAL:HB	1.96	0.46
1:A:668:G:O2'	15:O:46:HIS:ND1	2.46	0.46
1:A:1129:C:H5''	9:I:18:ARG:NH2	2.31	0.46
22:V:127:TRP:CH2	22:V:262:ILE:HD13	2.51	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:141:G:C4	1:A:142:G:C8	3.04	0.46
5:E:83:HIS:CG	8:H:96:MET:HE2	2.51	0.46
4:D:98:LEU:O	4:D:101:VAL:HG12	2.15	0.46
15:O:14:GLU:O	15:O:84:ARG:NH2	2.49	0.46
19:S:63:THR:HG22	19:S:64:ASP:N	2.30	0.46
1:A:625:U:H4'	16:P:16:PHE:CE2	2.51	0.46
11:K:16:VAL:HG13	11:K:17:SER:N	2.31	0.46
11:K:70:CYS:O	11:K:74:VAL:HG22	2.16	0.46
1:A:409:U:H5''	4:D:25:VAL:HG22	1.97	0.46
5:E:104:GLY:HA3	5:E:122:ASN:HA	1.97	0.46
22:V:507:LYS:NZ	22:V:591:LEU:HD12	2.31	0.46
22:V:583:TYR:CE1	22:V:585:ASP:HA	2.51	0.46
17:Q:76:VAL:HG23	17:Q:77:ARG:H	1.79	0.46
2:B:123:GLY:O	2:B:125:PHE:N	2.49	0.46
22:V:62:THR:OG1	24:V:801:GCP:O1G	2.33	0.46
1:A:746:A:H2'	1:A:747:A:C8	2.51	0.46
2:B:72:LYS:HZ2	2:B:204:ASP:HB3	1.81	0.46
1:A:428:G:C5	1:A:430:A:C6	3.04	0.46
7:G:54:SER:O	7:G:56:LYS:N	2.48	0.46
1:A:942:G:O2'	1:A:943:U:H5'	2.16	0.46
9:I:55:VAL:CA	9:I:94:LEU:HD23	2.46	0.45
1:A:481:G:OP1	1:A:481:G:H4'	2.14	0.45
1:A:502:A:H2'	1:A:503:C:C6	2.51	0.45
1:A:986:U:H2'	1:A:987:G:O4'	2.16	0.45
22:V:553:VAL:HG23	22:V:597:ALA:HB2	1.97	0.45
1:A:368:U:C5	22:V:362:ARG:HD3	2.51	0.45
3:C:83:ASP:O	3:C:87:LEU:HG	2.16	0.45
22:V:515:TYR:O	22:V:593:PHE:CZ	2.69	0.45
8:H:38:ASN:HA	8:H:49:PHE:HE1	1.81	0.45
14:N:27:LEU:HB3	14:N:31:ILE:HD12	1.97	0.45
1:A:1123:U:O2'	10:J:39:PRO:O	2.32	0.45
12:L:3:THR:HG22	12:L:5:ASN:H	1.80	0.45
1:A:730:G:O6	15:O:51:HIS:NE2	2.47	0.45
2:B:206:ILE:N	2:B:206:ILE:HD13	2.31	0.45
11:K:71:ALA:HB1	11:K:75:LYS:HD2	1.98	0.45
1:A:723:U:O2'	1:A:724:G:P	2.74	0.45
3:C:22:TRP:NE1	3:C:36:ASP:OD2	2.47	0.45
13:M:68:ASP:O	13:M:71:ARG:HB2	2.17	0.45
4:D:20:PHE:HB3	4:D:23:SER:OG	2.16	0.45
22:V:602:LYS:O	22:V:603:GLU:HB3	2.17	0.45
4:D:124:MET:CE	4:D:146:ARG:HG2	2.46	0.45
4:D:107:PHE:CE2	4:D:145:ILE:HG13	2.51	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:72:A:H2'	1:A:73:C:C5'	2.46	0.45
22:V:105:VAL:HG23	22:V:106:LEU:N	2.32	0.45
1:A:1014:A:N7	1:A:1015:G:C6	2.84	0.45
6:F:64:VAL:HG12	6:F:65:GLU:N	2.32	0.45
1:A:436:C:O2'	4:D:154:ARG:HG3	2.17	0.45
1:A:532:A:N7	3:C:192:THR:OG1	2.34	0.45
1:A:575:G:C6	1:A:821:G:N7	2.85	0.45
1:A:375:U:C4	1:A:376:G:N7	2.85	0.45
1:A:64:G:OP1	1:A:382:A:N6	2.50	0.45
7:G:111:ARG:HD2	7:G:119:ARG:HA	1.98	0.45
9:I:57:MET:CE	9:I:58:VAL:H	2.29	0.45
7:G:147:ALA:HB1	11:K:61:PHE:CE1	2.51	0.45
7:G:54:SER:C	7:G:56:LYS:H	2.19	0.45
1:A:449:G:N1	1:A:450:G:C6	2.85	0.45
3:C:155:GLY:O	3:C:156:ARG:HB2	2.17	0.45
1:A:560:A:H5'	1:A:566:G:N2	2.31	0.45
9:I:26:GLY:N	9:I:59:GLU:O	2.50	0.45
1:A:105:G:H2'	1:A:106:C:C6	2.52	0.45
16:P:23:ASP:OD2	16:P:25:ARG:NE	2.47	0.45
11:K:43:GLY:HA3	11:K:74:VAL:HG11	1.99	0.45
11:K:75:LYS:HE2	11:K:79:ILE:O	2.16	0.45
1:A:42:G:N2	1:A:401:C:C2	2.84	0.45
1:A:204:G:H3'	1:A:205:A:C5'	2.47	0.45
2:B:72:LYS:NZ	2:B:204:ASP:HB3	2.32	0.45
2:B:209:VAL:HG23	2:B:210:THR:N	2.31	0.45
1:A:1237:C:H1'	1:A:1334:G:O2'	2.16	0.45
10:J:48:ARG:NH1	10:J:66:GLU:OE1	2.50	0.45
2:B:140:LEU:O	2:B:143:LEU:N	2.49	0.45
22:V:104:ARG:NH2	22:V:408:ARG:H	2.15	0.45
1:A:913:A:H4'	1:A:914:A:O5'	2.17	0.45
1:A:1331:G:O2'	1:A:1332:A:P	2.74	0.45
1:A:1002:G:N2	1:A:1003:G:N3	2.64	0.45
13:M:29:ARG:NH2	13:M:33:ILE:HD11	2.31	0.45
3:C:20:SER:OG	3:C:40:ARG:NH2	2.49	0.45
21:U:19:PHE:CD1	21:U:19:PHE:O	2.70	0.45
10:J:56:HIS:O	10:J:57:VAL:HG12	2.16	0.45
19:S:34:TRP:CE2	19:S:57:HIS:HE1	2.35	0.45
5:E:39:VAL:HG22	5:E:67:ALA:HB1	1.99	0.45
11:K:101:ASN:HA	11:K:105:PHE:O	2.16	0.45
11:K:81:ASN:HB2	11:K:106:ARG:O	2.17	0.45
11:K:79:ILE:HG23	11:K:81:ASN:O	2.17	0.45
1:A:1087:G:O5'	1:A:1087:G:H8	1.99	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1277:C:O2'	1:A:1279:G:H8	1.99	0.45
1:A:1181:G:O2'	1:A:1182:G:N7	2.50	0.45
11:K:35:THR:HG23	11:K:36:ASP:N	2.31	0.45
3:C:118:ASP:O	3:C:121:THR:HG22	2.17	0.45
10:J:19:ASP:HA	10:J:22:THR:HG22	1.98	0.45
7:G:83:SER:HB2	7:G:85:TYR:CE2	2.52	0.45
13:M:2:ALA:CA	13:M:53:ILE:HD13	2.47	0.45
17:Q:55:ILE:C	17:Q:55:ILE:HD12	2.37	0.45
2:B:57:ASN:HB2	2:B:219:THR:CG2	2.46	0.45
1:A:747:A:N6	1:A:748:G:C6	2.85	0.45
1:A:1070:U:H2'	1:A:1071:C:C6	2.51	0.45
22:V:72:TRP:HB2	22:V:84:ILE:HD11	2.00	0.45
1:A:1171:A:C2	1:A:1172:C:C2	3.05	0.45
1:A:1088:G:H21	1:A:1167:A:N6	2.15	0.45
1:A:173:U:H6	1:A:198:G:HO2'	1.64	0.45
1:A:929:G:C6	1:A:930:C:C4	3.05	0.45
1:A:753:A:H4'	1:A:754:C:O5'	2.17	0.45
14:N:73:PHE:CZ	14:N:78:GLY:HA2	2.52	0.45
17:Q:62:ARG:HG2	17:Q:76:VAL:HG13	1.98	0.44
10:J:59:LYS:HG3	10:J:60:ASP:N	2.32	0.44
18:R:33:ILE:HA	18:R:40:VAL:HG23	1.99	0.44
1:A:441:A:H61	1:A:494:G:H22	1.64	0.44
14:N:20:TYR:O	14:N:23:LYS:HB3	2.16	0.44
22:V:63:ILE:HG21	22:V:468:ILE:HD12	1.99	0.44
17:Q:6:ARG:CZ	17:Q:6:ARG:HB3	2.47	0.44
22:V:197:ASP:O	22:V:199:GLY:N	2.50	0.44
8:H:105:SER:HB2	8:H:126:ILE:HD11	1.99	0.44
5:E:111:MET:HA	5:E:114:VAL:HG13	1.99	0.44
4:D:193:ALA:C	4:D:195:ILE:H	2.21	0.44
8:H:96:MET:SD	8:H:130:ALA:HB1	2.56	0.44
11:K:20:VAL:O	11:K:35:THR:HG22	2.18	0.44
1:A:1526:G:OP1	21:U:39:GLU:HB2	2.17	0.44
1:A:1038:C:H2'	1:A:1039:G:C8	2.52	0.44
18:R:63:ARG:HB3	18:R:70:TYR:CZ	2.52	0.44
9:I:34:SER:O	9:I:37:GLN:N	2.50	0.44
14:N:41:ARG:CG	14:N:42:TRP:N	2.80	0.44
1:A:1244:G:C6	1:A:1245:C:N4	2.86	0.44
1:A:68:G:C6	1:A:69:G:H1'	2.52	0.44
1:A:1413:A:H2'	1:A:1414:U:O4'	2.17	0.44
2:B:49:PHE:HB2	2:B:212:TYR:CE1	2.53	0.44
8:H:78:VAL:HG11	8:H:125:ILE:CD1	2.47	0.44
2:B:89:PHE:HB3	2:B:149:GLY:O	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:N:6:MET:HE2	14:N:63:ARG:HH22	1.82	0.44
3:C:123:GLN:HB3	3:C:128:VAL:HG11	1.99	0.44
7:G:23:LEU:HD21	7:G:47:LEU:HD21	1.99	0.44
1:A:620:C:H1'	4:D:132:ILE:CD1	2.47	0.44
20:T:58:VAL:HG13	20:T:72:ALA:HA	1.99	0.44
15:O:35:GLN:HB3	15:O:59:MET:HE1	2.00	0.44
4:D:161:LEU:HD22	4:D:161:LEU:H	1.82	0.44
1:A:408:A:OP1	4:D:110:THR:HG21	2.17	0.44
1:A:81:A:H5'	1:A:90:C:N4	2.32	0.44
13:M:57:ARG:CA	13:M:60:VAL:HG12	2.47	0.44
6:F:38:ARG:HG2	6:F:39:LEU:N	2.32	0.44
1:A:1314:C:OP2	19:S:6:LYS:HD2	2.17	0.44
6:F:5:GLU:OE2	18:R:24:LYS:HE2	2.17	0.44
19:S:64:ASP:N	19:S:64:ASP:OD1	2.50	0.44
1:A:77:A:H2'	1:A:78:A:H5'	1.99	0.44
1:A:598:U:H4'	8:H:86:TYR:CD2	2.53	0.44
1:A:602:A:H2'	1:A:603:U:C6	2.53	0.44
1:A:1273:C:H2'	1:A:1274:A:O4'	2.17	0.44
1:A:1193:G:OP2	3:C:167:TRP:HH2	2.01	0.44
7:G:95:ARG:NH2	7:G:99:LEU:HD21	2.33	0.44
11:K:68:GLU:C	11:K:70:CYS:H	2.15	0.44
22:V:632:ILE:HG23	22:V:642:LEU:CD2	2.47	0.44
3:C:42:TYR:HD2	3:C:43:LEU:HD12	1.82	0.44
6:F:10:VAL:HG12	6:F:11:HIS:N	2.33	0.44
22:V:227:ALA:HB1	22:V:234:MET:CB	2.48	0.44
1:A:1463:U:H2'	1:A:1464:U:C6	2.52	0.44
5:E:132:ASN:O	5:E:136:VAL:HG12	2.17	0.44
22:V:464:LEU:O	22:V:467:ASP:HB3	2.17	0.44
4:D:13:ARG:HG2	4:D:34:ILE:HA	2.00	0.44
7:G:145:ALA:C	7:G:147:ALA:H	2.20	0.44
22:V:200:VAL:HG23	22:V:201:THR:N	2.32	0.44
1:A:880:C:P	12:L:5:ASN:HD22	2.40	0.44
9:I:120:LYS:O	9:I:121:ALA:HB3	2.17	0.44
21:U:14:VAL:HG23	21:U:16:LEU:HG	1.99	0.44
1:A:1375:A:OP1	7:G:12:ILE:CD1	2.65	0.44
7:G:49:THR:O	7:G:53:ARG:HB2	2.17	0.44
1:A:1006:G:H2'	1:A:1007:U:C6	2.53	0.44
9:I:94:LEU:O	9:I:96:SER:N	2.45	0.44
1:A:72:A:C2'	1:A:73:C:H5''	2.48	0.44
10:J:6:ILE:HB	10:J:76:ILE:HB	2.00	0.44
2:B:30:ILE:CG2	2:B:32:GLY:H	2.31	0.44
2:B:212:TYR:HA	2:B:215:ALA:HB3	2.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:V:110:VAL:HG11	22:V:278:MET:SD	2.58	0.44
12:L:40:THR:HG22	12:L:41:THR:N	2.32	0.44
1:A:636:U:H2'	1:A:637:C:C6	2.53	0.44
22:V:90:PRO:HG2	22:V:98:GLU:HB2	2.00	0.44
1:A:1347:G:N2	1:A:1373:G:H2'	2.33	0.44
7:G:130:ASN:HB2	7:G:135:VAL:CG2	2.48	0.44
22:V:19:ILE:HD12	22:V:92:HIS:HA	1.99	0.44
5:E:114:VAL:CG1	5:E:137:VAL:HG23	2.48	0.44
13:M:114:LYS:CB	13:M:115:PRO:CD	2.96	0.44
1:A:114:U:O2'	1:A:115:G:H5'	2.17	0.44
22:V:666:TYR:CE2	22:V:670:LEU:HD22	2.52	0.44
3:C:129:MET:SD	3:C:132:ARG:HD2	2.58	0.44
1:A:909:A:H2'	1:A:910:C:O4'	2.18	0.44
1:A:1116:U:C4'	9:I:110:GLN:HE22	2.30	0.44
1:A:1026:G:H2'	1:A:1027:C:H5'	1.98	0.44
1:A:460:A:N3	1:A:460:A:H2'	2.33	0.44
7:G:51:ALA:HB1	7:G:57:SER:O	2.17	0.44
8:H:116:ALA:HA	8:H:121:LEU:HD11	2.00	0.44
2:B:86:CYS:C	2:B:88:GLN:H	2.21	0.44
13:M:13:LYS:HE3	13:M:17:ILE:HG22	1.99	0.44
2:B:67:LEU:CD2	2:B:69:VAL:HG13	2.48	0.44
20:T:67:ILE:HG13	20:T:71:LYS:HD3	2.00	0.44
1:A:1530:G:H2'	1:A:1531:A:C8	2.53	0.44
2:B:13:VAL:H	2:B:207:ARG:CZ	2.31	0.44
16:P:20:VAL:HG21	16:P:32:PHE:CG	2.53	0.44
7:G:113:ASP:O	7:G:119:ARG:NH2	2.50	0.43
4:D:29:ASP:OD1	4:D:30:THR:N	2.42	0.43
4:D:107:PHE:CD2	4:D:145:ILE:HG13	2.53	0.43
13:M:57:ARG:HG3	13:M:60:VAL:CG1	2.48	0.43
16:P:43:ALA:O	16:P:44:SER:C	2.56	0.43
17:Q:14:SER:HB3	17:Q:22:VAL:HG22	1.99	0.43
8:H:3:MET:CE	8:H:6:PRO:HA	2.48	0.43
2:B:79:VAL:O	2:B:83:ALA:HB3	2.18	0.43
4:D:60:LYS:HD2	4:D:195:ILE:HG22	2.00	0.43
6:F:26:THR:HG22	6:F:62:MET:HE3	2.00	0.43
13:M:49:SER:HB2	13:M:52:GLN:HB2	2.00	0.43
2:B:148:GLY:C	2:B:150:ILE:H	2.22	0.43
1:A:661:G:C2	1:A:745:G:C2	3.06	0.43
3:C:175:LEU:HD11	3:C:201:TRP:CD1	2.53	0.43
22:V:29:ARG:HA	22:V:29:ARG:NH1	2.33	0.43
1:A:827:U:C4	1:A:870:U:C2	3.06	0.43
21:U:34:ARG:CG	21:U:35:ARG:H	2.31	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:K:75:LYS:C	11:K:78:GLY:H	2.21	0.43
7:G:122:ASN:O	7:G:126:ASP:HB2	2.18	0.43
1:A:746:A:N1	1:A:747:A:N6	2.66	0.43
1:A:842:U:H3'	1:A:843:U:C5'	2.47	0.43
1:A:373:A:C1'	1:A:481:G:H1'	2.49	0.43
11:K:24:HIS:O	11:K:31:ILE:HG23	2.18	0.43
22:V:12:ASN:ND2	22:V:107:ASP:OD2	2.47	0.43
1:A:1240:U:H3'	1:A:1241:G:C5'	2.48	0.43
9:I:30:ILE:CD1	9:I:79:ILE:HD11	2.48	0.43
16:P:48:GLU:OE1	16:P:49:GLY:N	2.47	0.43
2:B:14:HIS:O	2:B:14:HIS:CG	2.71	0.43
9:I:56:ASP:N	9:I:57:MET:SD	2.91	0.43
1:A:922:G:C6	1:A:923:A:C6	3.06	0.43
1:A:267:C:OP2	17:Q:69:LYS:NZ	2.45	0.43
4:D:139:PRO:O	4:D:140:ASN:HB2	2.18	0.43
1:A:1330:U:O4	1:A:1331:G:C6	2.71	0.43
9:I:55:VAL:O	9:I:56:ASP:HB3	2.18	0.43
12:L:24:LEU:HD22	12:L:59:ASN:HB2	2.01	0.43
1:A:69:G:O6	1:A:98:A:N6	2.52	0.43
1:A:1181:G:O2'	1:A:1182:G:C8	2.72	0.43
6:F:26:THR:HG22	6:F:62:MET:CE	2.48	0.43
2:B:187:ASP:HB2	2:B:203:ASP:HB3	2.01	0.43
1:A:792:A:H4'	1:A:793:U:O5'	2.18	0.43
1:A:988:G:H1'	1:A:1015:G:H22	1.84	0.43
1:A:1119:C:OP1	9:I:85:ARG:NH1	2.52	0.43
1:A:543:U:P	4:D:14:ARG:HH21	2.42	0.43
1:A:978:A:C6	1:A:1318:A:C6	3.06	0.43
5:E:80:THR:HB	5:E:122:ASN:HD21	1.84	0.43
21:U:19:PHE:O	21:U:22:SER:HB3	2.18	0.43
2:B:119:GLN:HA	2:B:122:ASP:HB2	2.00	0.43
5:E:46:VAL:HG21	5:E:118:ALA:HB2	2.01	0.43
1:A:1051:C:C4	1:A:1052:U:C4	3.07	0.43
1:A:1163:A:C2	1:A:1174:G:C2	3.07	0.43
6:F:70:VAL:O	6:F:74:LEU:N	2.52	0.43
1:A:390:U:H4'	16:P:28:ARG:NH2	2.33	0.43
1:A:1306:A:H8	1:A:1306:A:O5'	2.02	0.43
22:V:18:HIS:ND1	22:V:122:GLN:HB2	2.33	0.43
2:B:32:GLY:HA2	2:B:39:ILE:HB	2.00	0.43
22:V:583:TYR:HD1	22:V:584:HIS:C	2.22	0.43
1:A:1226:C:P	13:M:90:ARG:HH12	2.42	0.43
5:E:83:HIS:CD2	8:H:96:MET:CE	3.02	0.43
2:B:99:MET:HA	2:B:106:VAL:HG21	1.99	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:122:G:C5	1:A:123:U:C5	3.07	0.43
22:V:505:HIS:O	22:V:506:ALA:HB3	2.19	0.43
18:R:57:ARG:O	18:R:61:ARG:HD2	2.18	0.43
2:B:32:GLY:O	2:B:33:ALA:CB	2.66	0.43
4:D:34:ILE:O	4:D:35:GLU:HB3	2.19	0.43
22:V:255:ARG:HG2	22:V:260:GLU:HB2	2.01	0.43
22:V:660:LEU:O	22:V:662:GLU:N	2.46	0.43
22:V:338:VAL:HG21	22:V:377:VAL:HG12	2.00	0.43
22:V:151:PHE:CE1	22:V:264:VAL:HG12	2.54	0.43
1:A:79:G:O4'	1:A:79:G:P	2.77	0.43
1:A:1305:G:O2'	1:A:1306:A:C8	2.72	0.43
8:H:106:THR:HG22	8:H:107:SER:N	2.34	0.43
12:L:24:LEU:HG	12:L:25:GLU:H	1.84	0.43
1:A:987:G:N2	1:A:1218:C:O2	2.46	0.43
16:P:4:ILE:N	16:P:4:ILE:HD12	2.34	0.43
22:V:549:TYR:CD2	22:V:593:PHE:CD2	3.07	0.43
22:V:657:GLU:OE1	22:V:686:LYS:NZ	2.51	0.43
2:B:98:GLY:C	2:B:100:LEU:H	2.21	0.43
1:A:688:G:C5	1:A:700:G:C2	3.07	0.43
22:V:75:MET:HE1	22:V:202:PHE:HZ	1.83	0.43
1:A:633:G:H2'	1:A:634:C:C6	2.54	0.43
1:A:109:A:C6	1:A:326:G:C6	3.07	0.43
2:B:58:LYS:NZ	2:B:62:ARG:HG3	2.33	0.43
1:A:1330:U:OP1	13:M:24:GLY:N	2.51	0.43
11:K:14:LYS:NZ	11:K:15:GLN:O	2.43	0.43
2:B:32:GLY:O	2:B:33:ALA:HB3	2.19	0.43
1:A:1496:C:C5	1:A:1497:G:C4	3.07	0.43
12:L:44:LYS:HB2	12:L:45:PRO:CD	2.49	0.43
1:A:689:C:OP1	11:K:46:THR:CB	2.66	0.43
13:M:48:LEU:HG	13:M:52:GLN:HB3	2.01	0.43
1:A:930:C:O2'	1:A:931:C:H5'	2.19	0.43
1:A:458:U:H2'	1:A:459:A:C8	2.54	0.43
2:B:61:SER:C	2:B:63:LYS:H	2.22	0.43
12:L:83:ARG:NH2	12:L:96:HIS:CD2	2.87	0.43
9:I:57:MET:HG2	9:I:58:VAL:N	2.34	0.43
1:A:1299:A:H2'	1:A:1299:A:N3	2.33	0.43
3:C:142:MET:HE2	3:C:148:GLY:HA2	2.00	0.43
13:M:10:PRO:O	13:M:11:ASP:HB2	2.19	0.43
9:I:9:THR:HG22	9:I:10:GLY:N	2.34	0.43
4:D:73:ARG:NH1	4:D:77:LYS:HE3	2.34	0.43
1:A:327:A:O2'	1:A:328:C:O4'	2.29	0.43
13:M:48:LEU:HD21	13:M:53:ILE:HA	2.01	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:123:GLN:HB3	3:C:128:VAL:CG1	2.49	0.43
22:V:142:ASN:OD1	22:V:143:LYS:N	2.45	0.43
15:O:41:GLY:O	15:O:44:ALA:HB2	2.19	0.43
15:O:16:GLY:C	15:O:18:ASP:H	2.22	0.43
1:A:981:U:O2'	14:N:61:ARG:NE	2.52	0.42
4:D:102:VAL:HG13	4:D:107:PHE:HB2	2.01	0.42
5:E:111:MET:CE	5:E:125:ALA:HB1	2.49	0.42
2:B:70:GLY:HA2	2:B:163:ILE:CG2	2.49	0.42
18:R:36:SER:HB3	21:U:4:ILE:CG1	2.50	0.42
1:A:1193:G:P	3:C:167:TRP:CH2	3.12	0.42
22:V:416:ILE:HG12	22:V:667:ALA:HB3	2.00	0.42
22:V:627:ASN:ND2	22:V:674:THR:HA	2.34	0.42
17:Q:15:ASP:OD1	17:Q:54:GLY:HA2	2.19	0.42
11:K:122:ARG:NH1	21:U:36:GLU:HG3	2.34	0.42
11:K:13:ARG:O	11:K:14:LYS:HB3	2.19	0.42
21:U:19:PHE:CD1	21:U:19:PHE:C	2.92	0.42
11:K:93:ARG:HH22	21:U:20:LYS:HD2	1.83	0.42
1:A:977:A:O2'	1:A:979:C:OP2	2.35	0.42
1:A:381:C:H2'	1:A:382:A:O4'	2.19	0.42
6:F:78:PHE:CD1	6:F:78:PHE:N	2.86	0.42
1:A:1059:C:O3'	14:N:85:ARG:NH2	2.52	0.42
1:A:1248:A:H4'	9:I:33:ARG:HH12	1.84	0.42
22:V:34:THR:HG21	22:V:70:ALA:CB	2.49	0.42
1:A:160:A:H2'	1:A:161:A:O4'	2.18	0.42
19:S:29:LYS:HB3	19:S:30:PRO:HD2	2.01	0.42
3:C:130:PHE:CG	3:C:131:ARG:N	2.87	0.42
4:D:147:GLU:HA	4:D:150:LYS:HD2	2.01	0.42
22:V:317:PHE:CE1	22:V:343:VAL:CG2	3.02	0.42
14:N:45:VAL:HG23	14:N:46:LEU:H	1.84	0.42
4:D:145:ILE:HG22	4:D:146:ARG:O	2.19	0.42
22:V:4:THR:CG2	22:V:378:ARG:CZ	2.98	0.42
17:Q:75:LEU:HD11	17:Q:77:ARG:O	2.19	0.42
13:M:50:GLU:HA	13:M:53:ILE:HD12	2.01	0.42
1:A:552:U:H5'	12:L:83:ARG:HH11	1.84	0.42
3:C:120:ILE:HD11	3:C:137:ALA:HB2	2.01	0.42
2:B:185:ILE:HA	2:B:199:ILE:HG13	2.01	0.42
12:L:30:LYS:O	12:L:82:ILE:HG22	2.18	0.42
22:V:272:ASN:O	22:V:276:GLN:NE2	2.52	0.42
1:A:1124:G:H3'	1:A:1145:A:N6	2.34	0.42
13:M:10:PRO:O	13:M:11:ASP:CB	2.67	0.42
1:A:1492:A:H5''	1:A:1492:A:N3	2.33	0.42
1:A:1225:A:H2'	1:A:1226:C:C5	2.54	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:I:129:LYS:HG3	9:I:130:ARG:N	2.35	0.42
1:A:328:C:O2	1:A:328:C:H2'	2.19	0.42
1:A:648:A:H2'	1:A:649:A:C8	2.54	0.42
1:A:949:A:OP1	13:M:100:GLN:HG2	2.19	0.42
3:C:126:ARG:HG2	3:C:126:ARG:O	2.20	0.42
13:M:57:ARG:O	13:M:60:VAL:HG12	2.19	0.42
8:H:106:THR:CG2	8:H:121:LEU:HD22	2.49	0.42
13:M:114:LYS:HB3	13:M:115:PRO:HD3	2.02	0.42
22:V:337:ARG:HA	22:V:382:ILE:HG22	2.00	0.42
4:D:174:ASP:O	4:D:175:ALA:HB2	2.19	0.42
1:A:293:G:C6	1:A:294:U:C4	3.08	0.42
2:B:41:ASN:ND2	2:B:44:LYS:HB2	2.34	0.42
11:K:86:VAL:HG21	21:U:17:ARG:HH22	1.84	0.42
1:A:1116:U:C3'	9:I:110:GLN:HE22	2.33	0.42
1:A:71:A:C2	1:A:72:A:C4	3.08	0.42
25:A:1839:HOH:O	5:E:126:LYS:HD2	2.20	0.42
4:D:36:GLN:O	4:D:37:ALA:HB2	2.20	0.42
22:V:586:VAL:HG22	22:V:587:ASP:H	1.84	0.42
19:S:3:ARG:O	19:S:4:SER:HB2	2.19	0.42
1:A:1059:C:O2'	10:J:53:ILE:O	2.34	0.42
1:A:16:A:C2'	1:A:17:U:H5'	2.50	0.42
15:O:39:LEU:O	15:O:42:HIS:N	2.53	0.42
8:H:59:LEU:HD21	8:H:61:LEU:HD21	2.02	0.42
9:I:50:GLN:N	9:I:51:PRO:HD2	2.35	0.42
11:K:100:LEU:HG	11:K:105:PHE:CB	2.50	0.42
1:A:42:G:HO2'	1:A:622:A:H2	1.65	0.42
1:A:1151:A:C2	1:A:1152:A:C5	3.07	0.42
13:M:60:VAL:CG2	13:M:65:VAL:HG12	2.49	0.42
22:V:632:ILE:HG23	22:V:642:LEU:HD22	2.01	0.42
1:A:1496:C:H2'	1:A:1497:G:O4'	2.19	0.42
1:A:35:G:H2'	1:A:36:C:C6	2.54	0.42
1:A:1284:C:C5	1:A:1285:A:C8	3.08	0.42
12:L:36:ARG:HD3	12:L:38:TYR:HE1	1.84	0.42
1:A:689:C:OP1	11:K:46:THR:OG1	2.37	0.42
1:A:142:G:H2'	1:A:142:G:N3	2.34	0.42
13:M:2:ALA:N	13:M:53:ILE:HD13	2.34	0.42
9:I:30:ILE:CD1	9:I:79:ILE:CD1	2.98	0.42
22:V:193:TRP:CH2	22:V:276:GLN:HB2	2.55	0.42
1:A:1343:G:H4'	9:I:124:ARG:HB3	2.00	0.42
2:B:18:GLN:HG2	2:B:189:ASN:OD1	2.20	0.42
1:A:270:A:H2'	1:A:271:C:C6	2.55	0.42
4:D:106:GLY:HA3	4:D:162:ALA:CB	2.50	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:204:TYR:CD1	4:D:204:TYR:N	2.86	0.42
15:O:46:HIS:C	15:O:48:LYS:N	2.72	0.42
22:V:342:VAL:HG22	22:V:378:ARG:HD2	2.01	0.42
4:D:182:PHE:HZ	4:D:186:PRO:HD3	1.84	0.42
7:G:4:ARG:O	7:G:6:VAL:N	2.50	0.42
22:V:627:ASN:C	22:V:629:GLY:H	2.23	0.42
9:I:20:PHE:CD2	9:I:64:TYR:HD2	2.37	0.42
1:A:1233:G:H2'	1:A:1234:C:C6	2.54	0.42
1:A:1216:A:H2'	1:A:1217:C:H6	1.84	0.42
17:Q:65:ARG:HG3	17:Q:66:PRO:HD2	2.02	0.42
1:A:31:G:H5'	1:A:306:A:C2	2.54	0.42
7:G:50:LEU:CD1	7:G:61:ALA:HB1	2.50	0.42
21:U:49:LYS:C	21:U:51:SER:N	2.73	0.42
1:A:1035:A:C8	1:A:1036:A:C8	3.07	0.42
1:A:858:G:O2'	1:A:859:G:H5'	2.20	0.42
1:A:858:G:C2'	1:A:859:G:H5'	2.49	0.42
1:A:1469:C:H2'	1:A:1470:U:C5'	2.50	0.42
1:A:1323:G:C6	1:A:1324:A:N6	2.88	0.42
4:D:87:GLY:HA2	4:D:201:VAL:HG21	2.01	0.42
22:V:4:THR:HG21	22:V:378:ARG:HG3	2.01	0.42
9:I:129:LYS:CG	9:I:130:ARG:H	2.31	0.42
7:G:46:ALA:O	7:G:50:LEU:HB2	2.19	0.42
6:F:98:GLU:HG3	6:F:99:ALA:N	2.35	0.42
1:A:1057:G:O3'	3:C:197:GLY:HA3	2.20	0.42
11:K:125:LYS:HZ1	21:U:36:GLU:H	1.68	0.42
8:H:106:THR:HG22	8:H:108:LYS:H	1.85	0.42
1:A:1264:U:H2'	1:A:1265:C:H6	1.85	0.42
1:A:1171:A:H2'	1:A:1172:C:C6	2.54	0.42
22:V:227:ALA:HB1	22:V:234:MET:HB2	2.01	0.42
1:A:270:A:C5	1:A:271:C:C4	3.07	0.42
22:V:218:TRP:N	22:V:218:TRP:CD1	2.86	0.42
14:N:9:ARG:O	14:N:13:ARG:HG3	2.19	0.42
2:B:52:ALA:O	2:B:56:LEU:HB2	2.20	0.42
1:A:946:A:O2'	1:A:1333:A:O2'	1.95	0.41
1:A:981:U:H5	1:A:982:U:HO2'	1.63	0.41
14:N:26:GLU:HG3	14:N:27:LEU:HD12	2.02	0.41
4:D:105:MET:HG2	4:D:171:LEU:HD13	2.01	0.41
11:K:55:SER:HA	11:K:57:LYS:NZ	2.34	0.41
22:V:4:THR:HG22	22:V:378:ARG:HG3	2.02	0.41
20:T:28:MET:O	20:T:32:ILE:HG13	2.20	0.41
21:U:14:VAL:CG2	21:U:16:LEU:HG	2.50	0.41
8:H:80:ARG:HH21	8:H:83:LEU:CB	2.33	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:85:ASN:HA	5:E:102:GLY:HA2	2.02	0.41
19:S:15:LEU:HD13	19:S:33:THR:HG21	2.02	0.41
19:S:41:PHE:HB3	19:S:42:PRO:HD2	2.02	0.41
1:A:938:A:C6	1:A:939:G:C5	3.08	0.41
22:V:20:ASP:O	22:V:21:ALA:HB3	2.20	0.41
1:A:1102:A:H2'	1:A:1103:C:C6	2.55	0.41
17:Q:14:SER:HB3	17:Q:22:VAL:CG2	2.50	0.41
10:J:92:LEU:O	10:J:93:ALA:CB	2.68	0.41
2:B:119:GLN:NE2	2:B:136:ARG:NH2	2.69	0.41
2:B:199:ILE:O	2:B:199:ILE:HG13	2.20	0.41
1:A:264:C:H4'	17:Q:65:ARG:HD2	2.02	0.41
1:A:414:A:H2'	1:A:415:A:O4'	2.20	0.41
6:F:81:ASN:OD1	6:F:83:ALA:N	2.49	0.41
1:A:1157:A:C6	1:A:1180:A:C6	3.08	0.41
1:A:807:A:C5	1:A:808:C:C4	3.08	0.41
10:J:8:ILE:CD1	10:J:76:ILE:HD11	2.49	0.41
13:M:14:HIS:HB2	13:M:17:ILE:HD12	2.01	0.41
18:R:32:TYR:HE2	18:R:47:THR:HG21	1.85	0.41
8:H:10:MET:HE1	8:H:33:LYS:HA	2.00	0.41
22:V:320:LEU:HD23	22:V:321:ALA:N	2.35	0.41
1:A:570:G:H1'	1:A:820:U:C4	2.55	0.41
4:D:168:PRO:HG2	4:D:171:LEU:HD11	2.03	0.41
1:A:71:A:N6	1:A:100:G:N7	2.68	0.41
1:A:72:A:H2'	1:A:73:C:H5'	2.02	0.41
1:A:658:C:O4'	15:O:22:THR:OG1	2.38	0.41
1:A:484:G:N7	1:A:486:U:H1'	2.35	0.41
9:I:34:SER:HB3	9:I:37:GLN:HG2	2.02	0.41
3:C:130:PHE:CE1	3:C:157:LEU:HD23	2.56	0.41
11:K:110:ILE:HG22	21:U:17:ARG:NH1	2.35	0.41
1:A:892:A:O2'	1:A:1415:G:H4'	2.20	0.41
1:A:1249:C:O2'	9:I:75:GLN:OE1	2.33	0.41
22:V:71:PHE:CE1	22:V:83:ARG:HG3	2.55	0.41
2:B:166:ASP:OD2	2:B:190:SER:HA	2.20	0.41
15:O:17:ARG:HH12	15:O:77:ARG:NH1	2.18	0.41
22:V:532:LYS:C	22:V:534:TYR:H	2.23	0.41
1:A:1404:C:H2'	1:A:1405:G:C8	2.55	0.41
1:A:1008:U:H2'	1:A:1009:U:H6	1.85	0.41
22:V:222:LEU:O	22:V:226:ALA:N	2.50	0.41
16:P:42:ILE:HG22	16:P:43:ALA:N	2.34	0.41
2:B:20:ARG:C	2:B:22:TRP:N	2.74	0.41
12:L:73:ASN:ND2	12:L:103:ASP:O	2.51	0.41
6:F:51:ILE:CG2	6:F:85:ILE:HD12	2.50	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:V:557:ILE:HG21	22:V:576:ILE:HD12	2.01	0.41
17:Q:59:VAL:CG2	17:Q:75:LEU:CD1	2.98	0.41
14:N:52:PRO:O	14:N:55:SER:HB3	2.21	0.41
12:L:38:TYR:HD2	12:L:52:VAL:HG23	1.86	0.41
13:M:48:LEU:HD21	13:M:52:GLN:C	2.41	0.41
19:S:41:PHE:CE1	19:S:67:VAL:O	2.73	0.41
1:A:1321:U:C4	1:A:1322:C:C5	3.08	0.41
9:I:91:ASP:CG	9:I:93:SER:HB3	2.41	0.41
20:T:51:PHE:C	20:T:51:PHE:CD1	2.94	0.41
11:K:81:ASN:HB3	11:K:106:ARG:O	2.18	0.41
9:I:94:LEU:O	9:I:98:LEU:N	2.48	0.41
1:A:1083:U:C5	1:A:1084:G:C6	3.09	0.41
1:A:1012:A:C6	1:A:1013:G:C6	3.09	0.41
22:V:645:GLN:O	22:V:646:GLU:C	2.59	0.41
4:D:192:SER:O	4:D:193:ALA:HB2	2.21	0.41
20:T:62:ALA:CA	20:T:67:ILE:HG22	2.51	0.41
1:A:591:U:C2	1:A:592:G:C8	3.09	0.41
20:T:42:GLY:O	20:T:44:LYS:N	2.53	0.41
10:J:11:LYS:CG	10:J:97:ASP:HB3	2.50	0.41
17:Q:5:ILE:O	17:Q:5:ILE:HG13	2.20	0.41
3:C:162:ILE:HD12	3:C:162:ILE:O	2.21	0.41
1:A:1236:A:H1'	1:A:1333:A:N1	2.36	0.41
1:A:1134:G:C2	1:A:1135:U:C2	3.08	0.41
1:A:978:A:C4	1:A:1319:A:C2	3.09	0.41
16:P:46:LYS:CG	16:P:47:GLU:H	2.30	0.41
12:L:43:LYS:HG2	12:L:44:LYS:H	1.84	0.41
3:C:7:PRO:HG2	3:C:184:TYR:CD2	2.55	0.41
10:J:50:THR:CG2	10:J:64:GLN:HG2	2.50	0.41
1:A:1181:G:O2'	1:A:1182:G:C5	2.69	0.41
11:K:92:GLY:O	11:K:96:THR:HB	2.21	0.41
3:C:14:ILE:O	3:C:15:VAL:HG22	2.21	0.41
22:V:338:VAL:O	22:V:380:GLY:N	2.39	0.41
22:V:5:THR:HG23	22:V:6:PRO:HD3	2.03	0.41
1:A:56:U:H2'	1:A:57:G:C8	2.56	0.41
1:A:57:G:C6	1:A:58:C:C4	3.09	0.41
15:O:6:GLU:HG3	15:O:7:ALA:N	2.36	0.41
1:A:1028:C:C5	1:A:1029:U:C2	3.08	0.41
1:A:1306:A:C6	1:A:1331:G:H1'	2.56	0.41
4:D:145:ILE:HD11	4:D:155:VAL:HG21	2.03	0.41
1:A:1086:U:O2'	1:A:1087:G:H5'	2.19	0.41
2:B:19:THR:HG23	2:B:36:LYS:O	2.20	0.41
1:A:452:A:H3'	1:A:452:A:C8	2.56	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:J:57:VAL:HG22	10:J:58:ASN:H	1.85	0.41
22:V:33:TYR:CE1	22:V:199:GLY:HA3	2.56	0.41
2:B:44:LYS:HE3	2:B:48:MET:HE2	2.03	0.41
15:O:72:ARG:NH2	15:O:73:LYS:HE2	2.35	0.41
11:K:89:PRO:HB3	21:U:29:LEU:HD13	2.03	0.41
19:S:66:MET:SD	19:S:74:PHE:HZ	2.42	0.41
1:A:460:A:N1	1:A:462:G:C8	2.89	0.41
1:A:868:C:N4	1:A:869:G:C2	2.89	0.41
13:M:29:ARG:HH22	13:M:33:ILE:HD11	1.86	0.41
13:M:29:ARG:NH1	13:M:33:ILE:HD11	2.36	0.41
10:J:87:LEU:O	10:J:91:ASP:OD2	2.39	0.41
3:C:22:TRP:HB3	3:C:59:ARG:HB2	2.03	0.41
17:Q:59:VAL:CG2	17:Q:75:LEU:HD13	2.50	0.41
8:H:10:MET:HG3	8:H:27:MET:SD	2.60	0.41
22:V:488:VAL:HG21	22:V:661:SER:HB3	2.02	0.41
22:V:85:ASN:ND2	22:V:382:ILE:HG13	2.35	0.41
1:A:1284:C:C5	1:A:1285:A:H8	2.39	0.41
6:F:21:MET:HE2	6:F:21:MET:HB3	1.84	0.41
20:T:68:HIS:HB3	20:T:69:LYS:NZ	2.36	0.41
12:L:63:VAL:HG21	12:L:95:TYR:CE1	2.55	0.41
21:U:14:VAL:CG2	21:U:16:LEU:CD2	2.99	0.41
9:I:30:ILE:HA	9:I:65:ILE:O	2.21	0.41
1:A:949:A:H1'	1:A:1364:U:C5	2.56	0.41
11:K:23:ILE:HD11	11:K:86:VAL:HG22	2.01	0.41
2:B:217:ALA:O	2:B:221:ARG:HB2	2.21	0.41
1:A:429:U:O3'	4:D:22:LYS:NZ	2.54	0.41
1:A:200:G:N2	1:A:218:U:C2	2.89	0.41
22:V:498:VAL:CG2	22:V:608:ALA:HB2	2.51	0.41
22:V:504:LYS:HA	22:V:516:GLY:O	2.20	0.41
1:A:672:U:H2'	1:A:673:A:C8	2.55	0.41
9:I:57:MET:CG	9:I:58:VAL:H	2.34	0.41
22:V:585:ASP:O	22:V:586:VAL:CB	2.68	0.41
12:L:25:GLU:HB2	12:L:27:CYS:SG	2.61	0.41
12:L:36:ARG:HD3	12:L:38:TYR:CE1	2.56	0.41
1:A:701:U:H4'	1:A:702:A:O5'	2.20	0.41
19:S:63:THR:CG2	19:S:64:ASP:N	2.84	0.41
1:A:1193:G:P	3:C:167:TRP:HH2	2.45	0.41
6:F:74:LEU:HG	6:F:78:PHE:CZ	2.56	0.41
1:A:707:U:H2'	1:A:708:C:C6	2.55	0.41
1:A:263:A:OP1	20:T:74:ARG:NH1	2.49	0.41
4:D:125:VAL:O	4:D:127:GLY:N	2.49	0.41
1:A:33:A:H2'	1:A:34:C:C6	2.56	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:26:A:N6	1:A:558:G:O2'	2.47	0.41
9:I:35:LEU:HG	9:I:36:GLU:N	2.36	0.41
7:G:75:VAL:HG11	7:G:144:MET:HG3	2.01	0.41
13:M:9:ILE:HG13	13:M:9:ILE:O	2.21	0.40
13:M:33:ILE:HD13	13:M:59:GLU:HB3	2.04	0.40
20:T:62:ALA:HB1	20:T:69:LYS:H	1.84	0.40
22:V:188:MET:HE3	22:V:218:TRP:CD1	2.57	0.40
1:A:1185:G:C6	1:A:1186:G:C5	3.09	0.40
12:L:99:ARG:HB2	12:L:117:TYR:HA	2.03	0.40
1:A:920:U:H2'	1:A:921:U:C6	2.56	0.40
14:N:28:LYS:HA	14:N:31:ILE:HB	2.03	0.40
13:M:57:ARG:O	13:M:61:ALA:N	2.54	0.40
20:T:85:LYS:C	20:T:87:ALA:H	2.25	0.40
14:N:20:TYR:O	14:N:24:ARG:N	2.54	0.40
8:H:59:LEU:HD21	8:H:61:LEU:CD2	2.52	0.40
6:F:97:THR:O	6:F:98:GLU:HG2	2.21	0.40
21:U:29:LEU:C	21:U:29:LEU:HD23	2.41	0.40
1:A:520:A:N1	1:A:536:C:H1'	2.36	0.40
8:H:64:LYS:HB3	8:H:71:VAL:HG21	2.02	0.40
1:A:959:A:O2'	1:A:984:C:O2'	2.35	0.40
3:C:134:MET:SD	3:C:153:VAL:CG1	3.09	0.40
1:A:1459:G:C6	1:A:1460:C:C4	3.09	0.40
7:G:97:ASN:OD1	7:G:97:ASN:N	2.55	0.40
16:P:78:VAL:O	16:P:78:VAL:HG12	2.21	0.40
9:I:84:THR:HG21	9:I:103:PHE:HB3	2.03	0.40
1:A:1033:G:C2'	1:A:1034:G:H5'	2.49	0.40
1:A:1508:A:H2'	1:A:1509:C:O4'	2.22	0.40
2:B:32:GLY:CA	2:B:39:ILE:H	2.31	0.40
1:A:476:U:O2'	1:A:477:C:H5'	2.22	0.40
11:K:107:ILE:HG12	21:U:12:PHE:HZ	1.87	0.40
18:R:55:LEU:O	18:R:59:ILE:N	2.32	0.40
13:M:34:LEU:CD1	13:M:41:GLU:HA	2.51	0.40
22:V:407:GLU:O	22:V:408:ARG:HB3	2.22	0.40
1:A:1051:C:H5"	22:V:543:GLY:HA3	2.02	0.40
4:D:147:GLU:O	4:D:148:LYS:C	2.59	0.40
3:C:47:LEU:CD1	3:C:68:ILE:HD13	2.51	0.40
22:V:578:LEU:HD13	22:V:579:HIS:H	1.86	0.40
22:V:212:VAL:O	22:V:216:ASN:N	2.50	0.40
1:A:781:A:C4	1:A:802:A:C2	3.09	0.40
20:T:20:HIS:CE1	20:T:24:ARG:HD3	2.57	0.40
1:A:1188:A:H2'	1:A:1189:U:O4'	2.21	0.40
1:A:188:C:H2'	1:A:189:A:O4'	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:V:421:GLU:O	22:V:481:ALA:HB1	2.21	0.40
4:D:59:GLN:O	4:D:63:ARG:HG3	2.21	0.40
18:R:34:THR:HG22	18:R:38:LYS:O	2.22	0.40
1:A:1252:A:H61	1:A:1285:A:N6	2.20	0.40
1:A:654:G:C2	1:A:753:A:C4	3.09	0.40
1:A:1193:G:OP1	3:C:167:TRP:CH2	2.74	0.40
1:A:1034:G:N2	1:A:1035:A:C6	2.89	0.40
4:D:105:MET:HB3	4:D:107:PHE:HE1	1.85	0.40
19:S:36:ARG:C	19:S:38:SER:H	2.25	0.40
10:J:40:ILE:HB	10:J:73:LEU:HB3	2.03	0.40
1:A:1392:G:C5	1:A:1393:U:C5	3.10	0.40
22:V:24:THR:OG1	22:V:88:ASP:OD2	2.39	0.40
7:G:18:PHE:CE1	7:G:58:GLU:HG2	2.56	0.40
1:A:158:G:H2'	1:A:159:G:C5'	2.52	0.40
1:A:661:G:N3	1:A:745:G:N2	2.70	0.40
22:V:30:ILE:O	22:V:34:THR:HG22	2.21	0.40
3:C:191:THR:HG21	3:C:196:ILE:HD12	2.03	0.40
1:A:662:U:H2'	1:A:663:A:C8	2.56	0.40
20:T:4:ILE:HG22	20:T:4:ILE:O	2.21	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 X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	216/241 (90%)	149 (69%)	55 (26%)	12 (6%)	3	8
3	C	204/233 (88%)	183 (90%)	16 (8%)	5 (2%)	9	32
4	D	203/206 (98%)	159 (78%)	35 (17%)	9 (4%)	4	15
5	E	148/167 (89%)	122 (82%)	22 (15%)	4 (3%)	8	30
6	F	98/135 (73%)	75 (76%)	18 (18%)	5 (5%)	3	10
7	G	149/179 (83%)	122 (82%)	25 (17%)	2 (1%)	18	54
8	H	127/130 (98%)	111 (87%)	16 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	125/130 (96%)	98 (78%)	21 (17%)	6 (5%)	4	12
10	J	96/103 (93%)	73 (76%)	19 (20%)	4 (4%)	4	16
11	K	115/129 (89%)	87 (76%)	24 (21%)	4 (4%)	6	23
12	L	121/124 (98%)	97 (80%)	15 (12%)	9 (7%)	2	4
13	M	112/118 (95%)	91 (81%)	14 (12%)	7 (6%)	2	6
14	N	92/101 (91%)	70 (76%)	20 (22%)	2 (2%)	10	37
15	O	86/89 (97%)	70 (81%)	14 (16%)	2 (2%)	10	36
16	P	80/82 (98%)	61 (76%)	15 (19%)	4 (5%)	3	11
17	Q	78/84 (93%)	57 (73%)	16 (20%)	5 (6%)	2	6
18	R	53/75 (71%)	43 (81%)	10 (19%)	0	100	100
19	S	77/92 (84%)	68 (88%)	9 (12%)	0	100	100
20	T	83/87 (95%)	68 (82%)	14 (17%)	1 (1%)	19	57
21	U	49/71 (69%)	24 (49%)	22 (45%)	3 (6%)	2	7
22	V	685/704 (97%)	556 (81%)	91 (13%)	38 (6%)	3	8
All	All	2997/3280 (91%)	2384 (80%)	491 (16%)	122 (4%)	4	17

All (122) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	40	ILE
2	B	72	LYS
2	B	119	GLN
3	C	101	ILE
4	D	25	VAL
4	D	29	ASP
4	D	35	GLU
4	D	175	ALA
4	D	193	ALA
6	F	98	GLU
7	G	130	ASN
9	I	121	ALA
9	I	129	LYS
10	J	28	THR
10	J	57	VAL
10	J	93	ALA
11	K	81	ASN
12	L	24	LEU

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Mol	Chain	Res	Type
12	L	34	CYS
12	L	44	LYS
12	L	76	GLU
12	L	78	SER
13	M	4	ILE
13	M	11	ASP
13	M	66	GLU
13	M	114	LYS
16	P	44	SER
17	Q	13	VAL
17	Q	51	ASN
17	Q	53	CYS
20	T	4	ILE
21	U	11	PRO
22	V	5	THR
22	V	7	ILE
22	V	24	THR
22	V	93	VAL
22	V	94	ASP
22	V	195	ASP
22	V	198	GLN
22	V	200	VAL
22	V	204	TYR
22	V	300	ASP
22	V	304	ASP
22	V	409	MET
22	V	423	LYS
22	V	454	ASN
22	V	506	ALA
22	V	527	PRO
22	V	544	VAL
22	V	586	VAL
22	V	647	SER
2	B	17	HIS
2	B	33	ALA
2	B	75	ALA
2	B	163	ILE
4	D	36	GLN
4	D	125	VAL
5	E	110	ALA
5	E	138	ARG
5	E	158	GLY

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Mol	Chain	Res	Type
9	I	58	VAL
11	K	41	ALA
11	K	69	ARG
12	L	3	THR
12	L	88	LYS
14	N	92	GLU
15	O	18	ASP
15	O	46	HIS
16	P	42	ILE
22	V	118	GLY
22	V	197	ASP
22	V	202	PHE
22	V	509	SER
22	V	649	VAL
22	V	662	GLU
22	V	698	VAL
3	C	61	ALA
6	F	56	LYS
7	G	146	GLU
12	L	123	LYS
13	M	105	ASN
16	P	80	LYS
17	Q	52	GLU
22	V	500	ASP
2	B	21	TYR
2	B	135	MET
3	C	66	VAL
5	E	102	GLY
6	F	94	HIS
6	F	99	ALA
9	I	120	LYS
10	J	74	VAL
12	L	74	LEU
13	M	5	ALA
13	M	47	GLU
17	Q	6	ARG
21	U	38	TYR
22	V	305	THR
22	V	323	LYS
22	V	408	ARG
22	V	413	GLU
22	V	646	GLU

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Mol	Chain	Res	Type
22	V	648	GLU
2	B	200	PRO
3	C	146	ALA
4	D	37	ALA
6	F	7	VAL
9	I	107	ASP
11	K	17	SER
16	P	77	GLU
22	V	308	GLU
22	V	550	ILE
9	I	96	SER
14	N	62	ASN
22	V	6	PRO
2	B	32	GLY
3	C	15	VAL
21	U	27	GLY
2	B	154	GLY
4	D	168	PRO
22	V	91	GLY
22	V	120	GLN

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 X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	180/199 (90%)	170 (94%)	10 (6%)	30	66
3	C	170/190 (90%)	164 (96%)	6 (4%)	48	85
4	D	172/173 (99%)	163 (95%)	9 (5%)	32	71
5	E	113/126 (90%)	106 (94%)	7 (6%)	26	61
6	F	87/116 (75%)	85 (98%)	2 (2%)	63	92
7	G	124/147 (84%)	123 (99%)	1 (1%)	89	97
8	H	104/105 (99%)	98 (94%)	6 (6%)	28	65
9	I	105/107 (98%)	99 (94%)	6 (6%)	29	66
10	J	86/90 (96%)	83 (96%)	3 (4%)	48	85
11	K	90/99 (91%)	82 (91%)	8 (9%)	14	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	103/104 (99%)	94 (91%)	9 (9%)	15	41
13	M	92/96 (96%)	92 (100%)	0	100	100
14	N	79/84 (94%)	77 (98%)	2 (2%)	60	91
15	O	76/77 (99%)	74 (97%)	2 (3%)	59	90
16	P	65/65 (100%)	63 (97%)	2 (3%)	52	88
17	Q	74/78 (95%)	69 (93%)	5 (7%)	22	55
18	R	48/65 (74%)	48 (100%)	0	100	100
19	S	70/79 (89%)	67 (96%)	3 (4%)	40	78
20	T	65/66 (98%)	60 (92%)	5 (8%)	18	47
21	U	44/61 (72%)	42 (96%)	2 (4%)	38	77
22	V	557/578 (96%)	507 (91%)	50 (9%)	14	39
All	All	2504/2705 (93%)	2366 (94%)	138 (6%)	30	68

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	49	PHE
2	B	56	LEU
2	B	63	LYS
2	B	94	ARG
2	B	124	THR
2	B	143	LEU
2	B	174	GLU
2	B	186	VAL
2	B	206	ILE
2	B	207	ARG
3	C	3	GLN
3	C	14	ILE
3	C	29	PHE
3	C	121	THR
3	C	144	LEU
3	C	153	VAL
4	D	32	CYS
4	D	33	LYS
4	D	48	LEU
4	D	73	ARG
4	D	93	LEU
4	D	101	VAL

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Mol	Chain	Res	Type
4	D	146	ARG
4	D	161	LEU
4	D	198	HIS
5	E	70	ASN
5	E	72	ILE
5	E	114	VAL
5	E	115	LEU
5	E	136	VAL
5	E	148	ASN
5	E	153	VAL
6	F	7	VAL
6	F	55	HIS
7	G	22	LEU
8	H	67	GLN
8	H	77	ARG
8	H	90	ASP
8	H	94	LYS
8	H	99	LEU
8	H	121	LEU
9	I	14	SER
9	I	38	TYR
9	I	46	MET
9	I	57	MET
9	I	63	LEU
9	I	88	MET
10	J	57	VAL
10	J	92	LEU
10	J	102	LEU
11	K	31	ILE
11	K	57	LYS
11	K	70	CYS
11	K	74	VAL
11	K	82	LEU
11	K	96	THR
11	K	97	ILE
11	K	125	LYS
12	L	7	LEU
12	L	14	ARG
12	L	20	ASN
12	L	29	GLN
12	L	33	VAL
12	L	59	ASN

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Mol	Chain	Res	Type
12	L	78	SER
12	L	90	LEU
12	L	102	LEU
14	N	31	ILE
14	N	85	ARG
15	O	64	ARG
15	O	87	LEU
16	P	1	MET
16	P	6	LEU
17	Q	28	PHE
17	Q	33	ILE
17	Q	38	ILE
17	Q	55	ILE
17	Q	61	ILE
19	S	13	LEU
19	S	23	VAL
19	S	64	ASP
20	T	12	ILE
20	T	49	LYS
20	T	51	PHE
20	T	54	MET
20	T	69	LYS
21	U	20	LYS
21	U	34	ARG
22	V	5	THR
22	V	19	ILE
22	V	23	LYS
22	V	29	ARG
22	V	77	LYS
22	V	83	ARG
22	V	95	PHE
22	V	96	THR
22	V	101	ARG
22	V	104	ARG
22	V	106	LEU
22	V	160	THR
22	V	182	VAL
22	V	200	VAL
22	V	202	PHE
22	V	204	TYR
22	V	220	GLN
22	V	232	GLU

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Mol	Chain	Res	Type
22	V	254	GLN
22	V	266	CYS
22	V	286	LEU
22	V	303	LYS
22	V	336	PHE
22	V	370	LYS
22	V	409	MET
22	V	418	ILE
22	V	431	MET
22	V	446	ARG
22	V	482	ASN
22	V	487	GLN
22	V	488	VAL
22	V	494	ILE
22	V	504	LYS
22	V	508	GLN
22	V	512	ARG
22	V	515	TYR
22	V	522	MET
22	V	532	LYS
22	V	555	LYS
22	V	578	LEU
22	V	594	LYS
22	V	602	LYS
22	V	618	LYS
22	V	646	GLU
22	V	660	LEU
22	V	675	LYS
22	V	677	ARG
22	V	681	THR
22	V	685	LEU
22	V	699	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	57	ASN
4	D	116	GLN
7	G	52	GLN
9	I	81	HIS
9	I	110	GLN
10	J	56	HIS

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Mol	Chain	Res	Type
11	K	81	ASN
11	K	109	ASN
12	L	59	ASN
12	L	96	HIS
15	O	40	GLN
19	S	52	HIS
19	S	57	HIS
20	T	20	HIS
22	V	55	GLN
22	V	122	GLN
22	V	465	HIS
22	V	579	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1532/1542 (99%)	273 (17%)	18 (1%)

All (273) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	5	U
1	A	7	A
1	A	9	G
1	A	32	A
1	A	39	G
1	A	40	C
1	A	47	C
1	A	48	C
1	A	51	A
1	A	52	C
1	A	70	U
1	A	71	A
1	A	72	A
1	A	73	C
1	A	75	G
1	A	76	G
1	A	77	A
1	A	78	A
1	A	79	G

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Mol	Chain	Res	Type
1	A	80	A
1	A	81	A
1	A	82	G
1	A	83	C
1	A	85	U
1	A	86	G
1	A	89	U
1	A	90	C
1	A	92	U
1	A	98	A
1	A	116	A
1	A	121	U
1	A	122	G
1	A	130	A
1	A	131	A
1	A	141	G
1	A	143	A
1	A	144	G
1	A	159	G
1	A	163	C
1	A	164	G
1	A	166	U
1	A	173	U
1	A	177	G
1	A	182	A
1	A	183	C
1	A	191	G
1	A	205	A
1	A	208	U
1	A	209	U
1	A	210	C
1	A	211	G
1	A	240	G
1	A	245	U
1	A	247	G
1	A	251	G
1	A	258	G
1	A	266	G
1	A	267	C
1	A	273	U
1	A	285	C
1	A	289	G

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Mol	Chain	Res	Type
1	A	321	A
1	A	328	C
1	A	329	A
1	A	330	C
1	A	332	G
1	A	344	A
1	A	345	C
1	A	346	G
1	A	347	G
1	A	352	C
1	A	354	G
1	A	367	U
1	A	372	C
1	A	373	A
1	A	384	G
1	A	392	C
1	A	406	G
1	A	408	A
1	A	411	A
1	A	412	A
1	A	413	G
1	A	421	U
1	A	423	G
1	A	424	G
1	A	429	U
1	A	430	A
1	A	435	A
1	A	441	A
1	A	452	A
1	A	455	G
1	A	457	G
1	A	458	U
1	A	459	A
1	A	461	A
1	A	462	G
1	A	463	U
1	A	466	A
1	A	467	U
1	A	468	A
1	A	481	G
1	A	482	A
1	A	484	G

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Mol	Chain	Res	Type
1	A	485	U
1	A	486	U
1	A	497	G
1	A	498	A
1	A	500	G
1	A	508	U
1	A	509	A
1	A	511	C
1	A	518	C
1	A	521	G
1	A	527	G
1	A	532	A
1	A	533	A
1	A	547	A
1	A	556	C
1	A	559	A
1	A	562	U
1	A	564	C
1	A	572	A
1	A	573	A
1	A	576	C
1	A	577	G
1	A	579	A
1	A	588	G
1	A	596	A
1	A	604	G
1	A	650	G
1	A	653	U
1	A	665	A
1	A	675	A
1	A	702	A
1	A	721	G
1	A	723	U
1	A	724	G
1	A	731	G
1	A	748	G
1	A	755	G
1	A	777	A
1	A	793	U
1	A	794	A
1	A	802	A
1	A	815	A

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Mol	Chain	Res	Type
1	A	817	C
1	A	828	U
1	A	829	G
1	A	841	C
1	A	843	U
1	A	845	A
1	A	846	G
1	A	859	G
1	A	902	G
1	A	914	A
1	A	926	G
1	A	927	G
1	A	932	C
1	A	934	C
1	A	935	A
1	A	960	U
1	A	966	G
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	983	A
1	A	993	G
1	A	1003	G
1	A	1004	A
1	A	1008	U
1	A	1018	G
1	A	1022	A
1	A	1027	C
1	A	1029	U
1	A	1030	U
1	A	1031	C
1	A	1033	G
1	A	1034	G
1	A	1037	C
1	A	1050	G
1	A	1054	C
1	A	1065	U
1	A	1066	C
1	A	1086	U

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Mol	Chain	Res	Type
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1102	A
1	A	1104	G
1	A	1108	G
1	A	1124	G
1	A	1125	U
1	A	1130	A
1	A	1133	G
1	A	1135	U
1	A	1136	C
1	A	1137	C
1	A	1139	G
1	A	1142	G
1	A	1159	U
1	A	1160	G
1	A	1167	A
1	A	1168	U
1	A	1169	A
1	A	1181	G
1	A	1182	G
1	A	1183	U
1	A	1196	A
1	A	1197	A
1	A	1202	U
1	A	1212	U
1	A	1213	A
1	A	1226	C
1	A	1227	A
1	A	1238	A
1	A	1240	U
1	A	1249	C
1	A	1250	A
1	A	1253	G
1	A	1256	A
1	A	1279	G
1	A	1280	A
1	A	1286	U
1	A	1287	A
1	A	1292	G
1	A	1293	C

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Mol	Chain	Res	Type
1	A	1299	A
1	A	1302	C
1	A	1303	C
1	A	1305	G
1	A	1316	G
1	A	1317	C
1	A	1318	A
1	A	1322	C
1	A	1323	G
1	A	1332	A
1	A	1336	C
1	A	1337	G
1	A	1346	A
1	A	1353	G
1	A	1364	U
1	A	1371	G
1	A	1380	U
1	A	1398	A
1	A	1406	U
1	A	1411	C
1	A	1412	C
1	A	1419	G
1	A	1441	A
1	A	1446	A
1	A	1452	C
1	A	1453	G
1	A	1454	G
1	A	1469	C
1	A	1470	U
1	A	1476	A
1	A	1487	G
1	A	1492	A
1	A	1493	A
1	A	1494	G
1	A	1497	G
1	A	1499	A
1	A	1503	A
1	A	1506	U
1	A	1517	G
1	A	1519	A
1	A	1529	G
1	A	1530	G

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Mol	Chain	Res	Type
1	A	1534	A

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	51	A
1	A	80	A
1	A	115	G
1	A	250	A
1	A	429	U
1	A	484	G
1	A	499	A
1	A	701	U
1	A	913	A
1	A	1030	U
1	A	1049	U
1	A	1101	A
1	A	1136	C
1	A	1201	A
1	A	1331	G
1	A	1336	C
1	A	1451	U
1	A	1452	C

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 45 ligands modelled in this entry, 44 are monoatomic - leaving 1 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	$\# Z > 2$
24	GCP	V	801	23	34,34,34	2.46	9 (26%)	51,54,54	2.38	9 (17%)

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
24	GCP	V	801	23	-	0/20/38/38	0/1/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	V	801	GCP	C2-N2	8.18	1.45	1.32
24	V	801	GCP	C2'-C1'	-5.14	1.46	1.53
24	V	801	GCP	PG-C3B	4.71	1.83	1.79
24	V	801	GCP	O4'-C1'	4.57	1.48	1.41
24	V	801	GCP	PB-C3B	4.17	1.83	1.79
24	V	801	GCP	C2'-C3'	-3.85	1.42	1.53
24	V	801	GCP	C1'-N9	-2.57	1.40	1.48
24	V	801	GCP	C3'-C4'	-2.45	1.46	1.53
24	V	801	GCP	O4'-C4'	2.02	1.49	1.45

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	V	801	GCP	C6-C5-N7	-8.47	133.00	134.14
24	V	801	GCP	C4'-O4'-C1'	-6.18	103.03	109.75
24	V	801	GCP	N3-C4-N9	5.19	134.53	126.91
24	V	801	GCP	PB-C3B-PG	-4.89	110.58	117.62
24	V	801	GCP	PA-O3A-PB	-4.52	118.16	131.74
24	V	801	GCP	O4'-C1'-N9	4.17	112.32	108.44
24	V	801	GCP	C2-N3-C4	4.05	120.78	115.09
24	V	801	GCP	C5-C4-N3	-3.83	120.39	125.94
24	V	801	GCP	C3'-C2'-C1'	3.57	106.50	100.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1533/1542 (99%)	-0.16	12 (0%) 83 89	15, 41, 72, 90	0
2	B	218/241 (90%)	-0.72	2 (0%) 81 88	33, 51, 67, 73	0
3	C	206/233 (88%)	-0.64	2 (0%) 79 86	21, 40, 56, 66	0
4	D	205/206 (99%)	0.04	18 (8%) 10 13	25, 47, 61, 79	0
5	E	150/167 (89%)	-0.46	2 (1%) 74 82	21, 37, 54, 67	0
6	F	100/135 (74%)	-0.60	1 (1%) 79 86	31, 51, 64, 71	0
7	G	151/179 (84%)	-0.46	3 (1%) 62 71	32, 48, 62, 68	0
8	H	129/130 (99%)	-0.55	2 (1%) 68 78	23, 35, 51, 69	0
9	I	127/130 (97%)	-0.39	1 (0%) 83 89	29, 55, 70, 75	0
10	J	98/103 (95%)	-0.58	0 100 100	30, 51, 69, 78	0
11	K	117/129 (90%)	-0.44	4 (3%) 43 51	23, 50, 70, 74	0
12	L	123/124 (99%)	-0.24	7 (5%) 23 28	21, 37, 55, 63	0
13	M	114/118 (96%)	-0.36	5 (4%) 33 40	42, 63, 72, 75	0
14	N	96/101 (95%)	-0.16	4 (4%) 35 41	27, 47, 64, 70	0
15	O	88/89 (98%)	-0.49	2 (2%) 57 66	22, 39, 53, 70	0
16	P	82/82 (100%)	-0.57	1 (1%) 75 83	22, 39, 62, 71	0
17	Q	80/84 (95%)	-0.36	2 (2%) 54 64	27, 41, 51, 57	0
18	R	55/75 (73%)	-0.28	3 (5%) 24 29	26, 40, 55, 64	0
19	S	79/92 (85%)	-0.36	4 (5%) 27 33	43, 58, 70, 74	0
20	T	85/87 (97%)	0.08	7 (8%) 12 15	23, 38, 53, 56	0
21	U	51/71 (71%)	0.24	6 (11%) 5 7	40, 57, 67, 71	0
22	V	689/704 (97%)	-0.32	25 (3%) 41 48	32, 56, 70, 80	0
All	All	4576/4822 (94%)	-0.31	113 (2%) 56 64	15, 46, 69, 90	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	2	ALA	12.0
7	G	83	SER	5.4
4	D	77	LYS	5.1
7	G	81	GLY	4.9
13	M	100	GLN	4.8
15	O	58	ARG	4.8
13	M	98	ARG	4.8
8	H	2	SER	4.8
21	U	30	ALA	4.7
22	V	461	MET	4.7
22	V	126	VAL	4.4
22	V	451	GLU	4.3
4	D	66	GLY	4.2
12	L	16	VAL	4.1
20	T	16	LYS	4.1
4	D	21	LEU	4.1
21	U	36	GLU	4.0
22	V	246	ALA	4.0
2	B	131	LYS	3.9
22	V	352	SER	3.9
20	T	32	ILE	3.9
22	V	125	THR	3.9
1	A	1323	G	3.9
4	D	4	TYR	3.7
21	U	34	ARG	3.7
22	V	353	VAL	3.7
15	O	54	ARG	3.6
22	V	396	THR	3.6
18	R	71	THR	3.5
21	U	31	GLU	3.5
22	V	351	ASN	3.5
12	L	19	SER	3.4
4	D	129	VAL	3.4
1	A	1253	G	3.4
11	K	126	LYS	3.4
22	V	546	PRO	3.3
22	V	414	PRO	3.3
22	V	300	ASP	3.3
4	D	98	LEU	3.3
12	L	84	GLY	3.2
4	D	99	ASP	3.2
22	V	669	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
22	V	359	ARG	3.1
11	K	129	VAL	3.1
3	C	163	ALA	3.0
12	L	86	ARG	3.0
22	V	16	SER	3.0
22	V	607	LYS	3.0
4	D	206	LYS	3.0
20	T	29	ARG	2.9
4	D	7	PRO	2.8
17	Q	26	GLU	2.8
18	R	74	HIS	2.8
1	A	587	G	2.8
4	D	128	ARG	2.7
20	T	13	GLN	2.7
1	A	1018	G	2.7
13	M	35	ALA	2.7
4	D	3	ARG	2.7
18	R	72	ASP	2.7
22	V	37	ASN	2.7
20	T	11	ALA	2.7
14	N	15	ALA	2.7
22	V	123	SER	2.6
19	S	69	HIS	2.6
1	A	1155	A	2.6
6	F	50	PRO	2.6
19	S	66	MET	2.6
22	V	368	ALA	2.6
11	K	116	ILE	2.4
13	M	82	ASP	2.4
4	D	36	GLN	2.4
21	U	33	ARG	2.4
11	K	117	PRO	2.4
22	V	391	VAL	2.4
14	N	28	LYS	2.3
20	T	33	LYS	2.3
22	V	392	THR	2.3
5	E	139	ALA	2.3
3	C	162	ILE	2.3
12	L	23	ALA	2.3
1	A	970	C	2.3
4	D	80	ALA	2.3
1	A	877	G	2.3

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Mol	Chain	Res	Type	RSRZ
14	N	17	ALA	2.3
1	A	1320	C	2.3
1	A	1403	C	2.3
19	S	3	ARG	2.2
4	D	65	TYR	2.2
12	L	24	LEU	2.2
12	L	85	GLY	2.2
21	U	32	VAL	2.2
5	E	92	SER	2.2
20	T	14	SER	2.2
14	N	25	ALA	2.2
22	V	555	LYS	2.2
4	D	75	TYR	2.1
1	A	552	U	2.1
22	V	589	SER	2.1
2	B	166	ASP	2.1
8	H	76	GLN	2.1
4	D	163	GLU	2.1
17	Q	43	LYS	2.1
9	I	32	GLN	2.1
1	A	1402	C	2.1
7	G	93	PRO	2.0
4	D	71	GLN	2.0
13	M	97	VAL	2.0
1	A	510	A	2.0
22	V	332	ASN	2.0
16	P	10	GLY	2.0
22	V	415	VAL	2.0
19	S	72	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
23	MG	A	1601	1/1	0.48	28.43	38,38,38,38	0
23	MG	A	1621	1/1	0.32	19.00	29,29,29,29	0
23	MG	A	1609	1/1	0.21	7.35	29,29,29,29	0
23	MG	A	1605	1/1	0.26	6.63	39,39,39,39	0
23	MG	A	1634	1/1	0.23	5.46	24,24,24,24	0
23	MG	A	1613	1/1	0.16	4.23	41,41,41,41	0
23	MG	T	101	1/1	0.30	4.18	41,41,41,41	0
23	MG	A	1604	1/1	0.28	2.18	27,27,27,27	0
23	MG	A	1633	1/1	0.28	2.05	52,52,52,52	0
23	MG	A	1629	1/1	0.39	1.78	17,17,17,17	0
23	MG	A	1603	1/1	0.13	1.62	38,38,38,38	0
23	MG	A	1627	1/1	0.17	1.54	24,24,24,24	0
23	MG	A	1640	1/1	0.21	1.52	15,15,15,15	0
23	MG	A	1639	1/1	0.18	1.34	20,20,20,20	0
23	MG	A	1628	1/1	0.15	1.04	30,30,30,30	0
23	MG	A	1619	1/1	0.14	0.65	34,34,34,34	0
23	MG	A	1638	1/1	0.15	0.07	26,26,26,26	0
23	MG	A	1622	1/1	0.15	0.00	36,36,36,36	0
23	MG	A	1632	1/1	0.13	-0.19	25,25,25,25	0
23	MG	A	1626	1/1	0.13	-0.37	32,32,32,32	0
23	MG	A	1612	1/1	0.11	-0.38	8,8,8,8	0
24	GCP	V	801	32/32	0.11	-0.62	24,48,54,56	0
23	MG	A	1625	1/1	0.13	-0.86	22,22,22,22	0
23	MG	A	1635	1/1	0.10	-1.00	17,17,17,17	0
23	MG	A	1606	1/1	0.13	-1.00	17,17,17,17	0
23	MG	A	1637	1/1	0.10	-1.08	47,47,47,47	0
23	MG	A	1610	1/1	0.09	-1.27	13,13,13,13	0
23	MG	A	1611	1/1	0.10	-1.33	20,20,20,20	0
23	MG	A	1602	1/1	0.12	-1.48	48,48,48,48	0
23	MG	A	1608	1/1	0.11	-1.88	14,14,14,14	0
23	MG	A	1617	1/1	0.11	-1.94	62,62,62,62	0
23	MG	A	1623	1/1	0.10	-2.05	18,18,18,18	0
23	MG	A	1616	1/1	0.10	-2.45	33,33,33,33	0
23	MG	A	1630	1/1	0.09	-2.46	40,40,40,40	0
23	MG	A	1631	1/1	0.08	-3.42	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	MG	A	1615	1/1	0.09	-3.43	38,38,38,38	0
23	MG	A	1607	1/1	0.10	-4.29	11,11,11,11	0
23	MG	V	802	1/1	0.05	-4.31	38,38,38,38	0
23	MG	E	201	1/1	0.09	-4.82	39,39,39,39	0
23	MG	A	1636	1/1	0.05	-5.89	21,21,21,21	0
23	MG	A	1618	1/1	0.05	-6.03	19,19,19,19	0
23	MG	A	1614	1/1	0.07	-12.27	37,37,37,37	0
23	MG	A	1624	1/1	0.06	-16.09	14,14,14,14	0
23	MG	C	401	1/1	0.69	-	49,49,49,49	0
23	MG	A	1620	1/1	0.03	-	14,14,14,14	0

6.5 Other polymers ⓘ

There are no such residues in this entry.