



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:20 AM UTC

PDB ID : 4GKK / pdb_00004gkk
Title : Structure of the *Thermus thermophilus* 30S ribosomal subunit complexed with a human mitochondrial anticodon stem loop (ASL) of transfer RNA Methionine (TRNAMET) bound to an mRNA with an AUA-codon in the A-site and paromomycin
Authors : Cantara, W.A.; Murphy IV, F.V.; Spears, J.L.; Demirci, H.; Agris, P.F.
Deposited on : 2012-08-11
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references](#) ①) were used in the production of this report:

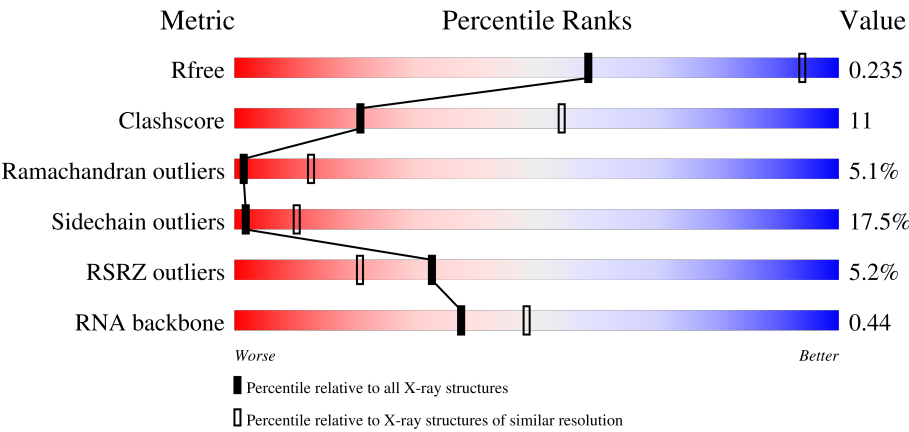
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1513	2% 56%34%9% .
2	B	234	6% 50%38%11% .
3	C	206	7% 53%38%8% .
4	D	208	13% 54%34%11%

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Mol	Chain	Length	Quality of chain
5	E	150	
6	F	101	
7	G	155	
8	H	138	
9	I	127	
10	J	98	
11	K	119	
12	L	124	
13	M	125	
14	N	60	
15	O	88	
16	P	83	
17	Q	104	
18	R	73	
19	S	80	
20	T	99	
21	V	24	
22	W	6	
23	X	17	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	RSQ	X	34	-	-	X	-
24	MG	A	1628	-	-	-	X
24	MG	A	1648	-	-	-	X
24	MG	A	1656	-	-	-	X
24	MG	A	1671	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	MG	A	1674	-	-	-	X
24	MG	A	1677	-	-	-	X
24	MG	A	1678	-	-	-	X
24	MG	A	1717	-	-	-	X
24	MG	A	1723	-	-	-	X
24	MG	A	1724	-	-	-	X
24	MG	A	1730	-	-	-	X
24	MG	A	1731	-	-	-	X
24	MG	A	1752	-	-	-	X
24	MG	A	1762	-	-	-	X

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 52188 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	1513	Total	C	N	O	P	22	0	0
			32515	14472	6016	10514	1513			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1005	C	-	expression tag	GB 48256
A	1013	G	-	expression tag	GB 48256
A	1225	C	-	expression tag	GB 48256
A	1226	A	-	expression tag	GB 48256
A	1517	U	C	conflict	GB 48256
A	1519	U	C	conflict	GB 48256

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- 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
			1612	1016	314	281	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- 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
			1146	724	217	201	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	0	0	0
			1011	639	198	174			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	58	ARG	HIS	conflict	UNP P80374

- 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
			794	499	156	138	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- 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
			734	459	147	126	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	96	GLN	GLU	conflict	UNP Q5SHP7

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	73	Total	C	N	O	0	0	0
			597	380	118	99			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	60	GLY	ALA	conflict	UNP Q5SLQ0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	80	Total	C	N	O	S	0	0	0
			647	414	119	112	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	41	VAL	ILE	conflict	UNP P80380

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	V	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 22 is a RNA chain called mRNA A-site fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	W	4	Total	C	N	O	P	0	0	0
			86	39	17	26	4			

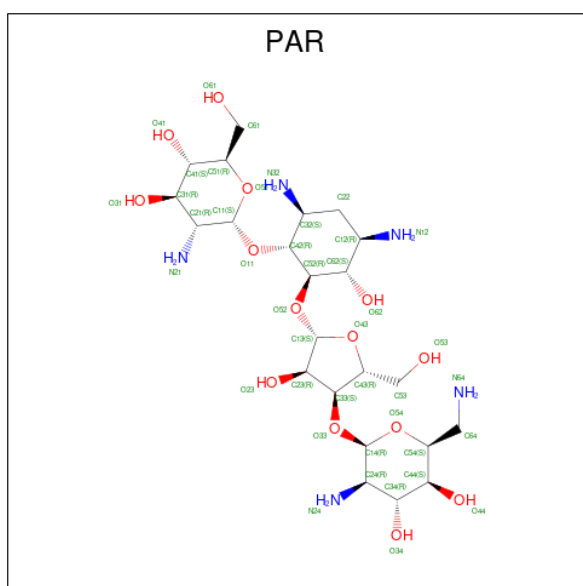
- Molecule 23 is a RNA chain called tRNA ASL human mitochondrial Met.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	X	6	Total	C	N	O	P	0	0	0
			126	57	21	42	6			

- Molecule 24 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	184	Total	Mg	0	0
			184	184		
24	B	1	Total	Mg	0	0
			1	1		
24	T	1	Total	Mg	0	0
			1	1		

- Molecule 25 is PAROMOMYCIN (CCD ID: PAR) (formula: C₂₃H₄₅N₅O₁₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			42	23	5	14		

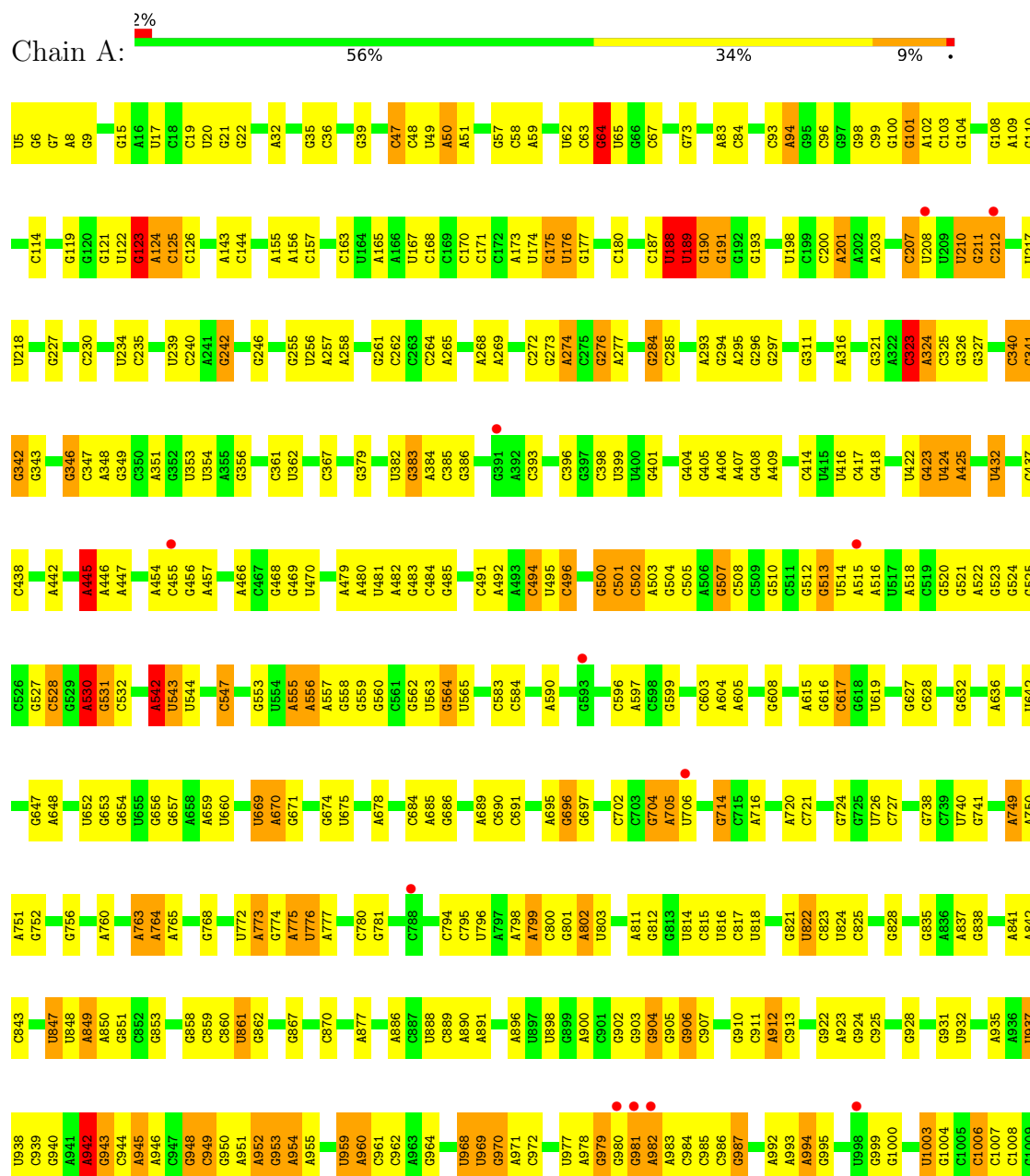
- Molecule 26 is ZINC ION (CCD ID: ZN) (formula: Zn).

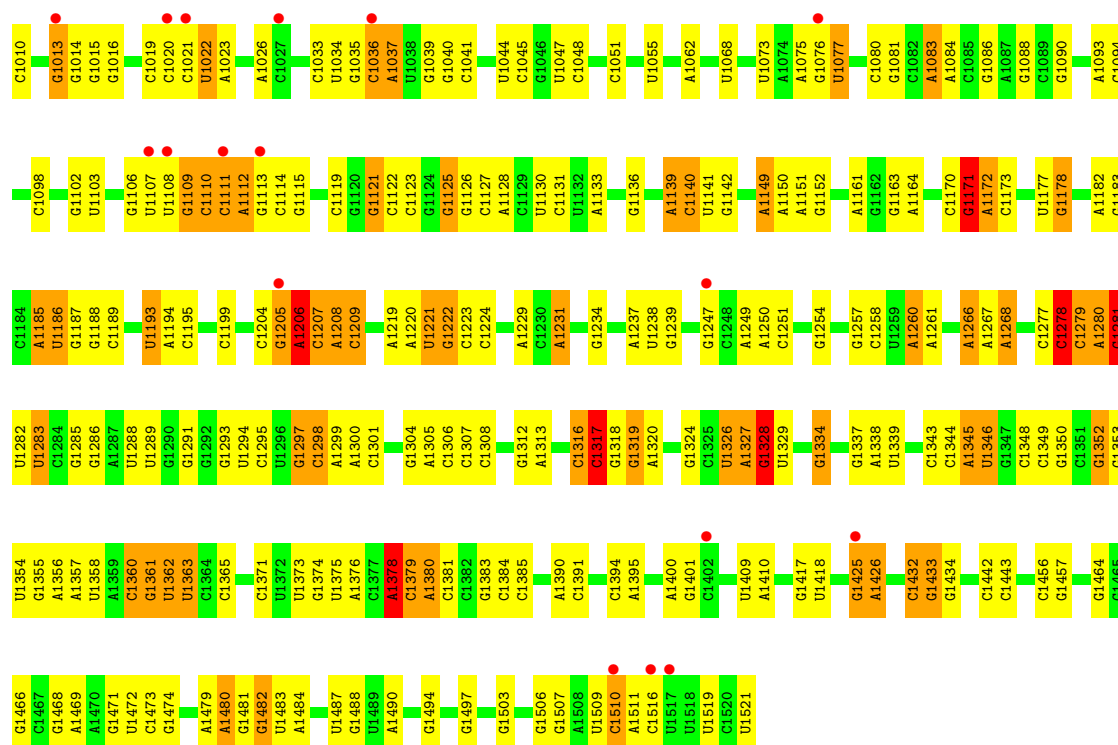
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	D	1	Total	Zn	0	0
			1	1		
26	N	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

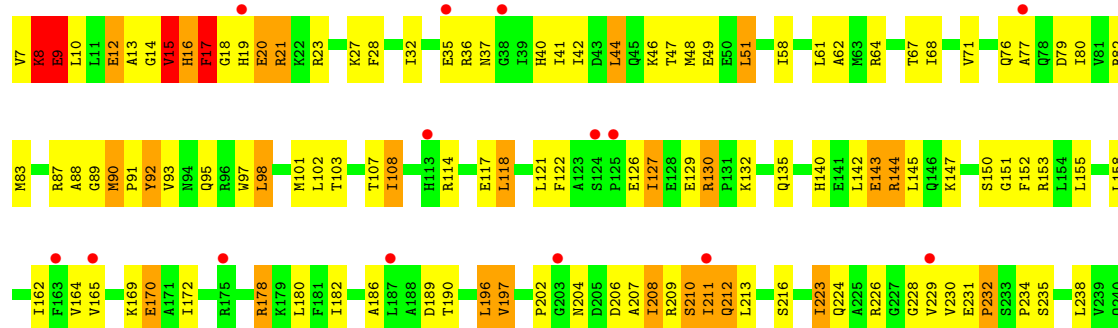
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

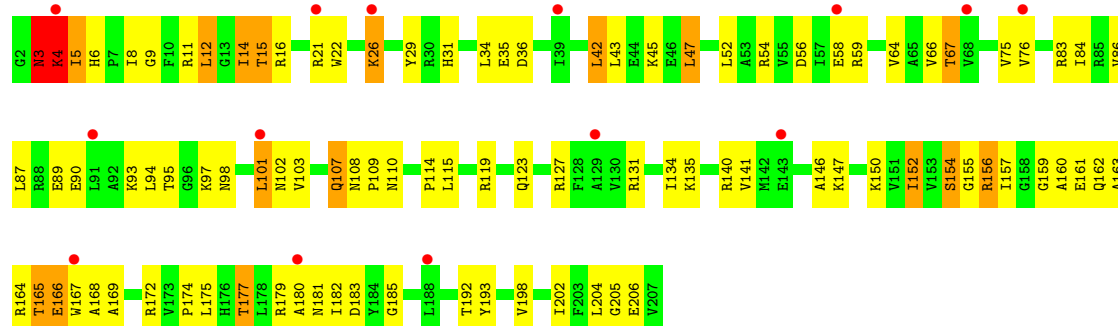




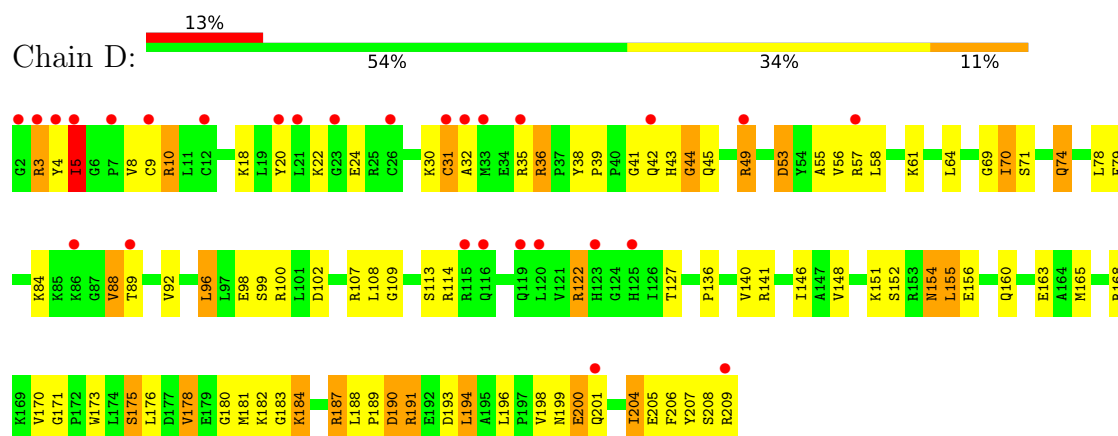
• Molecule 2: 30S ribosomal protein S2



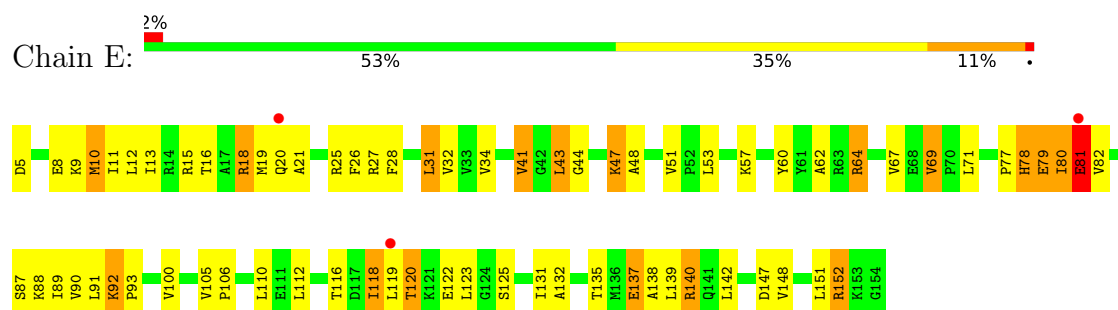
• Molecule 3: 30S ribosomal protein S3



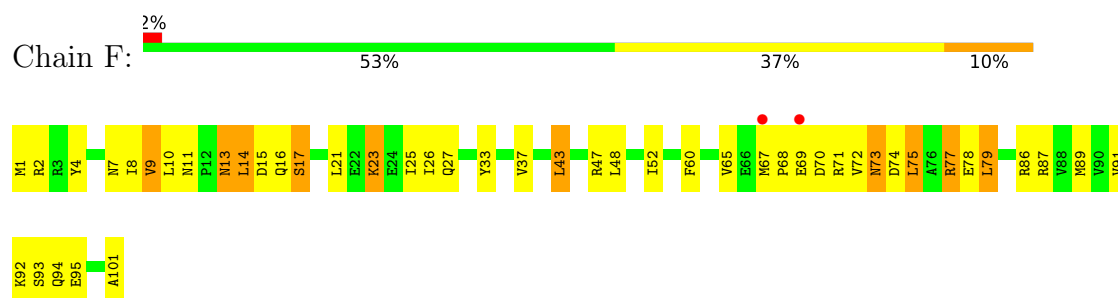
- Molecule 4: 30S ribosomal protein S4



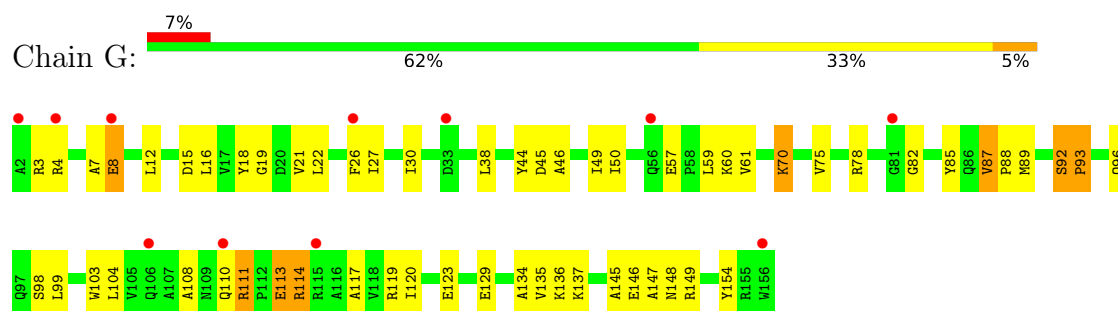
- Molecule 5: 30S ribosomal protein S5



- Molecule 6: 30S ribosomal protein S6

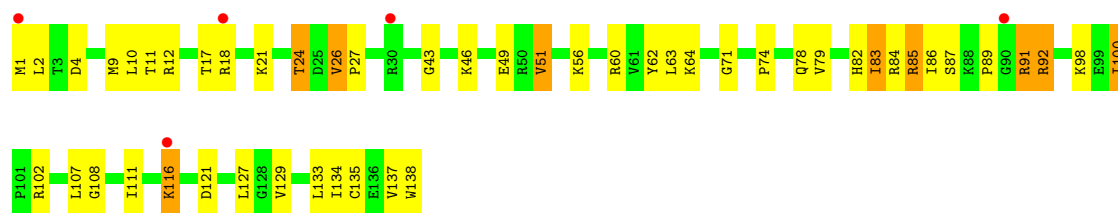


- Molecule 7: 30S ribosomal protein S7

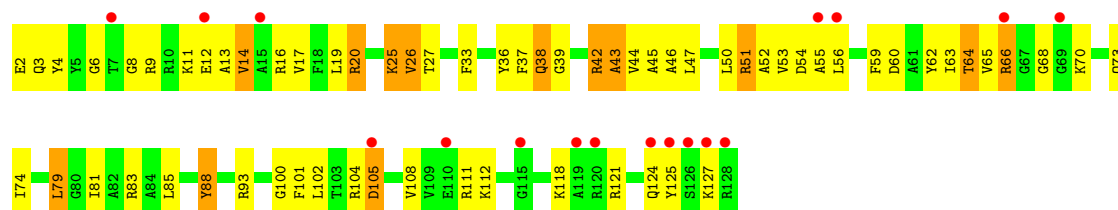


- Molecule 8: 30S ribosomal protein S8

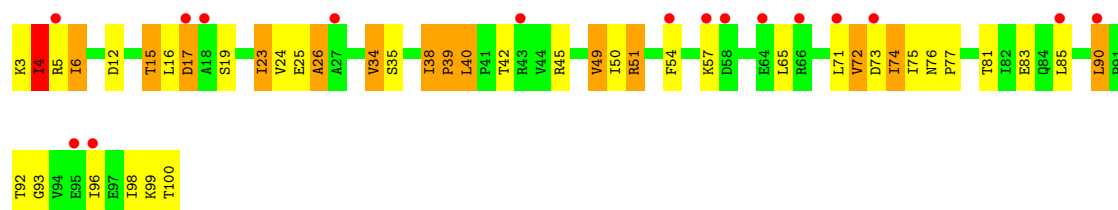




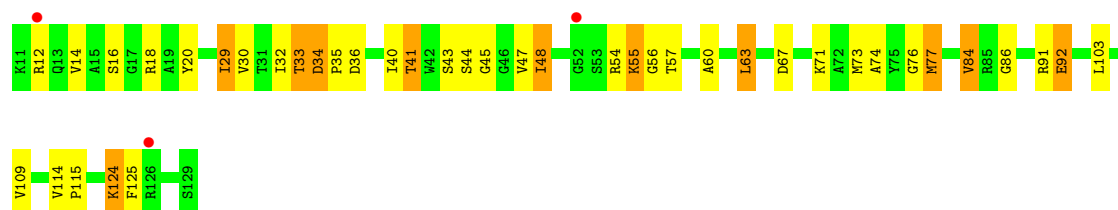
• Molecule 9: 30S ribosomal protein S9



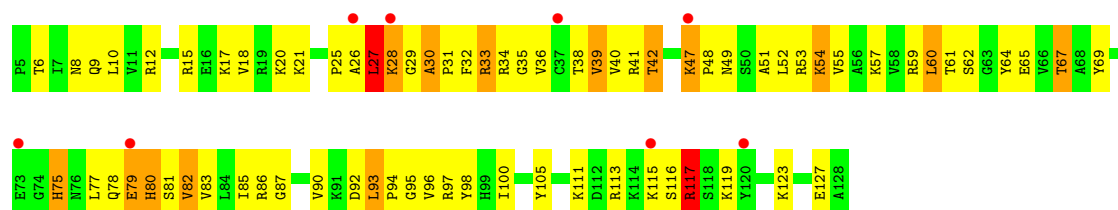
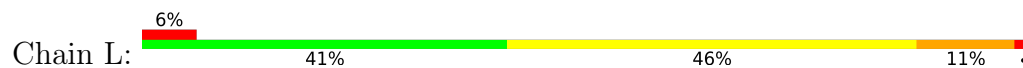
• Molecule 10: 30S ribosomal protein S10



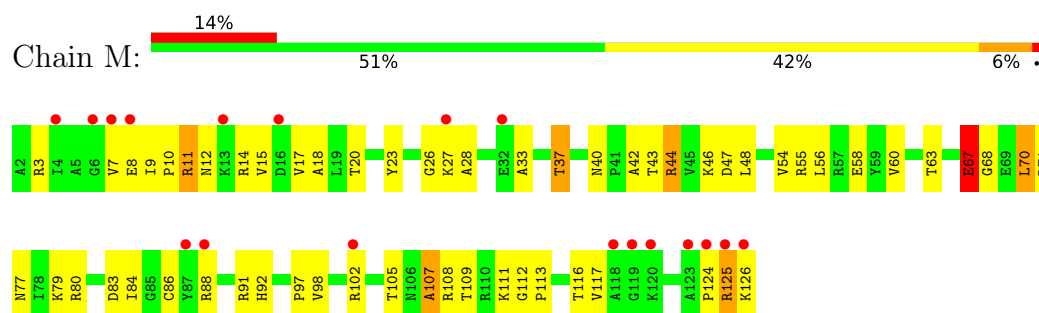
• Molecule 11: 30S ribosomal protein S11



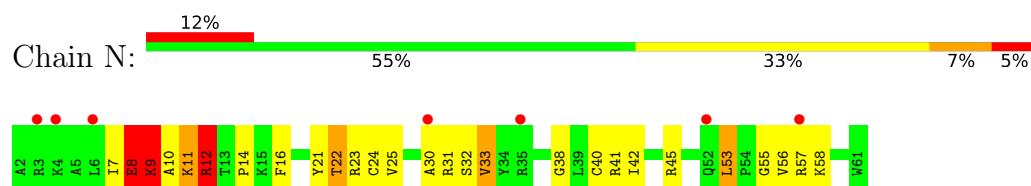
• Molecule 12: 30S ribosomal protein S12



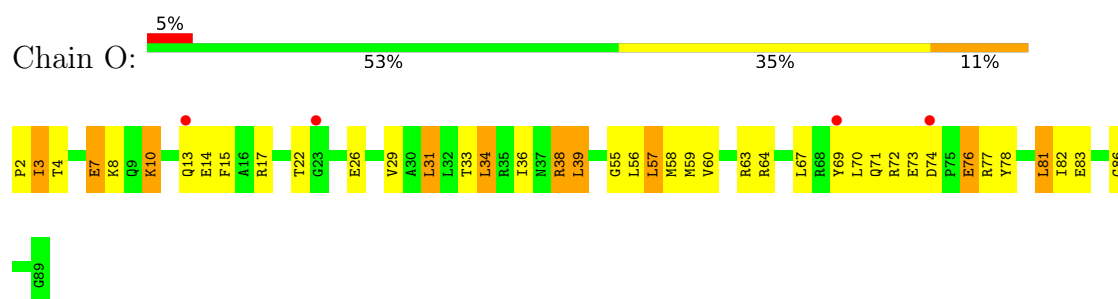
- Molecule 13: 30S ribosomal protein S13



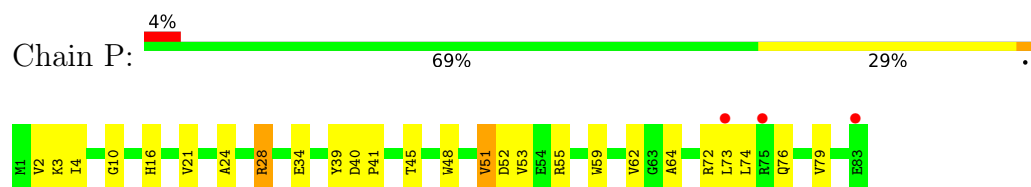
- Molecule 14: 30S ribosomal protein S14 type Z



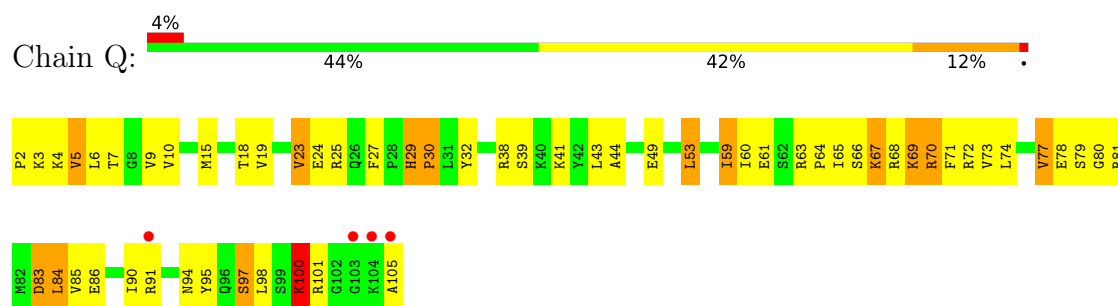
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17

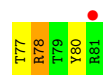
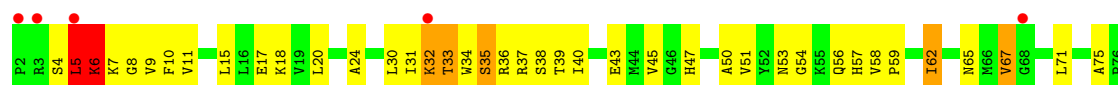


- Molecule 18: 30S ribosomal protein S18

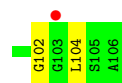
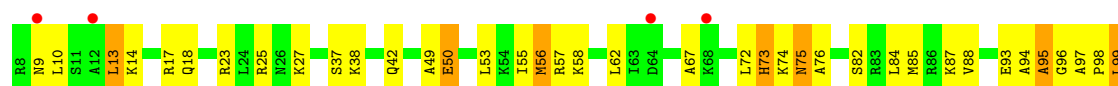




• Molecule 19: 30S ribosomal protein S19



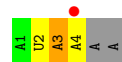
• Molecule 20: 30S ribosomal protein S20



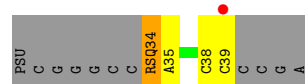
• Molecule 21: 30S ribosomal protein Thx



• Molecule 22: mRNA A-site fragment



• Molecule 23: tRNA ASL human mitochondrial Met



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	402.37Å 402.37Å 175.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.47 – 3.20 73.47 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.3 (73.47-3.20) 98.3 (73.47-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.195 , 0.236 0.194 , 0.235	Depositor DCC
R_{free} test set	11793 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	99.7	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 197.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	52188	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: RSQ, PAR, ZN, 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	0.42	0/36395	0.64	33/56801 (0.1%)
2	B	0.51	0/1935	0.98	4/2609 (0.2%)
3	C	0.54	0/1636	0.94	2/2205 (0.1%)
4	D	0.59	0/1733	0.96	4/2318 (0.2%)
5	E	0.73	0/1162	1.16	7/1564 (0.4%)
6	F	0.46	0/856	0.92	1/1154 (0.1%)
7	G	0.54	0/1276	0.97	5/1709 (0.3%)
8	H	0.78	0/1136	1.16	3/1527 (0.2%)
9	I	0.49	0/1029	0.94	3/1378 (0.2%)
10	J	0.65	0/807	1.10	4/1085 (0.4%)
11	K	0.64	0/900	1.01	1/1213 (0.1%)
12	L	0.64	0/986	1.17	5/1320 (0.4%)
13	M	0.57	0/1008	1.04	4/1347 (0.3%)
14	N	0.49	0/501	1.09	5/664 (0.8%)
15	O	0.63	0/745	0.92	0/992
16	P	0.74	0/716	1.00	1/963 (0.1%)
17	Q	0.68	0/870	1.11	5/1159 (0.4%)
18	R	0.55	0/603	1.04	1/799 (0.1%)
19	S	0.52	0/661	1.02	4/890 (0.4%)
20	T	0.71	0/764	1.08	3/1006 (0.3%)
21	V	0.46	0/212	0.90	0/277
22	W	0.50	0/96	0.73	0/147
23	X	0.46	0/115	0.59	0/176
All	All	0.49	0/56142	0.78	95/83303 (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
14	N	0	1

There are no bond length outliers.

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	92	SER	CA-C-N	9.31	131.48	119.84
7	G	92	SER	C-N-CA	9.31	131.48	119.84
14	N	9	LYS	N-CA-C	-9.04	101.68	112.89
19	S	54	GLY	N-CA-C	-8.79	104.23	114.69
5	E	64	ARG	N-CA-C	-8.43	99.18	110.55
12	L	47	LYS	CA-C-N	-8.42	109.31	119.84
12	L	47	LYS	C-N-CA	-8.42	109.31	119.84
12	L	26	ALA	N-CA-C	-8.23	104.25	112.97
10	J	38	ILE	CA-C-N	8.03	129.88	119.84
10	J	38	ILE	C-N-CA	8.03	129.88	119.84
14	N	53	LEU	CA-C-N	7.99	127.99	119.76
14	N	53	LEU	C-N-CA	7.99	127.99	119.76
5	E	48	ALA	CA-C-N	7.91	127.47	119.24
5	E	48	ALA	C-N-CA	7.91	127.47	119.24
10	J	17	ASP	N-CA-C	-7.83	104.33	114.04
19	S	80	TYR	N-CA-C	7.67	122.06	109.24
12	L	117	ARG	N-CA-C	7.49	120.32	111.71
12	L	119	LYS	N-CA-C	-7.45	99.46	110.48
8	H	100	ILE	CA-C-N	7.43	127.41	119.76
8	H	100	ILE	C-N-CA	7.43	127.41	119.76
2	B	23	ARG	N-CA-C	-7.20	102.06	111.71
1	A	542	A	P-O3'-C3'	6.89	130.53	120.20
9	I	127	LYS	N-CA-C	6.82	118.16	108.54
5	E	81	GLU	N-CA-C	-6.66	98.98	109.50
1	A	123	G	C4'-C3'-O3'	6.60	119.31	109.40
2	B	152	PHE	N-CA-C	-6.56	105.41	113.41
1	A	542	A	C4'-C3'-O3'	6.55	119.22	109.40
20	T	13	LEU	N-CA-C	-6.42	104.70	113.30
20	T	76	ALA	N-CA-C	-6.38	104.24	111.07
13	M	112	GLY	CA-C-N	6.37	127.80	119.84
13	M	112	GLY	C-N-CA	6.37	127.80	119.84
4	D	39	PRO	N-CA-C	6.21	116.43	110.47
2	B	182	ILE	CA-C-N	6.14	127.52	119.84
2	B	182	ILE	C-N-CA	6.14	127.52	119.84
19	S	32	LYS	N-CA-C	6.06	118.78	110.24
1	A	1432	C	P-O3'-C3'	6.04	129.26	120.20
11	K	40	ILE	N-CA-C	-6.03	106.38	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	U	P-O3'-C3'	5.91	129.07	120.20
1	A	64	G	C4'-C3'-O3'	5.85	118.17	109.40
4	D	163	GLU	N-CA-C	-5.83	105.66	112.89
10	J	51	ARG	N-CA-C	5.80	117.27	111.07
13	M	107	ALA	N-CA-C	-5.78	104.89	112.41
13	M	11	ARG	N-CA-C	5.74	117.79	109.07
1	A	1317	C	P-O3'-C3'	5.72	128.78	120.20
5	E	105	VAL	CA-C-N	-5.69	113.76	119.56
5	E	105	VAL	C-N-CA	-5.69	113.76	119.56
1	A	189	U	C2'-C3'-O3'	5.68	118.02	109.50
18	R	46	GLU	N-CA-C	-5.65	105.02	111.07
9	I	63	ILE	N-CA-C	5.64	116.19	107.78
1	A	1326	U	P-O3'-C3'	5.63	128.65	120.20
1	A	1378	A	C4'-C3'-O3'	5.63	117.84	109.40
1	A	861	U	P-O3'-C3'	5.62	128.63	120.20
1	A	188	U	C4'-C3'-O3'	5.56	117.74	109.40
1	A	1281	G	P-O3'-C3'	5.53	128.50	120.20
1	A	861	U	C4'-C3'-O3'	5.52	117.68	109.40
14	N	33	VAL	N-CA-C	5.51	114.54	106.55
1	A	1317	C	C2'-C3'-O3'	5.50	117.76	109.50
14	N	38	GLY	N-CA-C	-5.50	107.67	115.43
9	I	125	TYR	N-CA-C	5.50	116.33	108.74
6	F	14	LEU	CB-CA-C	-5.48	108.47	116.53
1	A	847	U	C4'-C3'-O3'	5.46	117.60	109.40
4	D	141	ARG	CA-C-N	-5.44	113.04	119.84
4	D	141	ARG	C-N-CA	-5.44	113.04	119.84
20	T	75	ASN	N-CA-C	-5.43	106.03	113.30
1	A	1278	C	C2'-C3'-O3'	5.42	117.63	109.50
1	A	123	G	P-O3'-C3'	5.41	128.32	120.20
1	A	1326	U	C2'-C3'-O3'	5.41	117.61	109.50
1	A	942	A	C2'-C3'-O3'	5.39	117.58	109.50
17	Q	29	HIS	CA-C-N	5.39	126.58	119.84
17	Q	29	HIS	C-N-CA	5.39	126.58	119.84
17	Q	67	LYS	N-CA-C	-5.38	103.79	110.41
1	A	1171	G	C4'-C3'-O3'	5.36	117.44	109.40
17	Q	27	PHE	N-CA-C	5.30	114.95	108.11
1	A	323	C	C2'-C3'-O3'	5.29	117.43	109.50
1	A	530	A	P-O3'-C3'	5.29	128.13	120.20
1	A	323	C	P-O3'-C3'	5.26	128.09	120.20
1	A	1281	G	C4'-C3'-O3'	5.24	117.26	109.40
1	A	1206	A	C2'-C3'-O3'	5.23	117.35	109.50
1	A	50	A	C4'-C3'-O3'	5.23	117.25	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	41	VAL	CB-CA-C	-5.23	101.35	110.71
1	A	500	G	C2'-C3'-O3'	5.23	117.34	109.50
1	A	445	A	C2'-C3'-O3'	5.20	117.31	109.50
1	A	1171	G	P-O3'-C3'	5.18	127.97	120.20
3	C	4	LYS	N-CA-C	5.17	121.82	110.80
8	H	46	LYS	N-CA-C	-5.17	107.02	113.38
19	S	24	ALA	N-CA-C	-5.15	107.66	114.31
17	Q	25	ARG	N-CA-C	5.10	117.29	107.44
16	P	51	VAL	N-CA-C	5.10	119.95	109.34
1	A	1328	G	P-O3'-C3'	5.09	127.84	120.20
1	A	50	A	P-O3'-C3'	5.09	127.84	120.20
3	C	5	ILE	CB-CA-C	-5.08	102.97	111.29
1	A	188	U	P-O3'-C3'	5.07	127.80	120.20
7	G	87	VAL	N-CA-C	5.03	112.84	107.76
7	G	70	LYS	CA-C-N	5.01	125.45	120.14
7	G	70	LYS	C-N-CA	5.01	125.45	120.14

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	N	8	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32515	0	16411	388	0
2	B	1900	0	1951	77	0
3	C	1612	0	1677	63	0
4	D	1703	0	1764	62	0
5	E	1146	0	1207	44	0
6	F	843	0	857	26	0
7	G	1257	0	1296	36	0
8	H	1116	0	1177	31	0
9	I	1011	0	1043	42	0
10	J	794	0	840	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	885	0	904	27	0
12	L	970	0	1057	44	0
13	M	997	0	1072	34	0
14	N	492	0	529	17	0
15	O	734	0	771	27	0
16	P	700	0	720	12	0
17	Q	857	0	930	39	0
18	R	597	0	668	26	0
19	S	647	0	673	22	0
20	T	762	0	859	16	0
21	V	208	0	221	9	0
22	W	86	0	44	6	0
23	X	126	0	66	8	0
24	A	184	0	0	0	0
24	B	1	0	0	0	0
24	T	1	0	0	0	0
25	A	42	0	45	2	0
26	D	1	0	0	0	0
26	N	1	0	0	0	0
All	All	52188	0	36782	963	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (963) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:GLY:HA2	2:B:42:ILE:HG12	1.51	0.93
1:A:1479:A:H2	1:A:1482:G:H1	1.14	0.92
1:A:1279:C:OP2	7:G:114:ARG:NH2	2.02	0.92
2:B:12:GLU:HG3	2:B:213:LEU:HD11	1.53	0.88
1:A:647:G:H22	1:A:724:G:H1	1.17	0.88
8:H:24:THR:HG22	8:H:63:LEU:HD21	1.56	0.87
7:G:117:ALA:H	7:G:120:ILE:HD13	1.40	0.85
1:A:1267:A:H2'	1:A:1268:A:H4'	1.59	0.85
12:L:27:LEU:O	12:L:29:GLY:N	2.09	0.84
1:A:1231:A:H4'	9:I:68:GLY:H	1.42	0.83
3:C:36:ASP:OD2	3:C:59:ARG:NH2	2.11	0.83
1:A:432:U:H5'	4:D:155:LEU:HD21	1.61	0.82
1:A:422:U:OP2	4:D:36:ARG:NH2	2.13	0.82
1:A:1171:G:O2'	3:C:3:ASN:HB3	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:21:ARG:HH22	10:J:93:GLY:H	1.28	0.81
1:A:801:G:O2'	1:A:802:A:H5''	1.81	0.81
1:A:1068:U:H3	1:A:1081:G:H22	1.30	0.80
5:E:106:PRO:HB3	5:E:135:THR:HG21	1.62	0.80
12:L:36:VAL:HG12	12:L:82:VAL:HG23	1.64	0.79
10:J:24:VAL:HG22	10:J:34:VAL:HG11	1.65	0.79
12:L:33:ARG:HD3	12:L:62:SER:HB2	1.65	0.79
1:A:952:A:H4'	1:A:953:G:H5''	1.65	0.78
17:Q:53:LEU:HD13	17:Q:85:VAL:HG11	1.64	0.78
19:S:53:ASN:HB2	19:S:56:GLN:H	1.51	0.76
3:C:14:ILE:O	3:C:16:ARG:N	2.19	0.76
4:D:191:ARG:NH1	4:D:200:GLU:OE2	2.17	0.75
1:A:1055:U:OP2	5:E:57:LYS:NZ	2.21	0.74
1:A:1170:C:OP1	10:J:51:ARG:NH2	2.20	0.74
11:K:57:THR:HG23	11:K:60:ALA:H	1.53	0.74
1:A:1417:G:H2'	1:A:1418:U:C6	2.24	0.73
1:A:952:A:H5'	1:A:952:A:H8	1.52	0.73
2:B:132:LYS:HA	2:B:135:GLN:HB2	1.70	0.73
17:Q:6:LEU:HB3	17:Q:23:VAL:HG11	1.71	0.73
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.70	0.72
5:E:92:LYS:HB3	5:E:119:LEU:HB2	1.70	0.71
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.71	0.71
1:A:1374:G:H21	1:A:1479:A:H8	1.39	0.71
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.23	0.71
1:A:818:U:OP1	18:R:64:ARG:NH2	2.24	0.71
2:B:71:VAL:HB	2:B:164:VAL:HG12	1.73	0.71
18:R:32:ARG:HA	18:R:69:THR:HG21	1.72	0.71
4:D:154:ASN:OD1	4:D:154:ASN:N	2.23	0.71
12:L:86:ARG:NH1	12:L:87:GLY:O	2.22	0.71
1:A:653:G:H21	6:F:73:ASN:HD21	1.40	0.70
9:I:100:GLY:O	9:I:102:LEU:N	2.23	0.70
5:E:80:ILE:HD13	5:E:138:ALA:HB1	1.74	0.70
2:B:80:ILE:HD12	2:B:80:ILE:H	1.57	0.69
9:I:8:GLY:HA2	9:I:79:LEU:HD13	1.72	0.69
13:M:107:ALA:HB3	13:M:111:LYS:HD2	1.75	0.69
15:O:74:ASP:HB3	15:O:77:ARG:HB3	1.74	0.69
2:B:88:ALA:HA	2:B:226:ARG:HH22	1.58	0.69
1:A:1115:G:N2	1:A:1123:C:O2	2.24	0.68
1:A:942:A:O2'	1:A:943:G:OP2	2.11	0.68
18:R:38:GLU:HA	18:R:41:LYS:HE2	1.76	0.68
5:E:137:GLU:OE2	5:E:140:ARG:NH1	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1133:A:H5''	10:J:42:THR:HG23	1.76	0.67
15:O:39:LEU:HD13	15:O:56:LEU:HB2	1.75	0.67
4:D:175:SER:HB3	4:D:184:LYS:HB3	1.77	0.66
8:H:86:ILE:HG21	8:H:133:LEU:HD23	1.77	0.66
2:B:77:ALA:HB2	2:B:211:ILE:HD13	1.76	0.66
12:L:27:LEU:C	12:L:29:GLY:H	2.03	0.66
17:Q:24:GLU:HG3	17:Q:39:SER:HB3	1.78	0.66
18:R:88:LYS:OXT	18:R:88:LYS:NZ	2.26	0.66
1:A:406:A:N3	1:A:408:G:O2'	2.27	0.66
16:P:74:LEU:HD22	16:P:79:VAL:HG21	1.77	0.66
17:Q:100:LYS:HG2	17:Q:101:ARG:HE	1.59	0.66
2:B:18:GLY:HA3	2:B:41:ILE:HA	1.78	0.66
3:C:154:SER:OG	3:C:155:GLY:N	2.16	0.66
2:B:158:LEU:HD12	2:B:158:LEU:H	1.61	0.65
11:K:73:MET:HE2	11:K:103:LEU:HG	1.77	0.65
13:M:11:ARG:HD3	13:M:12:ASN:HB2	1.77	0.65
2:B:89:GLY:H	2:B:226:ARG:HH12	1.44	0.65
4:D:36:ARG:HG3	4:D:38:TYR:CZ	2.30	0.65
7:G:70:LYS:HD3	7:G:96:GLN:HB3	1.78	0.65
1:A:180:C:O3'	20:T:82:SER:HB3	1.96	0.65
15:O:4:THR:OG1	15:O:7:GLU:OE2	2.12	0.65
15:O:4:THR:N	15:O:7:GLU:OE1	2.30	0.65
7:G:15:ASP:OD1	7:G:44:TYR:OH	2.15	0.65
1:A:1390:A:N1	25:A:1785:PAR:O61	2.30	0.64
15:O:38:ARG:HB3	15:O:38:ARG:HH11	1.61	0.64
4:D:199:ASN:O	4:D:201:GLN:N	2.29	0.64
1:A:583:C:H2'	1:A:584:C:H6	1.62	0.64
1:A:660:U:H3	1:A:696:G:H22	1.45	0.64
2:B:20:GLU:OE1	2:B:21:ARG:NH2	2.29	0.64
9:I:9:ARG:HG3	9:I:14:VAL:HG13	1.78	0.64
2:B:7:VAL:O	2:B:8:LYS:NZ	2.19	0.64
3:C:16:ARG:NH1	3:C:183:ASP:OD2	2.31	0.64
1:A:1062:A:O3'	5:E:16:THR:OG1	2.15	0.64
13:M:26:GLY:O	13:M:28:ALA:N	2.31	0.64
1:A:294:G:H2'	1:A:295:A:C8	2.33	0.64
1:A:1209:C:H4'	13:M:116:THR:HA	1.80	0.63
3:C:174:PRO:HB2	3:C:177:THR:HG23	1.80	0.63
10:J:4:ILE:HA	10:J:100:THR:HG22	1.79	0.63
1:A:1207:C:OP2	13:M:91:ARG:NH1	2.30	0.63
7:G:57:GLU:H	7:G:60:LYS:HE2	1.63	0.63
9:I:42:ARG:O	9:I:44:VAL:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:969:U:H3	1:A:1026:A:H62	1.47	0.63
4:D:70:ILE:HD11	4:D:100:ARG:CZ	2.29	0.63
2:B:189:ASP:HB3	2:B:204:ASN:HA	1.80	0.62
4:D:190:ASP:OD2	4:D:190:ASP:N	2.29	0.62
1:A:1006:C:N3	1:A:1016:G:N2	2.47	0.62
1:A:1222:G:H2'	1:A:1223:C:C6	2.33	0.62
10:J:4:ILE:HG13	10:J:74:ILE:HG13	1.81	0.62
5:E:89:ILE:HG12	5:E:135:THR:HG22	1.80	0.62
1:A:1295:C:N4	19:S:4:SER:OG	2.32	0.62
1:A:1374:G:N2	1:A:1479:A:H8	1.96	0.62
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.81	0.62
1:A:1279:C:H4'	1:A:1280:A:O4'	1.99	0.62
3:C:109:PRO:HG2	3:C:110:ASN:HD22	1.64	0.62
1:A:507:G:H2'	1:A:508:C:C6	2.35	0.61
18:R:41:LYS:HA	18:R:44:LEU:HD13	1.82	0.61
1:A:1111:C:H4'	1:A:1112:A:OP2	2.01	0.61
1:A:1204:C:OP2	19:S:78:ARG:NH2	2.33	0.61
15:O:26:GLU:OE1	15:O:77:ARG:NH1	2.33	0.61
20:T:56:MET:HE2	20:T:88:VAL:HG11	1.82	0.61
2:B:62:ALA:HB1	2:B:226:ARG:HG3	1.81	0.61
3:C:156:ARG:H	3:C:163:ALA:HA	1.66	0.61
4:D:108:LEU:HD23	4:D:170:VAL:HG21	1.81	0.61
1:A:953:G:H5'	1:A:1339:U:O2'	2.01	0.61
17:Q:83:ASP:OD1	17:Q:83:ASP:N	2.33	0.61
18:R:38:GLU:N	18:R:38:GLU:OE1	2.33	0.61
12:L:40:VAL:HG21	12:L:77:LEU:O	2.01	0.60
1:A:8:A:N6	4:D:205:GLU:O	2.34	0.60
1:A:1307:C:OP2	21:V:6:ARG:NH1	2.34	0.60
18:R:19:LYS:NZ	18:R:20:ALA:O	2.34	0.60
1:A:522:A:H2'	1:A:523:G:C8	2.36	0.60
19:S:32:LYS:HB3	19:S:50:ALA:HB3	1.84	0.60
10:J:50:ILE:HB	14:N:41:ARG:HD2	1.84	0.60
1:A:1229:A:N3	9:I:70:LYS:NZ	2.48	0.60
1:A:775:A:H4'	1:A:776:U:O5'	2.01	0.60
1:A:949:C:OP1	10:J:57:LYS:NZ	2.31	0.60
10:J:65:LEU:HD13	14:N:56:VAL:HG22	1.82	0.60
18:R:53:ARG:NH1	18:R:58:LEU:O	2.33	0.60
3:C:11:ARG:HD3	3:C:180:ALA:HB3	1.84	0.60
3:C:95:THR:HG22	3:C:97:LYS:H	1.66	0.60
4:D:196:LEU:HB3	4:D:198:VAL:HG22	1.84	0.59
7:G:103:TRP:CD1	7:G:137:LYS:HD2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:26:GLU:HA	15:O:81:LEU:HD11	1.85	0.59
13:M:23:TYR:HB3	13:M:67:GLU:HA	1.85	0.59
1:A:1110:C:N4	1:A:1126:G:O6	2.32	0.59
2:B:18:GLY:O	2:B:19:HIS:ND1	2.35	0.59
3:C:6:HIS:HD2	3:C:8:ILE:H	1.50	0.59
9:I:4:TYR:HB2	9:I:19:LEU:HB2	1.83	0.59
16:P:34:GLU:OE2	16:P:55:ARG:HD3	2.03	0.59
1:A:1278:C:O2'	1:A:1279:C:OP2	2.18	0.59
13:M:125:ARG:O	13:M:125:ARG:NH1	2.34	0.59
1:A:35:G:H2'	1:A:36:C:C6	2.38	0.58
1:A:1487:U:H2'	1:A:1488:G:C8	2.38	0.58
1:A:173:A:H2'	1:A:174:U:C6	2.38	0.58
1:A:1222:G:H2'	1:A:1223:C:H6	1.68	0.58
10:J:49:VAL:HG13	14:N:41:ARG:HG3	1.85	0.58
1:A:212:C:O2'	1:A:455:C:N4	2.35	0.58
1:A:1110:C:OP1	9:I:66:ARG:NH2	2.36	0.58
4:D:98:GLU:OE2	4:D:107:ARG:NE	2.35	0.58
6:F:15:ASP:O	6:F:17:SER:N	2.36	0.58
1:A:501:C:H5''	1:A:502:C:H6	1.67	0.58
1:A:690:C:H2'	1:A:691:C:H6	1.68	0.58
7:G:146:GLU:O	7:G:149:ARG:N	2.35	0.58
12:L:78:GLN:O	12:L:80:HIS:N	2.35	0.58
15:O:74:ASP:O	15:O:77:ARG:N	2.36	0.58
2:B:16:HIS:CD2	2:B:209:ARG:HB3	2.39	0.58
20:T:23:ARG:O	20:T:27:LYS:HB2	2.03	0.58
10:J:6:ILE:HD11	10:J:23:ILE:HD13	1.86	0.58
2:B:204:ASN:ND2	2:B:206:ASP:O	2.37	0.57
5:E:8:GLU:HG2	5:E:34:VAL:HG12	1.86	0.57
5:E:64:ARG:H	5:E:64:ARG:HD2	1.68	0.57
1:A:1204:C:P	19:S:78:ARG:HH21	2.26	0.57
3:C:180:ALA:HB1	3:C:182:ILE:HG13	1.84	0.57
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.85	0.57
22:W:3:A:H61	23:X:34:RSQ:HN4	1.52	0.57
7:G:111:ARG:NH1	7:G:113:GLU:OE2	2.38	0.57
21:V:10:ARG:HG2	21:V:13:ILE:HD12	1.87	0.57
7:G:18:TYR:CD1	7:G:59:LEU:HB2	2.39	0.57
13:M:37:THR:O	13:M:55:ARG:NH1	2.36	0.57
19:S:50:ALA:HA	19:S:58:VAL:O	2.04	0.57
20:T:14:LYS:O	20:T:18:GLN:HG2	2.04	0.57
1:A:102:A:H2'	1:A:321:G:N2	2.19	0.57
1:A:501:C:H5''	1:A:502:C:C6	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1036:C:O2'	1:A:1037:A:O5'	2.22	0.57
17:Q:19:VAL:HG23	17:Q:44:ALA:HB3	1.86	0.57
1:A:925:C:OP1	13:M:109:THR:HG22	2.03	0.57
7:G:78:ARG:NH1	7:G:154:TYR:HB3	2.20	0.57
1:A:1381:C:C2	1:A:1479:A:N6	2.72	0.57
3:C:67:THR:HG23	3:C:102:ASN:HB2	1.85	0.57
22:W:2:U:H2'	22:W:3:A:C8	2.39	0.57
17:Q:66:SER:OG	17:Q:67:LYS:N	2.33	0.57
8:H:1:MET:HG2	8:H:2:LEU:H	1.70	0.56
1:A:1288:U:H2'	1:A:1289:U:C6	2.40	0.56
8:H:92:ARG:HH11	8:H:92:ARG:CG	2.19	0.56
9:I:25:LYS:N	9:I:60:ASP:OD1	2.38	0.56
13:M:88:ARG:HG2	13:M:98:VAL:HG13	1.87	0.56
16:P:51:VAL:O	16:P:52:ASP:HB3	2.05	0.56
22:W:2:U:H2'	22:W:3:A:H8	1.70	0.56
5:E:16:THR:HG23	5:E:27:ARG:HB3	1.88	0.56
1:A:952:A:H5'	1:A:952:A:C8	2.36	0.56
1:A:408:G:O6	4:D:36:ARG:NH1	2.39	0.56
6:F:9:VAL:HG23	6:F:87:ARG:HB2	1.87	0.56
9:I:53:VAL:HG21	9:I:85:LEU:HD21	1.88	0.56
2:B:82:ARG:HA	2:B:92:TYR:CE1	2.40	0.56
12:L:65:GLU:OE1	12:L:65:GLU:N	2.39	0.56
1:A:273:G:OP2	17:Q:41:LYS:NZ	2.35	0.56
17:Q:7:THR:O	17:Q:23:VAL:HG13	2.05	0.56
15:O:82:ILE:O	15:O:86:GLY:N	2.31	0.56
1:A:1328:G:N2	1:A:1355:G:H2'	2.19	0.55
2:B:101:MET:HA	2:B:108:ILE:HD12	1.88	0.55
5:E:80:ILE:HD12	5:E:91:LEU:HB2	1.88	0.55
6:F:13:ASN:OD1	6:F:13:ASN:N	2.35	0.55
1:A:985:C:N3	1:A:1000:G:N2	2.50	0.55
2:B:118:LEU:HB3	2:B:142:LEU:HD13	1.88	0.55
11:K:14:VAL:O	11:K:16:SER:N	2.38	0.55
1:A:1109:G:N1	1:A:1126:G:N7	2.50	0.55
2:B:92:TYR:CE2	2:B:151:GLY:HA3	2.41	0.55
1:A:944:C:H2'	1:A:945:A:N7	2.22	0.55
7:G:108:ALA:O	7:G:119:ARG:HD2	2.06	0.55
1:A:937:U:H1'	1:A:1204:C:H5'	1.89	0.55
1:A:669:U:H4'	1:A:670:A:OP1	2.07	0.55
1:A:1350:G:H5''	9:I:112:LYS:HB3	1.89	0.55
1:A:905:G:H5'	1:A:1510:C:OP1	2.07	0.55
2:B:208:ILE:HD12	2:B:209:ARG:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:119:ARG:HG2	3:C:140:ARG:HH12	1.72	0.55
1:A:35:G:H2'	1:A:36:C:H6	1.72	0.55
7:G:111:ARG:HD2	7:G:123:GLU:HB2	1.88	0.55
17:Q:59:ILE:HD12	17:Q:73:VAL:HA	1.89	0.55
1:A:125:C:H2'	1:A:126:C:C6	2.42	0.55
1:A:928:G:OP2	13:M:102:ARG:NH2	2.40	0.55
1:A:1360:C:H5	1:A:1361:G:C4	2.24	0.55
2:B:9:GLU:HB3	2:B:12:GLU:HB2	1.89	0.55
3:C:22:TRP:HB3	3:C:59:ARG:HB3	1.89	0.55
3:C:22:TRP:NE1	3:C:36:ASP:OD1	2.34	0.55
1:A:978:A:N1	1:A:979:G:N2	2.55	0.54
1:A:188:U:H1'	1:A:189:U:H5''	1.89	0.54
9:I:26:VAL:HB	9:I:33:PHE:HB2	1.89	0.54
13:M:23:TYR:CE2	13:M:71:ARG:HB3	2.41	0.54
1:A:1204:C:H3'	1:A:1205:G:H5''	1.89	0.54
3:C:6:HIS:CD2	3:C:8:ILE:H	2.25	0.54
4:D:199:ASN:C	4:D:199:ASN:HD22	2.07	0.54
1:A:816:U:H2'	1:A:817:C:C6	2.43	0.54
1:A:123:G:N3	1:A:189:U:H3'	2.22	0.54
1:A:656:G:H2'	1:A:657:G:C8	2.42	0.54
1:A:143:A:H2'	1:A:144:C:C6	2.43	0.54
1:A:563:U:H2'	1:A:564:G:O4'	2.08	0.54
1:A:1350:G:OP1	9:I:111:ARG:NH2	2.41	0.54
11:K:18:ARG:HB2	11:K:33:THR:HG22	1.89	0.54
17:Q:15:MET:HG2	17:Q:18:THR:HB	1.90	0.54
7:G:8:GLU:CD	7:G:8:GLU:H	2.12	0.54
7:G:18:TYR:HB3	7:G:59:LEU:HD22	1.89	0.54
12:L:28:LYS:C	12:L:30:ALA:H	2.14	0.54
13:M:14:ARG:HG3	13:M:44:ARG:NH1	2.22	0.54
1:A:1231:A:H4'	9:I:68:GLY:N	2.18	0.54
3:C:93:LYS:HG3	3:C:94:LEU:HD23	1.90	0.54
11:K:14:VAL:HG21	11:K:77:MET:HE2	1.90	0.54
1:A:858:G:P	12:L:12:ARG:HH22	2.31	0.54
6:F:33:TYR:HA	6:F:71:ARG:HH21	1.72	0.54
1:A:525:G:P	4:D:10:ARG:HH22	2.29	0.53
1:A:1221:U:H3'	1:A:1222:G:H5'	1.91	0.53
1:A:424:U:H1'	1:A:425:A:H5''	1.90	0.53
2:B:114:ARG:O	2:B:118:LEU:N	2.40	0.53
2:B:140:HIS:HA	2:B:143:GLU:HG3	1.89	0.53
4:D:9:CYS:HB3	4:D:32:ALA:HB2	1.89	0.53
1:A:505:C:OP2	12:L:69:TYR:OH	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1121:G:N2	1:A:1126:G:H1	2.07	0.53
1:A:1327:A:N1	1:A:1356:A:H5''	2.23	0.53
17:Q:4:LYS:HE3	17:Q:6:LEU:HD21	1.89	0.53
1:A:1051:C:O2'	1:A:1173:C:H1'	2.08	0.53
1:A:1456:C:H2'	1:A:1457:G:H8	1.73	0.53
1:A:1479:A:H2	1:A:1482:G:N1	1.93	0.53
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.73	0.53
1:A:608:G:H4'	16:P:16:HIS:CD2	2.44	0.53
1:A:1308:C:OP2	21:V:12:LYS:NZ	2.42	0.53
7:G:46:ALA:O	7:G:50:ILE:HG12	2.09	0.53
1:A:15:G:H1'	5:E:19:MET:HE2	1.90	0.53
1:A:702:C:H1'	18:R:49:LYS:HG2	1.89	0.53
11:K:48:ILE:HG21	11:K:63:LEU:HD13	1.91	0.53
12:L:54:LYS:HG2	12:L:75:HIS:CD2	2.44	0.53
1:A:583:C:H2'	1:A:584:C:C6	2.44	0.53
1:A:923:A:H2'	1:A:924:G:C8	2.43	0.53
1:A:1121:G:H22	1:A:1126:G:H22	1.57	0.53
2:B:20:GLU:HB2	2:B:190:THR:OG1	2.09	0.53
5:E:10:MET:HA	5:E:32:VAL:HA	1.90	0.53
1:A:922:G:C2	1:A:923:A:C8	2.96	0.53
2:B:223:ILE:HG13	2:B:226:ARG:HH21	1.74	0.53
6:F:69:GLU:CD	6:F:69:GLU:H	2.16	0.53
22:W:3:A:N6	23:X:34:RSQ:HN4	2.07	0.53
2:B:16:HIS:HB3	2:B:210:SER:OG	2.09	0.53
8:H:64:LYS:HG2	8:H:79:VAL:HG21	1.90	0.53
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.91	0.53
12:L:57:LYS:HD3	12:L:67:THR:HB	1.90	0.53
1:A:1206:A:O2'	1:A:1207:C:O5'	2.23	0.52
1:A:1394:C:H2'	1:A:1395:A:C8	2.43	0.52
2:B:178:ARG:NH1	8:H:71:GLY:O	2.42	0.52
1:A:773:A:H5''	1:A:774:G:OP2	2.10	0.52
1:A:1260:A:H2'	1:A:1260:A:N3	2.24	0.52
3:C:11:ARG:NH1	3:C:177:THR:O	2.42	0.52
9:I:66:ARG:HH11	9:I:66:ARG:HB3	1.74	0.52
6:F:67:MET:HE1	6:F:75:LEU:HG	1.91	0.52
1:A:1093:A:N1	3:C:177:THR:HB	2.24	0.52
1:A:1121:G:H21	1:A:1125:G:N2	2.06	0.52
3:C:34:LEU:HD22	14:N:25:VAL:HG21	1.91	0.52
21:V:5:ASP:O	21:V:8:THR:OG1	2.27	0.52
1:A:603:C:H2'	1:A:604:A:O4'	2.09	0.52
4:D:43:HIS:O	4:D:45:GLN:N	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:84:VAL:HG21	11:K:91:ARG:HD3	1.92	0.52
15:O:36:ILE:HG13	15:O:59:MET:HE3	1.92	0.52
17:Q:86:GLU:O	17:Q:90:ILE:HG13	2.09	0.52
3:C:147:LYS:HD3	3:C:205:GLY:HA2	1.91	0.52
4:D:18:LYS:HB3	4:D:20:TYR:CE2	2.45	0.52
9:I:38:GLN:OE1	9:I:39:GLY:N	2.43	0.52
11:K:124:LYS:HE2	11:K:125:PHE:CZ	2.45	0.52
12:L:8:ASN:O	12:L:12:ARG:HG3	2.10	0.52
1:A:125:C:H2'	1:A:126:C:H6	1.75	0.52
1:A:274:A:H5''	1:A:276:G:H5'	1.91	0.52
2:B:208:ILE:HD12	2:B:209:ARG:H	1.74	0.52
8:H:111:ILE:HG22	8:H:134:ILE:HD12	1.91	0.52
8:H:116:LYS:HG3	8:H:129:VAL:HG11	1.92	0.52
9:I:3:GLN:HE22	9:I:20:ARG:HH21	1.57	0.52
9:I:11:LYS:C	9:I:13:ALA:H	2.17	0.52
9:I:50:LEU:C	9:I:52:ALA:H	2.18	0.52
1:A:1206:A:HO2'	1:A:1207:C:P	2.33	0.52
12:L:78:GLN:C	12:L:80:HIS:H	2.17	0.52
20:T:67:ALA:HA	20:T:73:HIS:H	1.75	0.52
1:A:382:U:H5'	1:A:383:G:P	2.50	0.51
1:A:1298:C:O2	19:S:37:ARG:NH2	2.40	0.51
2:B:28:PHE:CD2	2:B:190:THR:HA	2.45	0.51
9:I:11:LYS:O	9:I:13:ALA:N	2.43	0.51
12:L:52:LEU:O	12:L:54:LYS:NZ	2.29	0.51
1:A:949:C:H4'	10:J:57:LYS:HB3	1.91	0.51
17:Q:81:ARG:NE	17:Q:84:LEU:HD11	2.25	0.51
1:A:987:G:H22	1:A:999:G:H1'	1.76	0.51
13:M:15:VAL:HG21	13:M:48:LEU:HD21	1.92	0.51
19:S:51:VAL:O	19:S:58:VAL:HG22	2.11	0.51
1:A:323:C:H2'	1:A:323:C:O2	2.10	0.51
1:A:720:A:H2'	1:A:721:C:C6	2.46	0.51
2:B:235:SER:O	2:B:238:LEU:HB2	2.10	0.51
17:Q:67:LYS:O	17:Q:69:LYS:N	2.37	0.51
1:A:67:C:O2'	1:A:165:A:N3	2.34	0.51
1:A:689:A:C4'	11:K:29:ILE:HD11	2.41	0.51
1:A:1080:C:H2'	1:A:1081:G:O4'	2.09	0.51
2:B:87:ARG:HD2	2:B:234:PRO:HD2	1.91	0.51
1:A:904:G:H4'	1:A:1480:A:N7	2.26	0.51
1:A:931:G:H2'	1:A:932:U:C6	2.45	0.51
11:K:54:ARG:O	11:K:57:THR:HG22	2.11	0.51
1:A:268:A:N6	1:A:269:A:C6	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:C:OP1	1:A:496:C:O2'	2.25	0.51
1:A:1139:A:H4'	1:A:1140:C:O5'	2.11	0.51
6:F:60:PHE:CZ	18:R:78:LEU:HD21	2.46	0.51
19:S:15:LEU:HA	19:S:18:LYS:HB3	1.92	0.51
1:A:1039:G:H5''	3:C:154:SER:HB2	1.92	0.51
1:A:1044:U:H2'	1:A:1045:C:C6	2.46	0.51
3:C:35:GLU:OE2	3:C:59:ARG:NH1	2.43	0.51
4:D:30:LYS:C	4:D:32:ALA:N	2.68	0.51
17:Q:5:VAL:HG22	17:Q:60:ILE:HD12	1.92	0.51
1:A:521:G:H2'	1:A:522:A:H8	1.76	0.50
1:A:1088:G:H5''	3:C:172:ARG:HG2	1.93	0.50
1:A:1172:A:H5''	3:C:4:LYS:HE2	1.93	0.50
6:F:37:VAL:HA	6:F:65:VAL:HG12	1.91	0.50
10:J:17:ASP:C	10:J:19:SER:H	2.19	0.50
15:O:71:GLN:HG3	15:O:78:TYR:CD2	2.46	0.50
1:A:484:C:H2'	1:A:485:G:H8	1.76	0.50
1:A:522:A:H2'	1:A:523:G:H8	1.75	0.50
1:A:993:A:N3	1:A:1199:C:O2'	2.40	0.50
6:F:21:LEU:O	6:F:25:ILE:HG13	2.12	0.50
13:M:54:VAL:O	13:M:58:GLU:HG2	2.11	0.50
1:A:520:G:OP1	12:L:113:ARG:NH2	2.43	0.50
1:A:1188:G:H2'	1:A:1189:C:H6	1.75	0.50
5:E:43:LEU:HD11	5:E:132:ALA:HB1	1.92	0.50
1:A:264:C:H2'	1:A:265:A:C8	2.46	0.50
1:A:814:U:H2'	1:A:815:C:H6	1.76	0.50
18:R:73:ALA:HB3	18:R:79:LEU:HD12	1.92	0.50
2:B:122:PHE:HA	2:B:127:ILE:HD13	1.93	0.50
2:B:178:ARG:HH22	8:H:74:PRO:HG3	1.75	0.50
7:G:145:ALA:O	7:G:147:ALA:N	2.43	0.50
10:J:75:ILE:HG22	10:J:76:ASN:HD22	1.76	0.50
1:A:530:A:H4'	1:A:531:G:O5'	2.11	0.50
1:A:531:G:H2'	1:A:532:C:C6	2.46	0.50
1:A:1409:U:H2'	1:A:1410:A:C8	2.46	0.50
1:A:1019:C:H2'	1:A:1020:C:C6	2.47	0.50
3:C:3:ASN:HB2	3:C:4:LYS:HD2	1.93	0.50
4:D:148:VAL:HB	4:D:181:MET:HB3	1.92	0.50
5:E:87:SER:HB3	5:E:131:ILE:HD13	1.93	0.50
12:L:115:LYS:O	12:L:117:ARG:N	2.42	0.50
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.92	0.50
5:E:135:THR:O	5:E:139:LEU:HG	2.12	0.50
18:R:74:ARG:HB3	18:R:81:PHE:CE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:G:H2'	1:A:22:G:C8	2.47	0.50
1:A:900:A:OP1	5:E:21:ALA:HB2	2.11	0.50
1:A:1014:G:H2'	1:A:1015:G:O4'	2.11	0.50
12:L:69:TYR:CD1	12:L:90:VAL:HG21	2.46	0.50
14:N:57:ARG:HG2	14:N:58:LYS:H	1.77	0.50
2:B:186:ALA:HB3	2:B:197:VAL:HG11	1.94	0.49
15:O:33:THR:HG23	15:O:63:ARG:NH1	2.27	0.49
1:A:695:A:H2'	1:A:696:G:O4'	2.12	0.49
1:A:1073:U:O2	1:A:1075:A:C8	2.66	0.49
7:G:26:PHE:O	7:G:30:ILE:HG13	2.12	0.49
1:A:1083:A:H4'	1:A:1084:A:O5'	2.13	0.49
1:A:1098:C:O2'	9:I:108:VAL:HG21	2.13	0.49
2:B:143:GLU:O	2:B:147:LYS:HG3	2.12	0.49
3:C:26:LYS:HZ3	10:J:45:ARG:HE	1.60	0.49
7:G:18:TYR:HD1	7:G:59:LEU:HD22	1.77	0.49
12:L:34:ARG:O	12:L:61:THR:HG23	2.12	0.49
12:L:54:LYS:HG2	12:L:75:HIS:HD2	1.76	0.49
1:A:1037:A:C6	1:A:1187:G:C5	3.00	0.49
4:D:79:PHE:HE1	4:D:204:ILE:HG12	1.78	0.49
6:F:7:ASN:HB2	6:F:89:MET:O	2.12	0.49
12:L:27:LEU:C	12:L:29:GLY:N	2.67	0.49
2:B:212:GLN:O	2:B:216:SER:OG	2.20	0.49
9:I:6:GLY:HA3	9:I:83:ARG:HB2	1.94	0.49
12:L:113:ARG:HH12	12:L:116:SER:H	1.61	0.49
1:A:124:A:H1'	1:A:258:A:O2'	2.11	0.49
1:A:242:G:OP2	17:Q:100:LYS:HB3	2.12	0.49
1:A:994:A:H2'	1:A:995:G:O4'	2.13	0.49
6:F:101:ALA:HA	18:R:28:GLU:HA	1.95	0.49
7:G:117:ALA:H	7:G:120:ILE:CD1	2.20	0.49
12:L:25:PRO:C	12:L:27:LEU:H	2.19	0.49
1:A:311:G:OP2	1:A:346:G:O2'	2.31	0.49
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.95	0.49
4:D:61:LYS:HD2	4:D:207:TYR:OH	2.13	0.49
4:D:71:SER:OG	4:D:74:GLN:HB2	2.12	0.49
1:A:619:U:H5'	17:Q:2:PRO:HG2	1.95	0.49
3:C:107:GLN:CD	3:C:107:GLN:H	2.20	0.49
1:A:398:C:O2'	4:D:122:ARG:NH1	2.46	0.48
1:A:886:A:OP1	12:L:21:LYS:HE3	2.13	0.48
1:A:951:A:OP2	14:N:41:ARG:NH1	2.33	0.48
1:A:1039:G:H5''	3:C:154:SER:CB	2.43	0.48
7:G:26:PHE:CD2	7:G:30:ILE:HD11	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:86:GLY:O	11:K:91:ARG:NH1	2.46	0.48
16:P:3:LYS:HG2	16:P:24:ALA:HB2	1.95	0.48
23:X:34:RSQ:H2'	23:X:35:A:H8	1.78	0.48
3:C:150:LYS:HE2	3:C:152:ILE:HD11	1.94	0.48
4:D:53:ASP:O	4:D:57:ARG:HG3	2.13	0.48
8:H:92:ARG:HH11	8:H:92:ARG:HG2	1.78	0.48
1:A:385:C:H2'	1:A:386:G:C8	2.48	0.48
1:A:642:U:OP2	15:O:8:LYS:NZ	2.29	0.48
1:A:821:G:H2'	1:A:822:U:H5''	1.93	0.48
1:A:959:U:H4'	1:A:960:A:O5'	2.14	0.48
11:K:54:ARG:O	11:K:56:GLY:N	2.46	0.48
1:A:230:C:H5'	17:Q:70:ARG:HG2	1.95	0.48
3:C:42:LEU:HD21	3:C:90:GLU:HG3	1.94	0.48
3:C:134:ILE:HG22	3:C:168:ALA:HB3	1.94	0.48
4:D:165:MET:SD	4:D:168:ARG:NH1	2.86	0.48
6:F:23:LYS:O	6:F:27:GLN:HG2	2.13	0.48
2:B:92:TYR:HE2	2:B:151:GLY:HA3	1.78	0.48
1:A:705:A:H2'	1:A:705:A:N3	2.28	0.48
1:A:726:U:H2'	1:A:727:C:C6	2.49	0.48
17:Q:67:LYS:C	17:Q:69:LYS:H	2.21	0.48
1:A:19:C:H2'	1:A:20:U:H6	1.78	0.48
1:A:1036:C:HO2'	1:A:1037:A:P	2.37	0.48
1:A:1039:G:H2'	1:A:1040:G:O4'	2.14	0.48
2:B:126:GLU:HA	2:B:129:GLU:HB2	1.95	0.48
3:C:177:THR:O	3:C:180:ALA:HB2	2.14	0.48
4:D:98:GLU:HG2	4:D:189:PRO:HG3	1.96	0.48
7:G:27:ILE:HA	7:G:30:ILE:HD12	1.96	0.48
8:H:9:MET:HG3	8:H:26:VAL:HG11	1.96	0.48
13:M:15:VAL:HG23	13:M:43:THR:O	2.14	0.48
1:A:1352:G:C2	1:A:1353:G:C8	3.02	0.48
3:C:6:HIS:HE2	3:C:8:ILE:HD12	1.79	0.48
10:J:3:LYS:C	10:J:4:ILE:HD13	2.38	0.48
1:A:780:C:H2'	1:A:781:G:H8	1.78	0.48
1:A:1383:G:C2	1:A:1384:C:H1'	2.49	0.48
11:K:34:ASP:O	11:K:36:ASP:N	2.47	0.48
14:N:24:CYS:HB2	14:N:40:CYS:HB3	1.95	0.48
19:S:5:LEU:HA	19:S:6:LYS:NZ	2.28	0.48
14:N:23:ARG:NH1	14:N:30:ALA:HB2	2.29	0.47
1:A:64:G:H3'	1:A:64:G:OP1	2.13	0.47
1:A:501:C:H4'	1:A:502:C:O5'	2.13	0.47
1:A:1130:U:H2'	1:A:1131:C:O4'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:50:LEU:O	9:I:52:ALA:N	2.43	0.47
10:J:3:LYS:HE3	10:J:3:LYS:HB2	1.77	0.47
1:A:122:U:O3'	1:A:123:G:H3'	2.14	0.47
1:A:274:A:OP2	17:Q:95:TYR:OH	2.29	0.47
1:A:689:A:O4'	11:K:29:ILE:HD11	2.14	0.47
1:A:968:U:O2	1:A:970:G:H8	1.97	0.47
1:A:985:C:H42	1:A:1000:G:H1	1.61	0.47
2:B:10:LEU:C	2:B:12:GLU:H	2.21	0.47
9:I:17:VAL:HG11	9:I:81:ILE:HG12	1.95	0.47
12:L:48:PRO:C	12:L:49:ASN:HD22	2.22	0.47
1:A:422:U:OP2	1:A:423:G:O2'	2.33	0.47
1:A:981:G:C5	1:A:982:A:N7	2.82	0.47
1:A:1409:U:H2'	1:A:1410:A:H8	1.79	0.47
12:L:35:GLY:HA3	12:L:60:LEU:HD13	1.96	0.47
1:A:96:C:OP1	20:T:17:ARG:NH1	2.45	0.47
3:C:83:ARG:HE	3:C:87:LEU:HD11	1.80	0.47
13:M:40:ASN:HD21	13:M:42:ALA:HB3	1.80	0.47
1:A:690:C:H2'	1:A:691:C:C6	2.48	0.47
3:C:159:GLY:HA2	3:C:193:TYR:CE1	2.50	0.47
8:H:10:LEU:HD23	8:H:10:LEU:HA	1.62	0.47
9:I:19:LEU:HB3	9:I:59:PHE:CE2	2.49	0.47
20:T:93:GLU:O	20:T:95:ALA:N	2.47	0.47
1:A:119:G:H4'	1:A:617:C:O2	2.15	0.47
1:A:121:G:O3'	17:Q:3:LYS:NZ	2.47	0.47
1:A:405:G:H2'	1:A:424:U:C5	2.50	0.47
1:A:491:C:H5'	4:D:209:ARG:HH12	1.79	0.47
1:A:696:G:H2'	1:A:697:G:C8	2.49	0.47
1:A:902:G:O2'	1:A:904:G:OP1	2.32	0.47
4:D:3:ARG:HD3	4:D:3:ARG:HA	1.54	0.47
9:I:43:ALA:C	9:I:45:ALA:H	2.22	0.47
18:R:61:LYS:O	18:R:65:ILE:HG13	2.15	0.47
1:A:170:C:H2'	1:A:171:C:H6	1.79	0.47
3:C:174:PRO:HB2	3:C:177:THR:CG2	2.45	0.47
13:M:70:LEU:O	13:M:73:GLU:HG3	2.15	0.47
1:A:1305:A:O4'	1:A:1343:C:H4'	2.15	0.47
3:C:156:ARG:HG3	3:C:156:ARG:HH11	1.79	0.47
4:D:88:VAL:O	4:D:92:VAL:HG23	2.14	0.47
9:I:51:ARG:HA	9:I:56:LEU:HD11	1.97	0.47
11:K:41:THR:HG21	11:K:71:LYS:HB3	1.96	0.47
15:O:57:LEU:HD12	15:O:57:LEU:HA	1.59	0.47
19:S:51:VAL:HG21	19:S:71:LEU:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:G:H2'	1:A:532:C:H6	1.77	0.46
1:A:555:A:H5'	1:A:556:A:OP2	2.15	0.46
1:A:1036:C:H5	23:X:34:RSQ:O4'	1.98	0.46
1:A:1185:A:H5'	1:A:1186:U:OP2	2.15	0.46
8:H:85:ARG:NE	8:H:87:SER:O	2.48	0.46
10:J:39:PRO:O	10:J:40:LEU:HB2	2.15	0.46
10:J:50:ILE:HD12	10:J:50:ILE:H	1.79	0.46
15:O:31:LEU:HD12	15:O:31:LEU:HA	1.71	0.46
1:A:93:C:H2'	1:A:94:A:C8	2.50	0.46
1:A:492:A:H5''	4:D:55:ALA:HB2	1.97	0.46
2:B:13:ALA:O	2:B:15:VAL:N	2.48	0.46
5:E:31:LEU:HA	5:E:31:LEU:HD23	1.65	0.46
12:L:6:THR:OG1	12:L:9:GLN:HG3	2.14	0.46
1:A:62:U:H2'	1:A:63:C:C6	2.51	0.46
1:A:399:U:H5'	4:D:122:ARG:HD2	1.97	0.46
1:A:653:G:H2'	1:A:654:G:O4'	2.15	0.46
1:A:1337:G:H2'	1:A:1338:A:C8	2.51	0.46
14:N:9:LYS:NZ	14:N:22:THR:HA	2.30	0.46
1:A:740:U:H2'	1:A:741:G:O4'	2.15	0.46
1:A:1036:C:C5	23:X:34:RSQ:O4'	2.69	0.46
3:C:3:ASN:ND2	3:C:3:ASN:H	2.14	0.46
5:E:47:LYS:HE3	5:E:47:LYS:HB2	1.74	0.46
7:G:70:LYS:HB2	7:G:96:GLN:HB3	1.98	0.46
19:S:15:LEU:HD13	19:S:33:THR:HG21	1.96	0.46
19:S:17:GLU:HA	19:S:20:LEU:HG	1.98	0.46
1:A:396:C:H1'	1:A:605:A:H1'	1.96	0.46
1:A:690:C:H4'	11:K:20:TYR:CD1	2.50	0.46
1:A:1345:A:H4'	1:A:1346:U:H2'	1.96	0.46
1:A:1480:A:H61	1:A:1510:C:H5'	1.80	0.46
2:B:98:LEU:HD23	2:B:98:LEU:N	2.30	0.46
4:D:199:ASN:ND2	4:D:201:GLN:HB3	2.31	0.46
10:J:5:ARG:HB3	10:J:99:LYS:H	1.79	0.46
20:T:85:MET:HG2	20:T:104:LEU:HD21	1.98	0.46
4:D:96:LEU:HD12	4:D:96:LEU:HA	1.77	0.46
1:A:484:C:H2'	1:A:485:G:C8	2.50	0.46
1:A:794:C:H4'	1:A:877:A:N6	2.31	0.46
9:I:70:LYS:HA	9:I:73:GLN:HB2	1.97	0.46
17:Q:60:ILE:HG13	17:Q:61:GLU:N	2.30	0.46
20:T:37:SER:O	20:T:38:LYS:C	2.59	0.46
1:A:859:C:O2'	1:A:860:C:H5'	2.16	0.46
1:A:1041:C:O3'	14:N:45:ARG:NH2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:VAL:HG12	2:B:170:GLU:HG2	1.98	0.46
17:Q:94:ASN:HA	17:Q:105:ALA:HB1	1.98	0.46
1:A:1286:G:N2	1:A:1312:G:H1'	2.31	0.46
5:E:81:GLU:OE1	5:E:88:LYS:HE2	2.15	0.46
6:F:75:LEU:O	6:F:79:LEU:HB2	2.15	0.46
19:S:11:VAL:HG22	19:S:39:THR:HB	1.98	0.46
1:A:293:A:H2'	1:A:294:G:O4'	2.16	0.46
1:A:596:C:H2'	1:A:597:A:C8	2.51	0.46
1:A:1077:U:P	1:A:1090:G:H1	2.39	0.46
1:A:1425:G:H5''	1:A:1426:A:H3'	1.97	0.46
1:A:1442:C:H2'	1:A:1443:C:O4'	2.16	0.46
3:C:156:ARG:HD3	3:C:156:ARG:HA	1.72	0.46
18:R:21:LYS:HE2	18:R:54:ARG:O	2.15	0.46
18:R:40:LEU:HB3	18:R:79:LEU:HD11	1.98	0.46
1:A:616:G:H2'	1:A:617:C:C6	2.50	0.45
1:A:772:U:O2'	1:A:774:G:N7	2.45	0.45
2:B:46:LYS:HA	2:B:49:GLU:HG2	1.96	0.45
2:B:77:ALA:HA	2:B:80:ILE:HD13	1.97	0.45
10:J:50:ILE:HB	14:N:41:ARG:CD	2.46	0.45
1:A:83:A:H5''	1:A:84:C:OP2	2.16	0.45
1:A:110:G:O6	1:A:284:G:H1'	2.16	0.45
1:A:674:G:H2'	1:A:675:U:C6	2.51	0.45
1:A:952:A:H4'	1:A:953:G:C5'	2.43	0.45
1:A:982:A:N6	1:A:1019:C:H42	2.14	0.45
1:A:1224:C:H5''	21:V:8:THR:HG22	1.98	0.45
2:B:223:ILE:HG21	2:B:230:VAL:HG22	1.98	0.45
3:C:119:ARG:O	3:C:123:GLN:HG3	2.16	0.45
18:R:45:SER:N	18:R:49:LYS:O	2.44	0.45
19:S:8:GLY:O	19:S:10:PHE:N	2.49	0.45
20:T:87:LYS:HB2	20:T:87:LYS:HE3	1.64	0.45
1:A:200:C:H2'	1:A:201:A:H5''	1.97	0.45
1:A:1013:G:H2'	1:A:1014:G:C8	2.51	0.45
1:A:1472:U:H2'	1:A:1473:C:C6	2.51	0.45
3:C:164:ARG:HG2	3:C:165:THR:H	1.81	0.45
4:D:30:LYS:C	4:D:32:ALA:H	2.23	0.45
10:J:6:ILE:HG23	10:J:72:VAL:HB	1.98	0.45
22:W:3:A:H5''	22:W:4:A:OP2	2.15	0.45
1:A:408:G:H2'	1:A:423:G:N2	2.31	0.45
1:A:1187:G:C6	1:A:1188:G:C5	3.04	0.45
1:A:1247:G:N2	1:A:1250:A:OP2	2.40	0.45
4:D:152:SER:O	4:D:155:LEU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1020:C:H2'	1:A:1021:C:H5'	1.99	0.45
11:K:48:ILE:HA	11:K:48:ILE:HD12	1.68	0.45
1:A:1249:A:N3	1:A:1307:C:O2'	2.39	0.45
1:A:1400:A:H2'	1:A:1401:G:O4'	2.16	0.45
3:C:54:ARG:HD3	3:C:56:ASP:OD2	2.17	0.45
8:H:4:ASP:CG	8:H:85:ARG:HH11	2.22	0.45
13:M:124:PRO:C	13:M:126:LYS:H	2.25	0.45
1:A:284:G:C6	1:A:285:C:N4	2.85	0.45
1:A:1094:C:O2	3:C:179:ARG:N	2.43	0.45
1:A:1286:G:C4	1:A:1312:G:N2	2.85	0.45
1:A:1328:G:H3'	9:I:108:VAL:O	2.16	0.45
1:A:799:A:OP1	1:A:1503:G:O2'	2.28	0.45
1:A:912:A:C2	1:A:913:C:C2	3.05	0.45
1:A:1110:C:H4'	9:I:16:ARG:HH22	1.81	0.45
2:B:231:GLU:HB3	2:B:232:PRO:HD2	1.98	0.45
9:I:55:ALA:H	9:I:56:LEU:HD12	1.81	0.45
18:R:26:LEU:HD13	18:R:29:PHE:CE2	2.52	0.45
1:A:801:G:C2'	1:A:802:A:H5''	2.47	0.45
2:B:61:LEU:HD23	2:B:68:ILE:HD11	1.99	0.45
3:C:9:GLY:HA2	3:C:12:LEU:HD13	1.98	0.45
3:C:21:ARG:NH2	10:J:92:THR:HB	2.32	0.45
3:C:159:GLY:HA2	3:C:193:TYR:CZ	2.52	0.45
4:D:36:ARG:HG3	4:D:38:TYR:CE2	2.52	0.45
4:D:78:LEU:HD23	4:D:78:LEU:HA	1.67	0.45
8:H:26:VAL:HG23	8:H:27:PRO:O	2.17	0.45
1:A:198:U:O2'	20:T:57:ARG:HG3	2.17	0.44
9:I:16:ARG:N	9:I:64:THR:O	2.49	0.44
9:I:43:ALA:C	9:I:45:ALA:N	2.76	0.44
13:M:71:ARG:HA	13:M:74:VAL:HG12	1.99	0.44
18:R:47:THR:HA	18:R:83:GLU:HB2	1.98	0.44
20:T:56:MET:HG3	20:T:88:VAL:HG21	2.00	0.44
1:A:100:G:C2	1:A:101:G:H1'	2.52	0.44
1:A:437:C:H2'	1:A:438:C:C6	2.53	0.44
1:A:437:C:H2'	1:A:438:C:H6	1.82	0.44
1:A:1417:G:H2'	1:A:1418:U:H6	1.76	0.44
2:B:17:PHE:N	2:B:17:PHE:CD2	2.85	0.44
2:B:35:GLU:O	2:B:37:ASN:N	2.49	0.44
2:B:210:SER:O	2:B:213:LEU:N	2.50	0.44
8:H:108:GLY:HA3	8:H:138:TRP:HB3	1.99	0.44
10:J:81:THR:O	10:J:85:LEU:N	2.45	0.44
13:M:8:GLU:OE2	13:M:67:GLU:HG2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:71:LYS:O	18:R:74:ARG:HB2	2.18	0.44
19:S:35:SER:C	19:S:37:ARG:H	2.26	0.44
1:A:837:A:H2'	1:A:838:G:O4'	2.18	0.44
1:A:935:A:N3	1:A:962:C:O2'	2.43	0.44
1:A:1285:G:C6	1:A:1286:G:N1	2.85	0.44
1:A:1468:G:C5	25:A:1785:PAR:H21	2.52	0.44
2:B:17:PHE:H	2:B:17:PHE:HD2	1.63	0.44
3:C:114:PRO:HA	3:C:185:GLY:HA3	1.97	0.44
3:C:157:ILE:HD12	3:C:164:ARG:HB3	1.98	0.44
5:E:90:VAL:O	5:E:120:THR:HA	2.16	0.44
6:F:11:ASN:HD22	6:F:86:ARG:NH2	2.15	0.44
10:J:49:VAL:HG11	14:N:45:ARG:HB2	1.99	0.44
1:A:340:C:H4'	1:A:341:G:O5'	2.16	0.44
1:A:353:U:H2'	1:A:354:U:H6	1.83	0.44
1:A:1257:G:O5'	1:A:1257:G:H8	2.00	0.44
1:A:1348:C:H2'	1:A:1349:C:C6	2.53	0.44
5:E:10:MET:HB2	5:E:32:VAL:HG23	1.99	0.44
19:S:36:ARG:HH12	19:S:75:ALA:HB3	1.81	0.44
1:A:102:A:C6	1:A:321:G:C6	3.06	0.44
1:A:521:G:H2'	1:A:522:A:C8	2.53	0.44
16:P:39:TYR:CD2	16:P:73:LEU:HD11	2.51	0.44
1:A:750:A:H2'	1:A:751:A:O4'	2.18	0.44
5:E:110:LEU:HD13	5:E:118:ILE:HG21	1.99	0.44
7:G:15:ASP:HB3	7:G:19:GLY:N	2.32	0.44
7:G:26:PHE:CE2	7:G:30:ILE:HD11	2.53	0.44
12:L:87:GLY:H	12:L:98:TYR:HB3	1.83	0.44
13:M:79:LYS:O	13:M:83:ASP:N	2.51	0.44
5:E:69:VAL:HG21	5:E:139:LEU:HD13	2.00	0.44
6:F:4:TYR:CZ	6:F:72:VAL:HG21	2.52	0.44
8:H:49:GLU:HG2	8:H:62:TYR:HE2	1.82	0.44
9:I:9:ARG:HB3	9:I:104:ARG:NH2	2.32	0.44
23:X:34:RSQ:H2'	23:X:35:A:C8	2.52	0.44
1:A:510:G:O2'	1:A:518:A:N1	2.41	0.44
1:A:523:G:H2'	1:A:524:G:O4'	2.18	0.44
1:A:1384:C:H2'	1:A:1385:C:O4'	2.17	0.44
4:D:30:LYS:O	4:D:32:ALA:N	2.51	0.44
1:A:234:U:H5''	1:A:235:C:OP1	2.18	0.44
1:A:858:G:P	12:L:12:ARG:NH2	2.90	0.44
5:E:152:ARG:HB3	8:H:43:GLY:O	2.18	0.44
7:G:18:TYR:HD1	7:G:59:LEU:HB2	1.82	0.44
17:Q:65:ILE:HD12	17:Q:65:ILE:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:898:U:O2'	5:E:19:MET:O	2.31	0.43
1:A:1371:C:O5'	1:A:1371:C:H6	2.00	0.43
2:B:32:ILE:HG21	2:B:40:HIS:CD2	2.54	0.43
4:D:31:CYS:O	4:D:31:CYS:SG	2.76	0.43
10:J:12:ASP:OD1	10:J:15:THR:HB	2.18	0.43
15:O:14:GLU:HG3	15:O:15:PHE:CD1	2.53	0.43
20:T:49:ALA:O	20:T:53:LEU:HD12	2.17	0.43
1:A:951:A:P	14:N:41:ARG:HH22	2.41	0.43
1:A:1231:A:H2	1:A:1334:G:H21	1.63	0.43
1:A:1297:G:N2	1:A:1299:A:H3'	2.33	0.43
1:A:1357:A:H2'	1:A:1358:U:O4'	2.18	0.43
2:B:103:THR:HA	2:B:180:LEU:HD11	2.00	0.43
4:D:173:TRP:CD1	4:D:189:PRO:HD3	2.53	0.43
4:D:187:ARG:NE	4:D:188:LEU:H	2.16	0.43
15:O:3:ILE:HG21	15:O:34:LEU:HD11	1.99	0.43
20:T:55:ILE:O	20:T:58:LYS:N	2.51	0.43
1:A:255:G:H2'	1:A:256:U:C6	2.53	0.43
1:A:968:U:O4	1:A:1193:U:O2'	2.32	0.43
3:C:131:ARG:HD2	3:C:135:LYS:HE3	1.99	0.43
5:E:82:VAL:HG21	5:E:138:ALA:HA	2.00	0.43
1:A:721:C:H5''	6:F:69:GLU:HB3	2.01	0.43
1:A:1008:C:H42	1:A:1013:G:H1	1.65	0.43
1:A:1208:A:C2	13:M:117:VAL:HG21	2.53	0.43
2:B:196:LEU:HD23	2:B:196:LEU:HA	1.71	0.43
4:D:9:CYS:HB3	4:D:32:ALA:CB	2.48	0.43
6:F:1:MET:HE3	6:F:68:PRO:HD3	2.00	0.43
7:G:92:SER:HA	7:G:93:PRO:HD2	1.65	0.43
9:I:50:LEU:HB3	9:I:56:LEU:H	1.84	0.43
19:S:58:VAL:HA	19:S:59:PRO:HD3	1.91	0.43
1:A:445:A:O5'	1:A:445:A:H8	2.02	0.43
1:A:659:A:H1'	11:K:115:PRO:HB3	2.00	0.43
1:A:968:U:C5	1:A:1193:U:H1'	2.54	0.43
1:A:982:A:H5''	1:A:1003:U:C4	2.53	0.43
2:B:47:THR:O	2:B:51:LEU:HB2	2.18	0.43
4:D:3:ARG:C	4:D:5:ILE:H	2.26	0.43
6:F:48:LEU:HD13	6:F:52:ILE:HG13	2.01	0.43
15:O:69:TYR:CZ	15:O:73:GLU:HG3	2.53	0.43
20:T:50:GLU:HB2	20:T:99:LEU:HD13	1.99	0.43
1:A:888:U:H2'	1:A:889:C:C6	2.54	0.43
1:A:227:G:H1'	1:A:257:A:N1	2.33	0.43
1:A:385:C:H4'	16:P:28:ARG:NH2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:G:H1'	1:A:608:G:N2	2.34	0.43
2:B:17:PHE:N	2:B:17:PHE:HD2	2.17	0.43
15:O:2:PRO:C	15:O:38:ARG:HH22	2.27	0.43
1:A:49:U:C2	1:A:356:G:N2	2.87	0.43
1:A:143:A:H2'	1:A:144:C:H6	1.83	0.43
1:A:424:U:O2	1:A:425:A:C8	2.72	0.43
1:A:484:C:OP1	12:L:117:ARG:NH2	2.45	0.43
1:A:1291:G:OP1	13:M:80:ARG:NH2	2.52	0.43
3:C:21:ARG:HH12	10:J:93:GLY:HA3	1.83	0.43
7:G:45:ASP:O	7:G:49:ILE:HG13	2.18	0.43
11:K:124:LYS:HE2	11:K:125:PHE:CE1	2.53	0.43
1:A:714:G:OP1	1:A:749:A:H1'	2.19	0.43
2:B:47:THR:HA	2:B:202:PRO:HG2	2.01	0.43
4:D:199:ASN:C	4:D:199:ASN:ND2	2.77	0.43
5:E:118:ILE:HG12	5:E:119:LEU:N	2.34	0.43
7:G:57:GLU:O	7:G:61:VAL:HG23	2.18	0.43
8:H:89:PRO:C	8:H:91:ARG:H	2.27	0.43
17:Q:43:LEU:HD12	17:Q:68:ARG:HB3	1.99	0.43
1:A:353:U:H2'	1:A:354:U:C6	2.54	0.43
1:A:910:G:OP2	7:G:3:ARG:HB2	2.18	0.43
1:A:1173:C:O2	5:E:25:ARG:NH2	2.52	0.43
1:A:1354:U:H2'	1:A:1355:G:O4'	2.18	0.43
4:D:61:LYS:HD3	4:D:206:PHE:CE2	2.54	0.43
5:E:67:VAL:HG22	5:E:140:ARG:HE	1.83	0.43
6:F:26:ILE:HG23	6:F:79:LEU:HD11	2.01	0.43
1:A:627:G:C5	1:A:628:C:C5	3.07	0.42
1:A:1288:U:H5'	13:M:109:THR:HG21	2.00	0.42
1:A:1328:G:H22	1:A:1355:G:H2'	1.84	0.42
2:B:91:PRO:HG2	2:B:155:LEU:HG	2.00	0.42
4:D:109:GLY:HA3	4:D:165:MET:HE3	1.99	0.42
6:F:7:ASN:HB2	6:F:89:MET:HB3	2.01	0.42
12:L:59:ARG:HG3	12:L:65:GLU:HG3	2.00	0.42
13:M:67:GLU:HB3	13:M:68:GLY:H	1.55	0.42
16:P:4:ILE:HG13	16:P:64:ALA:HB1	2.01	0.42
1:A:954:A:H2'	1:A:955:A:H5''	2.01	0.42
1:A:1149:A:C6	1:A:1150:A:C6	3.07	0.42
5:E:92:LYS:HA	5:E:93:PRO:HD3	1.86	0.42
6:F:74:ASP:HA	6:F:77:ARG:HD2	2.00	0.42
8:H:84:ARG:HE	8:H:84:ARG:HB3	1.46	0.42
15:O:74:ASP:O	15:O:76:GLU:N	2.52	0.42
16:P:21:VAL:HG21	16:P:59:TRP:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:10:VAL:HB	17:Q:53:LEU:HA	2.01	0.42
1:A:108:G:H1'	1:A:109:A:N7	2.34	0.42
1:A:170:C:H2'	1:A:171:C:C6	2.53	0.42
1:A:207:C:H42	1:A:211:G:H1	1.67	0.42
1:A:849:A:O2'	1:A:850:A:H3'	2.19	0.42
1:A:888:U:OP1	12:L:95:GLY:HA2	2.19	0.42
1:A:1102:G:H2'	1:A:1103:U:C6	2.54	0.42
1:A:1348:C:H2'	1:A:1349:C:H6	1.85	0.42
4:D:4:TYR:C	4:D:5:ILE:HG13	2.43	0.42
8:H:82:HIS:ND1	8:H:138:TRP:CE2	2.88	0.42
11:K:45:GLY:C	11:K:55:LYS:HG2	2.43	0.42
17:Q:60:ILE:HG22	17:Q:72:ARG:O	2.19	0.42
18:R:58:LEU:HD13	18:R:62:GLU:HB3	2.02	0.42
1:A:542:A:H4'	1:A:543:U:O5'	2.19	0.42
1:A:704:G:H4'	1:A:705:A:O5'	2.19	0.42
1:A:841:A:H2'	1:A:842:A:C8	2.54	0.42
1:A:889:C:O2'	1:A:890:A:H5'	2.19	0.42
1:A:1306:C:H4'	21:V:17:THR:HG21	2.01	0.42
1:A:1319:G:C6	1:A:1320:A:C6	3.08	0.42
1:A:1381:C:C2	1:A:1383:G:C5	3.07	0.42
2:B:10:LEU:HD23	2:B:10:LEU:H	1.84	0.42
11:K:12:ARG:CZ	11:K:12:ARG:HA	2.49	0.42
22:W:3:A:N1	23:X:34:RSQ:N3	2.68	0.42
1:A:780:C:H2'	1:A:781:G:C8	2.54	0.42
1:A:1480:A:N6	1:A:1510:C:H5'	2.34	0.42
3:C:26:LYS:NZ	10:J:45:ARG:HE	2.17	0.42
6:F:8:ILE:HD13	6:F:26:ILE:HD13	2.00	0.42
10:J:24:VAL:O	10:J:26:ALA:N	2.50	0.42
19:S:45:VAL:HA	19:S:62:ILE:HD13	2.00	0.42
1:A:1019:C:H2'	1:A:1020:C:H6	1.84	0.42
1:A:1033:C:H2'	1:A:1034:U:H6	1.85	0.42
2:B:83:MET:SD	2:B:234:PRO:HB2	2.59	0.42
2:B:178:ARG:HH22	8:H:74:PRO:CG	2.32	0.42
6:F:2:ARG:NH1	6:F:69:GLU:HG2	2.35	0.42
8:H:91:ARG:NH1	17:Q:32:TYR:O	2.53	0.42
9:I:37:PHE:CE2	9:I:74:ILE:HG13	2.55	0.42
13:M:91:ARG:HA	13:M:91:ARG:HD2	1.82	0.42
17:Q:59:ILE:HG23	17:Q:71:PHE:CD1	2.55	0.42
1:A:1266:A:H4'	1:A:1267:A:O5'	2.20	0.42
2:B:32:ILE:HD13	2:B:40:HIS:CG	2.55	0.42
4:D:156:GLU:O	4:D:160:GLN:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:77:ARG:HG2	6:F:78:GLU:N	2.34	0.42
9:I:17:VAL:HG11	9:I:81:ILE:HA	2.02	0.42
10:J:5:ARG:O	10:J:98:ILE:HA	2.19	0.42
15:O:17:ARG:HG3	15:O:17:ARG:HH11	1.85	0.42
1:A:190:G:H4'	1:A:191:G:OP2	2.20	0.42
1:A:816:U:H2'	1:A:817:C:H6	1.81	0.42
1:A:1433:G:H2'	1:A:1434:G:O4'	2.20	0.42
6:F:9:VAL:CG2	6:F:87:ARG:HB2	2.50	0.42
8:H:11:THR:O	8:H:12:ARG:C	2.62	0.42
9:I:36:TYR:OH	9:I:73:GLN:NE2	2.47	0.42
17:Q:3:LYS:HD3	17:Q:61:GLU:O	2.20	0.42
1:A:906:G:C6	1:A:907:C:C4	3.08	0.42
1:A:1286:G:H5''	21:V:4:GLY:HA3	2.01	0.42
2:B:118:LEU:HD23	2:B:118:LEU:HA	1.93	0.42
13:M:17:VAL:O	13:M:20:THR:HB	2.20	0.42
1:A:849:A:C8	1:A:851:G:C8	3.08	0.42
1:A:1083:A:H8	2:B:172:ILE:HD13	1.84	0.42
1:A:1277:C:H5''	13:M:14:ARG:HD2	2.01	0.42
3:C:76:VAL:HG11	3:C:103:VAL:HG21	2.02	0.42
5:E:78:HIS:HB2	5:E:79:GLU:H	1.71	0.42
8:H:86:ILE:HG12	8:H:135:CYS:HA	2.01	0.42
15:O:3:ILE:HG21	15:O:34:LEU:CD1	2.50	0.42
17:Q:29:HIS:CE1	17:Q:30:PRO:HG2	2.55	0.42
17:Q:43:LEU:HD23	17:Q:43:LEU:HA	1.91	0.42
1:A:272:C:H5'	17:Q:68:ARG:HH12	1.84	0.41
1:A:501:C:OP2	1:A:513:G:H4'	2.20	0.41
1:A:557:A:N3	1:A:860:C:H1'	2.35	0.41
1:A:1036:C:OP1	1:A:1178:G:OP2	2.37	0.41
11:K:74:ALA:C	11:K:76:GLY:H	2.28	0.41
17:Q:29:HIS:HA	17:Q:30:PRO:HD2	1.85	0.41
19:S:33:THR:OG1	19:S:34:TRP:N	2.51	0.41
1:A:47:C:OP2	1:A:361:C:N4	2.39	0.41
1:A:217:U:H2'	1:A:218:U:C6	2.55	0.41
1:A:1306:C:P	21:V:6:ARG:HH22	2.44	0.41
2:B:71:VAL:O	2:B:164:VAL:HA	2.20	0.41
2:B:90:MET:HA	2:B:91:PRO:HD3	1.82	0.41
4:D:108:LEU:HD13	4:D:183:GLY:HA3	2.01	0.41
7:G:87:VAL:HA	7:G:88:PRO:HD3	1.92	0.41
10:J:34:VAL:HG22	10:J:74:ILE:HG22	2.01	0.41
10:J:50:ILE:HD12	10:J:50:ILE:N	2.34	0.41
14:N:10:ALA:O	14:N:12:ARG:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:A:OP2	12:L:51:ALA:HB1	2.19	0.41
1:A:652:U:H2'	1:A:653:G:C8	2.54	0.41
1:A:842:A:HO2'	1:A:843:C:H5'	1.85	0.41
2:B:144:ARG:HG3	2:B:145:LEU:N	2.35	0.41
3:C:3:ASN:ND2	3:C:3:ASN:N	2.67	0.41
4:D:113:SER:OG	4:D:114:ARG:N	2.52	0.41
5:E:15:ARG:HD3	5:E:26:PHE:CD1	2.56	0.41
5:E:148:VAL:O	5:E:152:ARG:HG3	2.20	0.41
9:I:118:LYS:HB2	9:I:121:ARG:HB3	2.01	0.41
11:K:92:GLU:OE2	18:R:88:LYS:NZ	2.52	0.41
13:M:23:TYR:CB	13:M:67:GLU:HA	2.48	0.41
1:A:689:A:H4'	11:K:29:ILE:HD11	2.02	0.41
2:B:8:LYS:HB3	2:B:9:GLU:H	1.48	0.41
4:D:178:VAL:C	4:D:180:GLY:H	2.28	0.41
4:D:194:LEU:H	4:D:194:LEU:HD22	1.85	0.41
12:L:41:ARG:HH22	12:L:57:LYS:HE3	1.86	0.41
15:O:60:VAL:O	15:O:64:ARG:HG2	2.21	0.41
16:P:40:ASP:HA	16:P:41:PRO:HD3	1.87	0.41
1:A:17:U:H1'	1:A:1062:A:N3	2.34	0.41
1:A:341:G:H2'	1:A:342:G:O4'	2.20	0.41
1:A:512:G:H22	12:L:51:ALA:HB2	1.85	0.41
1:A:1374:G:O2'	1:A:1375:U:H5'	2.20	0.41
4:D:102:ASP:HB3	4:D:136:PRO:HB3	2.02	0.41
7:G:146:GLU:C	7:G:148:ASN:N	2.77	0.41
8:H:121:ASP:OD1	8:H:121:ASP:N	2.52	0.41
14:N:9:LYS:HG3	14:N:21:TYR:O	2.19	0.41
16:P:39:TYR:HA	16:P:48:TRP:O	2.21	0.41
1:A:752:G:H4'	1:A:1490:A:H4'	2.02	0.41
1:A:904:G:N2	1:A:1373:U:H1'	2.36	0.41
1:A:939:C:H2'	1:A:940:G:O4'	2.20	0.41
2:B:97:TRP:CZ2	2:B:102:LEU:HD13	2.53	0.41
3:C:15:THR:OG1	3:C:16:ARG:N	2.53	0.41
10:J:65:LEU:HD12	14:N:55:GLY:O	2.21	0.41
11:K:43:SER:OG	11:K:44:SER:N	2.52	0.41
17:Q:97:SER:OG	17:Q:98:LEU:HD12	2.20	0.41
1:A:64:G:H8	1:A:64:G:H2'	1.51	0.41
1:A:763:A:O2'	1:A:764:A:H5''	2.21	0.41
1:A:1390:A:H2'	1:A:1391:C:C6	2.54	0.41
2:B:230:VAL:HB	2:B:231:GLU:H	1.53	0.41
3:C:154:SER:O	3:C:165:THR:HA	2.21	0.41
5:E:88:LYS:HB3	5:E:123:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:92:ASP:O	12:L:94:PRO:HD3	2.21	0.41
13:M:46:LYS:H	13:M:46:LYS:HG3	1.56	0.41
1:A:187:C:C4	1:A:188:U:C4	3.09	0.41
1:A:424:U:O3'	4:D:22:LYS:NZ	2.53	0.41
1:A:1362:U:H4'	1:A:1363:U:O5'	2.21	0.41
2:B:32:ILE:HD13	2:B:40:HIS:CD2	2.56	0.41
3:C:141:VAL:HG11	3:C:202:ILE:HG12	2.03	0.41
7:G:85:TYR:HD2	7:G:85:TYR:HA	1.75	0.41
18:R:51:LEU:HA	18:R:52:PRO:HD3	1.82	0.41
18:R:76:LEU:HA	18:R:76:LEU:HD23	1.85	0.41
1:A:175:G:H4'	1:A:176:U:H5'	2.03	0.41
1:A:210:U:H4'	1:A:211:G:O5'	2.20	0.41
1:A:520:G:H2'	1:A:521:G:H8	1.85	0.41
1:A:525:G:H5'	4:D:41:GLY:HA3	2.02	0.41
1:A:527:G:C6	1:A:528:C:C4	3.09	0.41
1:A:617:C:O2	1:A:617:C:H2'	2.20	0.41
1:A:948:G:H4'	1:A:949:C:C5'	2.51	0.41
1:A:1324:G:H1'	9:I:121:ARG:NH2	2.36	0.41
2:B:82:ARG:HA	2:B:92:TYR:CD1	2.56	0.41
3:C:164:ARG:HD2	3:C:166:GLU:OE2	2.21	0.41
4:D:38:TYR:HB2	4:D:44:GLY:O	2.21	0.41
5:E:9:LYS:HA	5:E:9:LYS:HD2	1.83	0.41
5:E:28:PHE:CD2	5:E:51:VAL:HG22	2.56	0.41
5:E:78:HIS:HE1	5:E:142:LEU:HA	1.85	0.41
5:E:80:ILE:HD12	5:E:80:ILE:H	1.85	0.41
8:H:51:VAL:HG11	8:H:60:ARG:CZ	2.50	0.41
12:L:10:LEU:HD23	12:L:10:LEU:HA	1.69	0.41
13:M:33:ALA:O	13:M:37:THR:HB	2.21	0.41
15:O:3:ILE:HG23	15:O:38:ARG:NH2	2.36	0.41
15:O:29:VAL:HG11	15:O:67:LEU:HD21	2.01	0.41
15:O:33:THR:HA	15:O:36:ILE:HD12	2.03	0.41
17:Q:67:LYS:HA	17:Q:70:ARG:NH2	2.35	0.41
20:T:104:LEU:HD23	20:T:104:LEU:HA	1.90	0.41
1:A:57:G:H2'	1:A:58:C:C6	2.56	0.41
1:A:323:C:O2'	1:A:324:A:OP2	2.28	0.41
4:D:79:PHE:CE1	4:D:204:ILE:HG12	2.56	0.41
11:K:48:ILE:HD11	11:K:67:ASP:HB2	2.02	0.41
12:L:38:THR:O	12:L:39:VAL:HB	2.21	0.41
13:M:3:ARG:HH12	13:M:7:VAL:HA	1.86	0.41
1:A:950:G:O3'	14:N:41:ARG:NH2	2.52	0.40
1:A:1277:C:H4'	1:A:1283:U:C5	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:49:ARG:NE	4:D:49:ARG:H	2.19	0.40
1:A:103:C:H2'	1:A:104:G:O4'	2.21	0.40
1:A:406:A:H62	1:A:408:G:N2	2.20	0.40
1:A:494:C:H6	1:A:494:C:H2'	1.67	0.40
1:A:547:C:OP1	12:L:15:ARG:NE	2.50	0.40
1:A:615:A:H2'	1:A:616:G:O4'	2.21	0.40
1:A:1008:C:N4	1:A:1013:G:H1	2.19	0.40
1:A:1036:C:H41	23:X:34:RSQ:C1'	2.33	0.40
1:A:1139:A:C5	1:A:1161:A:C6	3.09	0.40
2:B:44:LEU:H	2:B:44:LEU:HG	1.70	0.40
4:D:140:VAL:HG11	4:D:146:ILE:HD11	2.03	0.40
5:E:131:ILE:HD13	5:E:131:ILE:HA	1.93	0.40
7:G:99:LEU:HD23	7:G:99:LEU:HA	1.87	0.40
7:G:137:LYS:HB2	7:G:137:LYS:HE3	1.86	0.40
8:H:1:MET:HG2	8:H:2:LEU:N	2.35	0.40
9:I:4:TYR:CE2	9:I:88:TYR:HA	2.56	0.40
12:L:31:PRO:HB2	12:L:32:PHE:CE2	2.55	0.40
12:L:41:ARG:HG2	12:L:42:THR:N	2.35	0.40
17:Q:53:LEU:O	17:Q:53:LEU:HD12	2.21	0.40
21:V:5:ASP:O	21:V:11:GLY:HA3	2.21	0.40
1:A:98:G:H2'	1:A:99:C:C6	2.56	0.40
1:A:398:C:OP1	4:D:136:PRO:HD2	2.20	0.40
1:A:1378:A:H2	5:E:19:MET:HG3	1.85	0.40
5:E:151:LEU:HD23	5:E:151:LEU:HA	1.93	0.40
7:G:8:GLU:OE2	7:G:8:GLU:N	2.46	0.40
8:H:17:THR:HB	8:H:78:GLN:OE1	2.21	0.40
11:K:34:ASP:C	11:K:36:ASP:H	2.30	0.40
15:O:55:GLY:HA2	15:O:58:MET:HE3	2.04	0.40
19:S:5:LEU:HA	19:S:6:LYS:HZ2	1.87	0.40
1:A:15:G:H21	5:E:18:ARG:HA	1.86	0.40
1:A:297:G:H5''	12:L:17:LYS:HE3	2.04	0.40
1:A:423:G:H4'	1:A:424:U:O5'	2.21	0.40
1:A:704:G:OP2	18:R:53:ARG:HG3	2.22	0.40
1:A:1317:C:O5'	1:A:1317:C:H6	2.03	0.40
2:B:93:VAL:HG11	2:B:97:TRP:CD1	2.56	0.40
5:E:44:GLY:HA3	5:E:62:ALA:HB2	2.03	0.40
7:G:120:ILE:N	7:G:120:ILE:HD12	2.36	0.40
12:L:93:LEU:HB2	12:L:96:VAL:CG2	2.51	0.40
1:A:675:U:H1'	1:A:678:A:N7	2.37	0.40
1:A:948:G:P	1:A:948:G:H3'	2.62	0.40
1:A:982:A:C8	1:A:1020:C:N3	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1022:U:C2	1:A:1023:A:C8	3.10	0.40
1:A:1281:G:C6	1:A:1316:C:C5	3.09	0.40
1:A:1379:C:H4'	1:A:1380:A:OP2	2.20	0.40
3:C:155:GLY:O	3:C:156:ARG:HB2	2.21	0.40
16:P:51:VAL:HG12	16:P:52:ASP:C	2.45	0.40
18:R:83:GLU:HB3	18:R:84:LYS:H	1.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	232/234 (99%)	184 (79%)	33 (14%)	15 (6%)	1	8
3	C	204/206 (99%)	147 (72%)	40 (20%)	17 (8%)	0	4
4	D	206/208 (99%)	172 (84%)	24 (12%)	10 (5%)	1	13
5	E	148/150 (99%)	126 (85%)	19 (13%)	3 (2%)	6	31
6	F	99/101 (98%)	88 (89%)	9 (9%)	2 (2%)	6	31
7	G	153/155 (99%)	130 (85%)	18 (12%)	5 (3%)	3	21
8	H	136/138 (99%)	117 (86%)	18 (13%)	1 (1%)	18	52
9	I	125/127 (98%)	96 (77%)	20 (16%)	9 (7%)	1	6
10	J	96/98 (98%)	67 (70%)	18 (19%)	11 (12%)	0	1
11	K	117/119 (98%)	99 (85%)	16 (14%)	2 (2%)	7	35
12	L	122/124 (98%)	96 (79%)	18 (15%)	8 (7%)	1	7
13	M	123/125 (98%)	98 (80%)	19 (15%)	6 (5%)	1	13
14	N	58/60 (97%)	49 (84%)	5 (9%)	4 (7%)	1	7
15	O	86/88 (98%)	75 (87%)	9 (10%)	2 (2%)	5	29
16	P	81/83 (98%)	72 (89%)	8 (10%)	1 (1%)	10	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Q	102/104 (98%)	85 (83%)	11 (11%)	6 (6%)	1	10
18	R	71/73 (97%)	63 (89%)	6 (8%)	2 (3%)	4	25
19	S	78/80 (98%)	60 (77%)	10 (13%)	8 (10%)	0	2
20	T	97/99 (98%)	75 (77%)	13 (13%)	9 (9%)	0	3
21	V	22/24 (92%)	20 (91%)	2 (9%)	0	100	100
All	All	2356/2396 (98%)	1919 (82%)	316 (13%)	121 (5%)	1	13

All (121) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	36	ARG
2	B	211	ILE
2	B	229	VAL
3	C	15	THR
3	C	160	ALA
4	D	31	CYS
4	D	36	ARG
4	D	171	GLY
5	E	77	PRO
7	G	134	ALA
9	I	12	GLU
9	I	101	PHE
11	K	55	LYS
12	L	27	LEU
12	L	28	LYS
12	L	47	LYS
13	M	27	LYS
13	M	86	CYS
14	N	11	LYS
17	Q	49	GLU
17	Q	100	LYS
19	S	9	VAL
20	T	73	HIS
20	T	99	LEU
2	B	8	LYS
2	B	14	GLY
2	B	17	PHE
2	B	210	SER
3	C	4	LYS
3	C	47	LEU

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Mol	Chain	Res	Type
3	C	64	VAL
3	C	98	ASN
3	C	101	LEU
3	C	154	SER
4	D	69	GLY
4	D	208	SER
7	G	4	ARG
7	G	93	PRO
9	I	42	ARG
9	I	43	ALA
9	I	93	ARG
10	J	4	ILE
10	J	34	VAL
10	J	54	PHE
10	J	90	LEU
12	L	39	VAL
12	L	79	GLU
19	S	5	LEU
19	S	6	LYS
20	T	9	ASN
20	T	94	ALA
2	B	20	GLU
2	B	207	ALA
3	C	43	LEU
3	C	66	VAL
3	C	127	ARG
3	C	146	ALA
3	C	181	ASN
4	D	5	ILE
5	E	71	LEU
6	F	16	GLN
9	I	51	ARG
9	I	54	ASP
9	I	88	TYR
10	J	73	ASP
12	L	105	TYR
13	M	113	PRO
15	O	10	LYS
17	Q	97	SER
18	R	47	THR
19	S	47	HIS
19	S	77	THR

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Mol	Chain	Res	Type
20	T	95	ALA
2	B	9	GLU
2	B	95	GLN
2	B	228	GLY
2	B	232	PRO
3	C	29	TYR
3	C	206	GLU
4	D	35	ARG
6	F	43	LEU
7	G	7	ALA
10	J	39	PRO
10	J	40	LEU
10	J	72	VAL
12	L	123	LYS
14	N	8	GLU
14	N	14	PRO
15	O	72	ARG
17	Q	30	PRO
18	R	45	SER
19	S	30	LEU
19	S	78	ARG
20	T	96	GLY
20	T	98	PRO
2	B	15	VAL
2	B	130	ARG
3	C	3	ASN
3	C	108	ASN
9	I	105	ASP
10	J	26	ALA
11	K	35	PRO
14	N	12	ARG
20	T	102	GLY
4	D	184	LYS
5	E	78	HIS
10	J	25	GLU
13	M	67	GLU
13	M	84	ILE
20	T	97	ALA
8	H	51	VAL
7	G	82	GLY
13	M	97	PRO
16	P	10	GLY

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Mol	Chain	Res	Type
17	Q	77	VAL
4	D	44	GLY
4	D	88	VAL
10	J	77	PRO
12	L	30	ALA
17	Q	80	GLY
19	S	67	VAL

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	202/202 (100%)	161 (80%)	41 (20%)	1	7
3	C	160/160 (100%)	129 (81%)	31 (19%)	1	8
4	D	180/180 (100%)	147 (82%)	33 (18%)	2	9
5	E	115/115 (100%)	86 (75%)	29 (25%)	0	3
6	F	90/90 (100%)	72 (80%)	18 (20%)	1	7
7	G	126/126 (100%)	109 (86%)	17 (14%)	4	19
8	H	119/119 (100%)	103 (87%)	16 (13%)	4	19
9	I	98/98 (100%)	83 (85%)	15 (15%)	3	14
10	J	88/88 (100%)	75 (85%)	13 (15%)	3	15
11	K	90/90 (100%)	75 (83%)	15 (17%)	2	11
12	L	104/104 (100%)	80 (77%)	24 (23%)	1	5
13	M	100/100 (100%)	85 (85%)	15 (15%)	3	15
14	N	49/49 (100%)	37 (76%)	12 (24%)	1	3
15	O	79/79 (100%)	65 (82%)	14 (18%)	2	10
16	P	72/72 (100%)	65 (90%)	7 (10%)	8	32
17	Q	96/96 (100%)	80 (83%)	16 (17%)	2	11
18	R	64/64 (100%)	56 (88%)	8 (12%)	4	21
19	S	71/71 (100%)	59 (83%)	12 (17%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	T	76/76 (100%)	65 (86%)	11 (14%)	3	16
21	V	19/19 (100%)	17 (90%)	2 (10%)	6	28
All	All	1998/1998 (100%)	1649 (82%)	349 (18%)	2	10

All (349) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	8	LYS
2	B	9	GLU
2	B	12	GLU
2	B	15	VAL
2	B	16	HIS
2	B	17	PHE
2	B	21	ARG
2	B	27	LYS
2	B	44	LEU
2	B	48	MET
2	B	51	LEU
2	B	58	ILE
2	B	64	ARG
2	B	67	THR
2	B	76	GLN
2	B	79	ASP
2	B	90	MET
2	B	92	TYR
2	B	98	LEU
2	B	107	THR
2	B	108	ILE
2	B	117	GLU
2	B	118	LEU
2	B	121	LEU
2	B	127	ILE
2	B	130	ARG
2	B	143	GLU
2	B	144	ARG
2	B	150	SER
2	B	153	ARG
2	B	162	ILE
2	B	165	VAL
2	B	169	LYS
2	B	170	GLU

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Mol	Chain	Res	Type
2	B	178	ARG
2	B	196	LEU
2	B	197	VAL
2	B	208	ILE
2	B	212	GLN
2	B	223	ILE
2	B	224	GLN
3	C	3	ASN
3	C	4	LYS
3	C	5	ILE
3	C	12	LEU
3	C	14	ILE
3	C	26	LYS
3	C	31	HIS
3	C	42	LEU
3	C	45	LYS
3	C	47	LEU
3	C	52	LEU
3	C	67	THR
3	C	75	VAL
3	C	84	ILE
3	C	86	VAL
3	C	89	GLU
3	C	101	LEU
3	C	107	GLN
3	C	115	LEU
3	C	152	ILE
3	C	156	ARG
3	C	161	GLU
3	C	162	GLN
3	C	165	THR
3	C	166	GLU
3	C	167	TRP
3	C	175	LEU
3	C	177	THR
3	C	192	THR
3	C	198	VAL
3	C	204	LEU
4	D	3	ARG
4	D	5	ILE
4	D	8	VAL
4	D	10	ARG

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Mol	Chain	Res	Type
4	D	24	GLU
4	D	42	GLN
4	D	49	ARG
4	D	53	ASP
4	D	56	VAL
4	D	58	LEU
4	D	64	LEU
4	D	70	ILE
4	D	74	GLN
4	D	84	LYS
4	D	89	THR
4	D	96	LEU
4	D	99	SER
4	D	122	ARG
4	D	127	THR
4	D	151	LYS
4	D	154	ASN
4	D	155	LEU
4	D	175	SER
4	D	176	LEU
4	D	178	VAL
4	D	182	LYS
4	D	187	ARG
4	D	190	ASP
4	D	191	ARG
4	D	193	ASP
4	D	194	LEU
4	D	200	GLU
4	D	204	ILE
5	E	5	ASP
5	E	10	MET
5	E	11	ILE
5	E	12	LEU
5	E	13	ILE
5	E	18	ARG
5	E	20	GLN
5	E	31	LEU
5	E	41	VAL
5	E	43	LEU
5	E	47	LYS
5	E	53	LEU
5	E	60	TYR

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Mol	Chain	Res	Type
5	E	69	VAL
5	E	79	GLU
5	E	80	ILE
5	E	81	GLU
5	E	92	LYS
5	E	100	VAL
5	E	112	LEU
5	E	116	THR
5	E	118	ILE
5	E	120	THR
5	E	122	GLU
5	E	125	SER
5	E	137	GLU
5	E	140	ARG
5	E	147	ASP
5	E	152	ARG
6	F	9	VAL
6	F	10	LEU
6	F	13	ASN
6	F	14	LEU
6	F	17	SER
6	F	23	LYS
6	F	43	LEU
6	F	47	ARG
6	F	70	ASP
6	F	73	ASN
6	F	75	LEU
6	F	77	ARG
6	F	79	LEU
6	F	91	VAL
6	F	92	LYS
6	F	93	SER
6	F	94	GLN
6	F	95	GLU
7	G	8	GLU
7	G	12	LEU
7	G	16	LEU
7	G	21	VAL
7	G	22	LEU
7	G	38	LEU
7	G	75	VAL
7	G	89	MET

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Mol	Chain	Res	Type
7	G	98	SER
7	G	104	LEU
7	G	110	GLN
7	G	111	ARG
7	G	113	GLU
7	G	114	ARG
7	G	129	GLU
7	G	135	VAL
7	G	136	LYS
8	H	18	ARG
8	H	21	LYS
8	H	24	THR
8	H	26	VAL
8	H	56	LYS
8	H	83	ILE
8	H	85	ARG
8	H	91	ARG
8	H	92	ARG
8	H	98	LYS
8	H	100	ILE
8	H	102	ARG
8	H	107	LEU
8	H	116	LYS
8	H	127	LEU
8	H	137	VAL
9	I	2	GLU
9	I	14	VAL
9	I	20	ARG
9	I	25	LYS
9	I	26	VAL
9	I	27	THR
9	I	38	GLN
9	I	47	LEU
9	I	62	TYR
9	I	64	THR
9	I	65	VAL
9	I	66	ARG
9	I	79	LEU
9	I	105	ASP
9	I	124	GLN
10	J	4	ILE
10	J	6	ILE

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Mol	Chain	Res	Type
10	J	15	THR
10	J	16	LEU
10	J	23	ILE
10	J	35	SER
10	J	38	ILE
10	J	49	VAL
10	J	71	LEU
10	J	74	ILE
10	J	83	GLU
10	J	90	LEU
10	J	96	ILE
11	K	29	ILE
11	K	30	VAL
11	K	32	ILE
11	K	33	THR
11	K	34	ASP
11	K	41	THR
11	K	47	VAL
11	K	48	ILE
11	K	63	LEU
11	K	77	MET
11	K	84	VAL
11	K	92	GLU
11	K	109	VAL
11	K	114	VAL
11	K	124	LYS
12	L	18	VAL
12	L	20	LYS
12	L	27	LEU
12	L	33	ARG
12	L	42	THR
12	L	53	ARG
12	L	54	LYS
12	L	55	VAL
12	L	60	LEU
12	L	64	TYR
12	L	67	THR
12	L	75	HIS
12	L	79	GLU
12	L	80	HIS
12	L	81	SER
12	L	82	VAL

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Mol	Chain	Res	Type
12	L	83	VAL
12	L	85	ILE
12	L	93	LEU
12	L	97	ARG
12	L	100	ILE
12	L	111	LYS
12	L	117	ARG
12	L	127	GLU
13	M	9	ILE
13	M	37	THR
13	M	44	ARG
13	M	47	ASP
13	M	56	LEU
13	M	60	VAL
13	M	63	THR
13	M	67	GLU
13	M	70	LEU
13	M	73	GLU
13	M	77	ASN
13	M	92	HIS
13	M	105	THR
13	M	108	ARG
13	M	125	ARG
14	N	7	ILE
14	N	8	GLU
14	N	9	LYS
14	N	11	LYS
14	N	12	ARG
14	N	16	PHE
14	N	22	THR
14	N	31	ARG
14	N	32	SER
14	N	33	VAL
14	N	42	ILE
14	N	53	LEU
15	O	3	ILE
15	O	7	GLU
15	O	10	LYS
15	O	13	GLN
15	O	22	THR
15	O	31	LEU
15	O	34	LEU

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Mol	Chain	Res	Type
15	O	38	ARG
15	O	39	LEU
15	O	57	LEU
15	O	70	LEU
15	O	76	GLU
15	O	81	LEU
15	O	83	GLU
16	P	2	VAL
16	P	28	ARG
16	P	45	THR
16	P	53	VAL
16	P	62	VAL
16	P	72	ARG
16	P	76	GLN
17	Q	5	VAL
17	Q	9	VAL
17	Q	23	VAL
17	Q	38	ARG
17	Q	53	LEU
17	Q	59	ILE
17	Q	69	LYS
17	Q	70	ARG
17	Q	74	LEU
17	Q	77	VAL
17	Q	78	GLU
17	Q	79	SER
17	Q	83	ASP
17	Q	84	LEU
17	Q	91	ARG
17	Q	100	LYS
18	R	21	LYS
18	R	26	LEU
18	R	28	GLU
18	R	47	THR
18	R	54	ARG
18	R	55	ARG
18	R	86	VAL
18	R	88	LYS
19	S	5	LEU
19	S	6	LYS
19	S	7	LYS
19	S	31	ILE

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Mol	Chain	Res	Type
19	S	33	THR
19	S	35	SER
19	S	38	SER
19	S	40	ILE
19	S	43	GLU
19	S	62	ILE
19	S	65	ASN
19	S	67	VAL
20	T	10	LEU
20	T	13	LEU
20	T	25	ARG
20	T	42	GLN
20	T	50	GLU
20	T	56	MET
20	T	62	LEU
20	T	72	LEU
20	T	74	LYS
20	T	75	ASN
20	T	84	LEU
21	V	8	THR
21	V	15	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	16	HIS
2	B	40	HIS
2	B	113	HIS
2	B	135	GLN
3	C	110	ASN
3	C	123	GLN
3	C	170	GLN
4	D	42	GLN
4	D	45	GLN
5	E	56	GLN
5	E	65	ASN
5	E	78	HIS
6	F	73	ASN
9	I	34	ASN
10	J	76	ASN
11	K	78	GLN
11	K	93	GLN

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Mol	Chain	Res	Type
12	L	49	ASN
13	M	77	ASN
16	P	16	HIS
16	P	76	GLN
16	P	82	GLN
17	Q	96	GLN
19	S	47	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1513/1513 (100%)	330 (21%)	73 (4%)
22	W	3/6 (50%)	1 (33%)	0
23	X	5/17 (29%)	2 (40%)	0
All	All	1521/1536 (99%)	333 (21%)	73 (4%)

All (333) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	9	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	59	A
1	A	65	U
1	A	73	G
1	A	94	A
1	A	114	C
1	A	123	G
1	A	124	A
1	A	125	C
1	A	156	A
1	A	157	C
1	A	163	C
1	A	167	U
1	A	168	C

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Mol	Chain	Res	Type
1	A	176	U
1	A	177	G
1	A	189	U
1	A	190	G
1	A	191	G
1	A	193	G
1	A	201	A
1	A	203	A
1	A	207	C
1	A	208	U
1	A	211	G
1	A	212	C
1	A	239	U
1	A	240	C
1	A	242	G
1	A	246	G
1	A	261	G
1	A	262	C
1	A	274	A
1	A	276	G
1	A	277	A
1	A	284	G
1	A	296	G
1	A	316	A
1	A	323	C
1	A	324	A
1	A	325	C
1	A	326	G
1	A	327	G
1	A	340	C
1	A	341	G
1	A	342	G
1	A	343	G
1	A	346	G
1	A	347	C
1	A	348	A
1	A	349	G
1	A	351	A
1	A	362	U
1	A	367	C
1	A	379	G
1	A	383	G

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Mol	Chain	Res	Type
1	A	384	A
1	A	393	C
1	A	401	G
1	A	404	G
1	A	407	A
1	A	409	A
1	A	416	U
1	A	417	C
1	A	418	G
1	A	424	U
1	A	425	A
1	A	432	U
1	A	442	A
1	A	445	A
1	A	446	A
1	A	447	A
1	A	454	A
1	A	456	G
1	A	457	A
1	A	466	A
1	A	469	G
1	A	470	U
1	A	479	A
1	A	480	A
1	A	481	U
1	A	483	G
1	A	494	C
1	A	495	U
1	A	496	C
1	A	500	G
1	A	501	C
1	A	502	C
1	A	504	G
1	A	507	G
1	A	513	G
1	A	514	U
1	A	515	A
1	A	516	A
1	A	528	C
1	A	530	A
1	A	531	G
1	A	542	A

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Mol	Chain	Res	Type
1	A	543	U
1	A	544	U
1	A	547	C
1	A	553	G
1	A	555	A
1	A	556	A
1	A	559	G
1	A	560	G
1	A	562	G
1	A	564	G
1	A	565	U
1	A	590	A
1	A	617	C
1	A	632	G
1	A	636	A
1	A	648	A
1	A	670	A
1	A	671	G
1	A	684	C
1	A	685	A
1	A	686	G
1	A	696	G
1	A	705	A
1	A	706	U
1	A	714	G
1	A	716	A
1	A	738	G
1	A	749	A
1	A	756	G
1	A	760	A
1	A	763	A
1	A	764	A
1	A	765	A
1	A	768	G
1	A	773	A
1	A	775	A
1	A	776	U
1	A	777	A
1	A	795	C
1	A	796	U
1	A	798	A
1	A	799	A

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Mol	Chain	Res	Type
1	A	800	C
1	A	802	A
1	A	803	U
1	A	811	A
1	A	812	G
1	A	822	U
1	A	823	C
1	A	824	U
1	A	825	C
1	A	828	G
1	A	835	G
1	A	847	U
1	A	848	U
1	A	849	A
1	A	853	G
1	A	861	U
1	A	862	G
1	A	867	G
1	A	870	C
1	A	891	A
1	A	896	A
1	A	903	G
1	A	904	G
1	A	906	G
1	A	911	C
1	A	912	A
1	A	937	U
1	A	938	U
1	A	943	G
1	A	945	A
1	A	946	A
1	A	948	G
1	A	949	C
1	A	952	A
1	A	953	G
1	A	954	A
1	A	960	A
1	A	961	C
1	A	964	G
1	A	968	U
1	A	969	U
1	A	970	G

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Mol	Chain	Res	Type
1	A	971	A
1	A	972	C
1	A	977	U
1	A	979	G
1	A	980	G
1	A	981	G
1	A	982	A
1	A	983	A
1	A	984	C
1	A	986	C
1	A	987	G
1	A	992	A
1	A	994	A
1	A	1003	U
1	A	1004	G
1	A	1006	C
1	A	1007	C
1	A	1010	C
1	A	1013	G
1	A	1022	U
1	A	1035	G
1	A	1036	C
1	A	1037	A
1	A	1047	U
1	A	1048	C
1	A	1076	G
1	A	1077	U
1	A	1083	A
1	A	1086	G
1	A	1106	G
1	A	1107	U
1	A	1108	U
1	A	1109	G
1	A	1111	C
1	A	1112	A
1	A	1113	G
1	A	1114	C
1	A	1119	C
1	A	1121	G
1	A	1122	C
1	A	1125	G
1	A	1127	C

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Mol	Chain	Res	Type
1	A	1128	A
1	A	1136	G
1	A	1139	A
1	A	1140	C
1	A	1141	U
1	A	1142	G
1	A	1149	A
1	A	1151	A
1	A	1152	G
1	A	1163	G
1	A	1164	A
1	A	1172	A
1	A	1177	U
1	A	1178	G
1	A	1182	A
1	A	1183	G
1	A	1185	A
1	A	1186	U
1	A	1193	U
1	A	1194	A
1	A	1195	C
1	A	1205	G
1	A	1206	A
1	A	1207	C
1	A	1208	A
1	A	1209	C
1	A	1219	A
1	A	1220	A
1	A	1221	U
1	A	1222	G
1	A	1231	A
1	A	1234	G
1	A	1237	A
1	A	1238	U
1	A	1239	G
1	A	1251	C
1	A	1254	G
1	A	1258	C
1	A	1260	A
1	A	1261	A
1	A	1266	A
1	A	1268	A

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Mol	Chain	Res	Type
1	A	1279	C
1	A	1280	A
1	A	1281	G
1	A	1282	U
1	A	1283	U
1	A	1293	G
1	A	1294	U
1	A	1297	G
1	A	1298	C
1	A	1300	A
1	A	1301	C
1	A	1304	G
1	A	1313	A
1	A	1316	C
1	A	1317	C
1	A	1318	G
1	A	1319	G
1	A	1326	U
1	A	1327	A
1	A	1328	G
1	A	1329	U
1	A	1334	G
1	A	1344	C
1	A	1345	A
1	A	1346	U
1	A	1352	G
1	A	1360	C
1	A	1361	G
1	A	1363	U
1	A	1365	C
1	A	1376	A
1	A	1379	C
1	A	1380	A
1	A	1425	G
1	A	1426	A
1	A	1433	G
1	A	1464	G
1	A	1466	G
1	A	1469	A
1	A	1471	G
1	A	1474	G
1	A	1480	A

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Mol	Chain	Res	Type
1	A	1481	G
1	A	1482	G
1	A	1483	U
1	A	1484	A
1	A	1494	G
1	A	1497	G
1	A	1506	G
1	A	1507	G
1	A	1509	U
1	A	1510	C
1	A	1511	A
1	A	1516	C
1	A	1519	U
1	A	1521	U
22	W	3	A
23	X	38	C
23	X	39	C

All (73) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	50	A
1	A	64	G
1	A	101	G
1	A	123	G
1	A	155	A
1	A	175	G
1	A	188	U
1	A	189	U
1	A	190	G
1	A	210	U
1	A	239	U
1	A	276	G
1	A	323	C
1	A	340	C
1	A	347	C
1	A	383	G
1	A	417	C
1	A	423	G
1	A	424	U
1	A	445	A

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Mol	Chain	Res	Type
1	A	468	G
1	A	469	G
1	A	479	A
1	A	482	A
1	A	494	C
1	A	500	G
1	A	501	C
1	A	530	A
1	A	542	A
1	A	558	G
1	A	669	U
1	A	670	A
1	A	684	C
1	A	704	G
1	A	705	A
1	A	776	U
1	A	795	C
1	A	798	A
1	A	802	A
1	A	847	U
1	A	861	U
1	A	937	U
1	A	942	A
1	A	948	G
1	A	959	U
1	A	969	U
1	A	1035	G
1	A	1036	C
1	A	1076	G
1	A	1110	C
1	A	1111	C
1	A	1139	A
1	A	1163	G
1	A	1171	G
1	A	1182	A
1	A	1194	A
1	A	1206	A
1	A	1220	A
1	A	1278	C
1	A	1279	C
1	A	1281	G
1	A	1316	C

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Mol	Chain	Res	Type
1	A	1317	C
1	A	1326	U
1	A	1328	G
1	A	1345	A
1	A	1362	U
1	A	1378	A
1	A	1379	C
1	A	1432	C
1	A	1481	G
1	A	1510	C

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
23	RSQ	X	34	-	19,23,24	2.74	4 (21%)	25,33,36	1.40	3 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	RSQ	X	34	-	-	2/9/27/28	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	X	34	RSQ	O30-C10	9.44	1.42	1.22
23	X	34	RSQ	C2-N1	4.94	1.50	1.40
23	X	34	RSQ	C10-C5	4.20	1.56	1.46
23	X	34	RSQ	O2-C2	-2.29	1.19	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	X	34	RSQ	O30-C10-C5	-4.13	114.29	125.12
23	X	34	RSQ	C1'-N1-C2	3.10	125.29	118.44
23	X	34	RSQ	C1'-N1-C6	-2.98	116.24	121.15

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	X	34	RSQ	O30-C10-C5-C4
23	X	34	RSQ	O30-C10-C5-C6

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	X	34	RSQ	8	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 189 ligands modelled in this entry, 188 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	$\# Z > 2$
25	PAR	A	1785	-	44,45,45	1.07	2 (4%)	63,67,67	1.69	12 (19%)

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
25	PAR	A	1785	-	-	6/18/94/94	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1785	PAR	C52-C42	3.67	1.59	1.52
25	A	1785	PAR	C22-C12	-2.38	1.48	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1785	PAR	O33-C14-C24	6.98	119.50	108.08
25	A	1785	PAR	C34-C24-N24	-3.46	103.96	111.05
25	A	1785	PAR	C14-O33-C33	-3.16	110.49	117.98
25	A	1785	PAR	O34-C34-C44	-3.00	103.31	110.38
25	A	1785	PAR	O11-C11-O51	2.97	118.50	110.69
25	A	1785	PAR	C13-O52-C52	-2.97	110.94	117.98
25	A	1785	PAR	O54-C54-C44	2.93	114.98	109.70
25	A	1785	PAR	O43-C13-C23	-2.81	101.41	104.98
25	A	1785	PAR	C11-O51-C51	2.54	118.68	113.72
25	A	1785	PAR	O34-C34-C24	-2.18	106.30	110.22
25	A	1785	PAR	O52-C13-O43	-2.15	109.17	111.37
25	A	1785	PAR	O51-C51-C61	2.13	111.71	106.44

There are no chirality outliers.

All (6) torsion outliers are listed below:

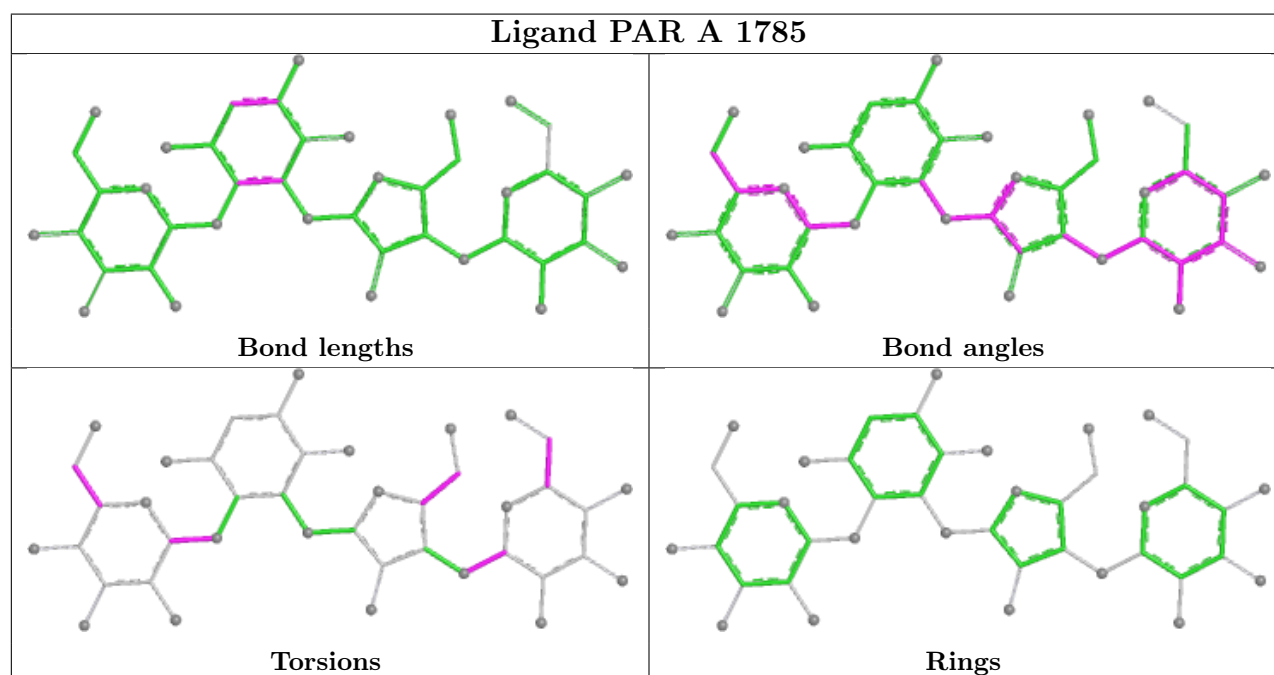
Mol	Chain	Res	Type	Atoms
25	A	1785	PAR	C44-C54-C64-N64
25	A	1785	PAR	O54-C54-C64-N64
25	A	1785	PAR	O51-C11-O11-C42
25	A	1785	PAR	C33-C43-C53-O53
25	A	1785	PAR	O54-C14-O33-C33
25	A	1785	PAR	O51-C51-C61-O61

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	1785	PAR	2	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	1512/1513 (99%)	-0.20	29 (1%) 66 46	40, 73, 157, 278	0
2	B	234/234 (100%)	0.33	14 (5%) 27 17	60, 107, 182, 222	0
3	C	206/206 (100%)	0.35	14 (6%) 23 15	64, 103, 161, 188	0
4	D	208/208 (100%)	0.52	28 (13%) 7 5	55, 83, 134, 205	0
5	E	150/150 (100%)	-0.16	3 (2%) 65 45	44, 63, 103, 123	0
6	F	101/101 (100%)	0.15	2 (1%) 65 45	66, 100, 135, 195	0
7	G	155/155 (100%)	0.38	11 (7%) 22 14	62, 94, 149, 222	0
8	H	138/138 (100%)	-0.08	5 (3%) 46 28	43, 61, 98, 138	0
9	I	127/127 (100%)	0.64	17 (13%) 7 6	65, 110, 155, 202	0
10	J	98/98 (100%)	0.95	16 (16%) 4 3	69, 129, 214, 238	0
11	K	119/119 (100%)	0.03	3 (2%) 58 39	45, 73, 122, 179	0
12	L	124/124 (100%)	0.27	8 (6%) 25 16	40, 70, 122, 195	0
13	M	125/125 (100%)	0.73	18 (14%) 6 5	70, 104, 151, 281	0
14	N	60/60 (100%)	0.52	7 (11%) 9 6	75, 91, 148, 195	0
15	O	88/88 (100%)	0.42	4 (4%) 38 24	48, 77, 130, 176	0
16	P	83/83 (100%)	0.19	3 (3%) 46 28	50, 59, 91, 147	0
17	Q	104/104 (100%)	0.16	4 (3%) 44 27	42, 68, 138, 202	0
18	R	73/73 (100%)	0.10	2 (2%) 56 36	55, 81, 157, 194	0
19	S	80/80 (100%)	0.59	6 (7%) 20 13	81, 127, 179, 205	0
20	T	99/99 (100%)	0.26	5 (5%) 33 21	55, 71, 131, 163	0
21	V	24/24 (100%)	0.51	3 (12%) 8 6	79, 96, 120, 141	0
22	W	4/6 (66%)	0.85	1 (25%) 2 2	69, 78, 80, 83	0
23	X	5/17 (29%)	0.80	1 (20%) 3 2	82, 85, 96, 112	0
All	All	3917/3932 (99%)	0.13	204 (5%) 33 21	40, 82, 157, 281	0

All (204) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	981	G	7.0
9	I	126	SER	6.8
1	A	208	U	6.5
4	D	3	ARG	6.5
13	M	8	GLU	5.5
13	M	126	LYS	5.3
12	L	26	ALA	5.3
19	S	2	PRO	5.3
10	J	57	LYS	5.0
2	B	35	GLU	4.9
9	I	128	ARG	4.9
7	G	4	ARG	4.8
17	Q	105	ALA	4.7
20	T	64	ASP	4.7
4	D	23	GLY	4.7
4	D	123	HIS	4.6
13	M	119	GLY	4.6
13	M	16	ASP	4.5
8	H	18	ARG	4.3
13	M	7	VAL	4.3
3	C	91	LEU	4.3
19	S	3	ARG	4.3
4	D	21	LEU	4.2
8	H	90	GLY	4.2
4	D	31	CYS	4.2
4	D	26	CYS	4.2
13	M	124	PRO	4.2
7	G	33	ASP	4.1
12	L	47	LYS	4.1
10	J	73	ASP	4.1
1	A	1111	C	4.0
9	I	124	GLN	4.0
13	M	4	ILE	4.0
10	J	58	ASP	4.0
1	A	1108	U	3.9
11	K	52	GLY	3.9
15	O	23	GLY	3.9
13	M	123	ALA	3.9
2	B	211	ILE	3.7
1	A	1516	C	3.7
10	J	90	LEU	3.6
1	A	706	U	3.5

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Mol	Chain	Res	Type	RSRZ
9	I	55	ALA	3.5
4	D	49	ARG	3.5
2	B	229	VAL	3.5
3	C	76	VAL	3.4
1	A	1402	C	3.4
13	M	88	ARG	3.4
2	B	77	ALA	3.4
4	D	32	ALA	3.4
8	H	30	ARG	3.3
12	L	28	LYS	3.3
1	A	1510	C	3.2
4	D	9	CYS	3.2
13	M	6	GLY	3.2
17	Q	104	LYS	3.2
4	D	42	GLN	3.2
13	M	125	ARG	3.2
20	T	68	LYS	3.1
7	G	115	ARG	3.1
2	B	19	HIS	3.1
1	A	1205	G	3.1
10	J	43	ARG	3.1
9	I	119	ALA	3.1
13	M	118	ALA	3.1
15	O	13	GLN	3.0
12	L	73	GLU	3.0
4	D	115	ARG	3.0
3	C	4	LYS	3.0
10	J	17	ASP	2.9
5	E	119	LEU	2.9
9	I	110	GLU	2.9
1	A	1076	G	2.9
9	I	127	LYS	2.8
10	J	18	ALA	2.8
17	Q	103	GLY	2.8
4	D	4	TYR	2.8
9	I	56	LEU	2.8
4	D	2	GLY	2.8
13	M	13	LYS	2.8
11	K	126	ARG	2.7
1	A	1021	C	2.7
2	B	163	PHE	2.7
1	A	593	G	2.7

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Mol	Chain	Res	Type	RSRZ
4	D	57	ARG	2.7
8	H	116	LYS	2.7
7	G	2	ALA	2.7
14	N	30	ALA	2.7
13	M	120	LYS	2.7
3	C	180	ALA	2.7
2	B	165	VAL	2.7
7	G	106	GLN	2.7
13	M	27	LYS	2.7
1	A	982	A	2.7
12	L	120	TYR	2.7
19	S	5	LEU	2.7
20	T	9	ASN	2.7
14	N	4	LYS	2.6
20	T	103	GLY	2.6
4	D	20	TYR	2.6
4	D	35	ARG	2.6
10	J	66	ARG	2.6
14	N	35	ARG	2.6
1	A	1027	C	2.6
17	Q	91	ARG	2.6
2	B	125	PRO	2.5
3	C	101	LEU	2.5
1	A	1247	G	2.5
7	G	156	TRP	2.5
6	F	67	MET	2.5
1	A	212	C	2.5
1	A	1036	C	2.5
9	I	120	ARG	2.5
10	J	27	ALA	2.5
3	C	143	GLU	2.5
18	R	83	GLU	2.5
10	J	85	LEU	2.5
21	V	24	ARG	2.5
7	G	8	GLU	2.4
1	A	391	G	2.4
3	C	68	VAL	2.4
9	I	115	GLY	2.4
3	C	39	ILE	2.4
4	D	86	LYS	2.4
2	B	187	LEU	2.4
1	A	455	C	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	129	ALA	2.4
1	A	998	U	2.4
1	A	1517	U	2.4
14	N	57	ARG	2.4
19	S	81	ARG	2.4
21	V	25	LYS	2.4
9	I	7	THR	2.4
9	I	105	ASP	2.4
9	I	66	ARG	2.4
10	J	54	PHE	2.4
1	A	980	G	2.4
12	L	37	CYS	2.4
1	A	515	A	2.4
6	F	69	GLU	2.4
13	M	32	GLU	2.4
15	O	69	TYR	2.3
5	E	81	GLU	2.3
2	B	203	GLY	2.3
20	T	12	ALA	2.3
9	I	125	TYR	2.3
4	D	201	GLN	2.3
7	G	56	GLN	2.3
1	A	1020	C	2.3
3	C	21	ARG	2.3
3	C	167	TRP	2.3
8	H	1	MET	2.3
4	D	120	LEU	2.3
1	A	1425	G	2.3
7	G	81	GLY	2.3
9	I	15	ALA	2.3
9	I	69	GLY	2.3
23	X	39	C	2.3
18	R	68	LYS	2.3
2	B	175	ARG	2.2
14	N	6	LEU	2.2
4	D	209	ARG	2.2
7	G	110	GLN	2.2
4	D	125	HIS	2.2
9	I	12	GLU	2.2
10	J	95	GLU	2.2
10	J	5	ARG	2.2
4	D	119	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
4	D	33	MET	2.2
19	S	32	LYS	2.2
1	A	1107	U	2.2
15	O	74	ASP	2.2
22	W	4	A	2.1
3	C	26	LYS	2.1
4	D	116	GLN	2.1
13	M	102	ARG	2.1
14	N	52	GLN	2.1
3	C	188	LEU	2.1
16	P	73	LEU	2.1
4	D	7	PRO	2.1
10	J	64	GLU	2.1
1	A	1113	G	2.1
12	L	115	LYS	2.1
4	D	5	ILE	2.1
11	K	12	ARG	2.1
14	N	3	ARG	2.1
16	P	75	ARG	2.1
2	B	124	SER	2.1
13	M	87	TYR	2.1
2	B	38	GLY	2.1
7	G	26	PHE	2.1
21	V	15	ARG	2.0
4	D	89	THR	2.0
19	S	68	GLY	2.0
1	A	788	C	2.0
1	A	1013	G	2.0
10	J	71	LEU	2.0
2	B	113	HIS	2.0
4	D	12	CYS	2.0
5	E	20	GLN	2.0
3	C	58	GLU	2.0
12	L	79	GLU	2.0
16	P	83	GLU	2.0
10	J	96	ILE	2.0

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

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. 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	RSQ	X	34	22/23	0.90	0.11	94,96,98,100	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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. 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	MG	A	1691	1/1	-0.15	0.28	156,156,156,156	0
24	MG	A	1716	1/1	0.41	0.17	106,106,106,106	0
24	MG	A	1628	1/1	0.43	0.46	78,78,78,78	0
24	MG	A	1731	1/1	0.52	0.52	108,108,108,108	0
24	MG	A	1702	1/1	0.61	0.11	90,90,90,90	0
24	MG	A	1678	1/1	0.62	0.93	75,75,75,75	0
24	MG	A	1781	1/1	0.63	0.10	92,92,92,92	0
24	MG	A	1753	1/1	0.64	0.32	87,87,87,87	0
24	MG	A	1603	1/1	0.71	0.35	61,61,61,61	0
24	MG	A	1752	1/1	0.71	0.52	62,62,62,62	0
24	MG	A	1648	1/1	0.71	0.47	41,41,41,41	0
24	MG	A	1717	1/1	0.71	1.22	109,109,109,109	0
24	MG	A	1641	1/1	0.72	0.33	87,87,87,87	0
24	MG	A	1656	1/1	0.73	0.41	52,52,52,52	0
24	MG	A	1750	1/1	0.74	0.24	72,72,72,72	0
24	MG	A	1766	1/1	0.74	0.40	77,77,77,77	0
24	MG	A	1677	1/1	0.74	0.65	99,99,99,99	0
24	MG	A	1724	1/1	0.75	0.42	84,84,84,84	0
24	MG	A	1644	1/1	0.76	0.37	87,87,87,87	0
24	MG	A	1723	1/1	0.76	0.51	68,68,68,68	0
24	MG	A	1692	1/1	0.76	0.14	122,122,122,122	0
24	MG	A	1782	1/1	0.77	0.35	62,62,62,62	0
24	MG	A	1674	1/1	0.78	0.49	57,57,57,57	0
24	MG	A	1624	1/1	0.78	0.12	120,120,120,120	0
24	MG	A	1730	1/1	0.78	0.53	73,73,73,73	0
24	MG	A	1602	1/1	0.78	0.33	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	MG	A	1658	1/1	0.78	0.18	101,101,101,101	0
24	MG	A	1671	1/1	0.79	0.59	84,84,84,84	0
24	MG	A	1633	1/1	0.79	0.12	90,90,90,90	0
24	MG	A	1762	1/1	0.79	0.53	75,75,75,75	0
24	MG	A	1695	1/1	0.80	0.20	101,101,101,101	0
24	MG	A	1758	1/1	0.80	0.24	43,43,43,43	0
24	MG	A	1616	1/1	0.80	0.28	83,83,83,83	0
24	MG	A	1629	1/1	0.80	0.29	65,65,65,65	0
24	MG	A	1776	1/1	0.80	0.44	82,82,82,82	0
24	MG	A	1645	1/1	0.80	0.32	58,58,58,58	0
24	MG	A	1604	1/1	0.80	0.13	105,105,105,105	0
24	MG	A	1618	1/1	0.81	0.37	72,72,72,72	0
24	MG	A	1660	1/1	0.81	0.47	41,41,41,41	0
24	MG	A	1739	1/1	0.81	0.69	53,53,53,53	1
24	MG	A	1775	1/1	0.82	0.19	80,80,80,80	0
24	MG	A	1632	1/1	0.82	0.59	51,51,51,51	0
24	MG	A	1725	1/1	0.82	0.17	58,58,58,58	0
24	MG	A	1755	1/1	0.82	0.49	86,86,86,86	0
24	MG	A	1619	1/1	0.83	0.51	73,73,73,73	0
24	MG	A	1733	1/1	0.83	0.33	77,77,77,77	0
24	MG	A	1698	1/1	0.83	0.28	74,74,74,74	0
24	MG	A	1699	1/1	0.83	0.18	82,82,82,82	0
24	MG	A	1621	1/1	0.83	0.19	70,70,70,70	0
24	MG	A	1705	1/1	0.83	0.24	58,58,58,58	0
24	MG	A	1713	1/1	0.83	0.39	81,81,81,81	0
24	MG	A	1760	1/1	0.84	0.53	52,52,52,52	0
24	MG	A	1700	1/1	0.84	0.40	81,81,81,81	0
24	MG	A	1609	1/1	0.84	0.38	66,66,66,66	0
24	MG	A	1771	1/1	0.84	0.23	60,60,60,60	0
24	MG	A	1672	1/1	0.84	0.72	50,50,50,50	0
24	MG	A	1615	1/1	0.84	0.47	43,43,43,43	0
24	MG	A	1608	1/1	0.84	0.41	96,96,96,96	0
24	MG	A	1665	1/1	0.84	0.22	82,82,82,82	0
24	MG	A	1712	1/1	0.85	0.26	59,59,59,59	0
24	MG	A	1601	1/1	0.85	0.12	59,59,59,59	0
24	MG	A	1683	1/1	0.85	0.33	66,66,66,66	0
24	MG	A	1706	1/1	0.85	0.36	56,56,56,56	0
24	MG	A	1749	1/1	0.86	0.27	59,59,59,59	0
24	MG	A	1710	1/1	0.86	0.32	64,64,64,64	0
24	MG	A	1659	1/1	0.86	0.31	55,55,55,55	0
24	MG	A	1638	1/1	0.86	0.26	72,72,72,72	0
24	MG	A	1735	1/1	0.86	0.36	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	MG	A	1780	1/1	0.86	0.51	81,81,81,81	0
24	MG	A	1707	1/1	0.86	0.41	52,52,52,52	0
24	MG	A	1742	1/1	0.86	0.24	90,90,90,90	0
24	MG	B	301	1/1	0.86	0.20	115,115,115,115	0
24	MG	A	1651	1/1	0.87	0.15	65,65,65,65	0
24	MG	A	1630	1/1	0.87	0.23	38,38,38,38	0
24	MG	A	1667	1/1	0.87	0.40	47,47,47,47	0
24	MG	A	1783	1/1	0.87	0.18	65,65,65,65	0
24	MG	A	1746	1/1	0.87	0.34	76,76,76,76	0
24	MG	A	1649	1/1	0.88	0.55	43,43,43,43	0
24	MG	A	1685	1/1	0.88	0.17	48,48,48,48	0
24	MG	A	1687	1/1	0.88	0.50	66,66,66,66	0
24	MG	A	1688	1/1	0.88	0.10	71,71,71,71	0
24	MG	A	1741	1/1	0.88	0.12	85,85,85,85	0
24	MG	A	1767	1/1	0.88	0.30	65,65,65,65	0
24	MG	A	1719	1/1	0.88	0.33	69,69,69,69	0
24	MG	A	1744	1/1	0.88	0.38	63,63,63,63	0
24	MG	A	1666	1/1	0.88	0.36	61,61,61,61	0
24	MG	A	1643	1/1	0.88	0.05	61,61,61,61	0
24	MG	A	1693	1/1	0.88	0.21	122,122,122,122	0
24	MG	A	1726	1/1	0.88	0.29	56,56,56,56	0
24	MG	A	1623	1/1	0.88	0.37	79,79,79,79	0
24	MG	A	1754	1/1	0.88	0.30	67,67,67,67	0
24	MG	T	201	1/1	0.88	0.05	99,99,99,99	0
24	MG	A	1759	1/1	0.89	0.31	52,52,52,52	0
24	MG	A	1697	1/1	0.89	0.91	81,81,81,81	0
24	MG	A	1611	1/1	0.89	0.55	44,44,44,44	0
24	MG	A	1642	1/1	0.89	0.52	57,57,57,57	0
24	MG	A	1610	1/1	0.89	0.23	89,89,89,89	0
24	MG	A	1711	1/1	0.89	0.27	39,39,39,39	0
24	MG	A	1626	1/1	0.89	0.48	81,81,81,81	0
24	MG	A	1625	1/1	0.90	0.79	64,64,64,64	0
24	MG	A	1620	1/1	0.90	0.24	68,68,68,68	0
24	MG	A	1773	1/1	0.90	0.32	64,64,64,64	0
24	MG	A	1774	1/1	0.90	0.12	67,67,67,67	0
24	MG	A	1756	1/1	0.90	0.26	81,81,81,81	0
24	MG	A	1734	1/1	0.90	0.48	58,58,58,58	0
24	MG	A	1655	1/1	0.90	0.47	49,49,49,49	0
24	MG	A	1738	1/1	0.90	0.20	48,48,48,48	0
24	MG	A	1761	1/1	0.90	0.26	57,57,57,57	0
24	MG	A	1639	1/1	0.90	0.23	56,56,56,56	0
24	MG	A	1764	1/1	0.90	0.72	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	MG	A	1704	1/1	0.90	0.09	61,61,61,61	0
24	MG	A	1640	1/1	0.91	0.17	105,105,105,105	0
24	MG	A	1684	1/1	0.91	0.34	63,63,63,63	0
24	MG	A	1736	1/1	0.91	0.18	62,62,62,62	0
24	MG	A	1636	1/1	0.91	0.37	59,59,59,59	0
24	MG	A	1662	1/1	0.91	0.42	41,41,41,41	0
24	MG	A	1709	1/1	0.91	0.27	82,82,82,82	0
24	MG	A	1664	1/1	0.91	0.11	47,47,47,47	0
24	MG	A	1622	1/1	0.91	0.13	85,85,85,85	0
24	MG	A	1745	1/1	0.91	0.71	55,55,55,55	0
24	MG	A	1701	1/1	0.91	0.53	63,63,63,63	0
24	MG	A	1607	1/1	0.91	0.13	76,76,76,76	0
24	MG	A	1715	1/1	0.91	0.28	53,53,53,53	0
24	MG	A	1743	1/1	0.92	0.27	43,43,43,43	0
24	MG	A	1718	1/1	0.92	0.30	65,65,65,65	0
24	MG	A	1690	1/1	0.92	0.88	90,90,90,90	0
24	MG	A	1679	1/1	0.92	0.44	63,63,63,63	0
24	MG	A	1732	1/1	0.92	0.31	91,91,91,91	0
24	MG	A	1769	1/1	0.92	0.37	43,43,43,43	0
24	MG	A	1647	1/1	0.92	0.33	67,67,67,67	0
24	MG	A	1772	1/1	0.92	0.20	96,96,96,96	0
24	MG	A	1708	1/1	0.92	0.12	74,74,74,74	0
24	MG	A	1681	1/1	0.93	0.58	59,59,59,59	0
24	MG	A	1727	1/1	0.93	0.23	64,64,64,64	0
24	MG	A	1779	1/1	0.93	0.49	97,97,97,97	0
24	MG	A	1657	1/1	0.93	0.36	66,66,66,66	0
24	MG	A	1748	1/1	0.93	0.51	77,77,77,77	0
24	MG	A	1722	1/1	0.93	0.16	76,76,76,76	0
24	MG	A	1634	1/1	0.93	0.21	56,56,56,56	0
24	MG	A	1613	1/1	0.93	0.17	64,64,64,64	0
24	MG	A	1680	1/1	0.93	0.42	53,53,53,53	0
25	PAR	A	1785	42/42	0.93	0.12	48,51,58,59	0
24	MG	A	1612	1/1	0.94	0.32	43,43,43,43	0
24	MG	A	1703	1/1	0.94	0.39	100,100,100,100	0
24	MG	A	1714	1/1	0.94	0.25	53,53,53,53	0
24	MG	A	1694	1/1	0.94	0.46	89,89,89,89	0
24	MG	A	1635	1/1	0.94	0.18	60,60,60,60	0
24	MG	A	1696	1/1	0.94	0.17	75,75,75,75	0
24	MG	A	1614	1/1	0.94	0.09	76,76,76,76	0
24	MG	A	1763	1/1	0.94	0.34	52,52,52,52	0
24	MG	A	1689	1/1	0.94	0.22	89,89,89,89	0
24	MG	A	1721	1/1	0.94	0.26	64,64,64,64	0

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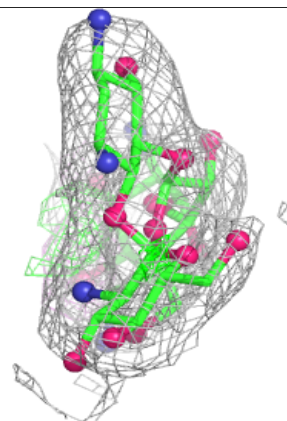
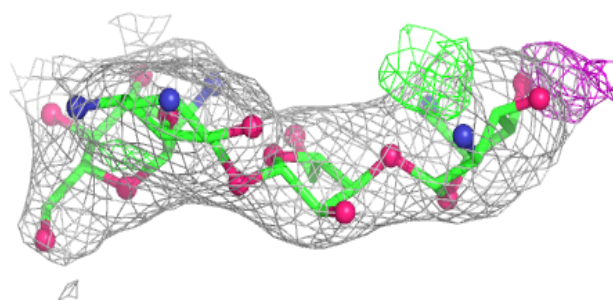
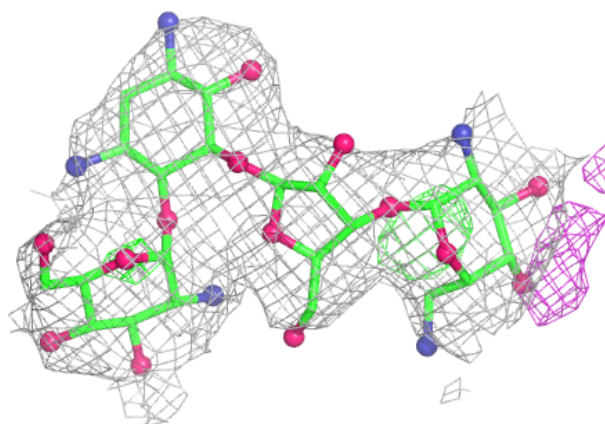
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	MG	A	1784	1/1	0.94	0.29	68,68,68,68	0
24	MG	A	1652	1/1	0.94	0.49	93,93,93,93	0
24	MG	A	1676	1/1	0.94	0.42	68,68,68,68	0
24	MG	A	1653	1/1	0.94	0.55	46,46,46,46	0
24	MG	A	1728	1/1	0.95	0.24	99,99,99,99	0
24	MG	A	1720	1/1	0.95	0.42	58,58,58,58	0
24	MG	A	1606	1/1	0.95	0.56	50,50,50,50	0
24	MG	A	1668	1/1	0.95	0.27	58,58,58,58	0
24	MG	A	1670	1/1	0.95	0.26	56,56,56,56	0
24	MG	A	1768	1/1	0.95	0.14	62,62,62,62	0
24	MG	A	1631	1/1	0.95	0.25	50,50,50,50	1
24	MG	A	1605	1/1	0.95	0.52	77,77,77,77	0
24	MG	A	1747	1/1	0.95	0.43	84,84,84,84	0
24	MG	A	1661	1/1	0.95	0.21	40,40,40,40	0
24	MG	A	1675	1/1	0.95	0.10	74,74,74,74	0
24	MG	A	1729	1/1	0.96	0.74	58,58,58,58	0
24	MG	A	1770	1/1	0.96	0.20	65,65,65,65	0
24	MG	A	1627	1/1	0.96	0.14	44,44,44,44	0
24	MG	A	1751	1/1	0.96	0.52	70,70,70,70	0
24	MG	A	1765	1/1	0.96	0.07	73,73,73,73	0
24	MG	A	1617	1/1	0.96	0.38	66,66,66,66	0
24	MG	A	1682	1/1	0.96	0.12	46,46,46,46	0
24	MG	A	1737	1/1	0.96	0.61	76,76,76,76	0
24	MG	A	1778	1/1	0.96	0.51	77,77,77,77	0
24	MG	A	1654	1/1	0.97	0.44	40,40,40,40	0
24	MG	A	1637	1/1	0.97	0.47	48,48,48,48	0
24	MG	A	1669	1/1	0.97	0.31	44,44,44,44	0
24	MG	A	1686	1/1	0.97	0.39	58,58,58,58	0
24	MG	A	1777	1/1	0.97	0.14	83,83,83,83	0
24	MG	A	1673	1/1	0.98	0.42	74,74,74,74	0
24	MG	A	1740	1/1	0.98	0.49	41,41,41,41	0
24	MG	A	1757	1/1	0.98	0.39	53,53,53,53	0
26	ZN	D	301	1/1	0.98	0.24	73,73,73,73	0
24	MG	A	1663	1/1	0.99	0.11	50,50,50,50	0
24	MG	A	1646	1/1	0.99	0.10	89,89,89,89	0
24	MG	A	1650	1/1	0.99	0.45	45,45,45,45	0
26	ZN	N	101	1/1	1.00	0.06	90,90,90,90	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PAR A 1785:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.