Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:03 AM UTC

PDB ID	:	6DTI / pdb_00006dti
Title	:	Structure of the Thermus thermophilus 30S ribosomal subunit complexed with an unmodifed anticodon stem loop (ASL) of Escherichia coli transfer RNA Arginine 2 (TRNAARG2) bound to an mRNA with an CGU-codon in the A-site and paromomycin
Authors	:	Cantara, W.A.; DeMirci, H.; Agris, P.F.
Deposited on	:	2018-06-16
Resolution	:	3.54 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:

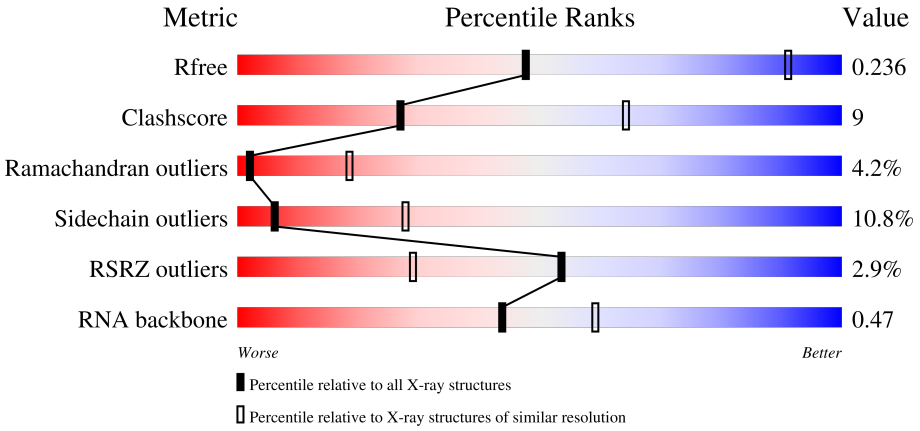
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 3.54 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	1008 (3.58-3.50)
Clashscore	190562	1062 (3.58-3.50)
Ramachandran outliers	187476	1033 (3.58-3.50)
Sidechain outliers	187428	1034 (3.58-3.50)
RSRZ outliers	180081	1007 (3.58-3.50)
RNA backbone	3983	1006 (4.02-3.06)

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 <=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	1507	2% 57% 35% 8%
2	B	256	% 54% 30% 7% 9%
3	C	239	3% 51% 31% • 14%
4	D	209	5% 57% 37% 5%

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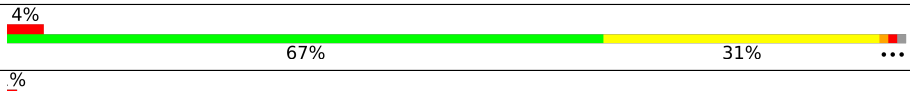
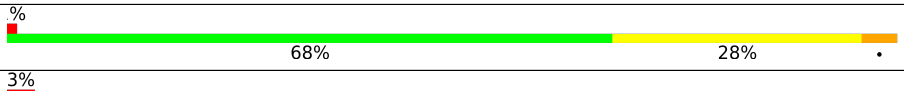
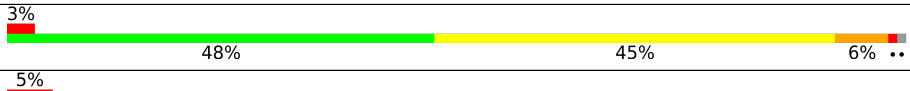
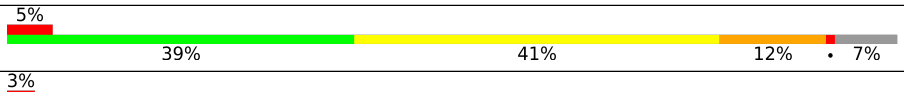
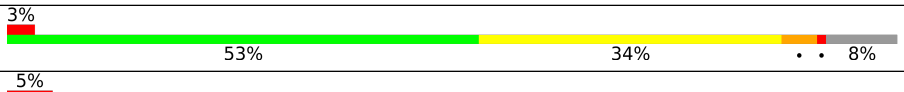
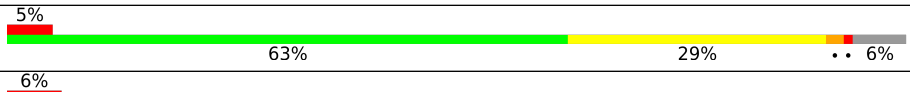
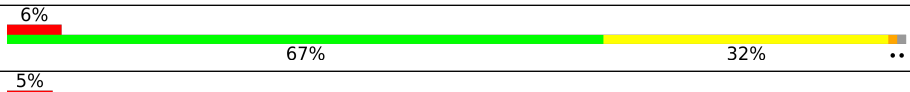
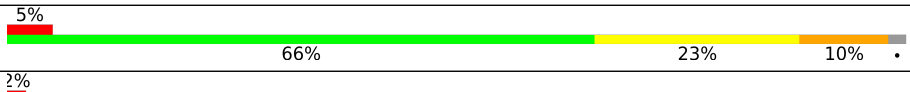
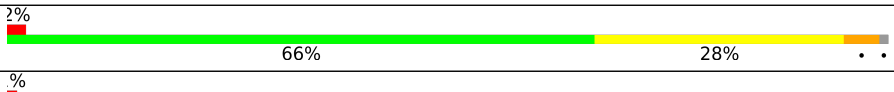
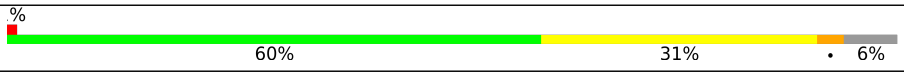
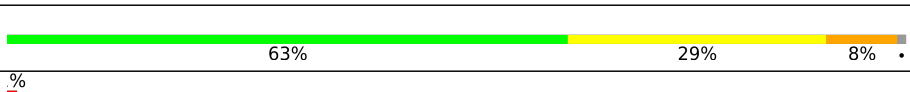
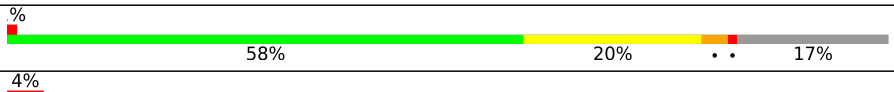
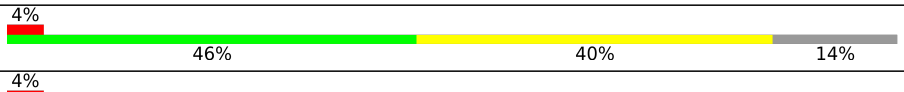
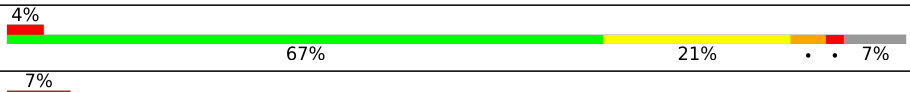
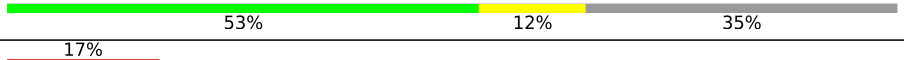
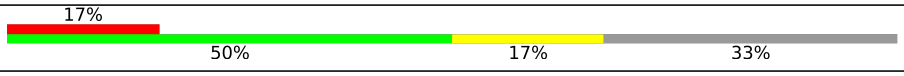
Mol	Chain	Length	Quality of chain
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	132	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	V	27	
22	X	17	
23	W	6	

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
25	MG	A	1632	-	-	-	X
25	MG	A	1654	-	-	-	X

2 Entry composition (i)

There are 25 unique types of molecules in this entry. The entry contains 52059 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
			Total	C	N	O	P			
1	A	1507	32380	14414	5990	10470	1506	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	206	1612	1016	314	281	1	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	150	1146	724	217	201	4	0	0	0

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

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

- 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
			792	498	156	137	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 P0DOY7

- 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			

- 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			

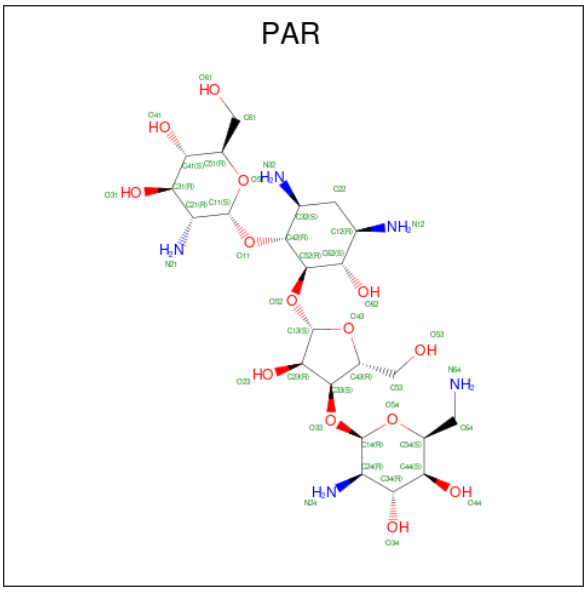
- Molecule 22 is a RNA chain called tRNA ASL Escherichia coli Arg2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	X	11	Total	C	N	O	P	0	0	0
			232	105	44	73	10			

- Molecule 23 is a RNA chain called mRNA A-site fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	4	Total	C	N	O	P	0	0	0
			82	38	15	26	3			

- Molecule 24 is PAROMOMYCIN (CCD ID: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



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

- Molecule 25 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

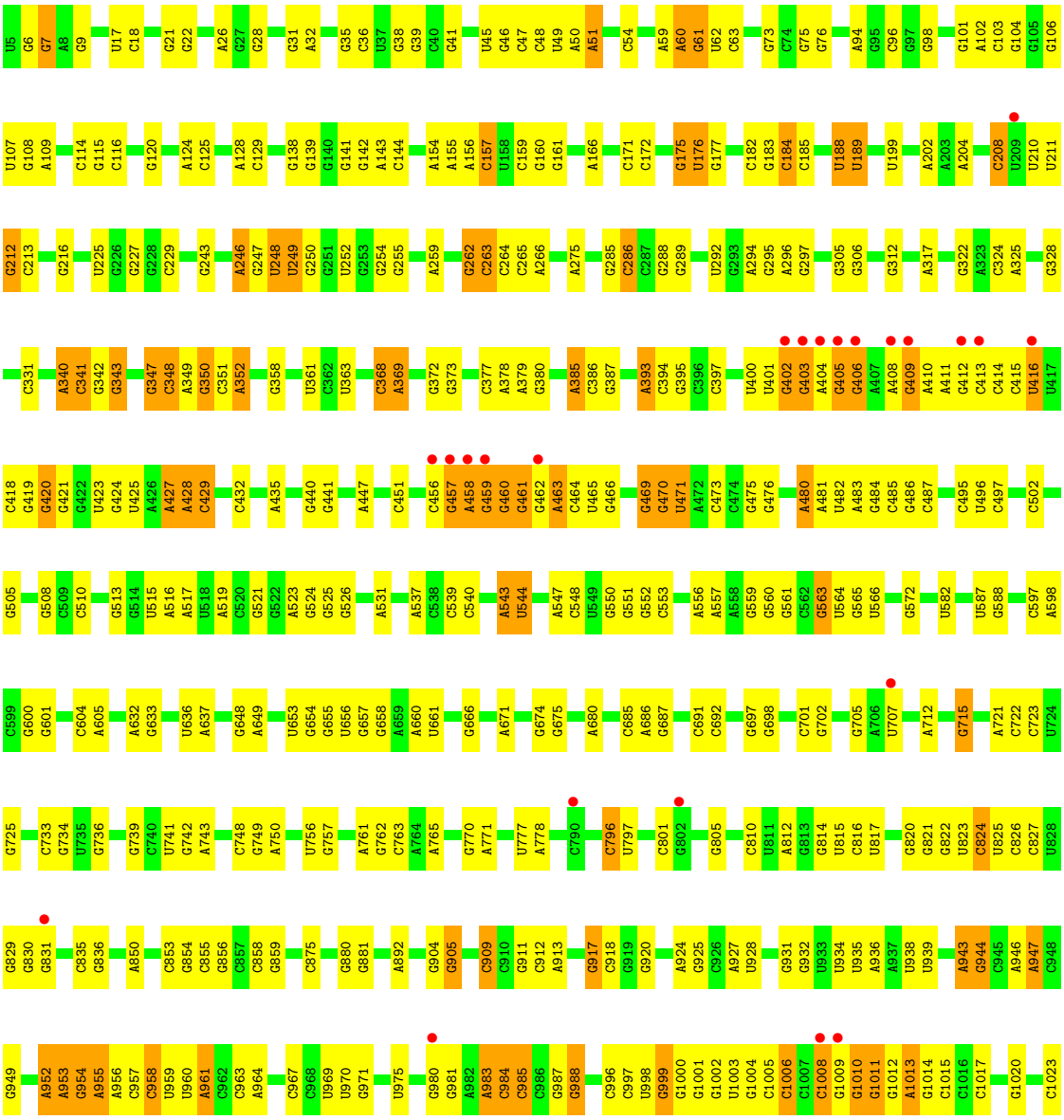
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	90	Total Mg 90 90	0	0
25	E	1	Total Mg 1 1	0	0
25	J	2	Total Mg 2 2	0	0
25	K	1	Total Mg 1 1	0	0

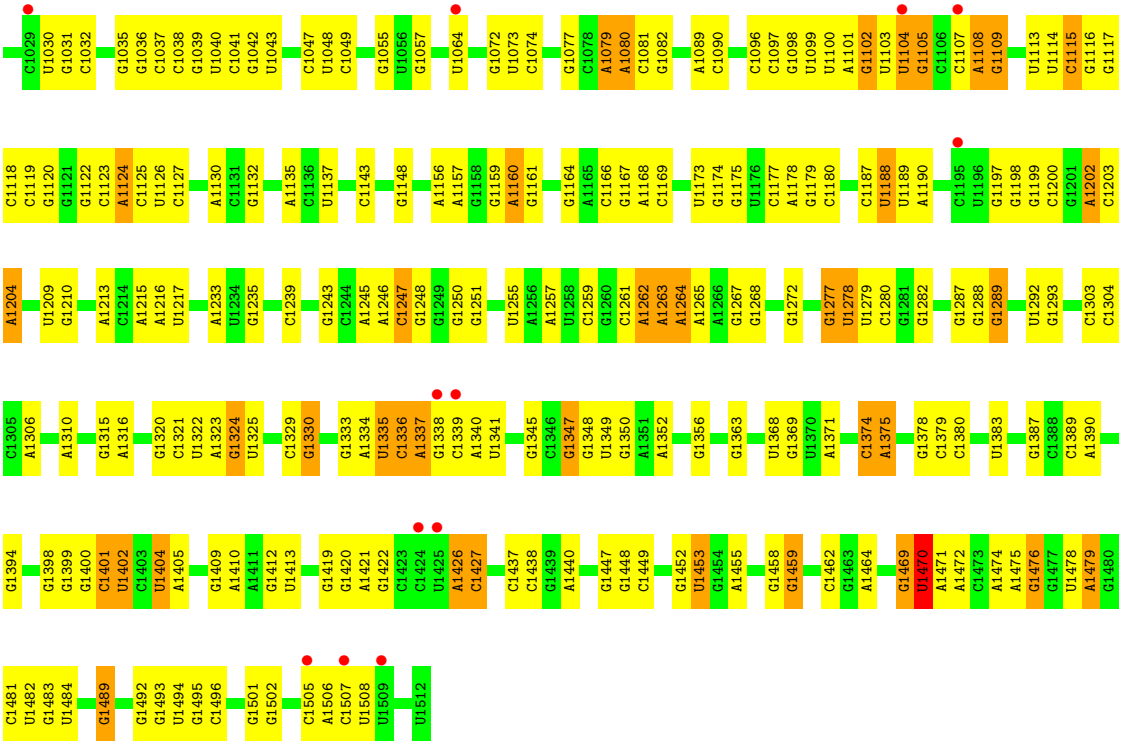
3 Residue-property plots (i)

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.

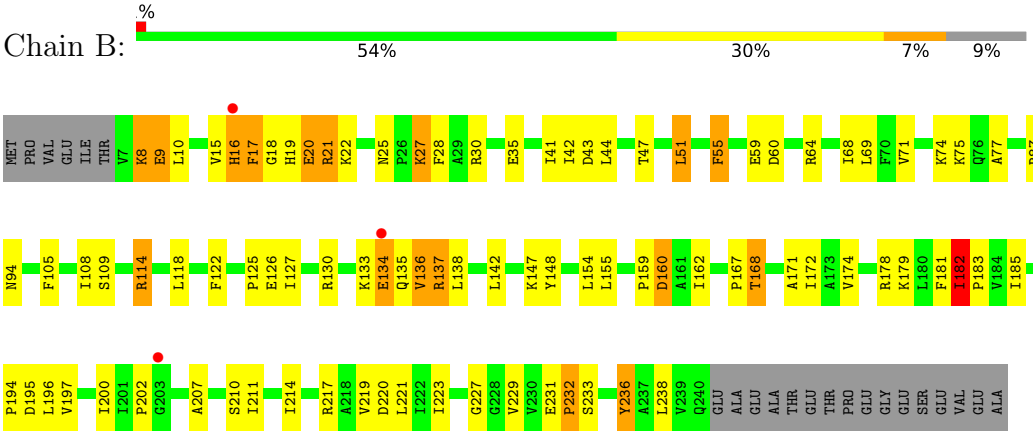
- Molecule 1: 16s rRNA

Chain A: 

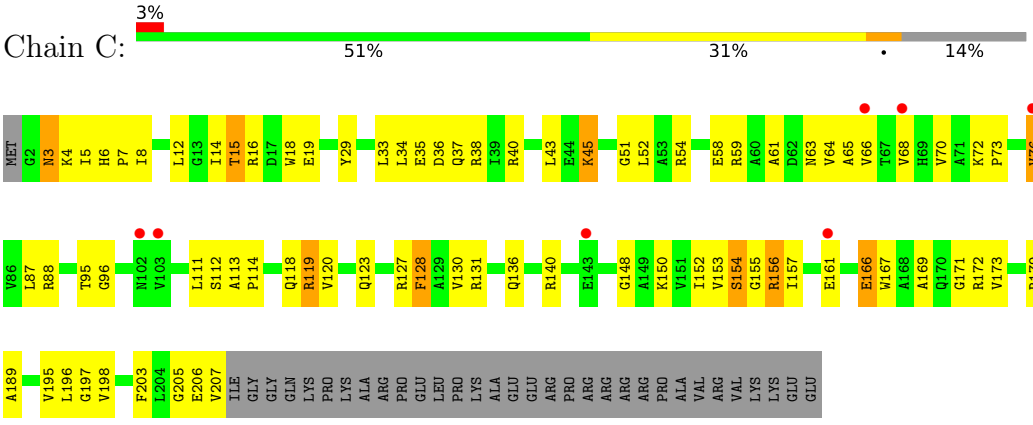




• Molecule 2: 30S ribosomal protein S2

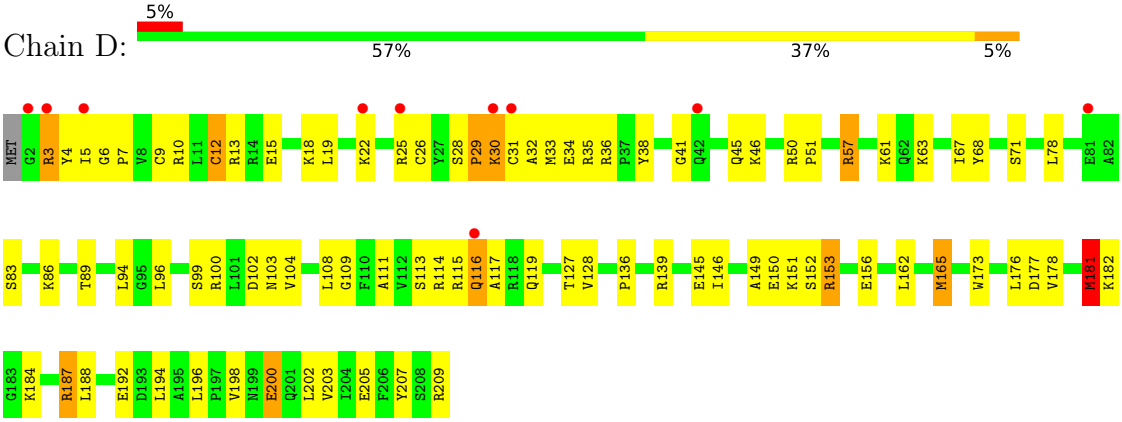


• Molecule 3: 30S ribosomal protein S3



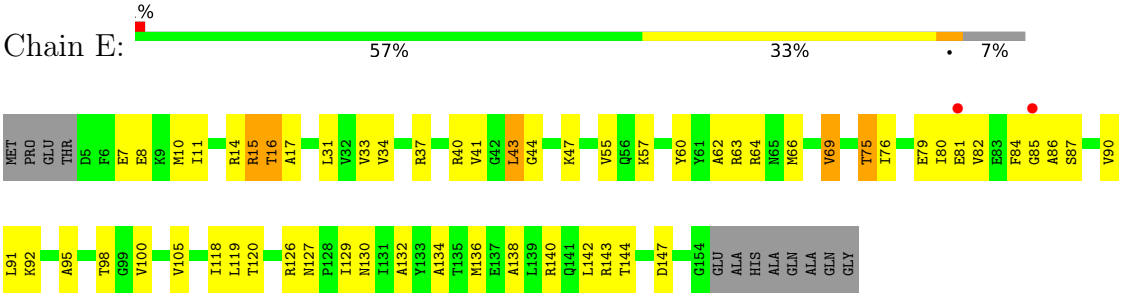
• Molecule 4: 30S ribosomal protein S4

Chain D:



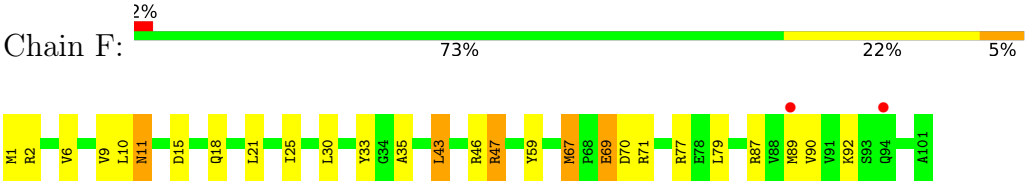
• Molecule 5: 30S ribosomal protein S5

Chain E:



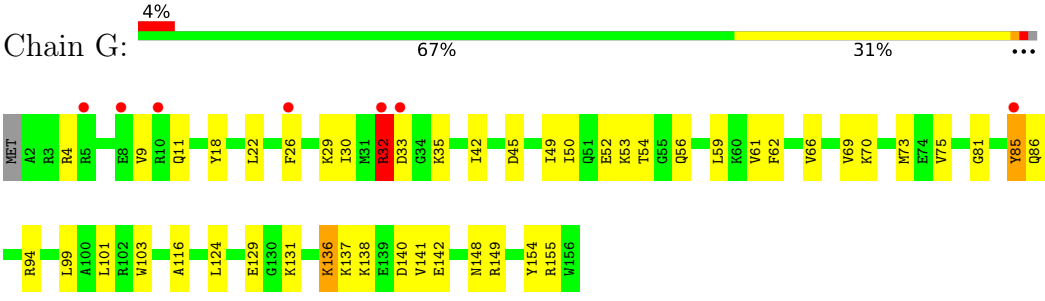
• Molecule 6: 30S ribosomal protein S6

Chain F:



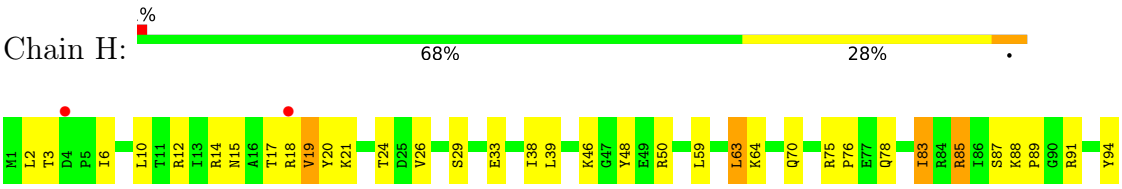
• Molecule 7: 30S ribosomal protein S7

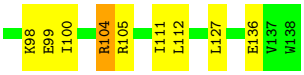
Chain G:



• Molecule 8: 30S ribosomal protein S8

Chain H:

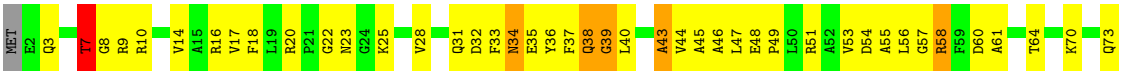


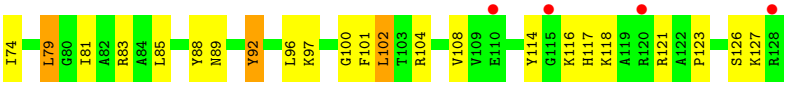


• Molecule 9: 30S ribosomal protein S9

Chain I:



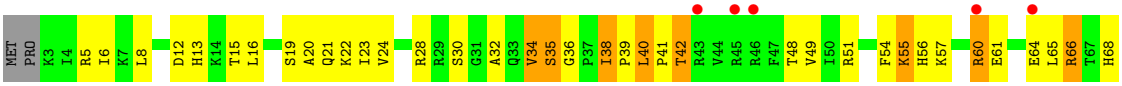


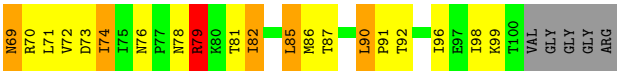


• Molecule 10: 30S ribosomal protein S10

Chain J:



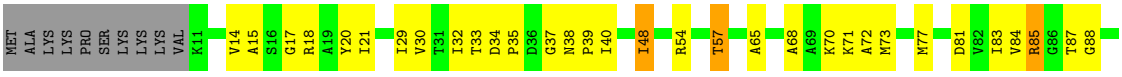


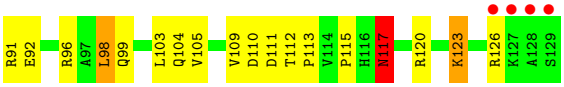


• Molecule 11: 30S ribosomal protein S11

Chain K:





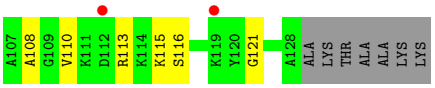


• Molecule 12: 30S ribosomal protein S12

Chain L:



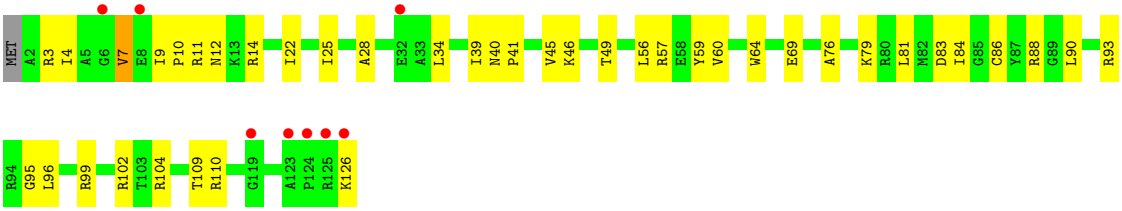




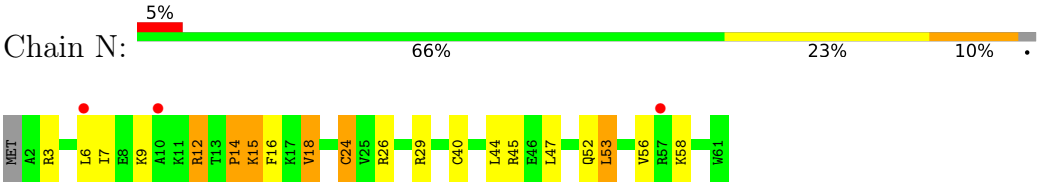
• Molecule 13: 30S ribosomal protein S13

Chain M:

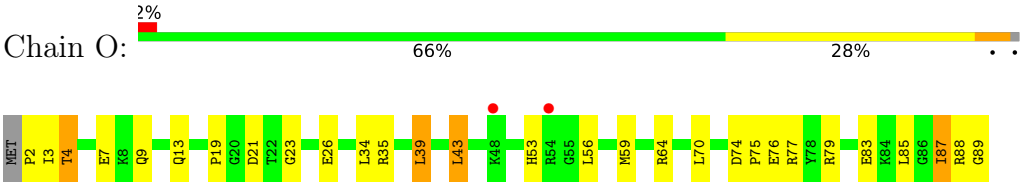




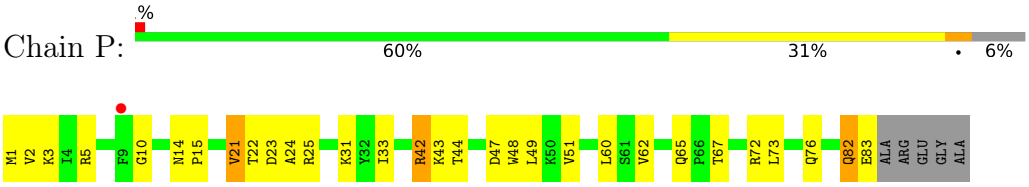
• Molecule 14: 30S ribosomal protein S14 type Z



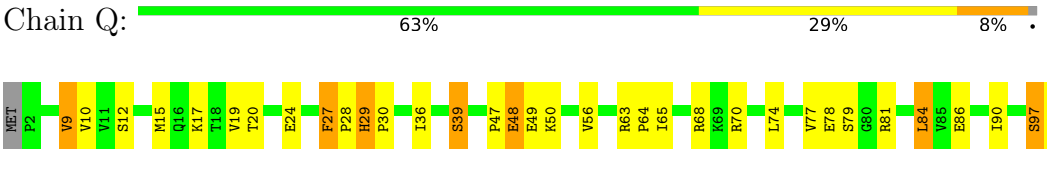
• Molecule 15: 30S ribosomal protein S15



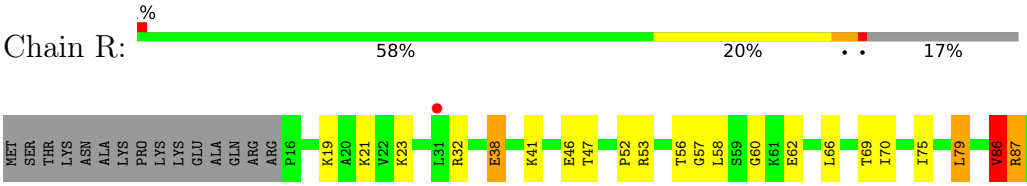
• Molecule 16: 30S ribosomal protein S16



• Molecule 17: 30S ribosomal protein S17

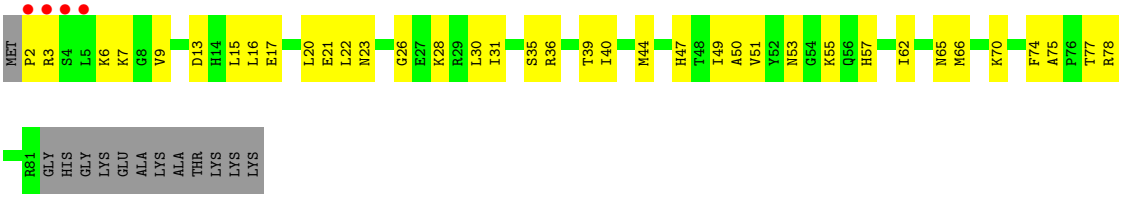


• Molecule 18: 30S ribosomal protein S18



• Molecule 19: 30S ribosomal protein S19





• Molecule 20: 30S ribosomal protein S20





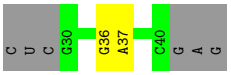
• Molecule 21: 30S ribosomal protein Thx





• Molecule 22: tRNA ASL Escherichia coli Arg2





• Molecule 23: mRNA A-site fragment





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	404.54Å 404.54Å 176.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.34 – 3.54 49.34 – 3.54	Depositor EDS
% Data completeness (in resolution range)	90.4 (49.34-3.54) 92.1 (49.34-3.54)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.197 , 0.236 0.200 , 0.236	Depositor DCC
R_{free} test set	1894 reflections (1.07%)	wwPDB-VP
Wilson B-factor (Å^2)	138.8	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 117.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	52059	wwPDB-VP
Average B, all atoms (Å^2)	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PAR, 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	0.25	0/36244	0.42	1/56567 (0.0%)
2	B	0.37	0/1935	0.85	4/2609 (0.2%)
3	C	0.41	0/1636	0.76	0/2205
4	D	0.41	0/1733	0.82	0/2318
5	E	0.45	0/1162	0.96	7/1564 (0.4%)
6	F	0.36	0/856	0.83	2/1154 (0.2%)
7	G	0.37	0/1276	0.78	2/1709 (0.1%)
8	H	0.44	0/1136	0.93	5/1527 (0.3%)
9	I	0.38	0/1029	0.79	0/1378
10	J	0.43	0/805	1.08	4/1082 (0.4%)
11	K	0.43	0/900	0.91	2/1213 (0.2%)
12	L	0.42	0/986	0.86	1/1320 (0.1%)
13	M	0.38	0/1008	0.77	0/1347
14	N	0.40	0/501	0.80	0/664
15	O	0.39	0/745	0.80	0/992
16	P	0.42	0/716	0.73	0/963
17	Q	0.41	0/870	0.90	4/1159 (0.3%)
18	R	0.36	0/603	0.84	1/799 (0.1%)
19	S	0.35	0/661	0.91	0/890
20	T	0.43	0/764	0.86	2/1006 (0.2%)
21	V	0.36	0/212	0.72	0/277
22	X	0.18	0/259	0.31	0/402
23	W	0.27	0/91	0.37	0/140
All	All	0.31	0/56128	0.59	35/83285 (0.0%)

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
10	J	0	1

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	J	79	ARG	CD-NE-CZ	20.05	152.47	124.40
11	K	38	ASN	CA-C-N	7.86	127.79	119.85
11	K	38	ASN	C-N-CA	7.86	127.79	119.85
6	F	67	MET	N-CA-C	6.71	116.04	108.25
18	R	70	ILE	N-CA-C	-6.63	106.55	112.12
7	G	155	ARG	CB-CA-C	-6.48	109.12	116.63
2	B	130	ARG	CA-C-N	6.41	125.64	118.97
2	B	130	ARG	C-N-CA	6.41	125.64	118.97
5	E	127	ASN	CA-C-N	6.32	125.81	119.24
5	E	127	ASN	C-N-CA	6.32	125.81	119.24
12	L	29	GLY	N-CA-C	-6.27	106.59	115.30
10	J	79	ARG	CB-CG-CD	-6.23	96.97	111.30
8	H	100	ILE	CA-C-N	6.07	125.98	119.85
8	H	100	ILE	C-N-CA	6.07	125.98	119.85
8	H	19	VAL	N-CA-C	-6.01	106.46	112.17
7	G	87	VAL	N-CA-C	5.88	113.68	108.63
17	Q	29	HIS	CA-C-N	5.84	127.14	119.84
17	Q	29	HIS	C-N-CA	5.84	127.14	119.84
5	E	92	LYS	CA-C-N	5.76	125.73	120.03
5	E	92	LYS	C-N-CA	5.76	125.73	120.03
10	J	38	ILE	CA-C-N	5.58	126.81	119.84
10	J	38	ILE	C-N-CA	5.58	126.81	119.84
17	Q	27	PHE	CA-C-N	5.38	125.14	119.76
17	Q	27	PHE	C-N-CA	5.38	125.14	119.76
8	H	75	ARG	CA-C-N	5.37	125.31	119.78
8	H	75	ARG	C-N-CA	5.37	125.31	119.78
2	B	182	ILE	CA-C-N	5.37	126.55	119.84
2	B	182	ILE	C-N-CA	5.37	126.55	119.84
5	E	105	VAL	CA-C-N	-5.35	114.30	119.87
5	E	105	VAL	C-N-CA	-5.35	114.30	119.87
1	A	1470	U	C2'-C3'-O3'	5.32	117.47	109.50
20	T	97	ALA	CA-C-N	5.30	126.46	119.84
20	T	97	ALA	C-N-CA	5.30	126.46	119.84
5	E	69	VAL	N-CA-C	5.19	113.58	107.77
6	F	11	ASN	N-CA-C	5.10	115.46	109.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	J	79	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32380	0	16346	355	0
2	B	1900	0	1951	50	0
3	C	1612	0	1677	48	0
4	D	1703	0	1767	57	0
5	E	1146	0	1207	25	0
6	F	843	0	857	13	0
7	G	1257	0	1296	27	0
8	H	1116	0	1177	24	0
9	I	1011	0	1043	38	0
10	J	792	0	835	40	3
11	K	885	0	904	26	0
12	L	970	0	1057	27	0
13	M	997	0	1072	33	0
14	N	492	0	529	19	0
15	O	734	0	771	14	0
16	P	700	0	720	25	0
17	Q	857	0	930	16	0
18	R	597	0	668	11	0
19	S	647	0	673	22	0
20	T	762	0	856	15	0
21	V	208	0	221	6	0
22	X	232	0	122	3	0
23	W	82	0	44	2	0
24	A	42	0	45	0	0
25	A	90	0	0	0	0
25	E	1	0	0	0	0
25	J	2	0	0	0	0
25	K	1	0	0	0	0
All	All	52059	0	36768	804	3

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 9.

All (804) 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)
13:M:3:ARG:HE	13:M:7:VAL:HG13	1.36	0.91
1:A:403:G:O2'	1:A:427:A:OP1	1.92	0.86
4:D:18:LYS:HE3	4:D:31:CYS:HB3	1.58	0.85
1:A:405:G:H3'	1:A:427:A:H62	1.42	0.85
3:C:85:ARG:HA	3:C:88:ARG:HD3	1.59	0.85
1:A:648:G:H22	1:A:725:G:H1	1.27	0.82
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.62	0.81
1:A:405:G:N2	1:A:429:C:OP1	2.13	0.80
1:A:208:C:H42	1:A:212:G:H1	1.31	0.78
3:C:33:LEU:HD21	14:N:53:LEU:HD22	1.64	0.78
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.68	0.76
13:M:3:ARG:HG3	13:M:7:VAL:HA	1.67	0.76
4:D:13:ARG:NH1	4:D:38:TYR:O	2.20	0.74
1:A:1006:C:N4	1:A:1012:G:O6	2.20	0.74
1:A:1401:C:N3	1:A:1448:G:N1	2.31	0.73
1:A:931:G:N7	13:M:104:ARG:NH2	2.37	0.73
3:C:179:ARG:HD2	3:C:207:VAL:HG22	1.70	0.73
8:H:17:THR:HB	8:H:78:GLN:HE22	1.53	0.73
1:A:1064:U:H3	1:A:1077:G:H22	1.37	0.73
1:A:1303:C:OP2	21:V:6:ARG:NH1	2.22	0.73
8:H:14:ARG:HG2	8:H:18:ARG:HH21	1.54	0.72
9:I:37:PHE:O	9:I:39:GLY:N	2.22	0.72
1:A:1166:C:OP1	10:J:51:ARG:NH2	2.22	0.72
3:C:58:GLU:H	3:C:65:ALA:HB3	1.54	0.72
1:A:661:U:H3	1:A:697:G:H22	1.39	0.71
1:A:953:A:H4'	1:A:954:G:H5"	1.73	0.71
5:E:75:THR:OG1	5:E:76:ILE:N	2.19	0.71
5:E:43:LEU:HD11	5:E:132:ALA:HB1	1.73	0.71
7:G:54:THR:HG22	7:G:56:GLN:H	1.56	0.70
8:H:98:LYS:HG3	8:H:99:GLU:HG3	1.72	0.70
17:Q:48:GLU:O	17:Q:50:LYS:N	2.23	0.70
1:A:1369:G:H21	1:A:1474:A:H8	1.40	0.70
9:I:45:ALA:HA	9:I:48:GLU:HG2	1.74	0.69
10:J:38:ILE:HB	10:J:71:LEU:HB2	1.73	0.69
1:A:400:U:OP2	4:D:3:ARG:NH1	2.24	0.69
1:A:1008:C:OP1	1:A:1010:G:N2	2.26	0.69
1:A:952:A:OP2	14:N:29:ARG:NH2	2.25	0.69
2:B:114:ARG:HH12	2:B:138:LEU:HD11	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:65:ALA:HB1	11:K:98:LEU:HD13	1.75	0.68
9:I:43:ALA:O	9:I:45:ALA:N	2.25	0.68
17:Q:100:LYS:HE2	17:Q:101:ARG:HG2	1.75	0.68
1:A:932:G:H21	1:A:1204:A:H62	1.40	0.68
1:A:38:G:H22	1:A:393:A:H5'	1.58	0.68
1:A:1010:G:N7	1:A:1011:G:N2	2.41	0.68
1:A:521:G:OP1	12:L:113:ARG:NH2	2.26	0.67
4:D:63:LYS:HE3	4:D:198:VAL:HG12	1.75	0.67
6:F:15:ASP:HB3	6:F:18:GLN:HB2	1.75	0.67
1:A:526:G:OP1	4:D:10:ARG:NH2	2.28	0.67
4:D:28:SER:O	4:D:30:LYS:N	2.27	0.67
1:A:563:G:H5'	1:A:712:A:H1'	1.75	0.67
1:A:565:G:O3'	15:O:64:ARG:NH2	2.27	0.67
10:J:90:LEU:H	10:J:91:PRO:HD2	1.59	0.67
1:A:312:G:OP2	1:A:347:G:O2'	2.13	0.66
9:I:16:ARG:HE	9:I:64:THR:HB	1.59	0.66
20:T:75:ASN:OD1	20:T:75:ASN:N	2.27	0.66
1:A:1287:G:OP2	13:M:88:ARG:NH1	2.29	0.66
10:J:78:ASN:HB2	10:J:81:THR:HG23	1.77	0.66
1:A:722:C:OP2	6:F:92:LYS:NZ	2.25	0.65
2:B:87:ARG:NH2	2:B:220:ASP:OD1	2.26	0.65
1:A:1005:C:N4	1:A:1011:G:O6	2.30	0.65
2:B:16:HIS:CD2	2:B:210:SER:HB3	2.32	0.65
3:C:189:ALA:HB3	3:C:196:LEU:HB2	1.79	0.65
5:E:43:LEU:HB2	5:E:136:MET:HE2	1.79	0.64
9:I:22:GLY:HA3	9:I:60:ASP:HB2	1.78	0.64
1:A:405:G:H3'	1:A:427:A:N6	2.10	0.64
15:O:39:LEU:HB3	15:O:56:LEU:HD12	1.80	0.64
3:C:131:ARG:NH2	3:C:166:GLU:OE2	2.31	0.64
4:D:29:PRO:O	4:D:35:ARG:NH2	2.30	0.64
10:J:16:LEU:HA	10:J:20:ALA:HB3	1.80	0.64
3:C:51:GLY:H	3:C:70:VAL:HG13	1.62	0.64
1:A:1292:U:O2'	1:A:1337:A:N3	2.30	0.64
16:P:43:LYS:HG3	16:P:48:TRP:CD2	2.32	0.63
1:A:1245:A:N3	1:A:1303:C:O2'	2.29	0.63
7:G:138:LYS:NZ	7:G:142:GLU:OE1	2.31	0.63
1:A:1122:G:H21	1:A:1124:A:H62	1.46	0.63
12:L:74:GLY:O	12:L:102:ARG:NH2	2.31	0.63
19:S:28:LYS:HE3	19:S:47:HIS:HB3	1.79	0.63
1:A:155:A:N1	1:A:343:G:O2'	2.29	0.63
4:D:57:ARG:NH1	4:D:205:GLU:OE2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:50:ARG:HE	4:D:51:PRO:HD2	1.64	0.62
9:I:79:LEU:HD22	9:I:83:ARG:HD2	1.80	0.62
10:J:57:LYS:O	10:J:60:ARG:NH1	2.32	0.62
1:A:405:G:N2	1:A:427:A:O2'	2.32	0.62
1:A:1000:G:H2'	1:A:1001:G:H8	1.65	0.62
12:L:28:LYS:HD3	12:L:33:ARG:HH22	1.64	0.62
20:T:50:GLU:HA	20:T:100:ILE:HD12	1.81	0.62
1:A:28:G:O2'	1:A:292:U:OP1	2.17	0.62
1:A:461:G:O6	1:A:464:C:N4	2.32	0.62
2:B:19:HIS:CD2	2:B:20:GLU:H	2.18	0.62
11:K:14:VAL:HG21	11:K:34:ASP:HB2	1.81	0.62
1:A:406:G:OP2	1:A:427:A:N6	2.33	0.61
16:P:10:GLY:HA3	16:P:14:ASN:O	2.00	0.61
10:J:65:LEU:HD23	14:N:56:VAL:HG22	1.80	0.61
1:A:458:A:H8	16:P:83:GLU:HG2	1.65	0.61
11:K:15:ALA:O	11:K:77:MET:HA	2.00	0.61
3:C:154:SER:OG	3:C:155:GLY:N	2.32	0.61
6:F:70:ASP:OD1	6:F:70:ASP:N	2.32	0.61
1:A:537:A:O2'	12:L:29:GLY:O	2.18	0.61
1:A:1400:G:N2	1:A:1449:C:O2	2.33	0.61
2:B:105:PHE:HA	2:B:108:ILE:HG22	1.82	0.61
4:D:109:GLY:HA3	4:D:165:MET:HE3	1.81	0.61
2:B:91:PRO:HG2	2:B:155:LEU:HG	1.83	0.61
15:O:39:LEU:HD13	15:O:56:LEU:HB2	1.83	0.61
3:C:118:GLN:O	3:C:120:VAL:N	2.34	0.60
5:E:80:ILE:HG22	8:H:104:ARG:HH21	1.64	0.60
1:A:821:G:H1	1:A:827:C:H42	1.50	0.60
7:G:9:VAL:HG13	7:G:94:ARG:HH21	1.66	0.60
9:I:97:LYS:HA	9:I:102:LEU:HD11	1.82	0.60
10:J:61:GLU:OE2	14:N:45:ARG:NH1	2.31	0.60
18:R:32:ARG:HA	18:R:69:THR:HG21	1.81	0.60
2:B:43:ASP:O	2:B:47:THR:OG1	2.12	0.60
12:L:70:ILE:HG12	12:L:100:ILE:HD12	1.82	0.60
1:A:415:C:OP1	1:A:497:C:O2'	2.18	0.60
1:A:1102:G:H3'	1:A:1123:C:N4	2.16	0.60
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.83	0.60
1:A:1383:U:O2	1:A:1489:G:N2	2.33	0.59
1:A:183:G:H21	1:A:184:C:H2'	1.67	0.59
1:A:1409:G:O2'	1:A:1440:A:N6	2.35	0.59
16:P:22:THR:HA	16:P:33:ILE:HD13	1.84	0.59
1:A:458:A:H1'	1:A:459:G:N2	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:GLY:HA3	2:B:41:ILE:HA	1.85	0.59
15:O:74:ASP:HB3	15:O:77:ARG:HG3	1.83	0.59
1:A:1043:U:C5	1:A:1167:G:H1'	2.37	0.59
1:A:1264:A:H2'	1:A:1265:A:C8	2.38	0.59
20:T:97:ALA:O	20:T:99:LEU:N	2.35	0.59
1:A:1109:G:OP1	9:I:3:GLN:NE2	2.35	0.59
11:K:17:GLY:HA2	11:K:35:PRO:HD3	1.84	0.58
21:V:13:ILE:HG22	21:V:22:ARG:CZ	2.33	0.58
1:A:405:G:H21	1:A:427:A:H8	1.51	0.58
10:J:6:ILE:HG13	10:J:98:ILE:HG23	1.85	0.58
13:M:4:ILE:HA	13:M:57:ARG:HG2	1.85	0.58
1:A:460:G:H2'	1:A:461:G:H4'	1.85	0.58
6:F:43:LEU:HD12	6:F:46:ARG:HD2	1.86	0.58
7:G:66:VAL:HG12	7:G:70:LYS:HE3	1.85	0.58
22:X:36:G:H1	23:W:1:C:H42	1.52	0.58
1:A:372:G:H5"	16:P:5:ARG:HB2	1.85	0.58
10:J:69:ASN:OD1	10:J:69:ASN:N	2.36	0.58
1:A:475:G:H2'	1:A:476:G:H8	1.67	0.58
10:J:76:ASN:O	10:J:76:ASN:ND2	2.36	0.58
1:A:1398:G:H2'	1:A:1399:G:C8	2.39	0.58
11:K:54:ARG:O	11:K:57:THR:OG1	2.20	0.58
1:A:1042:G:H21	1:A:1167:G:H2'	1.69	0.58
1:A:1035:G:H2'	1:A:1036:G:O4'	2.03	0.57
1:A:1101:A:H4'	10:J:36:GLY:HA3	1.86	0.57
10:J:32:ALA:HA	10:J:76:ASN:HD21	1.69	0.57
1:A:75:G:H2'	1:A:76:G:H8	1.69	0.57
1:A:1369:G:N2	1:A:1474:A:H8	2.02	0.57
3:C:153:VAL:HG23	3:C:198:VAL:HG12	1.86	0.57
1:A:397:C:O2'	1:A:605:A:N3	2.38	0.57
1:A:1368:U:H2'	1:A:1369:G:C8	2.39	0.57
1:A:1100:U:O4	1:A:1101:A:N6	2.37	0.57
4:D:12:CYS:SG	4:D:31:CYS:SG	3.02	0.57
3:C:19:GLU:O	3:C:40:ARG:NH2	2.38	0.57
8:H:85:ARG:NE	8:H:87:SER:O	2.38	0.57
1:A:1119:C:H2'	1:A:1120:G:H8	1.69	0.57
5:E:81:GLU:HB2	5:E:90:VAL:HG22	1.85	0.57
19:S:40:ILE:HG23	19:S:44:MET:HE2	1.86	0.56
1:A:225:U:O2'	16:P:23:ASP:OD2	2.22	0.56
1:A:403:G:H1	1:A:480:A:HO2'	1.53	0.56
1:A:1035:G:H5"	3:C:154:SER:HB2	1.86	0.56
4:D:113:SER:HB3	4:D:116:GLN:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:17:GLU:HA	19:S:20:LEU:HG	1.86	0.56
20:T:57:ARG:HH21	20:T:102:GLY:HA3	1.70	0.56
1:A:358:G:N2	1:A:361:U:OP2	2.38	0.56
5:E:84:PHE:O	5:E:86:ALA:N	2.38	0.56
5:E:82:VAL:HG21	5:E:138:ALA:HA	1.88	0.56
15:O:79:ARG:O	15:O:83:GLU:HG2	2.05	0.56
1:A:106:G:H1'	1:A:350:G:H5'	1.87	0.56
1:A:660:A:H1'	11:K:115:PRO:HB3	1.87	0.56
1:A:1261:C:H3'	1:A:1262:A:H8	1.70	0.56
1:A:1306:A:P	13:M:28:ALA:HB3	2.45	0.56
16:P:42:ARG:HB2	16:P:44:THR:HG23	1.88	0.56
2:B:134:GLU:O	2:B:138:LEU:N	2.39	0.56
10:J:30:SER:HB3	10:J:81:THR:HA	1.87	0.56
14:N:3:ARG:HH21	14:N:6:LEU:HD11	1.71	0.56
1:A:156:A:C5	1:A:157:C:H1'	2.40	0.56
4:D:187:ARG:NH1	4:D:188:LEU:H	2.04	0.56
7:G:129:GLU:HB2	7:G:131:LYS:HE2	1.87	0.56
1:A:1079:A:N7	2:B:172:ILE:HD11	2.21	0.56
1:A:936:A:N3	1:A:963:C:O2'	2.35	0.56
3:C:6:HIS:CE1	3:C:8:ILE:HB	2.42	0.55
3:C:153:VAL:HG22	3:C:196:LEU:HD12	1.88	0.55
6:F:9:VAL:HB	6:F:87:ARG:HB2	1.87	0.55
9:I:31:GLN:HB3	9:I:35:GLU:HB2	1.87	0.55
16:P:15:PRO:HD2	16:P:42:ARG:HD3	1.89	0.55
1:A:1119:C:H2'	1:A:1120:G:C8	2.41	0.55
1:A:35:G:H2'	1:A:36:C:C6	2.42	0.55
3:C:150:LYS:HA	3:C:169:ALA:HB1	1.89	0.55
7:G:52:GLU:HG3	7:G:53:LYS:HG3	1.89	0.55
12:L:59:ARG:HG2	12:L:65:GLU:HB3	1.89	0.55
19:S:13:ASP:HA	19:S:16:LEU:HG	1.88	0.55
10:J:54:PHE:HD2	10:J:55:LYS:HG2	1.70	0.55
1:A:636:U:O4	1:A:736:G:O2'	2.24	0.55
12:L:27:LEU:C	12:L:29:GLY:H	2.15	0.55
13:M:99:ARG:HH12	19:S:2:PRO:HG3	1.71	0.55
12:L:102:ARG:HH11	12:L:102:ARG:HB3	1.71	0.55
1:A:21:G:H2'	1:A:22:G:C8	2.42	0.54
1:A:1217:U:C2	7:G:32:ARG:HD3	2.41	0.54
1:A:1265:A:N3	1:A:1329:C:O2'	2.38	0.54
9:I:9:ARG:HG2	9:I:14:VAL:HG22	1.88	0.54
1:A:1324:G:N2	1:A:1350:G:H2'	2.22	0.54
4:D:19:LEU:HD22	4:D:67:ILE:HD13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:3:LYS:HG3	16:P:24:ALA:HB2	1.89	0.54
1:A:1293:G:H4'	14:N:18:VAL:HG11	1.89	0.54
2:B:174:VAL:O	2:B:178:ARG:HG2	2.07	0.54
4:D:153:ARG:HD2	4:D:181:MET:HE3	1.90	0.54
6:F:6:VAL:HG22	6:F:90:VAL:HG22	1.89	0.54
2:B:233:SER:HB3	2:B:236:TYR:HB2	1.89	0.54
10:J:64:GLU:OE2	10:J:66:ARG:NH1	2.41	0.54
1:A:470:G:O2'	1:A:471:U:OP2	2.21	0.54
1:A:953:A:H5'	1:A:953:A:H8	1.73	0.54
1:A:1289:G:N7	19:S:3:ARG:HB2	2.22	0.54
9:I:32:ASP:O	9:I:34:ASN:N	2.41	0.54
11:K:32:ILE:HD13	11:K:68:ALA:HB1	1.89	0.54
4:D:149:ALA:HB3	4:D:152:SER:HB3	1.89	0.54
1:A:457:G:H1	16:P:82:GLN:HA	1.73	0.53
1:A:587:U:H2'	1:A:588:G:C8	2.43	0.53
2:B:231:GLU:HG2	2:B:232:PRO:HD2	1.90	0.53
1:A:404:A:N6	4:D:25:ARG:HH21	2.06	0.53
1:A:822:G:C6	1:A:824:C:H1'	2.43	0.53
2:B:160:ASP:N	2:B:160:ASP:OD1	2.41	0.53
3:C:123:GLN:O	3:C:128:PHE:HB2	2.09	0.53
17:Q:24:GLU:HG2	17:Q:39:SER:HB3	1.91	0.53
1:A:817:U:H3	1:A:831:G:H1	1.55	0.53
3:C:51:GLY:N	3:C:70:VAL:HG13	2.22	0.53
1:A:458:A:C8	16:P:83:GLU:HG2	2.43	0.53
1:A:459:G:H1	16:P:83:GLU:HB2	1.72	0.53
1:A:464:C:H2'	1:A:465:U:O4'	2.08	0.53
4:D:153:ARG:HH11	4:D:181:MET:HE3	1.73	0.53
1:A:409:G:OP1	1:A:413:C:N4	2.42	0.53
4:D:7:PRO:HB2	4:D:10:ARG:HD2	1.91	0.53
8:H:46:LYS:HD3	8:H:64:LYS:HZ3	1.73	0.53
1:A:295:G:H2'	1:A:296:A:C8	2.44	0.53
1:A:924:A:O2'	1:A:1310:A:N3	2.38	0.53
11:K:84:VAL:HG11	11:K:91:ARG:HD2	1.89	0.53
12:L:27:LEU:O	12:L:29:GLY:N	2.42	0.53
20:T:53:LEU:HD12	20:T:102:GLY:H	1.74	0.53
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.90	0.53
1:A:1104:U:H3	1:A:1105:G:N2	2.07	0.52
1:A:1374:C:H4'	1:A:1375:A:OP2	2.10	0.52
1:A:1412:G:H2'	1:A:1413:U:C6	2.44	0.52
3:C:37:GLN:NE2	14:N:52:GLN:OE1	2.31	0.52
4:D:108:LEU:HD22	4:D:176:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:150:GLU:HA	4:D:153:ARG:HH21	1.73	0.52
12:L:6:THR:OG1	12:L:9:GLN:HG3	2.10	0.52
6:F:30:LEU:HB3	6:F:35:ALA:HB3	1.91	0.52
1:A:51:A:N7	1:A:107:U:O2'	2.42	0.52
14:N:24:CYS:HB3	14:N:29:ARG:H	1.73	0.52
1:A:928:U:OP2	13:M:102:ARG:HD2	2.09	0.52
1:A:1090:C:O2	3:C:179:ARG:HG2	2.10	0.52
2:B:168:THR:HA	2:B:171:ALA:HB2	1.90	0.52
19:S:36:ARG:NH2	19:S:75:ALA:O	2.43	0.52
1:A:427:A:O2'	1:A:428:A:H5'	2.10	0.52
4:D:103:ASN:OD1	4:D:114:ARG:NH2	2.42	0.52
1:A:414:C:H2'	1:A:415:C:C6	2.44	0.52
1:A:957:C:H3'	1:A:958:C:H5"	1.91	0.52
13:M:84:ILE:HG21	19:S:65:ASN:HD21	1.74	0.52
1:A:715:G:OP1	1:A:750:A:H1'	2.10	0.52
8:H:6:ILE:HB	8:H:85:ARG:NH1	2.25	0.52
19:S:39:THR:HG22	19:S:70:LYS:HG2	1.92	0.52
1:A:451:C:H42	1:A:461:G:H1'	1.74	0.52
7:G:75:VAL:HG21	7:G:86:GLN:HG3	1.91	0.52
1:A:1097:C:H42	1:A:1132:G:H1	1.58	0.52
1:A:1404:U:H2'	1:A:1405:A:C8	2.44	0.52
1:A:564:U:H2'	1:A:565:G:O4'	2.09	0.51
1:A:1203:C:N4	13:M:104:ARG:HG2	2.25	0.51
3:C:52:LEU:HD13	3:C:68:VAL:HG13	1.92	0.51
10:J:19:SER:HB3	10:J:91:PRO:HD3	1.92	0.51
11:K:85:ARG:HD2	11:K:111:ASP:O	2.10	0.51
1:A:1482:U:H2'	1:A:1483:G:C8	2.46	0.51
4:D:100:ARG:O	4:D:104:VAL:HG23	2.11	0.51
10:J:22:LYS:C	10:J:24:VAL:H	2.19	0.51
1:A:475:G:H2'	1:A:476:G:C8	2.46	0.51
15:O:43:LEU:HD11	15:O:53:HIS:HB2	1.92	0.51
17:Q:86:GLU:O	17:Q:90:ILE:HG12	2.11	0.51
1:A:188:U:O2'	1:A:189:U:H5'	2.11	0.51
1:A:1389:C:H2'	1:A:1390:A:C8	2.45	0.51
1:A:75:G:H2'	1:A:76:G:C8	2.45	0.51
1:A:523:A:H2'	1:A:524:G:C8	2.46	0.51
1:A:1315:G:C6	1:A:1316:A:C6	2.99	0.51
2:B:18:GLY:HA2	2:B:42:ILE:HG13	1.93	0.51
1:A:1250:G:C2	1:A:1251:G:H1'	2.46	0.50
1:A:1458:G:H2'	1:A:1459:G:O4'	2.11	0.50
1:A:934:U:H2'	1:A:935:U:O4'	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:21:ILE:HG12	11:K:30:VAL:HG12	1.93	0.50
1:A:124:A:N1	1:A:229:C:O2'	2.43	0.50
1:A:632:A:H2'	1:A:633:G:O4'	2.11	0.50
1:A:856:G:H5'	8:H:89:PRO:HG2	1.94	0.50
1:A:1042:G:N2	1:A:1167:G:H2'	2.26	0.50
1:A:160:G:H2'	1:A:161:G:H8	1.76	0.50
1:A:368:C:H1'	1:A:369:A:OP2	2.12	0.50
1:A:470:G:HO2'	1:A:471:U:P	2.34	0.50
1:A:954:G:OP2	1:A:1335:U:O2'	2.27	0.50
5:E:7:GLU:OE2	5:E:37:ARG:NE	2.40	0.50
11:K:72:ALA:HB1	11:K:77:MET:HG3	1.92	0.50
18:R:58:LEU:HD23	18:R:62:GLU:HB3	1.94	0.50
1:A:988:G:O6	1:A:999:G:N2	2.45	0.50
7:G:42:ILE:HD11	7:G:116:ALA:HB3	1.94	0.50
7:G:62:PHE:HD1	7:G:124:LEU:HD21	1.76	0.50
13:M:76:ALA:HA	13:M:79:LYS:HE2	1.92	0.50
1:A:924:A:H2'	1:A:925:G:C8	2.47	0.50
2:B:25:ASN:OD1	2:B:27:LYS:HB2	2.12	0.50
4:D:145:GLU:HA	4:D:184:LYS:HA	1.92	0.50
19:S:17:GLU:O	19:S:21:GLU:HB2	2.12	0.50
20:T:67:ALA:HA	20:T:73:HIS:H	1.76	0.50
7:G:99:LEU:HD22	7:G:103:TRP:CZ2	2.46	0.50
1:A:368:C:H4'	1:A:369:A:O5'	2.11	0.50
1:A:954:G:N7	1:A:1336:C:H1'	2.27	0.50
4:D:102:ASP:HB3	4:D:136:PRO:HB3	1.93	0.49
5:E:84:PHE:HB2	5:E:134:ALA:HB2	1.93	0.49
1:A:1035:G:H1	1:A:1180:C:H42	1.59	0.49
1:A:175:G:H4'	1:A:176:U:H5'	1.93	0.49
1:A:733:C:H2'	1:A:734:G:H8	1.77	0.49
1:A:597:C:H2'	1:A:598:A:C8	2.48	0.49
10:J:5:ARG:HE	10:J:99:LYS:HD2	1.77	0.49
11:K:33:THR:HA	11:K:39:PRO:HA	1.94	0.49
20:T:53:LEU:HB2	20:T:100:ILE:HD13	1.95	0.49
1:A:62:U:H2'	1:A:63:C:C6	2.48	0.49
1:A:1469:G:H2'	1:A:1470:U:H5'	1.94	0.49
4:D:6:GLY:H	4:D:115:ARG:HH22	1.61	0.49
12:L:75:HIS:HA	12:L:102:ARG:NH2	2.28	0.49
1:A:377:C:H2'	1:A:378:A:O4'	2.13	0.49
1:A:1469:G:C2'	1:A:1470:U:H5'	2.43	0.49
4:D:83:SER:HA	4:D:89:THR:OG1	2.13	0.49
13:M:99:ARG:NH1	19:S:2:PRO:HG3	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:22:LEU:HB2	19:S:28:LYS:HZ3	1.77	0.49
1:A:262:G:H5"	1:A:263:C:H5	1.78	0.49
2:B:91:PRO:HG3	2:B:154:LEU:HB2	1.94	0.49
7:G:22:LEU:HD11	7:G:101:LEU:HD21	1.95	0.49
21:V:3:LYS:HA	21:V:11:GLY:HA2	1.95	0.49
1:A:1233:A:N6	1:A:1255:U:O4'	2.44	0.49
2:B:219:VAL:C	2:B:221:LEU:H	2.20	0.49
4:D:111:ALA:HB3	4:D:117:ALA:HB2	1.94	0.49
7:G:85:TYR:HD2	7:G:154:TYR:HE2	1.61	0.49
1:A:657:G:H2'	1:A:658:G:C8	2.48	0.48
20:T:60:GLU:HG3	20:T:81:LYS:HD3	1.95	0.48
1:A:138:G:H1	1:A:172:C:H42	1.61	0.48
1:A:262:G:H5'	1:A:264:C:H41	1.78	0.48
1:A:955:A:H2'	1:A:956:A:H5"	1.94	0.48
7:G:136:LYS:O	7:G:140:ASP:N	2.45	0.48
8:H:19:VAL:HG13	8:H:21:LYS:HG2	1.94	0.48
10:J:8:LEU:O	10:J:70:ARG:N	2.46	0.48
11:K:18:ARG:HH21	11:K:37:GLY:HA2	1.77	0.48
15:O:87:ILE:O	15:O:89:GLY:N	2.45	0.48
1:A:587:U:H2'	1:A:588:G:H8	1.78	0.48
10:J:78:ASN:O	10:J:81:THR:OG1	2.22	0.48
1:A:45:U:H2'	1:A:46:G:C8	2.49	0.48
1:A:288:G:C5	1:A:289:G:H1'	2.48	0.48
1:A:405:G:H2'	1:A:405:G:N3	2.27	0.48
1:A:470:G:O2'	1:A:471:U:P	2.72	0.48
8:H:17:THR:HB	8:H:78:GLN:NE2	2.25	0.48
1:A:26:A:O2'	4:D:209:ARG:NH1	2.46	0.48
10:J:86:MET:HE3	10:J:87:THR:OG1	2.13	0.48
1:A:116:C:O2'	1:A:286:C:O2	2.29	0.48
1:A:544:U:H5'	1:A:550:G:N2	2.29	0.48
1:A:820:G:C6	1:A:829:G:C6	3.02	0.48
4:D:15:GLU:HB3	4:D:63:LYS:HG2	1.95	0.48
4:D:61:LYS:HG3	4:D:203:VAL:HG13	1.96	0.48
1:A:17:U:H2'	1:A:18:C:C6	2.49	0.48
1:A:1108:A:OP2	1:A:1109:G:H8	1.97	0.48
9:I:20:ARG:HG3	9:I:60:ASP:HB3	1.95	0.48
1:A:60:A:H4'	1:A:61:G:O5'	2.14	0.48
1:A:958:C:H5'	1:A:959:U:C5	2.49	0.48
10:J:55:LYS:HB2	10:J:56:HIS:H	1.52	0.48
12:L:11:VAL:HG23	17:Q:29:HIS:CD2	2.49	0.48
1:A:513:G:O6	12:L:49:ASN:ND2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:953:A:H5'	1:A:953:A:C8	2.48	0.48
6:F:21:LEU:O	6:F:25:ILE:HG12	2.13	0.48
9:I:100:GLY:O	9:I:102:LEU:N	2.47	0.48
10:J:12:ASP:HB3	10:J:15:THR:HG22	1.96	0.48
12:L:32:PHE:HB3	12:L:84:LEU:HD11	1.95	0.48
17:Q:100:LYS:H	17:Q:100:LYS:HD3	1.79	0.48
1:A:457:G:C2	16:P:82:GLN:HB3	2.49	0.47
3:C:148:GLY:HA3	3:C:172:ARG:H	1.78	0.47
4:D:9:CYS:HB3	4:D:32:ALA:HB2	1.96	0.47
7:G:73:MET:SD	7:G:90:GLU:HA	2.53	0.47
9:I:48:GLU:N	9:I:49:PRO:HD2	2.28	0.47
19:S:53:ASN:HD21	19:S:55:LYS:HB3	1.78	0.47
2:B:27:LYS:HB3	2:B:194:PRO:HD2	1.96	0.47
12:L:54:LYS:HD2	12:L:54:LYS:N	2.29	0.47
1:A:393:A:O2'	1:A:395:G:OP2	2.31	0.47
3:C:4:LYS:HA	3:C:4:LYS:HD3	1.68	0.47
20:T:32:ALA:O	20:T:36:LEU:HB2	2.14	0.47
1:A:691:C:H2'	1:A:692:C:C6	2.49	0.47
1:A:1320:G:H2'	1:A:1321:C:C6	2.49	0.47
7:G:18:TYR:CD2	7:G:59:LEU:HB2	2.49	0.47
7:G:26:PHE:CE2	7:G:30:ILE:HD11	2.50	0.47
1:A:1001:G:H2'	1:A:1002:G:H5'	1.96	0.47
1:A:1380:C:H1'	1:A:1472:A:N1	2.30	0.47
2:B:147:LYS:HE3	2:B:148:TYR:CE1	2.49	0.47
1:A:1167:G:H5"	3:C:3:ASN:HB2	1.96	0.47
9:I:36:TYR:OH	9:I:73:GLN:NE2	2.45	0.47
11:K:87:THR:OG1	11:K:88:GLY:N	2.38	0.47
13:M:57:ARG:C	13:M:59:TYR:H	2.23	0.47
18:R:52:PRO:O	18:R:56:THR:HG23	2.14	0.47
1:A:697:G:H2'	1:A:698:G:C8	2.49	0.47
1:A:702:G:H5'	11:K:117:ASN:HB2	1.97	0.47
1:A:796:C:OP1	1:A:881:G:H1'	2.15	0.47
1:A:1243:G:N2	1:A:1246:A:OP2	2.47	0.47
4:D:207:TYR:C	4:D:209:ARG:H	2.22	0.47
1:A:1030:U:H2'	1:A:1177:C:H41	1.79	0.47
2:B:17:PHE:HB3	2:B:44:LEU:HD21	1.96	0.47
11:K:30:VAL:HG21	11:K:65:ALA:HA	1.96	0.47
18:R:38:GLU:H	18:R:38:GLU:HG3	1.47	0.47
1:A:96:C:P	20:T:17:ARG:HH21	2.38	0.46
1:A:853:C:H1'	8:H:15:ASN:HD21	1.78	0.46
1:A:909:C:H42	1:A:1363:G:H1	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1042:G:O2'	1:A:1167:G:N2	2.47	0.46
7:G:50:ILE:HG21	7:G:61:VAL:HG11	1.96	0.46
9:I:34:ASN:N	9:I:34:ASN:OD1	2.48	0.46
10:J:82:ILE:HG22	10:J:86:MET:HB2	1.97	0.46
1:A:103:C:H2'	1:A:104:G:O4'	2.16	0.46
1:A:154:A:H2'	1:A:155:A:O4'	2.15	0.46
1:A:252:U:H5'	17:Q:17:LYS:NZ	2.31	0.46
1:A:1000:G:H2'	1:A:1001:G:C8	2.48	0.46
1:A:1481:C:H2'	1:A:1482:U:O4'	2.16	0.46
2:B:159:PRO:HG2	2:B:162:ILE:HD11	1.98	0.46
8:H:33:GLU:CD	8:H:50:ARG:HH21	2.23	0.46
10:J:74:ILE:HD13	10:J:74:ILE:H	1.80	0.46
1:A:403:G:N1	1:A:480:A:O2'	2.44	0.46
1:A:1079:A:H4'	1:A:1080:A:O5'	2.15	0.46
13:M:22:ILE:HB	13:M:25:ILE:HB	1.97	0.46
15:O:85:LEU:HD23	15:O:87:ILE:HD12	1.97	0.46
1:A:835:C:H2'	1:A:836:G:O4'	2.15	0.46
1:A:1426:A:H5'	1:A:1427:C:H5	1.79	0.46
5:E:63:ARG:HA	5:E:66:MET:HE2	1.97	0.46
11:K:20:TYR:CZ	11:K:83:ILE:HD12	2.51	0.46
13:M:79:LYS:O	13:M:83:ASP:HB2	2.16	0.46
1:A:1125:C:O2	9:I:16:ARG:NH1	2.49	0.46
1:A:1245:A:H2'	1:A:1246:A:C8	2.50	0.46
4:D:30:LYS:HB3	4:D:35:ARG:HH22	1.79	0.46
21:V:15:ARG:HA	21:V:15:ARG:HD3	1.72	0.46
1:A:98:G:OP2	20:T:18:GLN:NE2	2.48	0.46
1:A:143:A:H2'	1:A:144:C:C6	2.49	0.46
1:A:1055:G:H1	5:E:47:LYS:NZ	2.14	0.46
4:D:61:LYS:HD2	4:D:207:TYR:OH	2.16	0.46
15:O:35:ARG:HH21	15:O:59:MET:HE2	1.80	0.46
1:A:1496:C:OP1	11:K:120:ARG:NH2	2.49	0.46
3:C:73:PRO:O	3:C:76:VAL:HG22	2.15	0.46
1:A:810:C:H4'	8:H:12:ARG:HG3	1.98	0.46
1:A:1104:U:O2'	1:A:1105:G:OP1	2.32	0.46
1:A:1277:G:O2'	1:A:1278:U:P	2.74	0.46
5:E:140:ARG:O	5:E:143:ARG:NH2	2.49	0.46
1:A:486:G:H2'	1:A:487:C:O4'	2.16	0.46
1:A:1390:A:H2	1:A:1459:G:H22	1.61	0.46
4:D:9:CYS:HA	4:D:12:CYS:HB2	1.98	0.46
4:D:187:ARG:CZ	4:D:188:LEU:H	2.29	0.46
1:A:485:C:H2'	1:A:486:G:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:18:PHE:O	9:I:61:ALA:HA	2.16	0.46
1:A:457:G:N3	1:A:457:G:H2'	2.31	0.45
1:A:543:A:OP1	5:E:126:ARG:NH2	2.48	0.45
1:A:1057:G:O3'	5:E:14:ARG:NH2	2.49	0.45
2:B:181:PHE:HD2	8:H:70:GLN:HB3	1.81	0.45
3:C:59:ARG:HG3	3:C:63:ASN:O	2.16	0.45
3:C:130:VAL:HG21	3:C:157:ILE:HG23	1.98	0.45
9:I:53:VAL:HG21	9:I:85:LEU:HD21	1.97	0.45
12:L:33:ARG:HA	12:L:33:ARG:HD3	1.75	0.45
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.98	0.45
1:A:35:G:H2'	1:A:36:C:H6	1.82	0.45
1:A:1262:A:H4'	1:A:1263:A:O5'	2.16	0.45
1:A:1483:G:H2'	1:A:1484:U:O4'	2.16	0.45
8:H:24:THR:HG22	8:H:63:LEU:HD21	1.98	0.45
10:J:16:LEU:HD13	10:J:70:ARG:HG2	1.98	0.45
1:A:386:C:H2'	1:A:387:G:C8	2.51	0.45
9:I:17:VAL:HG11	9:I:81:ILE:HG12	1.98	0.45
12:L:89:ARG:HH21	12:L:97:ARG:HD2	1.82	0.45
1:A:1209:U:OP1	9:I:126:SER:OG	2.34	0.45
8:H:20:TYR:CE1	8:H:76:PRO:HD2	2.50	0.45
1:A:128:A:N6	16:P:25:ARG:HH21	2.14	0.45
1:A:458:A:H1'	1:A:459:G:H22	1.79	0.45
1:A:1268:G:O2'	9:I:38:GLN:O	2.31	0.45
2:B:8:LYS:HD3	2:B:9:GLU:HG3	1.98	0.45
7:G:85:TYR:HB3	7:G:86:GLN:H	1.59	0.45
11:K:48:ILE:HA	11:K:48:ILE:HD13	1.77	0.45
14:N:40:CYS:O	14:N:44:LEU:HB2	2.16	0.45
1:A:1387:G:H1	1:A:1462:C:H42	1.62	0.45
10:J:12:ASP:OD1	10:J:13:HIS:N	2.49	0.45
1:A:262:G:H5"	1:A:263:C:C5	2.51	0.45
12:L:82:VAL:N	12:L:106:ASP:OD2	2.46	0.45
1:A:254:G:H2'	1:A:255:G:H8	1.82	0.45
19:S:28:LYS:HG2	19:S:47:HIS:HA	1.98	0.45
1:A:373:G:OP1	16:P:3:LYS:HD3	2.16	0.45
1:A:636:U:C2	1:A:736:G:N2	2.85	0.45
1:A:855:C:H5"	8:H:88:LYS:HD2	1.99	0.45
1:A:1036:G:H2'	1:A:1037:C:O4'	2.17	0.45
1:A:1394:G:O2'	1:A:1455:A:N6	2.50	0.45
7:G:26:PHE:HD1	7:G:101:LEU:HD22	1.82	0.45
1:A:402:G:C8	1:A:480:A:C6	3.04	0.45
1:A:405:G:C2	1:A:429:C:H5'	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:653:U:H2'	1:A:654:G:C8	2.52	0.45
1:A:654:G:H2'	1:A:655:G:O4'	2.17	0.45
1:A:680:A:N3	1:A:770:G:O2'	2.46	0.45
1:A:1476:G:OP1	1:A:1479:A:H4'	2.17	0.45
2:B:87:ARG:HB2	2:B:219:VAL:HG11	1.99	0.45
6:F:33:TYR:HA	6:F:71:ARG:NH2	2.32	0.45
1:A:762:G:O5'	1:A:762:G:H8	2.00	0.44
1:A:762:G:H2'	1:A:763:C:O4'	2.17	0.44
1:A:943:A:O2'	1:A:944:G:OP2	2.28	0.44
1:A:1089:A:O2'	2:B:133:LYS:NZ	2.35	0.44
11:K:98:LEU:HD12	11:K:98:LEU:HA	1.76	0.44
16:P:47:ASP:OD2	16:P:47:ASP:N	2.50	0.44
1:A:124:A:H1'	1:A:259:A:O2'	2.17	0.44
1:A:1116:G:C8	1:A:1118:C:H1'	2.53	0.44
1:A:1261:C:H3'	1:A:1262:A:C8	2.51	0.44
2:B:8:LYS:HB2	2:B:9:GLU:H	1.51	0.44
2:B:68:ILE:O	2:B:90:MET:HB3	2.17	0.44
2:B:118:LEU:HD21	2:B:138:LEU:HG	1.99	0.44
17:Q:27:PHE:HA	17:Q:28:PRO:HD3	1.79	0.44
1:A:1495:G:OP1	11:K:123:LYS:NZ	2.30	0.44
4:D:177:ASP:HB3	4:D:182:LYS:HG3	1.99	0.44
18:R:86:VAL:HB	18:R:87:ARG:H	1.49	0.44
1:A:1126:U:H2'	1:A:1127:C:O4'	2.18	0.44
2:B:90:MET:HA	2:B:91:PRO:HD3	1.87	0.44
19:S:28:LYS:HZ1	19:S:31:ILE:HD11	1.82	0.44
1:A:469:G:H4'	1:A:470:G:O5'	2.17	0.44
1:A:1246:A:H5'	21:V:19:GLY:HA2	1.99	0.44
1:A:1347:G:H2'	1:A:1348:G:H8	1.82	0.44
3:C:45:LYS:HD2	3:C:45:LYS:HA	1.78	0.44
4:D:30:LYS:HB3	4:D:35:ARG:HH12	1.82	0.44
9:I:85:LEU:HD12	9:I:85:LEU:HA	1.76	0.44
10:J:86:MET:HB3	10:J:86:MET:HE2	1.75	0.44
19:S:31:ILE:HB	19:S:49:ILE:HG23	1.99	0.44
3:C:35:GLU:HA	3:C:38:ARG:HB2	1.99	0.44
3:C:196:LEU:HB3	3:C:197:GLY:H	1.62	0.44
4:D:45:GLN:O	4:D:46:LYS:HG3	2.18	0.44
4:D:176:LEU:HD12	4:D:182:LYS:O	2.17	0.44
5:E:142:LEU:HD23	5:E:142:LEU:HA	1.83	0.44
14:N:24:CYS:HB2	14:N:40:CYS:HB3	1.87	0.44
17:Q:12:SER:HB3	17:Q:20:THR:HB	2.00	0.44
18:R:46:GLU:CD	18:R:46:GLU:H	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:53:ARG:NH2	18:R:60:GLY:HA2	2.32	0.44
1:A:400:U:H2'	1:A:401:U:H6	1.82	0.44
1:A:1102:G:H5'	10:J:35:SER:O	2.18	0.44
1:A:1159:G:H4'	1:A:1160:A:H5'	1.99	0.44
1:A:1166:C:H5"	3:C:5:ILE:HD13	2.00	0.44
2:B:223:ILE:O	2:B:227:GLY:N	2.50	0.44
13:M:110:ARG:HE	13:M:110:ARG:HB2	1.50	0.44
1:A:1040:U:H2'	1:A:1041:C:C6	2.53	0.44
1:A:1401:C:H5'	1:A:1402:U:OP2	2.17	0.44
4:D:57:ARG:HD2	4:D:202:LEU:HD22	1.98	0.44
6:F:2:ARG:NE	6:F:69:GLU:HG2	2.33	0.44
13:M:3:ARG:N	13:M:9:ILE:HG12	2.32	0.44
3:C:7:PRO:HG2	3:C:184:TYR:HB2	1.99	0.44
12:L:82:VAL:HG13	12:L:105:TYR:HB3	1.99	0.44
14:N:26:ARG:HG3	14:N:47:LEU:HD11	2.00	0.44
1:A:182:C:C2	1:A:183:G:H8	2.36	0.43
1:A:741:U:H2'	1:A:742:G:O4'	2.16	0.43
1:A:829:G:H2'	1:A:830:G:C8	2.53	0.43
7:G:26:PHE:O	7:G:30:ILE:HG13	2.18	0.43
9:I:55:ALA:O	9:I:58:ARG:HB2	2.17	0.43
13:M:3:ARG:NE	13:M:7:VAL:HG13	2.17	0.43
13:M:34:LEU:HD13	13:M:41:PRO:HA	2.00	0.43
13:M:90:LEU:HD12	13:M:93:ARG:HD2	2.00	0.43
19:S:66:MET:HE3	19:S:74:PHE:CE2	2.53	0.43
1:A:905:G:N2	1:A:1368:U:H1'	2.33	0.43
1:A:999:G:H2'	1:A:1000:G:H8	1.83	0.43
1:A:1400:G:C2	1:A:1401:C:H1'	2.53	0.43
14:N:7:ILE:HG22	14:N:9:LYS:HG2	2.00	0.43
16:P:48:TRP:CD1	16:P:48:TRP:H	2.36	0.43
19:S:44:MET:HG3	19:S:62:ILE:HD12	2.00	0.43
1:A:510:C:OP2	12:L:91:LYS:HE2	2.19	0.43
1:A:1452:G:C6	1:A:1453:U:C4	3.07	0.43
3:C:14:ILE:C	3:C:16:ARG:H	2.24	0.43
3:C:29:TYR:HE1	3:C:33:LEU:HD22	1.83	0.43
9:I:89:ASN:O	9:I:92:TYR:HB2	2.18	0.43
1:A:7:G:H5'	1:A:294:A:O4'	2.18	0.43
1:A:1404:U:H2'	1:A:1405:A:H8	1.82	0.43
4:D:162:LEU:HD21	4:D:181:MET:HB3	2.00	0.43
9:I:127:LYS:HD3	13:M:126:LYS:HE3	2.01	0.43
14:N:12:ARG:O	14:N:14:PRO:HD3	2.19	0.43
1:A:159:C:H2'	1:A:160:G:H8	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:C:H2'	1:A:540:C:C6	2.53	0.43
1:A:547:A:O2'	1:A:550:G:O2'	2.25	0.43
1:A:756:U:H2'	1:A:757:G:C8	2.53	0.43
1:A:796:C:H6	1:A:796:C:H2'	1.58	0.43
11:K:70:LYS:HA	11:K:73:MET:HG2	2.00	0.43
16:P:72:ARG:O	16:P:76:GLN:HB2	2.18	0.43
1:A:604:C:H2'	1:A:605:A:O4'	2.19	0.43
1:A:1272:G:O2'	13:M:14:ARG:NH1	2.52	0.43
2:B:9:GLU:OE2	2:B:217:ARG:NH2	2.51	0.43
4:D:128:VAL:HG22	4:D:146:ILE:HG12	2.01	0.43
5:E:95:ALA:O	5:E:98:THR:OG1	2.30	0.43
13:M:11:ARG:HA	13:M:45:VAL:HB	2.00	0.43
16:P:43:LYS:HG3	16:P:48:TRP:CE2	2.53	0.43
1:A:1200:C:P	19:S:78:ARG:HH21	2.42	0.43
1:A:1400:G:N2	1:A:1401:C:H1'	2.34	0.43
2:B:122:PHE:HA	2:B:127:ILE:HG22	2.00	0.43
3:C:16:ARG:NH2	3:C:183:ASP:OD1	2.52	0.43
12:L:27:LEU:C	12:L:29:GLY:N	2.77	0.43
13:M:12:ASN:HA	13:M:46:LYS:HB2	2.01	0.43
3:C:136:GLN:HG3	3:C:140:ARG:HH12	1.84	0.43
1:A:340:A:H5'	1:A:341:C:C5	2.54	0.43
1:A:547:A:H2'	1:A:551:G:C8	2.54	0.43
1:A:1263:A:H2'	1:A:1264:A:H4'	2.01	0.43
1:A:1329:C:H2'	1:A:1330:G:C8	2.54	0.43
1:A:1493:G:H2'	1:A:1494:U:O4'	2.19	0.43
2:B:167:PRO:HG3	2:B:188:ALA:HB2	2.01	0.43
4:D:194:LEU:HD23	4:D:196:LEU:HD12	2.01	0.43
13:M:95:GLY:C	13:M:96:LEU:HD12	2.44	0.43
17:Q:104:LYS:HA	17:Q:104:LYS:HD2	1.75	0.43
1:A:96:C:O2'	1:A:166:A:N1	2.40	0.43
3:C:150:LYS:HA	3:C:169:ALA:CB	2.49	0.43
12:L:44:THR:HA	12:L:45:PRO:HD3	1.77	0.43
13:M:4:ILE:HG23	13:M:57:ARG:HA	1.99	0.43
15:O:2:PRO:HB2	15:O:3:ILE:H	1.65	0.43
15:O:75:PRO:O	15:O:79:ARG:HB2	2.19	0.43
1:A:249:U:H2'	1:A:250:G:C8	2.54	0.42
1:A:996:C:H2'	1:A:997:C:O4'	2.19	0.42
1:A:1098:G:H2'	1:A:1099:U:C6	2.54	0.42
7:G:32:ARG:HB3	7:G:33:ASP:H	1.49	0.42
8:H:38:ILE:HD12	8:H:111:ILE:HG23	2.01	0.42
16:P:5:ARG:NH2	16:P:24:ALA:HA	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:A:H2'	1:A:379:A:C8	2.54	0.42
1:A:440:G:H2'	1:A:441:G:H8	1.83	0.42
1:A:722:C:H2'	1:A:723:C:H6	1.84	0.42
1:A:1038:C:P	14:N:45:ARG:HH22	2.41	0.42
4:D:94:LEU:HD11	4:D:200:GLU:HG2	2.01	0.42
10:J:42:THR:HB	10:J:68:HIS:HA	2.00	0.42
3:C:12:LEU:HD13	3:C:18:TRP:NE1	2.34	0.42
9:I:116:LYS:HA	9:I:123:PRO:HD3	2.00	0.42
12:L:28:LYS:HB3	12:L:30:ALA:HB2	2.02	0.42
18:R:19:LYS:HE2	18:R:19:LYS:HB3	1.93	0.42
1:A:305:G:H2'	1:A:306:G:H8	1.84	0.42
1:A:653:U:H2'	1:A:654:G:H8	1.84	0.42
1:A:1398:G:H1'	1:A:1452:G:N2	2.34	0.42
5:E:31:LEU:HD12	5:E:44:GLY:O	2.20	0.42
5:E:144:THR:HG22	5:E:147:ASP:CG	2.45	0.42
11:K:99:GLN:HG2	11:K:105:VAL:HG21	2.02	0.42
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	2.00	0.42
1:A:199:U:O4'	20:T:103:GLY:HA2	2.20	0.42
1:A:351:C:H2'	1:A:352:A:O4'	2.20	0.42
1:A:963:C:H2'	1:A:964:A:C8	2.54	0.42
1:A:999:G:H2'	1:A:1000:G:C8	2.53	0.42
1:A:1333:G:H2'	1:A:1334:A:C8	2.55	0.42
8:H:6:ILE:HB	8:H:85:ARG:HH12	1.85	0.42
9:I:16:ARG:NE	9:I:64:THR:HB	2.32	0.42
16:P:42:ARG:H	16:P:42:ARG:HG2	1.43	0.42
17:Q:15:MET:HE3	17:Q:15:MET:HB2	1.96	0.42
1:A:526:G:H5'	4:D:41:GLY:HA3	2.02	0.42
1:A:1401:C:H3'	1:A:1402:U:O4'	2.19	0.42
4:D:31:CYS:C	4:D:33:MET:H	2.27	0.42
19:S:13:ASP:OD1	19:S:13:ASP:N	2.48	0.42
1:A:348:C:O2	1:A:351:C:N4	2.50	0.42
1:A:815:U:H2'	1:A:816:C:C6	2.55	0.42
1:A:1038:C:H2'	1:A:1039:G:H8	1.84	0.42
2:B:189:ASP:N	2:B:189:ASP:OD2	2.53	0.42
3:C:111:LEU:HD23	3:C:111:LEU:HA	1.83	0.42
5:E:40:ARG:HE	5:E:40:ARG:HB3	1.67	0.42
17:Q:10:VAL:HG13	17:Q:19:VAL:HB	2.01	0.42
7:G:45:ASP:O	7:G:49:ILE:HG12	2.20	0.42
9:I:32:ASP:H	9:I:35:GLU:HB2	1.85	0.42
10:J:34:VAL:HG12	10:J:36:GLY:H	1.85	0.42
12:L:89:ARG:HH21	12:L:97:ARG:CD	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:7:ILE:HG23	14:N:9:LYS:HE3	2.01	0.42
14:N:58:LYS:HD2	14:N:58:LYS:HA	1.86	0.42
20:T:48:LYS:HA	20:T:48:LYS:HD2	1.90	0.42
1:A:858:C:H2'	1:A:859:G:H8	1.85	0.42
1:A:999:G:N2	1:A:1000:G:O6	2.52	0.42
3:C:203:PHE:O	3:C:205:GLY:N	2.49	0.42
8:H:48:TYR:HD1	8:H:59:LEU:HD22	1.85	0.42
9:I:127:LYS:HD3	13:M:126:LYS:HG3	2.01	0.42
17:Q:97:SER:O	17:Q:99:SER:N	2.53	0.42
1:A:378:A:H2'	1:A:379:A:H8	1.85	0.42
1:A:1010:G:H2'	1:A:1011:G:O4'	2.20	0.42
1:A:1239:C:H42	1:A:1250:G:H1	1.68	0.42
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.60	0.42
10:J:49:VAL:O	10:J:60:ARG:HA	2.19	0.42
20:T:48:LYS:O	20:T:50:GLU:N	2.53	0.42
1:A:129:C:O2	16:P:1:MET:HB2	2.19	0.41
1:A:331:C:O2'	1:A:1410:A:N3	2.47	0.41
1:A:340:A:H5'	1:A:341:C:H5	1.84	0.41
1:A:423:U:OP2	4:D:36:ARG:NH1	2.51	0.41
1:A:725:G:H5"	15:O:59:MET:HE1	2.01	0.41
2:B:196:LEU:HD23	2:B:196:LEU:HA	1.84	0.41
3:C:36:ASP:HB2	3:C:59:ARG:NH2	2.35	0.41
1:A:432:C:H4'	4:D:156:GLU:HG2	2.01	0.41
1:A:544:U:H5'	1:A:550:G:C2	2.54	0.41
1:A:943:A:H5'	1:A:947:A:O4'	2.19	0.41
1:A:961:A:N1	1:A:1199:G:N2	2.66	0.41
1:A:983:A:H5"	1:A:984:C:C6	2.55	0.41
4:D:173:TRP:HB2	4:D:187:ARG:O	2.20	0.41
9:I:7:THR:HB	9:I:8:GLY:H	1.65	0.41
11:K:92:GLU:O	11:K:96:ARG:HG3	2.19	0.41
15:O:9:GLN:O	15:O:13:GLN:HG2	2.20	0.41
18:R:79:LEU:HD12	18:R:79:LEU:HA	1.79	0.41
1:A:141:G:C2	1:A:142:G:C8	3.08	0.41
1:A:925:G:O3'	13:M:109:THR:OG1	2.38	0.41
1:A:1324:G:O6	9:I:10:ARG:NH2	2.52	0.41
3:C:120:VAL:HG23	3:C:198:VAL:HG21	2.00	0.41
4:D:7:PRO:O	4:D:10:ARG:HG2	2.20	0.41
5:E:60:TYR:O	5:E:64:ARG:HG3	2.20	0.41
5:E:87:SER:OG	5:E:130:ASN:HB3	2.20	0.41
10:J:54:PHE:CD2	10:J:55:LYS:HG2	2.53	0.41
10:J:61:GLU:OE2	14:N:45:ARG:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:17:GLY:HA3	11:K:77:MET:HE1	2.02	0.41
1:A:351:C:H5'	1:A:385:A:OP2	2.20	0.41
1:A:1115:C:H4'	1:A:1116:G:N3	2.35	0.41
2:B:114:ARG:HH22	2:B:138:LEU:HD21	1.85	0.41
10:J:24:VAL:HG12	10:J:28:ARG:HD2	2.02	0.41
11:K:112:THR:HA	11:K:113:PRO:HD3	1.89	0.41
18:R:53:ARG:HD3	18:R:58:LEU:O	2.20	0.41
1:A:246:A:H1'	1:A:248:U:C5	2.55	0.41
1:A:985:C:N3	1:A:1000:G:N2	2.65	0.41
1:A:1288:G:H5"	19:S:3:ARG:HD2	2.02	0.41
3:C:148:GLY:HA2	3:C:171:GLY:HA3	2.02	0.41
4:D:22:LYS:O	4:D:25:ARG:HD3	2.19	0.41
1:A:459:G:N1	16:P:83:GLU:HB2	2.35	0.41
1:A:524:G:C6	1:A:525:G:C5	3.08	0.41
1:A:1247:C:H2'	1:A:1248:G:C8	2.56	0.41
1:A:1324:G:H3'	9:I:108:VAL:O	2.21	0.41
1:A:1349:U:H2'	1:A:1350:G:O4'	2.20	0.41
1:A:1398:G:H2'	1:A:1399:G:H8	1.82	0.41
3:C:70:VAL:HG12	3:C:72:LYS:H	1.84	0.41
12:L:102:ARG:HB3	12:L:102:ARG:NH1	2.35	0.41
14:N:15:LYS:HB3	14:N:16:PHE:H	1.76	0.41
15:O:4:THR:HB	15:O:7:GLU:HB2	2.03	0.41
3:C:19:GLU:HG2	3:C:54:ARG:HE	1.86	0.41
4:D:34:GLU:O	4:D:36:ARG:N	2.51	0.41
4:D:67:ILE:HG23	4:D:68:TYR:CD1	2.56	0.41
5:E:15:ARG:HD3	5:E:16:THR:O	2.20	0.41
10:J:71:LEU:HD23	10:J:71:LEU:HA	1.87	0.41
13:M:3:ARG:H	13:M:9:ILE:HG12	1.85	0.41
16:P:3:LYS:O	16:P:21:VAL:HA	2.21	0.41
1:A:139:G:H1	1:A:171:C:H42	1.67	0.41
1:A:721:A:H2'	1:A:722:C:C6	2.55	0.41
1:A:1037:C:O3'	14:N:45:ARG:NH2	2.53	0.41
1:A:1399:G:H2'	1:A:1400:G:H8	1.85	0.41
2:B:125:PRO:O	2:B:127:ILE:N	2.50	0.41
2:B:135:GLN:C	2:B:137:ARG:H	2.29	0.41
7:G:42:ILE:HD12	7:G:42:ILE:HA	1.87	0.41
9:I:25:LYS:HB2	9:I:60:ASP:OD1	2.20	0.41
9:I:56:LEU:HB3	9:I:57:GLY:H	1.60	0.41
20:T:36:LEU:HD23	20:T:36:LEU:HA	1.87	0.41
1:A:416:U:C5	1:A:420:G:H8	2.39	0.41
1:A:469:G:H5'	1:A:471:U:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:715:G:H5'	1:A:750:A:H4'	2.01	0.41
1:A:814:G:H2'	1:A:815:U:O4'	2.21	0.41
1:A:1013:A:C8	1:A:1014:G:C8	3.09	0.41
1:A:1096:C:OP1	9:I:9:ARG:HD2	2.21	0.41
1:A:1135:A:C6	1:A:1157:A:C6	3.08	0.41
1:A:1187:C:N4	1:A:1188:U:O4	2.54	0.41
1:A:1437:C:H2'	1:A:1438:C:O4'	2.21	0.41
2:B:22:LYS:NZ	2:B:35:GLU:OE1	2.53	0.41
2:B:28:PHE:CD2	2:B:190:THR:HA	2.55	0.41
2:B:35:GLU:H	2:B:35:GLU:HG2	1.65	0.41
2:B:47:THR:HG23	2:B:202:PRO:HG2	2.03	0.41
2:B:137:ARG:NH2	2:B:138:LEU:HD13	2.35	0.41
2:B:182:ILE:HA	2:B:183:PRO:HD2	1.78	0.41
4:D:150:GLU:O	4:D:153:ARG:HB2	2.20	0.41
5:E:118:ILE:HG12	5:E:119:LEU:N	2.36	0.41
6:F:47:ARG:CZ	6:F:47:ARG:H	2.33	0.41
13:M:40:ASN:HA	13:M:41:PRO:HD2	1.92	0.41
22:X:36:G:H1	23:W:1:C:N4	2.19	0.41
22:X:36:G:H2'	22:X:37:A:H8	1.85	0.41
1:A:582:U:H4'	8:H:94:TYR:CG	2.55	0.41
1:A:1047:C:O2'	1:A:1169:C:H1'	2.21	0.41
1:A:1080:A:H2'	1:A:1081:C:C6	2.56	0.41
2:B:55:PHE:HD2	2:B:55:PHE:HA	1.67	0.41
8:H:6:ILE:HD12	8:H:6:ILE:H	1.85	0.41
10:J:8:LEU:HD21	10:J:20:ALA:HB1	2.03	0.41
12:L:10:LEU:HD23	12:L:10:LEU:HA	1.85	0.41
16:P:49:LEU:HD22	16:P:73:LEU:HD22	2.02	0.41
17:Q:81:ARG:NE	17:Q:84:LEU:HD23	2.36	0.41
1:A:1038:C:O2	1:A:1175:G:C2	2.74	0.40
1:A:1096:C:H1'	1:A:1156:A:C4	2.56	0.40
1:A:1277:G:O2'	1:A:1280:C:N4	2.54	0.40
1:A:1378:G:C2	1:A:1379:C:H1'	2.56	0.40
3:C:43:LEU:C	3:C:45:LYS:H	2.29	0.40
3:C:113:ALA:N	3:C:114:PRO:HD2	2.36	0.40
3:C:156:ARG:NH2	3:C:161:GLU:HA	2.36	0.40
13:M:34:LEU:HD22	13:M:39:ILE:HB	2.03	0.40
18:R:23:LYS:HD2	18:R:57:GLY:O	2.21	0.40
1:A:115:G:N2	1:A:116:C:H1'	2.37	0.40
1:A:674:G:H2'	1:A:675:G:O4'	2.21	0.40
1:A:927:A:C2	1:A:1210:G:N3	2.89	0.40
1:A:1203:C:C4	13:M:104:ARG:HG2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:105:PHE:O	2:B:109:SER:OG	2.29	0.40
6:F:1:MET:HA	6:F:67:MET:O	2.21	0.40
7:G:90:GLU:H	7:G:90:GLU:HG2	1.77	0.40
7:G:137:LYS:O	7:G:141:VAL:HG23	2.21	0.40
8:H:127:LEU:HD23	8:H:127:LEU:HA	1.93	0.40
1:A:102:A:H2'	1:A:322:G:N2	2.36	0.40
1:A:265:C:H2'	1:A:266:A:C8	2.56	0.40
1:A:463:A:OP1	1:A:463:A:H4'	2.21	0.40
1:A:955:A:C2'	1:A:956:A:H5"	2.51	0.40
1:A:1197:G:H2'	1:A:1198:G:C8	2.57	0.40
2:B:51:LEU:HD11	2:B:214:ILE:HD11	2.02	0.40
2:B:69:LEU:HB3	2:B:162:ILE:CD1	2.51	0.40
5:E:34:VAL:HG12	5:E:62:ALA:HB1	2.03	0.40
12:L:102:ARG:NH1	12:L:108:ALA:O	2.53	0.40
13:M:3:ARG:O	13:M:57:ARG:HD3	2.21	0.40
17:Q:9:VAL:HG13	17:Q:56:VAL:HG22	2.02	0.40
21:V:18:TYR:CD1	21:V:24:ARG:HG2	2.57	0.40
1:A:917:G:C6	1:A:918:C:N4	2.90	0.40
1:A:1114:U:H5"	1:A:1115:C:C5	2.56	0.40
5:E:91:LEU:HB3	5:E:118:ILE:HD11	2.02	0.40
1:A:552:G:C6	1:A:553:C:N4	2.89	0.40
1:A:566:U:OP2	1:A:742:G:N1	2.47	0.40
1:A:748:C:H2'	1:A:749:G:O4'	2.22	0.40
1:A:829:G:H2'	1:A:830:G:H8	1.85	0.40
1:A:1202:A:H2'	1:A:1202:A:N3	2.37	0.40
1:A:1352:A:H4'	7:G:29:LYS:HE2	2.03	0.40
9:I:43:ALA:HA	9:I:74:ILE:HD13	2.02	0.40
10:J:40:LEU:HA	10:J:41:PRO:HD3	1.96	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:79:ARG:CD	10:J:79:ARG:NE[8_665]	1.46	0.74
10:J:79:ARG:CG	10:J:79:ARG:CD[8_665]	1.53	0.67
10:J:79:ARG:CG	10:J:79:ARG:CG[8_665]	2.05	0.15

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	232/256 (91%)	176 (76%)	44 (19%)	12 (5%)	1 14
3	C	204/239 (85%)	166 (81%)	27 (13%)	11 (5%)	1 13
4	D	206/209 (99%)	178 (86%)	22 (11%)	6 (3%)	3 25
5	E	148/162 (91%)	134 (90%)	11 (7%)	3 (2%)	6 32
6	F	99/101 (98%)	89 (90%)	10 (10%)	0	100 100
7	G	153/156 (98%)	137 (90%)	13 (8%)	3 (2%)	6 32
8	H	136/138 (99%)	124 (91%)	11 (8%)	1 (1%)	18 52
9	I	125/128 (98%)	98 (78%)	16 (13%)	11 (9%)	0 7
10	J	96/105 (91%)	65 (68%)	21 (22%)	10 (10%)	0 5
11	K	117/129 (91%)	98 (84%)	17 (14%)	2 (2%)	7 35
12	L	122/132 (92%)	98 (80%)	18 (15%)	6 (5%)	1 15
13	M	123/126 (98%)	91 (74%)	29 (24%)	3 (2%)	4 29
14	N	58/61 (95%)	45 (78%)	9 (16%)	4 (7%)	1 10
15	O	86/89 (97%)	79 (92%)	3 (4%)	4 (5%)	2 16
16	P	81/88 (92%)	71 (88%)	9 (11%)	1 (1%)	10 42
17	Q	102/105 (97%)	84 (82%)	11 (11%)	7 (7%)	1 10
18	R	71/88 (81%)	62 (87%)	6 (8%)	3 (4%)	2 18
19	S	78/93 (84%)	55 (70%)	19 (24%)	4 (5%)	1 15
20	T	97/106 (92%)	81 (84%)	9 (9%)	7 (7%)	1 9
21	V	22/27 (82%)	21 (96%)	1 (4%)	0	100 100
All	All	2356/2538 (93%)	1952 (83%)	306 (13%)	98 (4%)	2 18

All (98) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	232	PRO

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Mol	Chain	Res	Type
2	B	236	TYR
8	H	91	ARG
9	I	38	GLN
9	I	43	ALA
10	J	85	LEU
14	N	14	PRO
17	Q	47	PRO
17	Q	49	GLU
17	Q	79	SER
2	B	21	ARG
2	B	74	LYS
2	B	137	ARG
3	C	3	ASN
3	C	119	ARG
3	C	154	SER
3	C	167	TRP
4	D	4	TYR
4	D	29	PRO
5	E	85	GLY
7	G	4	ARG
9	I	39	GLY
9	I	101	PHE
9	I	121	ARG
10	J	23	ILE
10	J	72	VAL
10	J	73	ASP
10	J	90	LEU
12	L	116	SER
12	L	121	GLY
13	M	86	CYS
15	O	21	ASP
15	O	88	ARG
16	P	31	LYS
18	R	86	VAL
19	S	6	LYS
20	T	49	ALA
2	B	9	GLU
2	B	126	GLU
2	B	207	ALA
2	B	238	LEU
3	C	61	ALA
3	C	66	VAL

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Mol	Chain	Res	Type
3	C	156	ARG
3	C	206	GLU
4	D	30	LYS
4	D	153	ARG
4	D	181	MET
7	G	32	ARG
9	I	33	PHE
9	I	88	TYR
9	I	117	HIS
10	J	34	VAL
11	K	117	ASN
12	L	28	LYS
12	L	46	LYS
12	L	115	LYS
17	Q	98	LEU
19	S	23	ASN
20	T	73	HIS
20	T	98	PRO
2	B	77	ALA
3	C	96	GLY
5	E	16	THR
5	E	17	ALA
9	I	118	LYS
10	J	40	LEU
10	J	55	LYS
10	J	60	ARG
11	K	126	ARG
12	L	78	GLN
13	M	10	PRO
15	O	19	PRO
15	O	23	GLY
17	Q	97	SER
18	R	21	LYS
19	S	30	LEU
20	T	96	GLY
20	T	97	ALA
2	B	20	GLU
3	C	15	THR
9	I	7	THR
14	N	15	LYS
17	Q	99	SER
2	B	136	VAL

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Mol	Chain	Res	Type
14	N	24	CYS
17	Q	30	PRO
18	R	87	ARG
19	S	26	GLY
20	T	9	ASN
7	G	81	GLY
9	I	44	VAL
4	D	5	ILE
13	M	7	VAL
14	N	18	VAL
20	T	69	GLY
3	C	81	GLY
10	J	39	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	202/220 (92%)	172 (85%)	30 (15%)	3 17
3	C	160/188 (85%)	145 (91%)	15 (9%)	8 32
4	D	180/181 (99%)	161 (89%)	19 (11%)	6 28
5	E	115/123 (94%)	100 (87%)	15 (13%)	4 21
6	F	90/90 (100%)	83 (92%)	7 (8%)	11 37
7	G	126/127 (99%)	117 (93%)	9 (7%)	13 39
8	H	119/119 (100%)	107 (90%)	12 (10%)	7 29
9	I	98/99 (99%)	82 (84%)	16 (16%)	2 14
10	J	87/92 (95%)	76 (87%)	11 (13%)	4 22
11	K	90/99 (91%)	76 (84%)	14 (16%)	2 15
12	L	104/109 (95%)	96 (92%)	8 (8%)	12 38
13	M	100/101 (99%)	94 (94%)	6 (6%)	17 44
14	N	49/50 (98%)	47 (96%)	2 (4%)	27 53
15	O	79/80 (99%)	71 (90%)	8 (10%)	7 29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	P	72/74 (97%)	63 (88%)	9 (12%)	4 22
17	Q	96/97 (99%)	85 (88%)	11 (12%)	5 25
18	R	64/77 (83%)	57 (89%)	7 (11%)	6 27
19	S	71/80 (89%)	65 (92%)	6 (8%)	10 34
20	T	75/82 (92%)	65 (87%)	10 (13%)	4 21
21	V	19/22 (86%)	18 (95%)	1 (5%)	20 47
All	All	1996/2110 (95%)	1780 (89%)	216 (11%)	6 28

All (216) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	8	LYS
2	B	10	LEU
2	B	15	VAL
2	B	16	HIS
2	B	17	PHE
2	B	21	ARG
2	B	27	LYS
2	B	30	ARG
2	B	51	LEU
2	B	55	PHE
2	B	59	GLU
2	B	60	ASP
2	B	64	ARG
2	B	71	VAL
2	B	75	LYS
2	B	94	ASN
2	B	114	ARG
2	B	134	GLU
2	B	136	VAL
2	B	142	LEU
2	B	160	ASP
2	B	168	THR
2	B	179	LYS
2	B	182	ILE
2	B	185	ILE
2	B	195	ASP
2	B	197	VAL
2	B	200	ILE
2	B	211	ILE

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Mol	Chain	Res	Type
2	B	229	VAL
3	C	15	THR
3	C	34	LEU
3	C	45	LYS
3	C	64	VAL
3	C	76	VAL
3	C	87	LEU
3	C	95	THR
3	C	112	SER
3	C	119	ARG
3	C	127	ARG
3	C	128	PHE
3	C	152	ILE
3	C	166	GLU
3	C	173	VAL
3	C	195	VAL
4	D	3	ARG
4	D	12	CYS
4	D	57	ARG
4	D	71	SER
4	D	78	LEU
4	D	86	LYS
4	D	96	LEU
4	D	99	SER
4	D	116	GLN
4	D	119	GLN
4	D	127	THR
4	D	139	ARG
4	D	151	LYS
4	D	165	MET
4	D	178	VAL
4	D	181	MET
4	D	187	ARG
4	D	192	GLU
4	D	200	GLU
5	E	8	GLU
5	E	10	MET
5	E	11	ILE
5	E	15	ARG
5	E	33	VAL
5	E	41	VAL
5	E	43	LEU

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Mol	Chain	Res	Type
5	E	55	VAL
5	E	57	LYS
5	E	69	VAL
5	E	75	THR
5	E	79	GLU
5	E	100	VAL
5	E	120	THR
5	E	129	ILE
6	F	11	ASN
6	F	43	LEU
6	F	47	ARG
6	F	69	GLU
6	F	77	ARG
6	F	79	LEU
6	F	89	MET
7	G	11	GLN
7	G	32	ARG
7	G	35	LYS
7	G	69	VAL
7	G	85	TYR
7	G	91	VAL
7	G	136	LYS
7	G	148	ASN
7	G	149	ARG
8	H	2	LEU
8	H	3	THR
8	H	26	VAL
8	H	29	SER
8	H	39	LEU
8	H	63	LEU
8	H	83	ILE
8	H	85	ARG
8	H	104	ARG
8	H	105	ARG
8	H	112	LEU
8	H	136	GLU
9	I	7	THR
9	I	23	ASN
9	I	28	VAL
9	I	34	ASN
9	I	40	LEU
9	I	47	LEU

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Mol	Chain	Res	Type
9	I	51	ARG
9	I	54	ASP
9	I	58	ARG
9	I	70	LYS
9	I	79	LEU
9	I	92	TYR
9	I	96	LEU
9	I	102	LEU
9	I	104	ARG
9	I	114	TYR
10	J	21	GLN
10	J	35	SER
10	J	42	THR
10	J	48	THR
10	J	66	ARG
10	J	69	ASN
10	J	74	ILE
10	J	79	ARG
10	J	82	ILE
10	J	85	LEU
10	J	96	ILE
11	K	29	ILE
11	K	40	ILE
11	K	48	ILE
11	K	57	THR
11	K	71	LYS
11	K	81	ASP
11	K	85	ARG
11	K	98	LEU
11	K	103	LEU
11	K	104	GLN
11	K	109	VAL
11	K	110	ASP
11	K	117	ASN
11	K	123	LYS
12	L	23	LYS
12	L	28	LYS
12	L	40	VAL
12	L	46	LYS
12	L	55	VAL
12	L	81	SER
12	L	83	VAL

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Mol	Chain	Res	Type
12	L	110	VAL
13	M	49	THR
13	M	56	LEU
13	M	60	VAL
13	M	64	TRP
13	M	69	GLU
13	M	81	LEU
14	N	12	ARG
14	N	53	LEU
15	O	4	THR
15	O	26	GLU
15	O	34	LEU
15	O	39	LEU
15	O	43	LEU
15	O	70	LEU
15	O	76	GLU
15	O	87	ILE
16	P	2	VAL
16	P	21	VAL
16	P	42	ARG
16	P	51	VAL
16	P	60	LEU
16	P	62	VAL
16	P	65	GLN
16	P	67	THR
16	P	82	GLN
17	Q	9	VAL
17	Q	36	ILE
17	Q	39	SER
17	Q	48	GLU
17	Q	65	ILE
17	Q	68	ARG
17	Q	70	ARG
17	Q	74	LEU
17	Q	77	VAL
17	Q	78	GLU
17	Q	84	LEU
18	R	38	GLU
18	R	41	LYS
18	R	47	THR
18	R	66	LEU
18	R	75	ILE

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Mol	Chain	Res	Type
18	R	79	LEU
18	R	86	VAL
19	S	7	LYS
19	S	9	VAL
19	S	15	LEU
19	S	35	SER
19	S	51	VAL
19	S	77	THR
20	T	8	ARG
20	T	19	SER
20	T	30	LYS
20	T	36	LEU
20	T	48	LYS
20	T	73	HIS
20	T	75	ASN
20	T	84	LEU
20	T	87	LYS
20	T	100	ILE
21	V	9	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	16	HIS
2	B	19	HIS
2	B	94	ASN
2	B	224	GLN
3	C	170	GLN
8	H	15	ASN
10	J	33	GLN
10	J	76	ASN
11	K	93	GLN
12	L	49	ASN
14	N	49	HIS
15	O	53	HIS
15	O	71	GLN
17	Q	26	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1506/1507 (99%)	301 (19%)	25 (1%)
22	X	10/17 (58%)	0	0
23	W	3/6 (50%)	0	0
All	All	1519/1530 (99%)	301 (19%)	25 (1%)

All (301) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	9	G
1	A	31	G
1	A	32	A
1	A	39	G
1	A	41	G
1	A	47	C
1	A	48	C
1	A	49	U
1	A	50	A
1	A	51	A
1	A	54	C
1	A	59	A
1	A	61	G
1	A	73	G
1	A	94	A
1	A	101	G
1	A	109	A
1	A	114	C
1	A	120	G
1	A	125	C
1	A	157	C
1	A	176	U
1	A	177	G
1	A	184	C
1	A	185	C
1	A	188	U
1	A	189	U
1	A	202	A
1	A	204	A
1	A	208	C
1	A	210	U
1	A	211	U
1	A	212	G

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Mol	Chain	Res	Type
1	A	213	C
1	A	216	G
1	A	227	G
1	A	243	G
1	A	246	A
1	A	247	G
1	A	248	U
1	A	249	U
1	A	263	C
1	A	275	A
1	A	285	G
1	A	286	C
1	A	297	G
1	A	317	A
1	A	324	C
1	A	325	A
1	A	328	G
1	A	340	A
1	A	341	C
1	A	342	G
1	A	343	G
1	A	347	G
1	A	348	C
1	A	349	A
1	A	350	G
1	A	352	A
1	A	363	U
1	A	368	C
1	A	369	A
1	A	380	G
1	A	385	A
1	A	393	A
1	A	394	C
1	A	402	G
1	A	403	G
1	A	405	G
1	A	406	G
1	A	408	A
1	A	409	G
1	A	410	A
1	A	411	A
1	A	412	G

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Mol	Chain	Res	Type
1	A	416	U
1	A	418	C
1	A	419	G
1	A	420	G
1	A	421	G
1	A	425	U
1	A	427	A
1	A	428	A
1	A	429	C
1	A	435	A
1	A	447	A
1	A	456	C
1	A	457	G
1	A	458	A
1	A	459	G
1	A	460	G
1	A	461	G
1	A	462	G
1	A	463	A
1	A	466	G
1	A	470	G
1	A	471	U
1	A	473	C
1	A	480	A
1	A	481	A
1	A	482	U
1	A	483	A
1	A	484	G
1	A	495	C
1	A	496	U
1	A	502	C
1	A	505	G
1	A	508	G
1	A	515	U
1	A	516	A
1	A	517	A
1	A	519	A
1	A	531	A
1	A	543	A
1	A	544	U
1	A	548	C
1	A	556	A

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Mol	Chain	Res	Type
1	A	557	A
1	A	559	G
1	A	560	G
1	A	561	G
1	A	563	G
1	A	572	G
1	A	600	G
1	A	601	G
1	A	637	A
1	A	649	A
1	A	656	U
1	A	666	G
1	A	671	A
1	A	686	A
1	A	687	G
1	A	701	C
1	A	705	G
1	A	707	U
1	A	715	G
1	A	739	G
1	A	743	A
1	A	761	A
1	A	765	A
1	A	771	A
1	A	777	U
1	A	778	A
1	A	797	U
1	A	801	C
1	A	805	G
1	A	812	A
1	A	823	U
1	A	824	C
1	A	825	U
1	A	826	C
1	A	850	A
1	A	854	G
1	A	875	C
1	A	880	G
1	A	892	A
1	A	904	G
1	A	905	G
1	A	909	C

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Mol	Chain	Res	Type
1	A	911	G
1	A	912	C
1	A	913	A
1	A	917	G
1	A	920	G
1	A	938	U
1	A	939	U
1	A	944	G
1	A	946	A
1	A	947	A
1	A	949	G
1	A	952	A
1	A	953	A
1	A	954	G
1	A	955	A
1	A	958	C
1	A	960	U
1	A	961	A
1	A	967	C
1	A	969	U
1	A	970	U
1	A	971	G
1	A	975	U
1	A	980	G
1	A	981	G
1	A	983	A
1	A	984	C
1	A	985	C
1	A	987	G
1	A	988	G
1	A	998	U
1	A	999	G
1	A	1003	U
1	A	1004	G
1	A	1006	C
1	A	1008	C
1	A	1009	G
1	A	1010	G
1	A	1011	G
1	A	1013	A
1	A	1015	C
1	A	1017	C

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Mol	Chain	Res	Type
1	A	1020	G
1	A	1023	C
1	A	1031	G
1	A	1032	C
1	A	1048	U
1	A	1049	C
1	A	1072	G
1	A	1073	U
1	A	1074	C
1	A	1079	A
1	A	1080	A
1	A	1082	G
1	A	1102	G
1	A	1103	U
1	A	1104	U
1	A	1105	G
1	A	1107	C
1	A	1108	A
1	A	1109	G
1	A	1113	U
1	A	1115	C
1	A	1117	G
1	A	1124	A
1	A	1130	A
1	A	1137	U
1	A	1143	C
1	A	1148	G
1	A	1160	A
1	A	1161	G
1	A	1164	G
1	A	1168	A
1	A	1173	U
1	A	1174	G
1	A	1178	A
1	A	1179	G
1	A	1188	U
1	A	1189	U
1	A	1190	A
1	A	1202	A
1	A	1204	A
1	A	1213	A
1	A	1215	A

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Mol	Chain	Res	Type
1	A	1216	A
1	A	1235	G
1	A	1247	C
1	A	1257	A
1	A	1259	C
1	A	1263	A
1	A	1264	A
1	A	1267	G
1	A	1278	U
1	A	1279	U
1	A	1282	G
1	A	1289	G
1	A	1304	C
1	A	1322	U
1	A	1323	A
1	A	1324	G
1	A	1325	U
1	A	1330	G
1	A	1336	C
1	A	1337	A
1	A	1338	G
1	A	1339	C
1	A	1340	A
1	A	1341	U
1	A	1345	G
1	A	1347	G
1	A	1356	G
1	A	1371	A
1	A	1375	A
1	A	1401	C
1	A	1402	U
1	A	1404	U
1	A	1419	G
1	A	1420	G
1	A	1421	A
1	A	1422	G
1	A	1426	A
1	A	1427	C
1	A	1447	G
1	A	1453	U
1	A	1459	G
1	A	1464	A

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Mol	Chain	Res	Type
1	A	1469	G
1	A	1471	A
1	A	1475	A
1	A	1476	G
1	A	1478	U
1	A	1479	A
1	A	1489	G
1	A	1492	G
1	A	1501	G
1	A	1502	G
1	A	1505	C
1	A	1506	A
1	A	1507	C
1	A	1508	U

All (25) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	60	A
1	A	108	G
1	A	175	G
1	A	247	G
1	A	262	G
1	A	324	C
1	A	368	C
1	A	424	G
1	A	469	G
1	A	470	G
1	A	543	A
1	A	685	C
1	A	796	C
1	A	943	A
1	A	1079	A
1	A	1104	U
1	A	1160	A
1	A	1178	A
1	A	1262	A
1	A	1277	G
1	A	1323	A
1	A	1324	G
1	A	1335	U
1	A	1374	C

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Mol	Chain	Res	Type
1	A	1470	U

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 95 ligands modelled in this entry, 94 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	PAR	A	1601	-	44,45,45	1.31	7 (15%)	63,67,67	1.65	11 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PAR	A	1601	-	-	2/18/94/94	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1601	PAR	C52-C42	3.96	1.60	1.52
24	A	1601	PAR	C13-C23	2.45	1.56	1.52
24	A	1601	PAR	C62-C52	2.35	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1601	PAR	O54-C14	2.16	1.47	1.41
24	A	1601	PAR	C44-C54	2.10	1.57	1.53
24	A	1601	PAR	O43-C13	2.07	1.45	1.41
24	A	1601	PAR	O54-C54	2.05	1.49	1.44

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	1601	PAR	O33-C14-C24	6.51	118.73	108.08
24	A	1601	PAR	O54-C54-C44	3.66	116.30	109.70
24	A	1601	PAR	C34-C24-N24	-3.25	104.40	111.05
24	A	1601	PAR	O11-C11-O51	2.93	118.39	110.69
24	A	1601	PAR	C14-O33-C33	-2.77	111.41	117.98
24	A	1601	PAR	O34-C34-C44	-2.73	103.95	110.38
24	A	1601	PAR	O52-C13-O43	-2.60	108.72	111.37
24	A	1601	PAR	C13-O52-C52	-2.43	112.21	117.98
24	A	1601	PAR	O51-C51-C61	2.25	112.01	106.44
24	A	1601	PAR	C11-O51-C51	2.08	117.78	113.72
24	A	1601	PAR	C13-C23-C33	2.00	104.51	102.10

There are no chirality outliers.

All (2) torsion outliers are listed below:

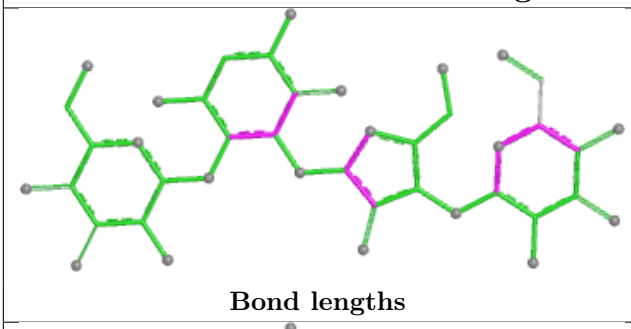
Mol	Chain	Res	Type	Atoms
24	A	1601	PAR	C44-C54-C64-N64
24	A	1601	PAR	C43-C33-O33-C14

There are no ring outliers.

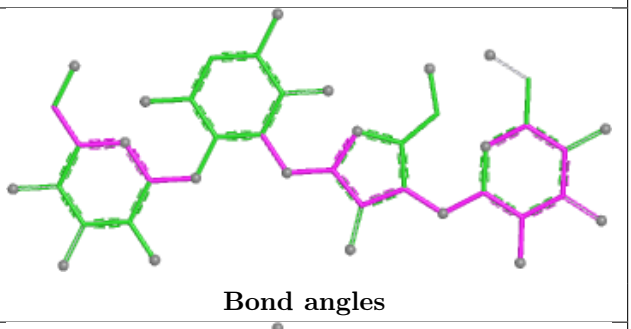
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

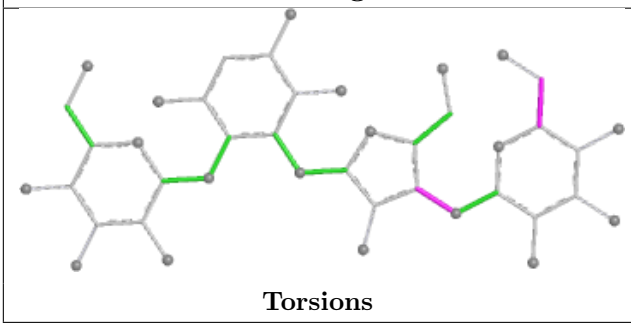
Ligand PAR A 1601



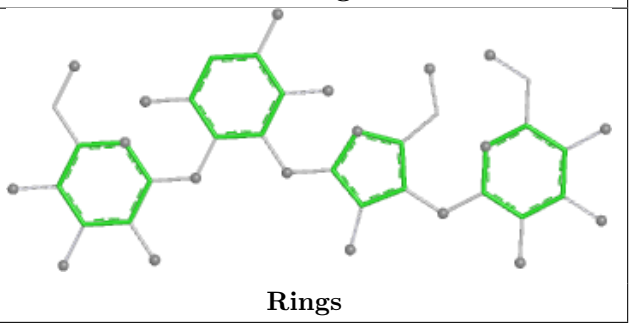
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1507/1507 (100%)	-0.16	35 (2%) 61 34	76, 119, 225, 386	0
2	B	234/256 (91%)	-0.02	3 (1%) 75 47	101, 165, 229, 356	0
3	C	206/239 (86%)	0.02	7 (3%) 48 26	95, 155, 226, 290	0
4	D	208/209 (99%)	0.08	10 (4%) 35 18	92, 136, 202, 274	0
5	E	150/162 (92%)	-0.20	2 (1%) 75 47	74, 112, 161, 210	0
6	F	101/101 (100%)	-0.24	2 (1%) 65 36	105, 146, 195, 230	0
7	G	155/156 (99%)	0.06	7 (4%) 38 19	99, 148, 210, 278	0
8	H	138/138 (100%)	-0.29	2 (1%) 73 45	70, 106, 154, 190	0
9	I	127/128 (99%)	-0.02	4 (3%) 51 28	93, 155, 204, 254	0
10	J	98/105 (93%)	0.37	5 (5%) 33 18	97, 180, 276, 303	0
11	K	119/129 (92%)	-0.09	4 (3%) 48 26	82, 125, 189, 228	0
12	L	124/132 (93%)	0.15	6 (4%) 35 18	73, 122, 194, 210	0
13	M	125/126 (99%)	0.14	8 (6%) 25 15	108, 155, 230, 324	0
14	N	60/61 (98%)	0.20	3 (5%) 34 18	107, 141, 201, 294	0
15	O	88/89 (98%)	0.05	2 (2%) 61 34	79, 128, 189, 237	0
16	P	83/88 (94%)	-0.12	1 (1%) 76 49	78, 110, 153, 255	0
17	Q	104/105 (99%)	-0.12	0 100 100	78, 111, 205, 265	0
18	R	73/88 (82%)	-0.14	1 (1%) 73 45	90, 131, 224, 248	0
19	S	80/93 (86%)	0.16	4 (5%) 34 18	114, 175, 217, 294	0
20	T	99/106 (93%)	0.15	4 (4%) 42 22	86, 117, 190, 214	0
21	V	24/27 (88%)	0.49	2 (8%) 17 11	107, 141, 190, 211	0
22	X	11/17 (64%)	0.90	0 100 100	135, 159, 256, 288	0
23	W	4/6 (66%)	0.58	1 (25%) 2 2	126, 126, 148, 152	0
All	All	3918/4068 (96%)	-0.05	113 (2%) 53 29	70, 131, 220, 386	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	S	2	PRO	8.3
19	S	3	ARG	7.4
1	A	1338	G	6.5
13	M	126	LYS	5.5
11	K	129	SER	5.5
7	G	33	ASP	5.2
2	B	16	HIS	4.9
11	K	128	ALA	4.8
13	M	124	PRO	4.7
12	L	89	ARG	4.5
4	D	116	GLN	4.4
1	A	1507	C	4.3
1	A	406	G	4.1
11	K	126	ARG	4.1
13	M	123	ALA	4.1
14	N	10	ALA	4.1
12	L	112	ASP	3.9
1	A	404	A	3.9
21	V	25	LYS	3.8
1	A	458	A	3.8
13	M	125	ARG	3.8
1	A	1009	G	3.8
1	A	402	G	3.7
1	A	1505	C	3.7
20	T	68	LYS	3.7
1	A	403	G	3.6
1	A	412	G	3.5
14	N	57	ARG	3.4
10	J	64	GLU	3.4
11	K	127	LYS	3.4
1	A	1195	C	3.3
1	A	1107	C	3.3
1	A	209	U	3.2
3	C	66	VAL	3.2
3	C	103	VAL	3.2
15	O	48	LYS	3.2
4	D	81	GLU	3.1
10	J	45	ARG	3.1
1	A	1064	U	3.1
4	D	31	CYS	3.0
19	S	5	LEU	3.0
3	C	68	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
7	G	32	ARG	2.9
12	L	47	LYS	2.9
1	A	457	G	2.9
9	I	110	GLU	2.9
1	A	802	G	2.9
4	D	3	ARG	2.8
3	C	143	GLU	2.8
9	I	115	GLY	2.8
4	D	30	LYS	2.8
1	A	413	C	2.7
1	A	1008	C	2.7
1	A	1104	U	2.7
15	O	54	ARG	2.7
3	C	76	VAL	2.7
1	A	409	G	2.7
20	T	64	ASP	2.7
1	A	456	C	2.7
1	A	1424	C	2.7
7	G	85	TYR	2.6
4	D	2	GLY	2.6
13	M	6	GLY	2.6
9	I	128	ARG	2.6
2	B	134	GLU	2.6
19	S	4	SER	2.6
1	A	1509	U	2.6
20	T	9	ASN	2.5
10	J	60	ARG	2.5
1	A	405	G	2.5
1	A	1339	C	2.5
5	E	85	GLY	2.5
1	A	459	G	2.5
1	A	416	U	2.5
8	H	18	ARG	2.5
7	G	8	GLU	2.4
21	V	24	ARG	2.4
13	M	32	GLU	2.4
10	J	43	ARG	2.4
10	J	46	ARG	2.4
6	F	89	MET	2.4
5	E	81	GLU	2.4
6	F	94	GLN	2.3
1	A	707	U	2.3

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Mol	Chain	Res	Type	RSRZ
23	W	4	A	2.3
2	B	203	GLY	2.3
12	L	26	ALA	2.3
1	A	1029	C	2.3
4	D	5	ILE	2.3
4	D	25	ARG	2.3
7	G	10	ARG	2.3
13	M	119	GLY	2.3
3	C	161	GLU	2.2
4	D	22	LYS	2.2
12	L	64	TYR	2.2
16	P	9	PHE	2.2
14	N	6	LEU	2.2
20	T	69	GLY	2.2
1	A	790	C	2.2
1	A	1425	U	2.2
12	L	119	LYS	2.1
13	M	8	GLU	2.1
1	A	980	G	2.1
3	C	102	ASN	2.1
7	G	26	PHE	2.1
7	G	5	ARG	2.1
4	D	42	GLN	2.0
1	A	462	G	2.0
1	A	831	G	2.0
9	I	120	ARG	2.0
8	H	4	ASP	2.0
18	R	31	LEU	2.0
1	A	408	A	2.0

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

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

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(Å^2)	Q<0.9
25	MG	A	1632	1/1	0.60	0.53	116,116,116,116	0
25	MG	A	1648	1/1	0.67	0.22	97,97,97,97	0
25	MG	A	1613	1/1	0.70	0.36	108,108,108,108	0
25	MG	A	1671	1/1	0.70	0.31	102,102,102,102	0
25	MG	A	1651	1/1	0.75	0.39	79,79,79,79	0
25	MG	A	1627	1/1	0.75	0.36	85,85,85,85	0
25	MG	A	1654	1/1	0.76	0.51	110,110,110,110	0
25	MG	A	1615	1/1	0.76	0.24	93,93,93,93	0
25	MG	A	1676	1/1	0.79	0.29	123,123,123,123	0
25	MG	A	1668	1/1	0.80	0.20	89,89,89,89	0
25	MG	A	1638	1/1	0.80	0.15	100,100,100,100	0
25	MG	A	1605	1/1	0.80	0.14	115,115,115,115	0
25	MG	A	1614	1/1	0.82	0.37	84,84,84,84	0
25	MG	A	1657	1/1	0.83	0.34	105,105,105,105	0
25	MG	A	1637	1/1	0.83	0.22	66,66,66,66	0
25	MG	K	201	1/1	0.83	0.52	89,89,89,89	0
25	MG	A	1603	1/1	0.84	0.32	96,96,96,96	0
25	MG	A	1682	1/1	0.84	0.20	85,85,85,85	0
25	MG	A	1626	1/1	0.84	0.31	73,73,73,73	0
25	MG	A	1681	1/1	0.85	0.21	100,100,100,100	0
25	MG	A	1609	1/1	0.85	0.43	93,93,93,93	0
25	MG	A	1687	1/1	0.85	0.31	93,93,93,93	0
25	MG	A	1691	1/1	0.85	0.32	104,104,104,104	0
25	MG	A	1669	1/1	0.85	0.29	91,91,91,91	0
25	MG	A	1630	1/1	0.86	0.48	86,86,86,86	0
25	MG	A	1616	1/1	0.86	0.34	68,68,68,68	0
25	MG	A	1620	1/1	0.86	0.40	89,89,89,89	0
25	MG	A	1679	1/1	0.86	0.07	87,87,87,87	0
25	MG	A	1680	1/1	0.86	0.20	88,88,88,88	0
25	MG	A	1666	1/1	0.87	0.22	109,109,109,109	0
25	MG	A	1649	1/1	0.87	0.34	88,88,88,88	0
25	MG	A	1645	1/1	0.88	0.21	73,73,73,73	0
25	MG	A	1631	1/1	0.88	0.26	89,89,89,89	0
25	MG	A	1639	1/1	0.89	0.38	94,94,94,94	0
25	MG	A	1663	1/1	0.89	0.19	91,91,91,91	0
25	MG	A	1610	1/1	0.90	0.05	99,99,99,99	0
25	MG	A	1674	1/1	0.90	0.27	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	MG	A	1635	1/1	0.91	0.22	89,89,89,89	0
25	MG	A	1622	1/1	0.91	0.24	67,67,67,67	0
25	MG	A	1690	1/1	0.91	0.18	83,83,83,83	0
25	MG	A	1608	1/1	0.91	0.11	89,89,89,89	0
25	MG	A	1634	1/1	0.91	0.23	85,85,85,85	0
25	MG	A	1662	1/1	0.92	0.10	105,105,105,105	0
25	MG	A	1678	1/1	0.92	0.21	114,114,114,114	0
25	MG	A	1606	1/1	0.92	0.29	81,81,81,81	0
24	PAR	A	1601	42/42	0.92	0.14	101,107,113,115	0
25	MG	A	1650	1/1	0.92	0.19	69,69,69,69	0
25	MG	A	1617	1/1	0.92	0.35	69,69,69,69	0
25	MG	A	1670	1/1	0.92	0.14	111,111,111,111	0
25	MG	A	1689	1/1	0.92	0.11	111,111,111,111	0
25	MG	A	1633	1/1	0.92	0.20	87,87,87,87	0
25	MG	A	1673	1/1	0.92	0.24	104,104,104,104	0
25	MG	E	201	1/1	0.92	0.31	69,69,69,69	0
25	MG	A	1619	1/1	0.92	0.31	66,66,66,66	0
25	MG	A	1643	1/1	0.93	0.42	67,67,67,67	0
25	MG	A	1629	1/1	0.93	0.21	86,86,86,86	0
25	MG	A	1647	1/1	0.93	0.21	69,69,69,69	0
25	MG	A	1672	1/1	0.93	0.12	89,89,89,89	0
25	MG	A	1652	1/1	0.93	0.45	72,72,72,72	0
25	MG	A	1625	1/1	0.93	0.07	85,85,85,85	0
25	MG	A	1628	1/1	0.94	0.10	100,100,100,100	0
25	MG	A	1611	1/1	0.94	0.32	94,94,94,94	0
25	MG	A	1686	1/1	0.94	0.28	90,90,90,90	0
25	MG	A	1602	1/1	0.94	0.07	105,105,105,105	0
25	MG	A	1664	1/1	0.94	0.08	95,95,95,95	0
25	MG	A	1640	1/1	0.94	0.10	99,99,99,99	0
25	MG	A	1618	1/1	0.94	0.30	71,71,71,71	0
25	MG	A	1644	1/1	0.94	0.43	73,73,73,73	0
25	MG	J	201	1/1	0.94	0.18	96,96,96,96	0
25	MG	A	1636	1/1	0.94	0.17	83,83,83,83	0
25	MG	A	1685	1/1	0.95	0.14	96,96,96,96	0
25	MG	A	1661	1/1	0.95	0.32	107,107,107,107	0
25	MG	A	1641	1/1	0.95	0.15	109,109,109,109	0
25	MG	A	1688	1/1	0.95	0.13	80,80,80,80	0
25	MG	A	1607	1/1	0.95	0.19	95,95,95,95	0
25	MG	A	1683	1/1	0.96	0.20	78,78,78,78	0
25	MG	A	1684	1/1	0.96	0.16	107,107,107,107	0
25	MG	A	1623	1/1	0.96	0.23	87,87,87,87	0
25	MG	A	1624	1/1	0.96	0.27	67,67,67,67	0

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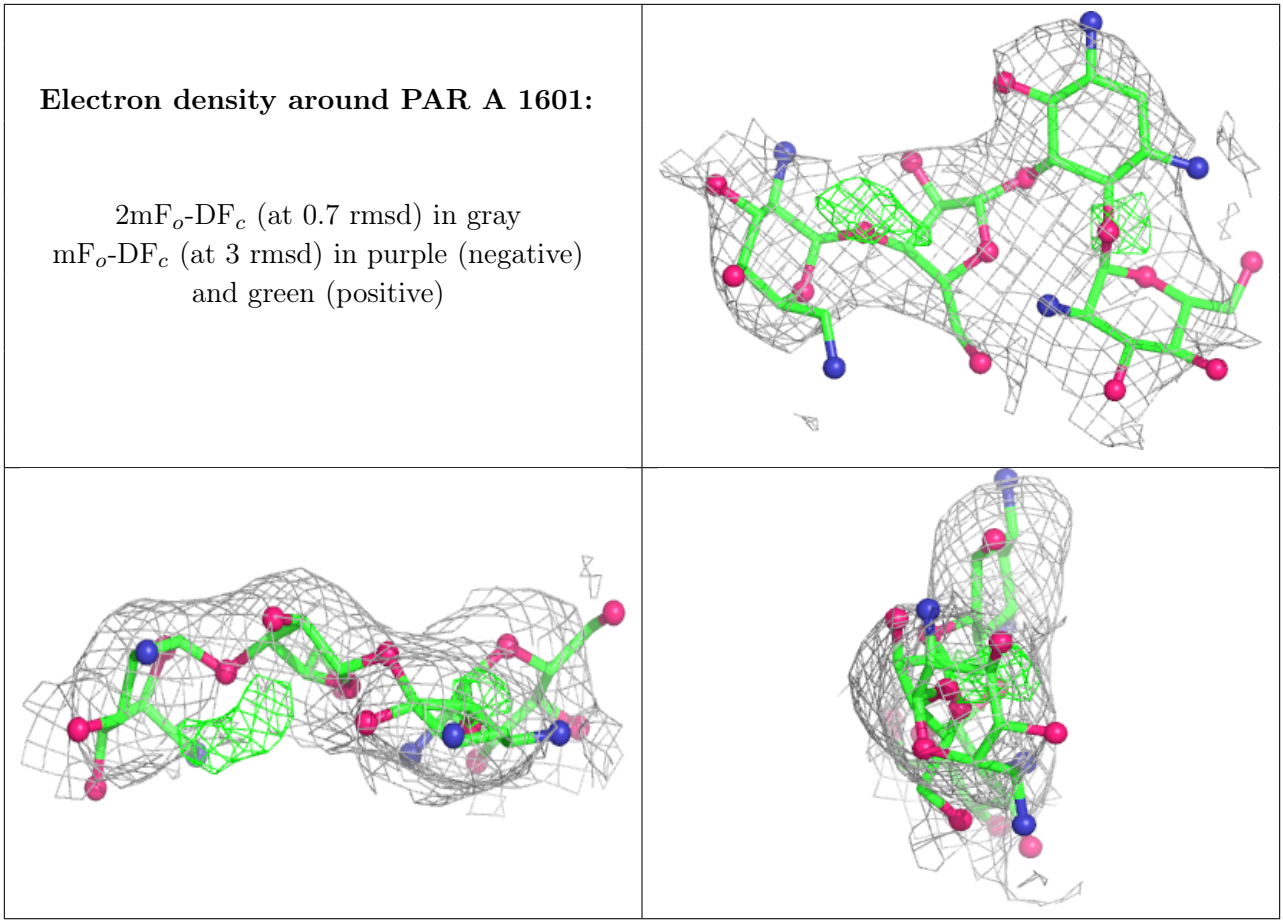
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	MG	A	1675	1/1	0.96	0.17	106,106,106,106	0
25	MG	A	1612	1/1	0.96	0.22	101,101,101,101	0
25	MG	A	1677	1/1	0.96	0.13	88,88,88,88	0
25	MG	A	1656	1/1	0.96	0.30	80,80,80,80	0
25	MG	A	1621	1/1	0.96	0.13	81,81,81,81	0
25	MG	A	1658	1/1	0.96	0.15	110,110,110,110	0
25	MG	A	1642	1/1	0.96	0.12	89,89,89,89	0
25	MG	J	202	1/1	0.96	0.10	97,97,97,97	0
25	MG	A	1604	1/1	0.96	0.26	86,86,86,86	0
25	MG	A	1665	1/1	0.97	0.35	71,71,71,71	0
25	MG	A	1655	1/1	0.97	0.14	67,67,67,67	0
25	MG	A	1646	1/1	0.97	0.11	70,70,70,70	0
25	MG	A	1667	1/1	0.98	0.08	140,140,140,140	0
25	MG	A	1660	1/1	0.99	0.07	86,86,86,86	0
25	MG	A	1653	1/1	0.99	0.10	84,84,84,84	0
25	MG	A	1659	1/1	0.99	0.05	77,77,77,77	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 1601:

$2mF_o$-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.