



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 06:59 PM EDT

PDB ID : 6WAN
Title : Structure of Acinetobacter baumannii Cap4 SAVED/CARF-domain containing receptor with the cyclic trinucleotide 3'3'3'-cAAA
Authors : Lowey, B.; Whiteley, A.T.; Keszei, A.F.A.; Morehouse, B.R.; Antine, S.P.; Cabrera, V.; Schwede, F.; Mekalanos, J.J.; Shao, S.; Lee, A.S.Y.; Kranzusch, P.J.
Deposited on : 2020-03-25
Resolution : 2.40 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

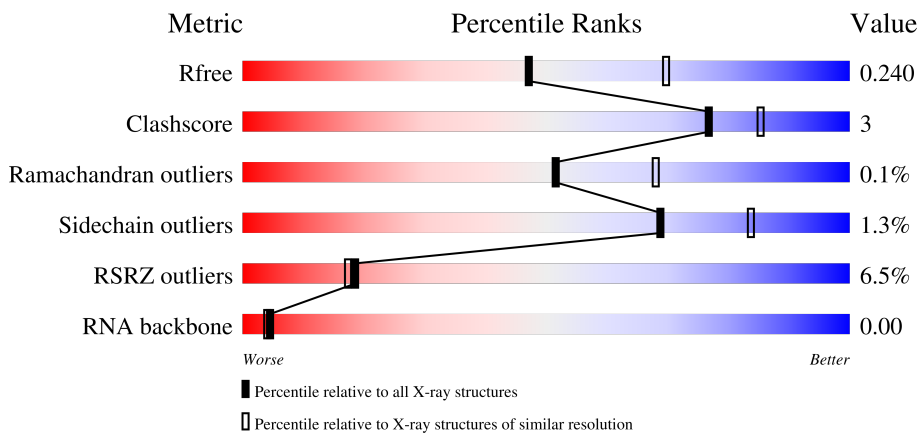
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)
RNA backbone	3102	1174 (2.80-2.00)

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	462	
1	B	462	
1	C	462	

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Mol	Chain	Length	Quality of chain
1	D	462	<p>8% 85% 9% 6%</p>
1	E	462	<p>3% 85% 10% 5%</p>
1	F	462	<p>10% 81% 8% 10%</p>
2	G	3	<p>33% 33% 33%</p>
2	H	3	<p>33% 33% 33%</p>
2	I	3	<p>33% 67%</p>
2	J	3	<p>33% 67%</p>
2	K	3	<p>33% 33% 33%</p>
2	L	3	<p>33% 67%</p>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 21812 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 protein called SAVED domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	438	Total 3518	C 2245	N 593	O 669	S 11	0	0	0
1	B	438	Total 3518	C 2245	N 593	O 669	S 11	0	0	0
1	C	438	Total 3518	C 2245	N 593	O 669	S 11	0	0	0
1	D	435	Total 3489	C 2223	N 590	O 665	S 11	0	0	0
1	E	437	Total 3513	C 2242	N 592	O 668	S 11	0	0	0
1	F	415	Total 3338	C 2129	N 563	O 636	S 10	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP C0VHC9
B	1	SER	-	expression tag	UNP C0VHC9
C	1	SER	-	expression tag	UNP C0VHC9
D	1	SER	-	expression tag	UNP C0VHC9
E	1	SER	-	expression tag	UNP C0VHC9
F	1	SER	-	expression tag	UNP C0VHC9

- Molecule 2 is a RNA chain called Cyclic RNA (R(P*AP*AP*A)).

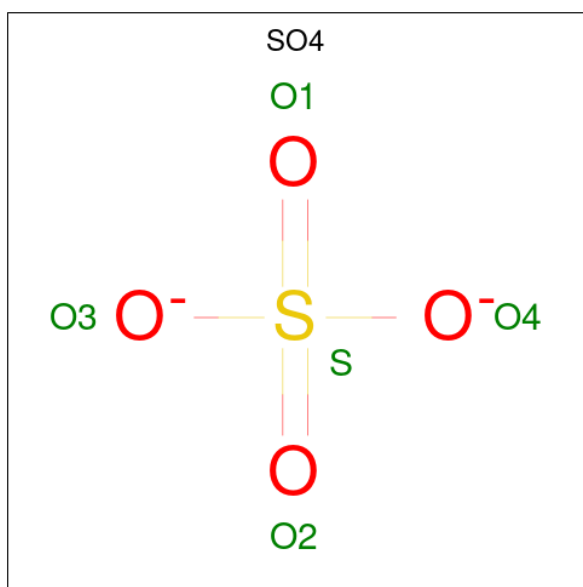
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	G	3	Total 66	C 30	N 15	O 18	P 3	0	0	0
2	H	3	Total 66	C 30	N 15	O 18	P 3	0	0	0
2	I	3	Total 66	C 30	N 15	O 18	P 3	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	J	3	Total	C	N	O	P	0	0	0
			66	30	15	18	3			
2	K	3	Total	C	N	O	P	0	0	0
			66	30	15	18	3			
2	L	3	Total	C	N	O	P	0	0	0
			66	30	15	18	3			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O S	0	0
			5	4 1		
3	B	1	Total	O S	0	0
			5	4 1		
3	C	1	Total	O S	0	0
			5	4 1		
3	D	1	Total	O S	0	0
			5	4 1		
3	E	1	Total	O S	0	0
			5	4 1		
3	F	1	Total	O S	0	0
			5	4 1		

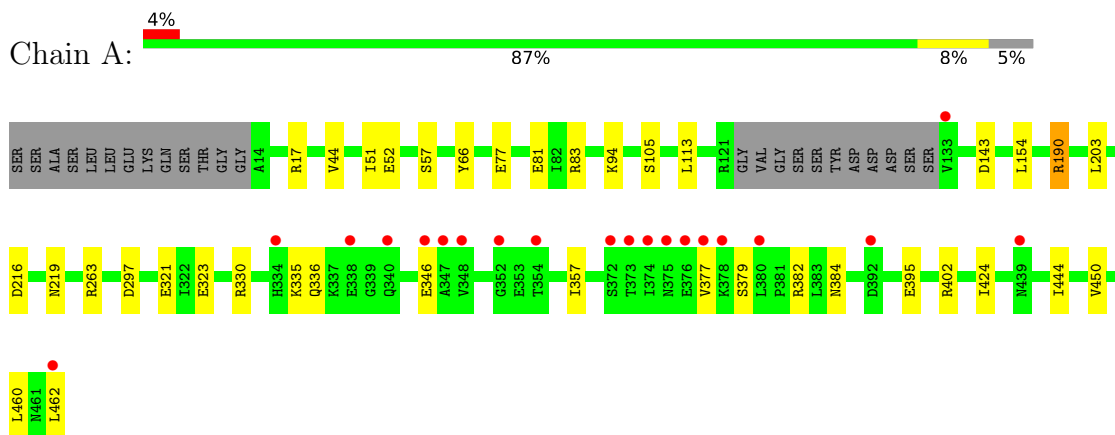
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	84	Total O 84 84	0	0
4	B	76	Total O 76 76	0	0
4	C	90	Total O 90 90	0	0
4	D	83	Total O 83 83	0	0
4	E	81	Total O 81 81	0	0
4	F	71	Total O 71 71	0	0
4	H	1	Total O 1 1	0	0
4	J	2	Total O 2 2	0	0
4	K	3	Total O 3 3	0	0
4	L	1	Total O 1 1	0	0

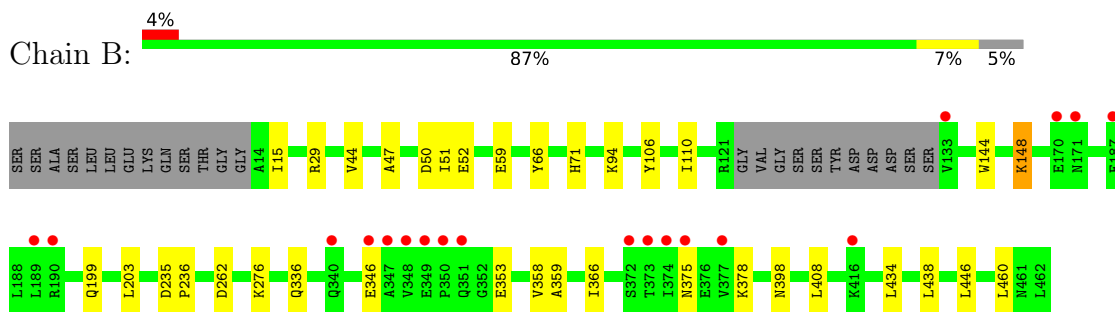
3 Residue-property plots [i](#)

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.

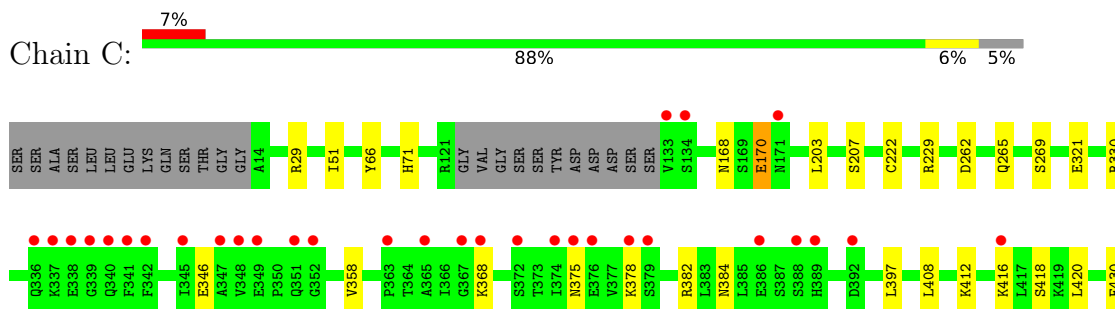
- Molecule 1: SAVED domain-containing protein



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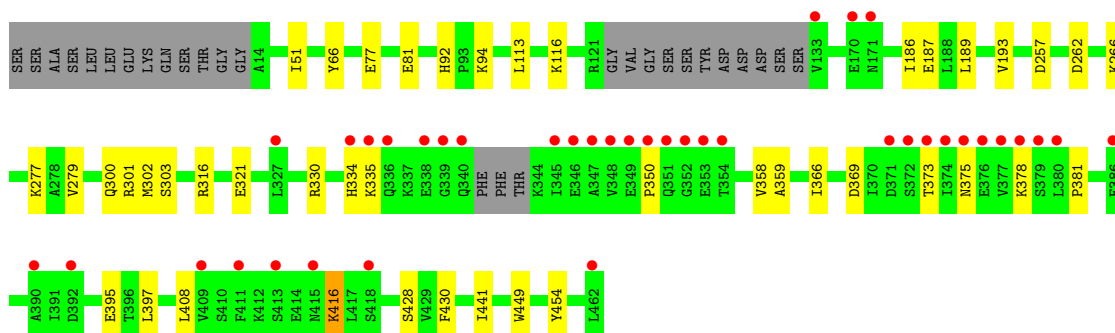
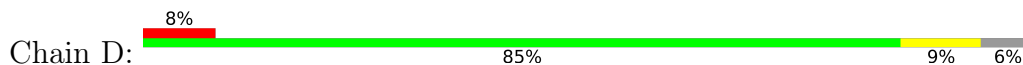


- Molecule 1: SAVED domain-containing protein

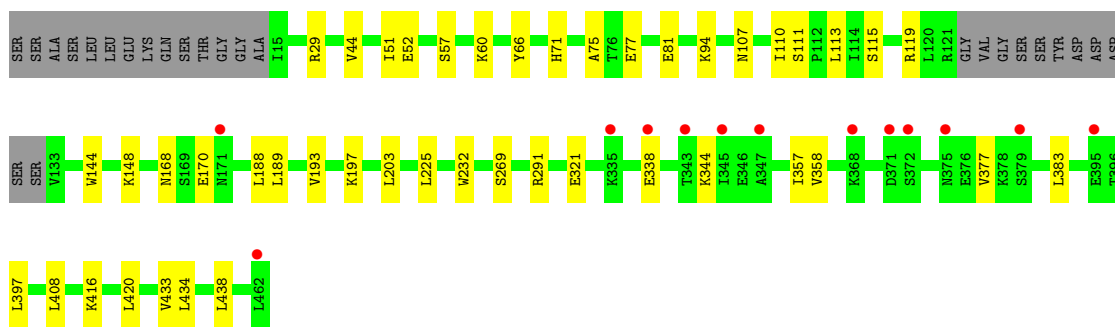
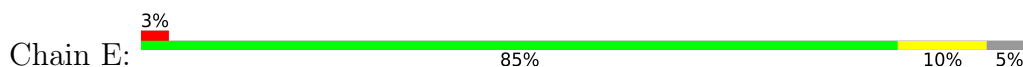




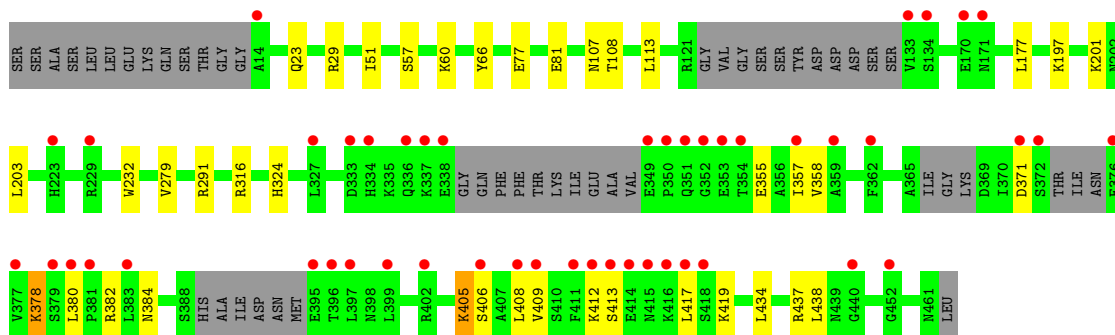
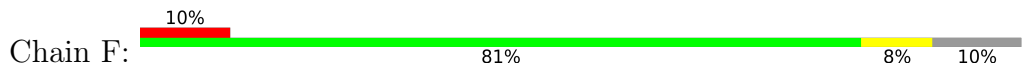
- Molecule 1: SAVED domain-containing protein



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- Molecule 1: SAVED domain-containing protein



- Molecule 2: Cyclic RNA (R(P*AP*AP*A))





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- Molecule 2: Cyclic RNA (R(P*AP*AP*A))



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.50Å 111.18Å 163.75Å 90.00° 100.36° 90.00°	Depositor
Resolution (Å)	38.80 – 2.40 38.80 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.9 (38.80-2.40) 91.5 (38.80-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.69 (at 2.39Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.208 , 0.240 0.208 , 0.240	Depositor DCC
R_{free} test set	2000 reflections (1.38%)	wwPDB-VP
Wilson B-factor (Å ²)	44.4	Xtrriage
Anisotropy	0.355	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21812	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0/3593	0.41	0/4856
1	B	0.24	0/3593	0.42	0/4856
1	C	0.25	0/3593	0.42	0/4856
1	D	0.24	0/3561	0.42	0/4811
1	E	0.24	0/3588	0.41	0/4849
1	F	0.24	0/3406	0.42	0/4599
2	G	7.33	34/74 (45.9%)	7.50	35/113 (31.0%)
2	H	7.33	34/74 (45.9%)	7.51	34/113 (30.1%)
2	I	7.27	34/74 (45.9%)	7.68	38/113 (33.6%)
2	J	7.34	34/74 (45.9%)	7.85	38/113 (33.6%)
2	K	7.22	32/74 (43.2%)	7.60	33/113 (29.2%)
2	L	7.32	34/74 (45.9%)	7.86	35/113 (31.0%)
All	All	1.07	202/21778 (0.9%)	1.23	213/29505 (0.7%)

All (202) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1	A	N7-C5	21.29	1.52	1.39
2	L	1	A	N7-C5	20.93	1.51	1.39
2	J	1	A	N7-C5	20.61	1.51	1.39
2	H	1	A	N7-C5	20.32	1.51	1.39
2	K	1	A	N7-C5	20.13	1.51	1.39
2	G	2	A	N7-C5	19.86	1.51	1.39
2	G	2	A	N9-C4	-18.90	1.26	1.37
2	J	1	A	N9-C4	-18.68	1.26	1.37
2	L	1	A	N9-C4	-18.65	1.26	1.37
2	L	1	A	C6-N6	18.56	1.48	1.33
2	H	1	A	N9-C4	-18.40	1.26	1.37
2	I	1	A	C6-N6	18.25	1.48	1.33
2	H	3	A	C6-N6	18.00	1.48	1.33
2	J	3	A	C6-N6	17.98	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	A	C6-N6	17.91	1.48	1.33
2	J	1	A	C6-N6	17.89	1.48	1.33
2	I	1	A	N9-C4	-17.85	1.27	1.37
2	K	1	A	N9-C4	-17.83	1.27	1.37
2	K	1	A	C6-N6	17.80	1.48	1.33
2	K	3	A	C6-N6	17.74	1.48	1.33
2	G	2	A	C6-N6	17.46	1.48	1.33
2	L	3	A	C6-N6	17.44	1.48	1.33
2	I	3	A	C6-N6	17.43	1.47	1.33
2	G	1	A	C6-N6	17.29	1.47	1.33
2	J	2	A	C6-N6	14.93	1.45	1.33
2	H	2	A	C8-N7	14.78	1.41	1.31
2	K	2	A	C8-N7	14.68	1.41	1.31
2	L	2	A	C6-N6	14.52	1.45	1.33
2	L	2	A	C8-N7	14.24	1.41	1.31
2	G	3	A	C8-N7	14.07	1.41	1.31
2	I	2	A	C8-N7	14.03	1.41	1.31
2	G	3	A	C6-N6	13.93	1.45	1.33
2	I	2	A	C6-N6	13.86	1.45	1.33
2	H	2	A	C6-N6	13.62	1.44	1.33
2	J	2	A	C8-N7	13.52	1.41	1.31
2	G	3	A	C6-N1	-13.33	1.26	1.35
2	J	1	A	N9-C8	-13.30	1.27	1.37
2	K	2	A	C6-N6	13.29	1.44	1.33
2	G	2	A	N9-C8	-13.16	1.27	1.37
2	H	3	A	N7-C5	13.11	1.47	1.39
2	H	2	A	C6-N1	-13.01	1.26	1.35
2	I	1	A	N9-C8	-13.00	1.27	1.37
2	J	2	A	C6-N1	-12.95	1.26	1.35
2	K	1	A	N9-C8	-12.93	1.27	1.37
2	H	1	A	N9-C8	-12.91	1.27	1.37
2	K	3	A	N7-C5	12.90	1.47	1.39
2	K	2	A	C6-N1	-12.81	1.26	1.35
2	L	1	A	N9-C8	-12.68	1.27	1.37
2	I	2	A	C6-N1	-12.67	1.26	1.35
2	L	2	A	C6-N1	-12.56	1.26	1.35
2	L	3	A	N7-C5	12.38	1.46	1.39
2	G	1	A	N7-C5	12.24	1.46	1.39
2	I	3	A	N7-C5	12.24	1.46	1.39
2	J	3	A	N7-C5	12.09	1.46	1.39
2	J	2	A	N1-C2	-11.99	1.23	1.34
2	G	3	A	N1-C2	-11.91	1.23	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	2	A	N1-C2	-11.69	1.23	1.34
2	L	2	A	N1-C2	-11.63	1.23	1.34
2	I	2	A	N1-C2	-11.42	1.24	1.34
2	K	2	A	N1-C2	-11.16	1.24	1.34
2	J	3	A	P-O5'	11.08	1.70	1.59
2	H	1	A	C8-N7	10.74	1.39	1.31
2	K	1	A	C8-N7	10.19	1.38	1.31
2	L	3	A	P-O5'	10.15	1.69	1.59
2	G	2	A	C8-N7	10.02	1.38	1.31
2	I	1	A	C8-N7	9.90	1.38	1.31
2	G	1	A	P-O5'	9.82	1.69	1.59
2	I	3	A	P-O5'	9.77	1.69	1.59
2	L	1	A	C8-N7	9.61	1.38	1.31
2	H	3	A	P-O5'	9.49	1.69	1.59
2	K	2	A	C3'-C2'	-9.03	1.42	1.52
2	K	3	A	P-O5'	8.96	1.68	1.59
2	J	2	A	C3'-C2'	-8.95	1.43	1.52
2	J	1	A	C8-N7	8.79	1.37	1.31
2	G	1	A	C8-N7	8.75	1.37	1.31
2	I	2	A	C3'-C2'	-8.75	1.43	1.52
2	K	3	A	C8-N7	8.71	1.37	1.31
2	J	2	A	O4'-C1'	8.69	1.52	1.41
2	H	2	A	C3'-C2'	-8.65	1.43	1.52
2	I	3	A	O4'-C1'	8.65	1.52	1.41
2	G	3	A	C3'-C2'	-8.58	1.43	1.52
2	H	3	A	O4'-C1'	8.53	1.52	1.41
2	G	3	A	O4'-C1'	8.36	1.52	1.41
2	L	2	A	O4'-C1'	8.34	1.52	1.41
2	J	3	A	O4'-C1'	8.32	1.52	1.41
2	I	2	A	O4'-C1'	8.30	1.52	1.41
2	L	3	A	O4'-C1'	8.28	1.52	1.41
2	G	2	A	C3'-C2'	-8.27	1.43	1.52
2	J	1	A	P-O5'	8.23	1.68	1.59
2	H	1	A	C3'-C2'	-8.19	1.43	1.52
2	J	2	A	C5-C4	8.15	1.44	1.38
2	L	1	A	C3'-C2'	-8.09	1.43	1.52
2	I	3	A	C8-N7	8.08	1.37	1.31
2	H	2	A	O4'-C1'	8.05	1.52	1.41
2	L	1	A	P-O5'	7.97	1.67	1.59
2	L	2	A	C5-C4	7.96	1.44	1.38
2	K	3	A	O4'-C1'	7.94	1.51	1.41
2	K	2	A	O4'-C1'	7.93	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	A	N9-C4	-7.87	1.33	1.37
2	J	1	A	C3'-C2'	-7.86	1.44	1.52
2	I	1	A	C3'-C2'	-7.82	1.44	1.52
2	G	3	A	N9-C8	7.76	1.44	1.37
2	I	2	A	C5-C4	7.74	1.44	1.38
2	L	3	A	C8-N7	7.74	1.36	1.31
2	I	2	A	N9-C8	7.73	1.44	1.37
2	I	1	A	P-O5'	7.72	1.67	1.59
2	H	1	A	P-O5'	7.71	1.67	1.59
2	H	2	A	N9-C8	7.69	1.44	1.37
2	L	2	A	C3'-C2'	-7.69	1.44	1.52
2	K	2	A	N9-C8	7.67	1.43	1.37
2	K	1	A	P-O5'	7.66	1.67	1.59
2	G	1	A	O4'-C1'	7.63	1.51	1.41
2	K	1	A	C3'-C2'	-7.59	1.44	1.52
2	G	1	A	C4'-C3'	-7.55	1.44	1.53
2	L	2	A	N9-C8	7.51	1.43	1.37
2	K	3	A	N9-C4	-7.51	1.33	1.37
2	J	3	A	C4'-C3'	-7.47	1.45	1.53
2	G	1	A	C3'-C2'	-7.45	1.44	1.52
2	K	3	A	N9-C8	-7.43	1.31	1.37
2	K	3	A	C3'-C2'	-7.38	1.44	1.52
2	H	2	A	C5-C4	7.37	1.44	1.38
2	G	3	A	C5-C4	7.35	1.43	1.38
2	G	1	A	O3'-P	7.32	1.70	1.61
2	H	3	A	C8-N7	7.28	1.36	1.31
2	G	3	A	C4'-O4'	7.22	1.54	1.45
2	I	2	A	C4'-O4'	7.19	1.54	1.45
2	I	3	A	N9-C4	-7.18	1.33	1.37
2	G	1	A	N9-C8	-7.16	1.32	1.37
2	J	2	A	N9-C8	7.16	1.43	1.37
2	I	3	A	N9-C8	-7.13	1.32	1.37
2	L	2	A	C4'-O4'	7.12	1.54	1.45
2	K	2	A	C4'-O4'	7.08	1.54	1.45
2	G	2	A	P-O5'	7.07	1.66	1.59
2	J	3	A	C8-N7	7.05	1.36	1.31
2	H	3	A	C4'-C3'	-7.03	1.45	1.53
2	I	1	A	C5-C4	7.01	1.43	1.38
2	H	3	A	N9-C8	-7.00	1.32	1.37
2	L	3	A	C3'-C2'	-6.99	1.45	1.52
2	H	3	A	C3'-C2'	-6.96	1.45	1.52
2	H	2	A	C2-N3	-6.94	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	3	A	C4'-O4'	6.92	1.54	1.45
2	K	3	A	C4'-C3'	-6.87	1.45	1.53
2	H	2	A	C4'-O4'	6.86	1.54	1.45
2	G	2	A	C5-C4	6.84	1.43	1.38
2	L	2	A	C2-N3	-6.84	1.27	1.33
2	I	3	A	C4'-O4'	6.83	1.54	1.45
2	J	1	A	O3'-P	6.83	1.69	1.61
2	H	1	A	C5-C4	6.77	1.43	1.38
2	J	2	A	C4'-O4'	6.76	1.54	1.45
2	L	1	A	O3'-P	6.76	1.69	1.61
2	J	3	A	N9-C8	-6.73	1.32	1.37
2	H	3	A	N9-C4	-6.71	1.33	1.37
2	J	2	A	C2-N3	-6.71	1.27	1.33
2	L	3	A	C4'-C3'	-6.68	1.45	1.53
2	G	2	A	O3'-P	6.67	1.69	1.61
2	G	3	A	C2-N3	-6.65	1.27	1.33
2	K	1	A	C5-C4	6.64	1.43	1.38
2	H	3	A	C4'-O4'	6.60	1.54	1.45
2	I	2	A	C2-N3	-6.59	1.27	1.33
2	K	3	A	C4'-O4'	6.59	1.54	1.45
2	K	1	A	O3'-P	6.58	1.69	1.61
2	H	1	A	O3'-P	6.55	1.69	1.61
2	K	2	A	C5-C4	6.50	1.43	1.38
2	J	3	A	C3'-C2'	-6.45	1.45	1.52
2	L	3	A	N9-C4	-6.43	1.33	1.37
2	K	2	A	C2-N3	-6.36	1.27	1.33
2	L	3	A	N9-C8	-6.29	1.32	1.37
2	J	1	A	C5-C4	6.16	1.43	1.38
2	I	3	A	C4'-C3'	-6.13	1.46	1.53
2	G	1	A	C4'-O4'	6.13	1.53	1.45
2	I	1	A	O3'-P	6.08	1.68	1.61
2	I	3	A	C3'-C2'	-6.07	1.46	1.52
2	J	1	A	O4'-C1'	6.00	1.49	1.41
2	J	3	A	N9-C4	-5.90	1.34	1.37
2	J	3	A	C4'-O4'	5.87	1.53	1.45
2	H	3	A	C5-C4	5.80	1.42	1.38
2	L	1	A	C5-C4	5.74	1.42	1.38
2	I	1	A	O4'-C1'	5.72	1.49	1.41
2	G	1	A	C2'-C1'	-5.68	1.47	1.53
2	J	2	A	C4'-C3'	-5.62	1.47	1.52
2	I	1	A	N3-C4	-5.54	1.31	1.34
2	H	2	A	C4'-C3'	-5.49	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	2	A	C4'-C3'	-5.47	1.47	1.52
2	I	2	A	C4'-C3'	-5.45	1.47	1.52
2	L	2	A	C5-C6	5.44	1.46	1.41
2	G	3	A	C4'-C3'	-5.34	1.47	1.52
2	H	1	A	O4'-C1'	5.34	1.48	1.41
2	L	1	A	O4'-C1'	5.32	1.48	1.41
2	L	1	A	N3-C4	-5.31	1.31	1.34
2	J	2	A	P-O5'	5.26	1.65	1.59
2	L	3	A	C2'-C1'	-5.26	1.47	1.53
2	I	2	A	C5-C6	5.22	1.45	1.41
2	K	1	A	O4'-C1'	5.19	1.48	1.41
2	J	2	A	C5-C6	5.18	1.45	1.41
2	L	3	A	C5-C4	5.18	1.42	1.38
2	J	3	A	C5-C4	5.18	1.42	1.38
2	H	2	A	P-O5'	5.15	1.64	1.59
2	K	1	A	N3-C4	-5.14	1.31	1.34
2	G	3	A	P-O5'	5.14	1.64	1.59
2	I	3	A	C5-C4	5.12	1.42	1.38
2	G	2	A	N3-C4	-5.11	1.31	1.34
2	H	2	A	C5-C6	5.03	1.45	1.41

All (213) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	1	A	C8-N9-C4	44.37	123.55	105.80
2	J	1	A	C8-N9-C4	42.73	122.89	105.80
2	I	1	A	C8-N9-C4	40.98	122.19	105.80
2	K	1	A	C8-N9-C4	39.78	121.71	105.80
2	H	1	A	C8-N9-C4	38.65	121.26	105.80
2	G	2	A	C8-N9-C4	38.03	121.01	105.80
2	K	3	A	C8-N9-C4	21.59	114.44	105.80
2	I	3	A	C8-N9-C4	20.86	114.14	105.80
2	L	3	A	C8-N9-C4	20.68	114.07	105.80
2	J	3	A	C2-N3-C4	20.38	120.79	110.60
2	G	1	A	C8-N9-C4	20.28	113.91	105.80
2	H	3	A	C2-N3-C4	20.23	120.71	110.60
2	H	3	A	C8-N9-C4	20.11	113.84	105.80
2	J	3	A	C8-N9-C4	20.07	113.83	105.80
2	K	3	A	C2-N3-C4	19.77	120.49	110.60
2	G	1	A	C2-N3-C4	19.74	120.47	110.60
2	L	3	A	C2-N3-C4	19.66	120.43	110.60
2	I	3	A	C2-N3-C4	19.61	120.40	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	1	A	N7-C8-N9	-19.33	104.14	113.80
2	H	1	A	C2-N3-C4	19.27	120.23	110.60
2	K	1	A	C2-N3-C4	18.86	120.03	110.60
2	L	1	A	C2-N3-C4	18.67	119.94	110.60
2	G	2	A	C2-N3-C4	18.28	119.74	110.60
2	J	1	A	N7-C8-N9	-18.27	104.66	113.80
2	I	1	A	C2-N3-C4	18.23	119.72	110.60
2	J	1	A	C2-N3-C4	17.56	119.38	110.60
2	I	1	A	N7-C8-N9	-17.19	105.21	113.80
2	K	1	A	N7-C8-N9	-16.83	105.38	113.80
2	L	2	A	C2-N3-C4	16.55	118.88	110.60
2	J	2	A	C2-N3-C4	16.11	118.66	110.60
2	H	1	A	N7-C8-N9	-16.02	105.79	113.80
2	G	3	A	C2-N3-C4	16.01	118.61	110.60
2	I	2	A	C2-N3-C4	16.00	118.60	110.60
2	L	1	A	N1-C2-N3	-15.94	121.33	129.30
2	K	2	A	C2-N3-C4	15.94	118.57	110.60
2	H	2	A	C2-N3-C4	15.83	118.52	110.60
2	J	1	A	N1-C2-N3	-15.72	121.44	129.30
2	G	3	A	N7-C8-N9	-15.51	106.05	113.80
2	G	2	A	N1-C2-N3	-15.39	121.60	129.30
2	I	1	A	N1-C2-N3	-15.38	121.61	129.30
2	H	1	A	N1-C2-N3	-15.15	121.73	129.30
2	H	2	A	N7-C8-N9	-15.11	106.25	113.80
2	K	1	A	N1-C2-N3	-14.91	121.84	129.30
2	K	2	A	N7-C8-N9	-14.65	106.47	113.80
2	G	2	A	N7-C8-N9	-14.64	106.48	113.80
2	L	2	A	N7-C8-N9	-14.30	106.65	113.80
2	J	3	A	C1'-O4'-C4'	-14.29	98.47	109.90
2	I	2	A	N7-C8-N9	-14.28	106.66	113.80
2	J	2	A	N7-C8-N9	-14.09	106.76	113.80
2	I	1	A	C4-C5-N7	-13.76	103.82	110.70
2	K	3	A	N1-C2-N3	-13.71	122.44	129.30
2	G	3	A	N3-C4-C5	-13.67	117.23	126.80
2	G	1	A	N1-C2-N3	-13.55	122.52	129.30
2	H	1	A	C4-C5-N7	-13.51	103.95	110.70
2	H	3	A	N1-C2-N3	-13.50	122.55	129.30
2	J	1	A	C4-C5-N7	-13.49	103.95	110.70
2	L	2	A	N3-C4-C5	-13.35	117.46	126.80
2	K	1	A	C4-C5-N7	-13.34	104.03	110.70
2	L	3	A	C1'-O4'-C4'	-13.32	99.24	109.90
2	J	2	A	N3-C4-C5	-13.27	117.51	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	3	A	N1-C2-N3	-13.12	122.74	129.30
2	I	3	A	N1-C2-N3	-13.11	122.75	129.30
2	H	2	A	N3-C4-C5	-13.10	117.63	126.80
2	J	3	A	N3-C4-C5	-13.05	117.66	126.80
2	K	2	A	N3-C4-C5	-12.81	117.83	126.80
2	H	2	A	C8-N9-C4	12.75	110.90	105.80
2	G	2	A	C4-C5-N7	-12.62	104.39	110.70
2	G	3	A	C8-N9-C4	12.61	110.85	105.80
2	J	3	A	N1-C2-N3	-12.61	122.99	129.30
2	I	2	A	N3-C4-C5	-12.50	118.05	126.80
2	L	1	A	C4-C5-N7	-12.33	104.53	110.70
2	G	3	A	N3-C4-N9	12.26	137.21	127.40
2	I	2	A	C1'-O4'-C4'	-12.19	100.15	109.90
2	H	3	A	C4-C5-N7	-11.97	104.71	110.70
2	I	3	A	N3-C4-C5	-11.81	118.53	126.80
2	L	2	A	C8-N9-C4	11.62	110.45	105.80
2	H	3	A	N3-C4-C5	-11.60	118.68	126.80
2	L	3	A	N3-C4-C5	-11.59	118.69	126.80
2	G	3	A	C1'-O4'-C4'	-11.59	100.63	109.90
2	H	2	A	N3-C4-N9	11.54	136.63	127.40
2	K	2	A	C1'-O4'-C4'	-11.51	100.69	109.90
2	K	3	A	N7-C8-N9	-11.44	108.08	113.80
2	I	3	A	N7-C8-N9	-11.37	108.12	113.80
2	L	2	A	N3-C4-N9	11.30	136.44	127.40
2	J	3	A	N3-C4-N9	11.27	136.41	127.40
2	I	3	A	C1'-O4'-C4'	-11.25	100.90	109.90
2	K	2	A	C8-N9-C4	11.17	110.27	105.80
2	I	3	A	C4-C5-N7	-11.14	105.13	110.70
2	J	3	A	C4-C5-N7	-11.13	105.14	110.70
2	J	3	A	N7-C8-N9	-11.10	108.25	113.80
2	G	1	A	N3-C4-C5	-11.08	119.04	126.80
2	H	3	A	C1'-O4'-C4'	-11.05	101.06	109.90
2	J	2	A	C8-N9-C4	11.02	110.21	105.80
2	I	2	A	C8-N9-C4	10.93	110.17	105.80
2	K	3	A	N3-C4-C5	-10.92	119.16	126.80
2	K	3	A	C4-C5-N7	-10.87	105.26	110.70
2	J	2	A	C1'-O4'-C4'	-10.85	101.22	109.90
2	L	3	A	N7-C8-N9	-10.83	108.38	113.80
2	H	2	A	C1'-O4'-C4'	-10.82	101.24	109.90
2	J	2	A	N3-C4-N9	10.80	136.04	127.40
2	H	3	A	N7-C8-N9	-10.66	108.47	113.80
2	I	1	A	C6-C5-N7	10.63	139.74	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	A	N7-C8-N9	-10.62	108.49	113.80
2	K	3	A	C1'-O4'-C4'	-10.61	101.42	109.90
2	L	1	A	N3-C4-N9	10.60	135.88	127.40
2	L	2	A	C1'-O4'-C4'	-10.60	101.42	109.90
2	G	1	A	C4-C5-N7	-10.50	105.45	110.70
2	G	1	A	C1'-O4'-C4'	-10.48	101.52	109.90
2	L	3	A	N3-C4-N9	10.46	135.77	127.40
2	K	2	A	N3-C4-N9	10.33	135.66	127.40
2	K	1	A	N3-C4-N9	10.29	135.63	127.40
2	J	1	A	C6-C5-N7	10.18	139.42	132.30
2	J	1	A	N3-C4-N9	10.12	135.49	127.40
2	I	2	A	N3-C4-N9	10.03	135.42	127.40
2	H	1	A	C6-C5-N7	10.02	139.31	132.30
2	I	3	A	N3-C4-N9	9.98	135.39	127.40
2	G	2	A	C6-C5-N7	9.86	139.20	132.30
2	K	1	A	C6-C5-N7	9.81	139.17	132.30
2	H	1	A	N3-C4-N9	9.81	135.25	127.40
2	L	3	A	C4-C5-N7	-9.70	105.85	110.70
2	I	1	A	N3-C4-N9	9.61	135.09	127.40
2	L	1	A	C6-C5-N7	9.60	139.02	132.30
2	H	3	A	N3-C4-N9	9.57	135.06	127.40
2	G	2	A	N3-C4-N9	9.35	134.88	127.40
2	K	3	A	N3-C4-N9	9.28	134.82	127.40
2	G	2	A	OP1-P-OP2	-9.19	105.82	119.60
2	G	1	A	N3-C4-N9	9.13	134.71	127.40
2	H	1	A	N3-C4-C5	-9.02	120.49	126.80
2	K	1	A	N3-C4-C5	-8.90	120.57	126.80
2	K	1	A	OP1-P-OP2	-8.71	106.54	119.60
2	G	1	A	OP1-P-OP2	-8.58	106.72	119.60
2	G	1	A	O3'-P-O5'	8.54	120.22	104.00
2	I	2	A	O4'-C1'-N9	8.54	115.03	108.20
2	K	3	A	C3'-C2'-C1'	8.50	108.30	101.50
2	I	1	A	OP1-P-OP2	-8.49	106.86	119.60
2	G	1	A	C3'-C2'-C1'	8.46	108.27	101.50
2	H	3	A	C3'-C2'-C1'	8.39	108.21	101.50
2	J	2	A	O3'-P-O5'	8.33	119.83	104.00
2	I	3	A	OP1-P-OP2	-8.12	107.42	119.60
2	G	2	A	N3-C4-C5	-8.09	121.14	126.80
2	I	3	A	C3'-C2'-C1'	8.08	107.96	101.50
2	J	2	A	C5-N7-C8	8.06	107.93	103.90
2	L	1	A	N9-C4-C5	-8.04	102.58	105.80
2	G	3	A	C5-N7-C8	7.97	107.88	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	3	A	C3'-C2'-C1'	7.96	107.87	101.50
2	L	1	A	OP1-P-OP2	-7.95	107.68	119.60
2	J	1	A	OP1-P-OP2	-7.88	107.79	119.60
2	I	1	A	N3-C4-C5	-7.84	121.31	126.80
2	H	1	A	OP1-P-OP2	-7.81	107.89	119.60
2	J	1	A	N3-C4-C5	-7.69	121.42	126.80
2	J	3	A	OP1-P-OP2	-7.65	108.13	119.60
2	K	3	A	OP1-P-OP2	-7.59	108.21	119.60
2	J	2	A	OP1-P-OP2	-7.59	108.22	119.60
2	K	2	A	OP1-P-OP2	-7.54	108.30	119.60
2	L	3	A	OP1-P-OP2	-7.53	108.30	119.60
2	I	2	A	C5-N7-C8	7.53	107.66	103.90
2	L	1	A	N3-C4-C5	-7.52	121.54	126.80
2	H	2	A	OP1-P-OP2	-7.50	108.36	119.60
2	G	3	A	OP1-P-OP2	-7.40	108.50	119.60
2	L	2	A	OP1-P-OP2	-7.39	108.52	119.60
2	K	1	A	O3'-P-O5'	7.36	117.98	104.00
2	H	3	A	OP1-P-OP2	-7.34	108.60	119.60
2	H	3	A	C6-C5-N7	7.31	137.42	132.30
2	L	2	A	O3'-P-O5'	7.31	117.89	104.00
2	I	1	A	O3'-P-O5'	7.26	117.79	104.00
2	G	2	A	C3'-C2'-C1'	7.25	107.30	101.50
2	I	2	A	OP1-P-OP2	-7.11	108.94	119.60
2	L	2	A	C5-N7-C8	7.09	107.45	103.90
2	L	1	A	C1'-O4'-C4'	-7.04	104.27	109.90
2	J	2	A	O4'-C1'-N9	6.93	113.74	108.20
2	H	1	A	O3'-P-O5'	6.89	117.09	104.00
2	K	2	A	O4'-C1'-N9	6.86	113.69	108.20
2	J	3	A	C3'-C2'-C1'	6.84	106.98	101.50
2	J	1	A	N9-C4-C5	-6.78	103.09	105.80
2	H	2	A	C5-N7-C8	6.69	107.24	103.90
2	J	1	A	O3'-P-O5'	6.58	116.50	104.00
2	K	3	A	C6-C5-N7	6.55	136.88	132.30
2	L	1	A	O3'-P-O5'	6.48	116.32	104.00
2	G	2	A	O3'-P-O5'	6.48	116.31	104.00
2	K	2	A	C5-N7-C8	6.44	107.12	103.90
2	J	3	A	O4'-C1'-N9	6.36	113.29	108.20
2	J	1	A	C1'-O4'-C4'	-6.35	104.82	109.90
2	G	1	A	C6-C5-N7	6.21	136.64	132.30
2	H	2	A	O3'-P-O5'	6.14	115.67	104.00
2	K	1	A	C3'-C2'-C1'	6.00	106.30	101.50
2	K	1	A	C1'-O4'-C4'	-5.93	105.16	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	3	A	C5-N7-C8	5.93	106.86	103.90
2	I	2	A	C6-C5-N7	5.88	136.41	132.30
2	I	2	A	O3'-P-O5'	5.86	115.13	104.00
2	J	2	A	C6-C5-N7	5.84	136.39	132.30
2	I	3	A	C6-C5-N7	5.83	136.38	132.30
2	I	1	A	C1'-O4'-C4'	-5.77	105.28	109.90
2	H	3	A	C5-N7-C8	5.63	106.71	103.90
2	J	1	A	C4-N9-C1'	-5.59	116.24	126.30
2	L	1	A	C4-N9-C1'	-5.58	116.25	126.30
2	I	1	A	N9-C4-C5	-5.50	103.60	105.80
2	G	1	A	O5'-C5'-C4'	-5.42	101.39	111.70
2	L	3	A	C5-C6-N1	5.42	120.41	117.70
2	G	1	A	C5-C6-N1	5.40	120.40	117.70
2	H	1	A	C3'-C2'-C1'	5.34	105.77	101.50
2	G	2	A	C5-C6-N1	5.33	120.37	117.70
2	G	1	A	C4'-C3'-C2'	5.32	107.92	102.60
2	L	3	A	C6-C5-N7	5.32	136.02	132.30
2	I	2	A	C6-N1-C2	5.31	121.79	118.60
2	I	3	A	C5-N7-C8	5.27	106.53	103.90
2	J	3	A	C5-C6-N6	-5.25	119.50	123.70
2	H	3	A	C5-C6-N1	5.25	120.33	117.70
2	I	1	A	C3'-C2'-C1'	5.18	105.65	101.50
2	J	2	A	C6-N1-C2	5.18	121.71	118.60
2	I	3	A	C5-C6-N1	5.12	120.26	117.70
2	L	3	A	O5'-C5'-C4'	-5.04	102.13	111.70
2	K	1	A	N9-C4-C5	-5.01	103.80	105.80
2	H	2	A	O4'-C1'-N9	5.01	112.20	108.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3518	0	3466	23	0
1	B	3518	0	3466	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3518	0	3466	15	0
1	D	3489	0	3440	26	0
1	E	3513	0	3461	24	0
1	F	3338	0	3278	20	0
2	G	66	0	33	1	0
2	H	66	0	33	1	0
2	I	66	0	33	0	0
2	J	66	0	33	3	0
2	K	66	0	33	1	0
2	L	66	0	33	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	1	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
4	A	84	0	0	5	0
4	B	76	0	0	4	0
4	C	90	0	0	0	0
4	D	83	0	0	6	0
4	E	81	0	0	2	0
4	F	71	0	0	0	0
4	H	1	0	0	0	0
4	J	2	0	0	0	0
4	K	3	0	0	0	0
4	L	1	0	0	0	0
All	All	21812	0	20775	127	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 3.

All (127) 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)
1:B:199:GLN:OE1	4:B:601:HOH:O	1.84	0.94
1:A:424:ILE:O	4:A:601:HOH:O	1.99	0.80
1:E:75:ALA:HA	1:E:110:ILE:HD11	1.65	0.79
1:E:416:LYS:NZ	4:E:602:HOH:O	2.18	0.77
1:A:263:ARG:NH2	4:A:604:HOH:O	2.21	0.73
1:A:105:SER:OG	4:A:602:HOH:O	2.10	0.69
1:F:279:VAL:HG22	1:F:316:ARG:HH22	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:375:ASN:HA	1:C:378:LYS:HG2	1.77	0.65
1:B:276:LYS:NZ	4:B:605:HOH:O	2.31	0.63
1:B:52:GLU:OE1	1:B:94:LYS:NZ	2.28	0.63
3:D:501:SO4:O1	4:D:601:HOH:O	2.14	0.62
1:B:51:ILE:HB	1:B:66:TYR:HB2	1.82	0.61
1:D:321:GLU:HG2	1:D:330:ARG:HG2	1.83	0.59
1:E:52:GLU:OE1	1:E:94:LYS:NZ	2.32	0.59
1:E:51:ILE:HB	1:E:66:TYR:HB2	1.85	0.59
1:F:382:ARG:NE	1:F:384:ASN:OD1	2.35	0.59
1:A:190:ARG:NH1	4:A:605:HOH:O	2.36	0.58
1:D:186:ILE:O	4:D:602:HOH:O	2.17	0.58
1:A:263:ARG:HH21	1:A:450:VAL:HG22	1.68	0.58
1:E:321:GLU:OE2	4:E:601:HOH:O	2.17	0.58
1:F:371:ASP:HA	1:F:378:LYS:HG3	1.87	0.57
1:B:262:ASP:HB2	4:B:607:HOH:O	2.05	0.56
1:D:300:GLN:O	2:J:3:A:H4'	2.06	0.54
1:F:412:LYS:HA	1:F:417:LEU:HD12	1.90	0.54
1:F:358:VAL:HG11	1:F:408:LEU:HD21	1.90	0.53
1:D:257:ASP:OD2	1:F:107:ASN:ND2	2.42	0.52
1:D:397:LEU:HD11	1:D:430:PHE:HA	1.91	0.52
1:C:51:ILE:HB	1:C:66:TYR:HB2	1.91	0.52
1:B:375:ASN:HA	1:B:378:LYS:HD3	1.91	0.52
1:E:168:ASN:HB3	1:E:170:GLU:OE1	2.10	0.52
1:A:382:ARG:HH11	1:A:384:ASN:HD21	1.59	0.51
1:B:358:VAL:HG11	1:B:408:LEU:HD21	1.92	0.51
1:D:373:THR:HG22	1:D:454:TYR:HB2	1.91	0.51
4:B:612:HOH:O	1:E:71:HIS:HD2	1.93	0.51
1:C:358:VAL:HG11	1:C:408:LEU:HD11	1.93	0.51
1:E:44:VAL:HB	1:E:52:GLU:HB2	1.92	0.51
1:D:335:LYS:HB3	1:D:395:GLU:HG2	1.93	0.51
1:F:51:ILE:HB	1:F:66:TYR:HB2	1.93	0.50
1:B:346:GLU:HG2	1:B:346:GLU:O	2.11	0.50
1:A:321:GLU:HG2	1:A:330:ARG:HG2	1.93	0.50
1:A:51:ILE:HB	1:A:66:TYR:HB2	1.93	0.50
1:A:143:ASP:OD1	4:A:603:HOH:O	2.19	0.50
1:D:279:VAL:HG22	1:D:316:ARG:HH22	1.76	0.50
1:F:355:GLU:HG2	1:F:419:LYS:HB3	1.95	0.49
1:D:359:ALA:HB1	1:D:366:ILE:HD12	1.94	0.49
1:A:335:LYS:HB3	1:A:395:GLU:HG2	1.94	0.49
1:C:382:ARG:NE	1:C:384:ASN:OD1	2.46	0.49
1:F:23:GLN:HB2	1:F:51:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:302:MET:HE1	1:D:428:SER:HA	1.95	0.48
1:A:203:LEU:HD21	1:A:216:ASP:HB3	1.95	0.48
1:E:77:GLU:O	1:E:81:GLU:HG2	2.14	0.48
1:F:232:TRP:CH2	1:F:291:ARG:HD2	2.48	0.48
1:D:92:HIS:CE1	1:D:94:LYS:HE2	2.49	0.48
1:D:116:LYS:NZ	4:D:608:HOH:O	2.41	0.48
1:E:397:LEU:HD21	1:E:433:VAL:HG21	1.96	0.47
1:F:406:SER:HA	1:F:409:VAL:HG22	1.97	0.47
2:G:3:A:N3	2:G:3:A:H2'	2.28	0.47
1:A:52:GLU:OE1	1:A:94:LYS:NZ	2.41	0.47
1:D:51:ILE:HB	1:D:66:TYR:HB2	1.97	0.47
1:A:44:VAL:HB	1:A:52:GLU:HB2	1.97	0.47
1:B:106:TYR:HB3	1:B:110:ILE:HD11	1.97	0.47
1:C:397:LEU:HD11	1:C:430:PHE:HA	1.95	0.47
1:E:107:ASN:HB2	1:E:110:ILE:HB	1.97	0.47
1:B:144:TRP:O	1:B:148:LYS:HD2	2.15	0.46
1:A:263:ARG:NH2	1:A:450:VAL:HG22	2.30	0.46
1:F:177:LEU:HD21	1:F:197:LYS:HD3	1.97	0.46
1:C:222:CYS:HB3	1:C:229:ARG:HD2	1.97	0.46
1:D:303:SER:HB2	4:D:624:HOH:O	2.15	0.46
1:E:57:SER:HB3	1:E:60:LYS:O	2.16	0.46
1:B:47:ALA:HB3	1:B:50:ASP:HB2	1.98	0.46
1:C:420:LEU:HD13	1:C:442:CYS:SG	2.56	0.46
1:B:434:LEU:O	1:B:438:LEU:HG	2.16	0.45
1:A:444:ILE:HB	1:A:460:LEU:HB2	1.97	0.45
1:C:71:HIS:CE1	1:E:269:SER:HB3	2.51	0.45
1:D:301:ARG:HA	2:J:3:A:O5'	2.17	0.45
1:F:434:LEU:HG	1:F:438:LEU:HD11	1.99	0.45
1:D:358:VAL:HG11	1:D:408:LEU:HD21	1.97	0.45
1:F:412:LYS:HG3	1:F:413:SER:N	2.32	0.44
1:E:408:LEU:HD22	1:E:420:LEU:HD13	1.99	0.44
1:B:144:TRP:CE2	1:B:148:LYS:HD3	2.52	0.44
1:A:83:ARG:HG3	1:A:154:LEU:HD11	2.00	0.44
1:E:144:TRP:CZ2	1:E:148:LYS:HD2	2.53	0.44
1:A:346:GLU:N	1:A:346:GLU:OE1	2.50	0.44
1:C:321:GLU:HG2	1:C:330:ARG:HG2	1.99	0.44
1:E:188:LEU:HD21	1:E:225:LEU:HD23	1.99	0.43
1:F:405:LYS:HD2	1:F:437:ARG:HB3	2.00	0.43
1:E:358:VAL:HG11	1:E:408:LEU:HD21	1.99	0.43
1:B:336:GLN:HG2	1:B:398:ASN:HB3	2.00	0.43
1:C:346:GLU:O	1:C:346:GLU:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:277:LYS:NZ	4:D:607:HOH:O	2.40	0.43
1:B:359:ALA:HB1	1:B:366:ILE:HD12	2.01	0.43
1:A:297:ASP:HA	1:A:323:GLU:HG2	2.00	0.42
1:B:71:HIS:CE1	1:C:269:SER:HB3	2.53	0.42
1:A:336:GLN:HE22	1:A:402:ARG:HE	1.67	0.42
1:C:368:LYS:HA	1:C:368:LYS:HD3	1.64	0.42
1:E:115:SER:O	1:E:119:ARG:HG2	2.20	0.42
1:E:232:TRP:CH2	1:E:291:ARG:HD2	2.54	0.42
1:B:44:VAL:HB	1:B:52:GLU:HB2	2.01	0.42
2:J:2:A:N3	2:J:2:A:H2'	2.35	0.42
1:D:77:GLU:O	1:D:81:GLU:HG2	2.20	0.42
1:D:369:ASP:HB3	1:D:449:TRP:CZ3	2.55	0.42
1:E:344:LYS:HG3	1:E:383:LEU:HD11	2.01	0.42
1:E:357:ILE:HD11	1:E:377:VAL:O	2.19	0.42
1:F:357:ILE:HG13	1:F:380:LEU:HB2	2.00	0.42
1:A:357:ILE:HD11	1:A:377:VAL:HG12	2.01	0.42
1:A:379:SER:O	1:A:379:SER:OG	2.34	0.42
1:D:350:PRO:HA	1:D:381:PRO:HG3	2.02	0.42
2:K:2:A:N3	2:K:2:A:H2'	2.34	0.41
1:B:15:ILE:HG23	1:F:201:LYS:HE2	2.03	0.41
1:B:446:LEU:HD11	1:B:460:LEU:HD11	2.02	0.41
1:B:235:ASP:HA	1:B:236:PRO:HD3	1.94	0.41
1:D:262:ASP:OD2	1:F:108:THR:HG22	2.20	0.41
1:E:189:LEU:O	1:E:193:VAL:HG23	2.20	0.41
1:D:189:LEU:O	1:D:193:VAL:HG23	2.20	0.41
1:E:434:LEU:O	1:E:438:LEU:HG	2.21	0.41
1:F:77:GLU:O	1:F:81:GLU:HG2	2.21	0.41
1:D:187:GLU:HA	4:D:606:HOH:O	2.20	0.41
1:A:77:GLU:O	1:A:81:GLU:HG2	2.21	0.41
1:E:197:LYS:HE2	1:E:197:LYS:HB3	1.95	0.41
1:F:60:LYS:HA	1:F:60:LYS:HD2	1.74	0.41
2:H:2:A:N3	2:H:2:A:H2'	2.36	0.41
1:C:168:ASN:HB3	1:C:170:GLU:OE2	2.21	0.40
1:D:416:LYS:HD3	1:D:416:LYS:HA	1.91	0.40
1:A:17:ARG:CZ	1:C:207:SER:HB2	2.52	0.40
1:D:257:ASP:HB3	1:D:266:LYS:HE3	2.03	0.40
1:C:262:ASP:O	1:C:265:GLN:HG2	2.22	0.40
1:D:375:ASN:OD1	1:D:378:LYS:HE3	2.22	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	
1	A	434/462 (94%)	422 (97%)	12 (3%)	0	100	100
1	B	434/462 (94%)	421 (97%)	13 (3%)	0	100	100
1	C	434/462 (94%)	417 (96%)	16 (4%)	1 (0%)	47	62
1	D	429/462 (93%)	417 (97%)	11 (3%)	1 (0%)	47	62
1	E	433/462 (94%)	417 (96%)	16 (4%)	0	100	100
1	F	403/462 (87%)	389 (96%)	14 (4%)	0	100	100
All	All	2567/2772 (93%)	2483 (97%)	82 (3%)	2 (0%)	51	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	416	LYS
1	D	441	ILE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	
1	A	392/411 (95%)	387 (99%)	5 (1%)	69	84
1	B	392/411 (95%)	387 (99%)	5 (1%)	69	84
1	C	392/411 (95%)	387 (99%)	5 (1%)	69	84
1	D	389/411 (95%)	386 (99%)	3 (1%)	81	91
1	E	392/411 (95%)	387 (99%)	5 (1%)	69	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	373/411 (91%)	366 (98%)	7 (2%)	57 75
All	All	2330/2466 (94%)	2300 (99%)	30 (1%)	69 84

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	SER
1	A	113	LEU
1	A	190	ARG
1	A	219	ASN
1	A	462	LEU
1	B	29	ARG
1	B	59	GLU
1	B	148	LYS
1	B	203	LEU
1	B	353	GLU
1	C	29	ARG
1	C	170	GLU
1	C	203	LEU
1	C	412	LYS
1	C	418	SER
1	D	113	LEU
1	D	334	HIS
1	D	416	LYS
1	E	29	ARG
1	E	111	SER
1	E	113	LEU
1	E	203	LEU
1	E	338	GLU
1	F	29	ARG
1	F	57	SER
1	F	113	LEU
1	F	203	LEU
1	F	324	HIS
1	F	378	LYS
1	F	405	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	231	GLN

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Mol	Chain	Res	Type
1	D	181	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	G	2/3 (66%)	1 (50%)	1 (50%)
2	H	2/3 (66%)	2 (100%)	1 (50%)
2	I	2/3 (66%)	2 (100%)	0
2	J	2/3 (66%)	2 (100%)	1 (50%)
2	K	2/3 (66%)	2 (100%)	0
2	L	2/3 (66%)	2 (100%)	0
All	All	12/18 (66%)	11 (91%)	3 (25%)

All (11) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	G	3	A
2	H	2	A
2	H	3	A
2	I	2	A
2	I	3	A
2	J	2	A
2	J	3	A
2	K	2	A
2	K	3	A
2	L	2	A
2	L	3	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	G	2	A
2	H	2	A
2	J	2	A

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	F	501	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	D	501	-	4,4,4	0.12	0	6,6,6	0.08	0
3	SO4	E	501	-	4,4,4	0.13	0	6,6,6	0.09	0
3	SO4	C	501	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	A	501	-	4,4,4	0.14	0	6,6,6	0.04	0
3	SO4	B	501	-	4,4,4	0.14	0	6,6,6	0.04	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	501	SO4	1	0

5.7 Other polymers [i](#)

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 i

6.1 Protein, DNA and RNA chains i

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	438/462 (94%)	0.03	20 (4%) 32 31	37, 55, 102, 135	0
1	B	438/462 (94%)	0.04	19 (4%) 35 33	41, 59, 100, 117	0
1	C	438/462 (94%)	0.14	32 (7%) 15 13	38, 59, 118, 158	0
1	D	435/462 (94%)	0.34	39 (8%) 9 8	37, 62, 133, 170	0
1	E	437/462 (94%)	0.01	13 (2%) 50 49	36, 55, 98, 122	0
1	F	415/462 (89%)	0.39	48 (11%) 4 4	38, 61, 121, 152	0
2	G	3/3 (100%)	-0.34	0 100 100	54, 54, 55, 58	0
2	H	3/3 (100%)	-0.55	0 100 100	58, 58, 60, 62	0
2	I	3/3 (100%)	-0.46	0 100 100	66, 66, 69, 72	0
2	J	3/3 (100%)	-0.09	0 100 100	75, 75, 77, 80	0
2	K	3/3 (100%)	-0.97	0 100 100	56, 56, 59, 60	0
2	L	3/3 (100%)	-0.79	0 100 100	67, 67, 72, 72	0
All	All	2619/2790 (93%)	0.15	171 (6%) 18 17	36, 58, 117, 170	0

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	348	VAL	10.4
1	F	411	PHE	9.3
1	D	347	ALA	7.6
1	B	347	ALA	6.4
1	B	348	VAL	6.4
1	F	352	GLY	6.4
1	D	352	GLY	6.2
1	C	348	VAL	6.1
1	B	372	SER	5.9
1	D	350	PRO	5.8
1	A	373	THR	5.7

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Mol	Chain	Res	Type	RSRZ
1	B	373	THR	5.7
1	F	416	LYS	5.5
1	D	462	LEU	5.5
1	A	347	ALA	5.5
1	D	373	THR	5.4
1	A	372	SER	5.3
1	C	340	GLN	5.3
1	C	372	SER	5.3
1	F	409	VAL	5.2
1	D	379	SER	5.1
1	C	133	VAL	5.1
1	F	171	ASN	4.9
1	D	372	SER	4.9
1	B	133	VAL	4.8
1	F	133	VAL	4.7
1	F	354	THR	4.7
1	F	380	LEU	4.6
1	F	351	GLN	4.6
1	C	347	ALA	4.5
1	D	351	GLN	4.5
1	D	374	ILE	4.5
1	D	339	GLY	4.4
1	D	375	ASN	4.4
1	F	334	HIS	4.4
1	C	368	LYS	4.2
1	F	336	GLN	4.2
1	A	374	ILE	4.2
1	F	413	SER	4.2
1	E	372	SER	4.2
1	D	133	VAL	4.1
1	C	134	SER	4.1
1	B	171	ASN	4.1
1	E	171	ASN	4.0
1	A	375	ASN	4.0
1	C	352	GLY	4.0
1	F	414	GLU	4.0
1	D	376	GLU	4.0
1	F	440	GLY	3.9
1	C	462	LEU	3.9
1	F	377	VAL	3.9
1	D	338	GLU	3.8
1	F	353	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	F	327	LEU	3.8
1	A	377	VAL	3.8
1	E	347	ALA	3.7
1	F	371	ASP	3.7
1	A	133	VAL	3.6
1	D	340	GLN	3.6
1	F	399	LEU	3.5
1	F	383	LEU	3.3
1	F	170	GLU	3.3
1	D	345	ILE	3.3
1	B	374	ILE	3.3
1	C	386	GLU	3.3
1	F	134	SER	3.3
1	D	353	GLU	3.2
1	C	376	GLU	3.2
1	F	338	GLU	3.2
1	F	379	SER	3.2
1	C	416	LYS	3.2
1	B	349	GLU	3.2
1	E	379	SER	3.2
1	F	415	ASN	3.2
1	A	352	GLY	3.2
1	A	378	LYS	3.2
1	B	375	ASN	3.1
1	D	377	VAL	3.1
1	A	338	GLU	3.1
1	D	413	SER	3.1
1	F	418	SER	3.1
1	A	380	LEU	3.1
1	F	412	LYS	3.1
1	F	372	SER	3.0
1	D	409	VAL	3.0
1	C	345	ILE	3.0
1	D	378	LYS	3.0
1	F	396	THR	3.0
1	A	348	VAL	3.0
1	C	336	GLN	2.9
1	C	374	ILE	2.9
1	E	345	ILE	2.9
1	A	354	THR	2.9
1	C	389	HIS	2.9
1	C	351	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	462	LEU	2.9
1	C	379	SER	2.8
1	C	365	ALA	2.8
1	F	376	GLU	2.8
1	D	390	ALA	2.8
1	D	171	ASN	2.8
1	D	415	ASN	2.8
1	C	342	PHE	2.7
1	F	333	ASP	2.7
1	C	171	ASN	2.7
1	C	375	ASN	2.7
1	A	376	GLU	2.7
1	F	350	PRO	2.7
1	D	327	LEU	2.7
1	C	338	GLU	2.6
1	F	417	LEU	2.6
1	C	367	GLY	2.6
1	D	335	LYS	2.6
1	E	343	THR	2.6
1	B	377	VAL	2.6
1	B	170	GLU	2.6
1	D	418	SER	2.5
1	D	380	LEU	2.5
1	D	392	ASP	2.5
1	A	340	GLN	2.4
1	F	402	ARG	2.4
1	D	349	GLU	2.4
1	D	411	PHE	2.4
1	B	346	GLU	2.4
1	B	187	GLU	2.4
1	C	363	PRO	2.3
1	F	408	LEU	2.3
1	B	189	LEU	2.3
1	B	190	ARG	2.3
1	E	338	GLU	2.3
1	A	392	ASP	2.3
1	F	395	GLU	2.3
1	F	357	ILE	2.2
1	D	386	GLU	2.2
1	B	416	LYS	2.2
1	F	337	LYS	2.2
1	D	170	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	346	GLU	2.2
1	F	349	GLU	2.2
1	F	362	PHE	2.2
1	E	335	LYS	2.2
1	F	359	ALA	2.2
1	B	351	GLN	2.2
1	C	341	PHE	2.2
1	A	439	ASN	2.2
1	F	406	SER	2.2
1	F	452	GLY	2.2
1	B	350	PRO	2.2
1	C	388	SER	2.2
1	C	339	GLY	2.1
1	F	229	ARG	2.1
1	F	14	ALA	2.1
1	A	334	HIS	2.1
1	F	223	HIS	2.1
1	C	378	LYS	2.1
1	E	368	LYS	2.1
1	C	392	ASP	2.1
1	F	397	LEU	2.1
1	D	336	GLN	2.1
1	D	371	ASP	2.1
1	E	371	ASP	2.1
1	A	462	LEU	2.1
1	E	375	ASN	2.1
1	B	340	GLN	2.1
1	F	381	PRO	2.0
1	D	354	THR	2.0
1	C	337	LYS	2.0
1	A	346	GLU	2.0
1	D	334	HIS	2.0
1	C	349	GLU	2.0
1	E	395	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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
3	SO4	D	501	5/5	0.96	0.12	53,57,58,68	0
3	SO4	C	501	5/5	0.97	0.13	48,56,64,69	0
3	SO4	B	501	5/5	0.97	0.12	60,64,69,69	0
3	SO4	A	501	5/5	0.98	0.10	59,63,66,74	0
3	SO4	F	501	5/5	0.98	0.11	56,62,68,70	0
3	SO4	E	501	5/5	0.99	0.14	58,60,64,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.