Full wwPDB X-ray Structure Validation Report

Aug 8, 2020 – 04:51 AM BST

PDB ID	:	6VM6
Title	:	Structure of Acinetobacter baumannii Cap4 SAVED/CARF-domain containing receptor with the cyclic trinucleotide 2'3'3'-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	:	2020-01-27
Resolution	:	2.10 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 (i) symbol.

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

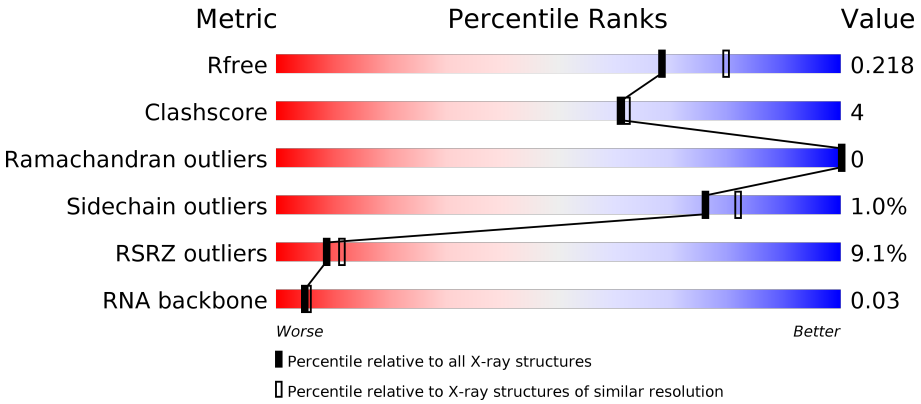
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)
RNA backbone	3102	1000 (2.54-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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	462	6% 86% 9% 5%
1	B	462	4% 85% 11% 5%
1	C	462	10% 87% 7% 5%
1	D	462	4% 88% 7% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	462	11% 83% 11% 6%
1	F	462	17% 84% 10% 5%
2	G	3	33% 67%
2	H	3	100%
2	I	3	67% 33%
2	J	3	67% 33%
2	K	3	33% 67% 33%

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
3	SO4	B	501	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23004 atoms, of which 66 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
1	A	438	Total	C	N	O	S	0	0	0
			3518	2245	593	669	11			
1	B	440	Total	C	N	O	S	0	0	0
			3528	2250	595	672	11			
1	C	439	Total	C	N	O	S	0	0	0
			3522	2247	594	670	11			
1	D	440	Total	C	N	O	S	0	0	0
			3528	2250	595	672	11			
1	E	432	Total	C	N	O	S	0	0	0
			3472	2217	586	658	11			
1	F	437	Total	C	N	O	S	0	0	0
			3510	2239	592	668	11			

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 2'-5'-Linked Cyclic RNA (5'-R(P*AP*AP*A)-3').

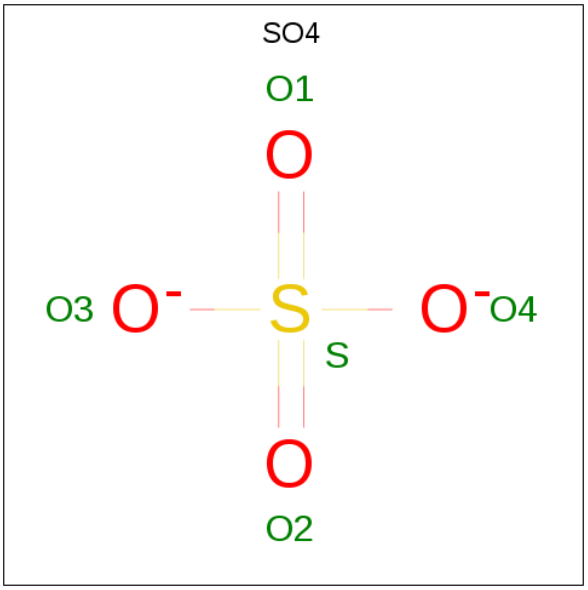
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	G	3	Total	C	N	O	P		0	0	0
			66	30	15	18	3				
2	H	3	Total	C	H	N	O	P	0	0	0
			99	30	33	15	18	3			
2	I	3	Total	C	N	O	P		0	0	0
			66	30	15	18	3				

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	J	3	Total C N O P 66 30 15 18 3	0	0	0
2	K	3	Total C H N O P 99 30 33 15 18 3	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is water.

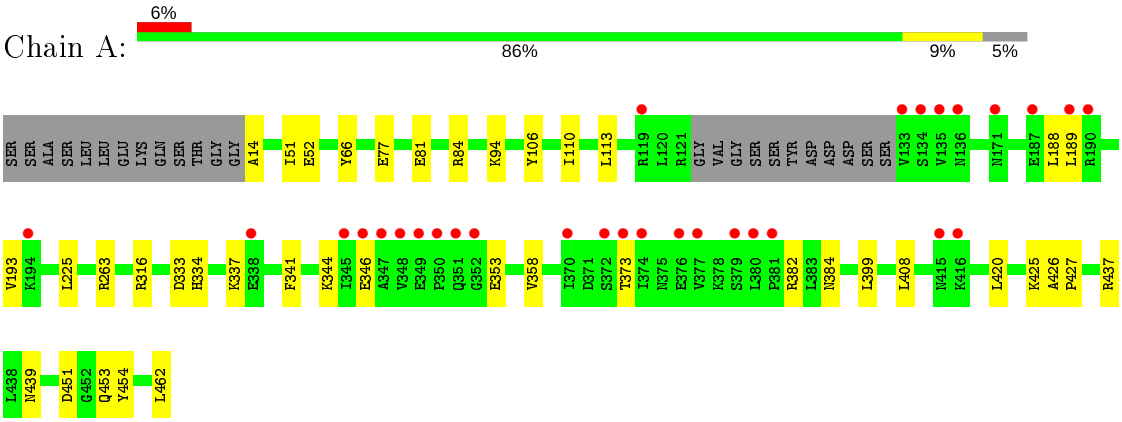
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	237	Total O 237 237	0	0
4	B	277	Total O 277 277	0	0
4	C	242	Total O 242 242	0	0
4	D	272	Total O 272 272	0	0
4	E	229	Total O 229 229	0	0
4	F	220	Total O 220 220	0	0
4	G	7	Total O 7 7	0	0
4	H	3	Total O 3 3	0	0
4	J	3	Total O 3 3	0	0

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.

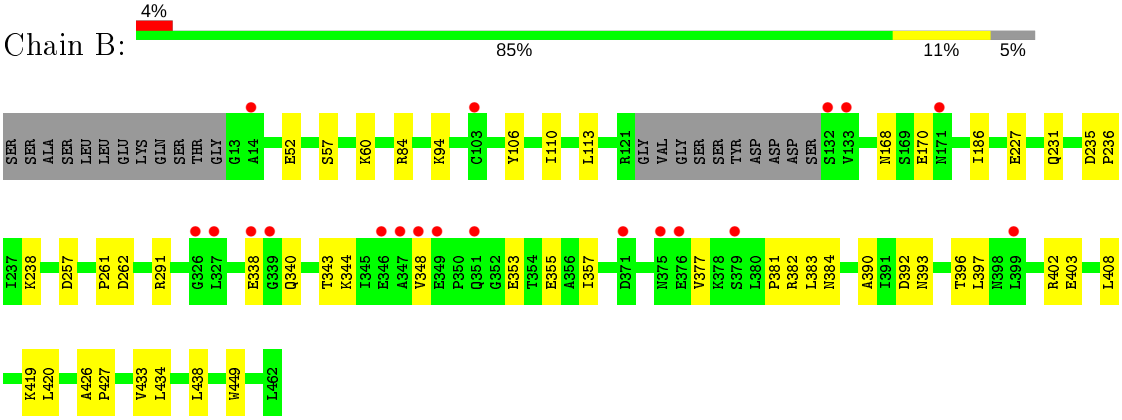
- Molecule 1: SAVED domain-containing protein

Chain A:



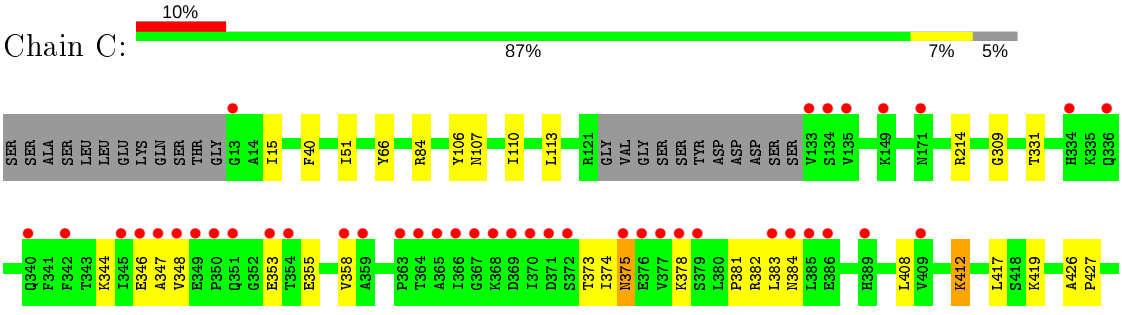
- Molecule 1: SAVED domain-containing protein

Chain B:



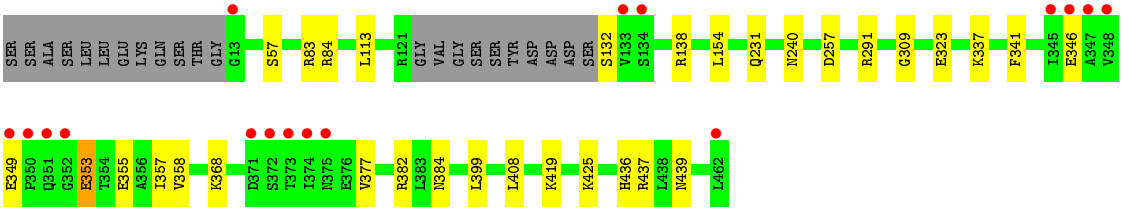
- Molecule 1: SAVED domain-containing protein

Chain C:



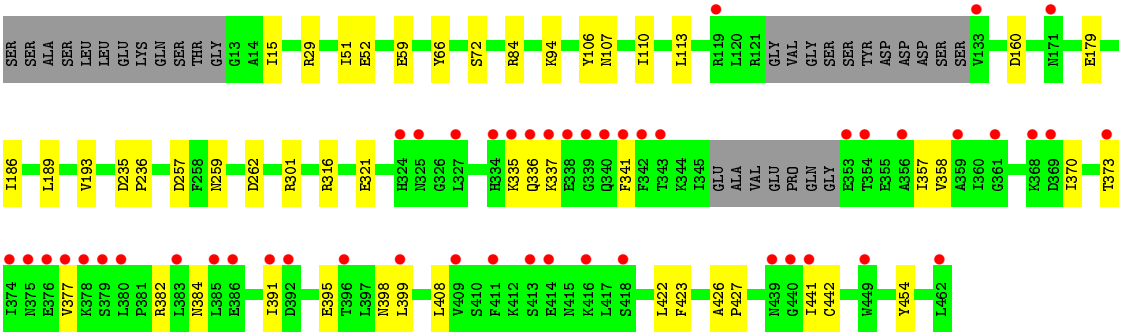
• Molecule 1: SAVED domain-containing protein

Chain D:



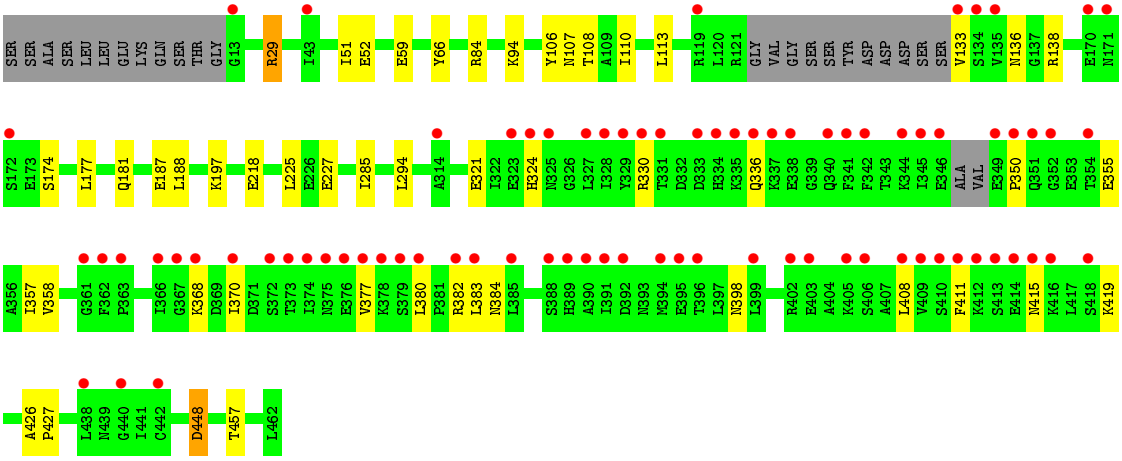
• Molecule 1: SAVED domain-containing protein

Chain E:



• Molecule 1: SAVED domain-containing protein

Chain F:



• Molecule 2: 2'-5'-Linked Cyclic RNA (5'-R(P*AP*AP*A)-3')

Chain G:

• Molecule 2: 2'-5'-Linked Cyclic RNA (5'-R(P*AP*AP*A)-3')

Chain H:

• Molecule 2: 2'-5'-Linked Cyclic RNA (5'-R(P*AP*AP*A)-3')

Chain I:

• Molecule 2: 2'-5'-Linked Cyclic RNA (5'-R(P*AP*AP*A)-3')

Chain J:

• Molecule 2: 2'-5'-Linked Cyclic RNA (5'-R(P*AP*AP*A)-3')

Chain K:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	106.58Å 111.46Å 164.83Å 90.00° 100.21° 90.00°	Depositor
Resolution (Å)	49.21 – 2.10 49.21 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.1 (49.21-2.10) 98.1 (49.21-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.185 , 0.219 0.185 , 0.218	Depositor DCC
R_{free} test set	2000 reflections (0.92%)	wwPDB-VP
Wilson B-factor (Å^2)	39.9	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 42.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	23004	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: 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	0.26	0/3593	0.44	0/4856
1	B	0.27	0/3603	0.44	0/4869
1	C	0.27	0/3597	0.44	0/4861
1	D	0.27	0/3603	0.45	0/4869
1	E	0.27	0/3545	0.45	0/4788
1	F	0.26	0/3584	0.44	0/4841
2	G	7.87	26/74 (35.1%)	9.89	52/113 (46.0%)
2	H	7.98	26/74 (35.1%)	10.39	56/113 (49.6%)
2	I	8.02	30/74 (40.5%)	9.90	51/113 (45.1%)
2	J	8.01	29/74 (39.2%)	9.88	51/113 (45.1%)
2	K	8.05	26/74 (35.1%)	10.58	54/113 (47.8%)
All	All	1.07	137/21895 (0.6%)	1.47	264/29649 (0.9%)

All (137) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	2	A	N7-C5	29.72	1.57	1.39
2	H	2	A	N7-C5	28.97	1.56	1.39
2	G	2	A	N7-C5	28.29	1.56	1.39
2	J	2	A	N7-C5	28.14	1.56	1.39
2	I	2	A	N7-C5	28.12	1.56	1.39
2	K	3	A	C6-N6	25.35	1.54	1.33
2	H	3	A	C6-N6	24.76	1.53	1.33
2	J	3	A	C6-N6	23.92	1.53	1.33
2	I	3	A	C6-N6	23.79	1.52	1.33
2	G	3	A	C6-N6	23.54	1.52	1.33
2	K	2	A	C6-N6	21.16	1.50	1.33
2	H	2	A	C6-N6	20.62	1.50	1.33
2	K	1	A	C6-N6	20.08	1.50	1.33
2	H	1	A	C6-N6	19.94	1.50	1.33
2	G	1	A	C6-N6	19.58	1.49	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	1	A	C6-N6	19.53	1.49	1.33
2	H	3	A	N7-C5	19.48	1.50	1.39
2	I	1	A	C6-N6	19.37	1.49	1.33
2	G	1	A	N7-C5	19.27	1.50	1.39
2	K	1	A	N7-C5	19.15	1.50	1.39
2	I	1	A	N7-C5	19.09	1.50	1.39
2	J	1	A	N7-C5	19.03	1.50	1.39
2	J	2	A	C6-N6	19.01	1.49	1.33
2	H	1	A	N7-C5	18.85	1.50	1.39
2	G	2	A	C6-N6	18.85	1.49	1.33
2	I	2	A	C6-N6	18.82	1.49	1.33
2	G	3	A	N7-C5	18.26	1.50	1.39
2	I	3	A	N7-C5	17.88	1.50	1.39
2	J	3	A	N7-C5	17.69	1.49	1.39
2	K	3	A	N7-C5	17.66	1.49	1.39
2	I	2	A	N9-C4	-16.98	1.27	1.37
2	G	2	A	N9-C4	-16.80	1.27	1.37
2	J	2	A	N9-C4	-16.64	1.27	1.37
2	H	2	A	N9-C4	-14.32	1.29	1.37
2	I	3	A	C5-C4	13.73	1.48	1.38
2	J	3	A	C5-C4	13.68	1.48	1.38
2	K	2	A	N9-C4	-13.37	1.29	1.37
2	J	2	A	C5-C4	12.54	1.47	1.38
2	K	2	A	C5-C4	12.35	1.47	1.38
2	I	2	A	C5-C4	12.16	1.47	1.38
2	J	2	A	N9-C8	-12.15	1.28	1.37
2	G	2	A	C5-C4	12.15	1.47	1.38
2	K	2	A	N9-C8	-12.03	1.28	1.37
2	H	2	A	N9-C8	-12.02	1.28	1.37
2	G	3	A	C5-C4	11.94	1.47	1.38
2	H	2	A	C5-C4	11.90	1.47	1.38
2	G	2	A	N9-C8	-11.79	1.28	1.37
2	I	3	A	C2'-O2'	11.73	1.56	1.41
2	I	2	A	N9-C8	-11.70	1.28	1.37
2	J	3	A	C2'-O2'	11.62	1.56	1.41
2	H	3	A	C5-C4	10.80	1.46	1.38
2	G	3	A	C2'-O2'	10.61	1.55	1.41
2	K	3	A	C5-C4	10.25	1.46	1.38
2	I	1	A	P-O5'	10.20	1.70	1.59
2	J	1	A	P-O5'	10.08	1.69	1.59
2	K	3	A	C2'-O2'	9.89	1.54	1.41
2	H	3	A	C2'-O2'	9.59	1.54	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	1	A	C5-C4	9.03	1.45	1.38
2	K	1	A	P-O5'	8.96	1.68	1.59
2	H	1	A	C5-C4	8.75	1.44	1.38
2	I	1	A	C5-C4	8.72	1.44	1.38
2	G	1	A	C5-C4	8.62	1.44	1.38
2	J	1	A	C5-C4	8.60	1.44	1.38
2	G	1	A	P-O5'	8.52	1.68	1.59
2	I	3	A	P-O5'	8.14	1.67	1.59
2	K	3	A	P-O5'	8.02	1.67	1.59
2	H	3	A	C8-N7	7.75	1.36	1.31
2	H	1	A	P-O5'	7.73	1.67	1.59
2	H	3	A	P-O5'	7.60	1.67	1.59
2	G	3	A	P-O5'	7.60	1.67	1.59
2	J	3	A	C3'-C2'	7.53	1.61	1.52
2	J	3	A	P-O5'	7.47	1.67	1.59
2	K	3	A	C8-N7	7.45	1.36	1.31
2	I	3	A	C3'-O3'	7.39	1.52	1.42
2	G	1	A	C8-N7	7.35	1.36	1.31
2	K	1	A	O3'-P	7.26	1.69	1.61
2	G	1	A	O3'-P	7.26	1.69	1.61
2	H	1	A	N9-C8	-7.21	1.31	1.37
2	J	1	A	C8-N7	7.14	1.36	1.31
2	G	2	A	O4'-C1'	7.14	1.50	1.41
2	K	1	A	C8-N7	7.11	1.36	1.31
2	H	1	A	O3'-P	7.02	1.69	1.61
2	G	3	A	C8-N7	7.00	1.36	1.31
2	I	2	A	O4'-C1'	6.99	1.50	1.41
2	I	1	A	O3'-P	6.98	1.69	1.61
2	J	2	A	O4'-C1'	6.97	1.50	1.41
2	I	1	A	C8-N7	6.97	1.36	1.31
2	H	1	A	C8-N7	6.89	1.36	1.31
2	K	1	A	N9-C8	-6.83	1.32	1.37
2	I	3	A	O4'-C1'	6.67	1.50	1.41
2	J	1	A	O3'-P	6.66	1.69	1.61
2	J	3	A	O4'-C1'	6.55	1.50	1.41
2	K	2	A	C5-C6	-6.54	1.35	1.41
2	J	1	A	N9-C8	-6.48	1.32	1.37
2	I	1	A	N9-C8	-6.41	1.32	1.37
2	G	1	A	N9-C8	-6.35	1.32	1.37
2	J	3	A	N9-C8	-6.34	1.32	1.37
2	K	1	A	O4'-C1'	6.32	1.49	1.41
2	K	2	A	O3'-P	6.13	1.68	1.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2	A	O3'-P	6.12	1.68	1.61
2	H	2	A	C5-C6	-6.07	1.35	1.41
2	J	3	A	C3'-O3'	6.05	1.50	1.42
2	H	1	A	C3'-C2'	-6.01	1.46	1.52
2	K	1	A	C3'-C2'	-5.86	1.46	1.52
2	I	3	A	C8-N7	5.84	1.35	1.31
2	I	1	A	C3'-C2'	-5.79	1.46	1.52
2	J	1	A	C3'-C2'	-5.77	1.46	1.52
2	I	2	A	C4'-O4'	5.76	1.53	1.45
2	G	2	A	O3'-P	5.75	1.68	1.61
2	H	2	A	O3'-P	5.74	1.68	1.61
2	K	2	A	P-O5'	5.73	1.65	1.59
2	G	1	A	C3'-C2'	-5.72	1.46	1.52
2	I	3	A	N9-C8	-5.67	1.33	1.37
2	H	1	A	O4'-C1'	5.63	1.49	1.41
2	J	2	A	O3'-P	5.61	1.67	1.61
2	I	3	A	C3'-C2'	5.57	1.59	1.52
2	G	2	A	P-O5'	5.52	1.65	1.59
2	K	2	A	C4'-O4'	5.49	1.52	1.45
2	G	2	A	C4'-O4'	5.48	1.52	1.45
2	K	3	A	N1-C2	5.46	1.39	1.34
2	H	3	A	C2'-C1'	5.44	1.59	1.53
2	J	2	A	C4'-O4'	5.43	1.52	1.45
2	I	3	A	N1-C2	5.42	1.39	1.34
2	H	2	A	C4'-O4'	5.37	1.52	1.45
2	G	2	A	C8-N7	5.35	1.35	1.31
2	J	2	A	P-O5'	5.34	1.65	1.59
2	J	3	A	C8-N7	5.33	1.35	1.31
2	J	3	A	N1-C2	5.32	1.39	1.34
2	J	2	A	C8-N7	5.28	1.35	1.31
2	I	2	A	P-O5'	5.27	1.65	1.59
2	G	2	A	C4'-C3'	-5.24	1.47	1.52
2	I	2	A	C4'-C3'	-5.21	1.47	1.52
2	H	3	A	N1-C2	5.15	1.39	1.34
2	I	3	A	N3-C4	5.11	1.38	1.34
2	G	3	A	N1-C2	5.09	1.39	1.34
2	K	2	A	C8-N7	5.06	1.35	1.31
2	H	3	A	O4'-C1'	5.01	1.48	1.41

All (264) bond angle outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	2	A	C8-N9-C4	55.54	128.02	105.80
2	H	2	A	C8-N9-C4	55.37	127.95	105.80
2	I	2	A	C8-N9-C4	54.26	127.50	105.80
2	J	2	A	C8-N9-C4	54.04	127.42	105.80
2	G	2	A	C8-N9-C4	53.45	127.18	105.80
2	G	1	A	C8-N9-C4	32.63	118.85	105.80
2	J	1	A	C8-N9-C4	32.46	118.78	105.80
2	I	1	A	C8-N9-C4	31.79	118.52	105.80
2	K	3	A	C8-N9-C4	31.74	118.50	105.80
2	G	3	A	C8-N9-C4	31.56	118.42	105.80
2	J	3	A	C8-N9-C4	30.63	118.05	105.80
2	H	1	A	C8-N9-C4	30.23	117.89	105.80
2	K	1	A	C8-N9-C4	30.01	117.81	105.80
2	H	3	A	C8-N9-C4	29.97	117.79	105.80
2	I	3	A	C8-N9-C4	29.80	117.72	105.80
2	K	2	A	N7-C8-N9	-24.70	101.45	113.80
2	H	2	A	N7-C8-N9	-24.58	101.51	113.80
2	I	2	A	N7-C8-N9	-23.27	102.16	113.80
2	G	2	A	N7-C8-N9	-22.94	102.33	113.80
2	J	2	A	N7-C8-N9	-22.88	102.36	113.80
2	K	3	A	N7-C8-N9	-21.72	102.94	113.80
2	G	3	A	C2-N3-C4	19.77	120.49	110.60
2	I	3	A	C2-N3-C4	19.72	120.46	110.60
2	J	3	A	C2-N3-C4	19.61	120.41	110.60
2	K	3	A	C1'-O4'-C4'	-19.47	94.32	109.90
2	H	3	A	C1'-O4'-C4'	-19.30	94.46	109.90
2	H	3	A	C2-N3-C4	19.18	120.19	110.60
2	G	3	A	N7-C8-N9	-19.01	104.29	113.80
2	K	3	A	C2-N3-C4	18.25	119.73	110.60
2	H	3	A	N7-C8-N9	-17.91	104.84	113.80
2	J	3	A	N3-C4-N9	17.84	141.67	127.40
2	J	1	A	N7-C8-N9	-17.59	105.00	113.80
2	K	2	A	C4-C5-N7	-17.39	102.00	110.70
2	G	1	A	N7-C8-N9	-17.37	105.12	113.80
2	I	3	A	N3-C4-N9	17.36	141.29	127.40
2	H	2	A	C4-C5-N7	-17.09	102.15	110.70
2	G	2	A	C4-C5-N7	-16.98	102.21	110.70
2	J	2	A	C4-C5-N7	-16.82	102.29	110.70
2	I	2	A	C4-C5-N7	-16.72	102.34	110.70
2	I	1	A	N7-C8-N9	-16.70	105.45	113.80
2	I	1	A	C2-N3-C4	16.50	118.85	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	1	A	C2-N3-C4	16.36	118.78	110.60
2	G	1	A	C2-N3-C4	16.14	118.67	110.60
2	H	3	A	C5-C6-N1	15.98	125.69	117.70
2	G	3	A	N3-C4-N9	15.86	140.09	127.40
2	H	2	A	C6-C5-N7	15.73	143.31	132.30
2	K	2	A	C6-C5-N7	15.59	143.22	132.30
2	H	1	A	N7-C8-N9	-15.44	106.08	113.80
2	K	1	A	N7-C8-N9	-15.43	106.08	113.80
2	K	3	A	C4-C5-N7	-15.34	103.03	110.70
2	I	3	A	N7-C8-N9	-15.26	106.17	113.80
2	K	3	A	O4'-C4'-C3'	15.26	119.26	104.00
2	J	3	A	N7-C8-N9	-15.25	106.17	113.80
2	K	3	A	C5-N7-C8	15.16	111.48	103.90
2	J	3	A	N3-C4-C5	-15.10	116.23	126.80
2	K	2	A	N9-C4-C5	-15.07	99.77	105.80
2	I	3	A	N3-C4-C5	-15.05	116.26	126.80
2	H	2	A	N9-C4-C5	-15.05	99.78	105.80
2	H	3	A	O4'-C1'-C2'	15.01	121.11	107.60
2	K	1	A	C2-N3-C4	14.92	118.06	110.60
2	K	3	A	O4'-C1'-C2'	14.83	120.95	107.60
2	H	1	A	C2-N3-C4	14.60	117.90	110.60
2	H	2	A	C5-C6-N1	14.57	124.98	117.70
2	H	3	A	O4'-C4'-C3'	14.38	118.38	104.00
2	G	2	A	C2-N3-C4	14.35	117.78	110.60
2	I	2	A	N9-C4-C5	-14.20	100.12	105.80
2	H	2	A	N3-C4-N9	14.19	138.75	127.40
2	I	2	A	N3-C4-N9	14.17	138.73	127.40
2	K	2	A	N3-C4-N9	14.08	138.66	127.40
2	J	2	A	N9-C4-C5	-14.06	100.17	105.80
2	K	3	A	N3-C4-N9	14.05	138.64	127.40
2	G	3	A	N3-C4-C5	-13.91	117.06	126.80
2	J	2	A	N3-C4-N9	13.88	138.50	127.40
2	I	3	A	C5'-C4'-C3'	-13.84	93.85	116.00
2	I	2	A	C2-N3-C4	13.75	117.48	110.60
2	G	2	A	C6-C5-N7	13.71	141.90	132.30
2	K	2	A	C5-C6-N1	13.69	124.55	117.70
2	H	3	A	N3-C4-N9	13.59	138.27	127.40
2	J	2	A	C2-N3-C4	13.56	117.38	110.60
2	K	3	A	N3-C4-C5	-13.56	117.31	126.80
2	G	2	A	N3-C4-N9	13.48	138.18	127.40
2	H	2	A	C2-N3-C4	13.39	117.30	110.60
2	G	2	A	N9-C4-C5	-13.32	100.47	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	3	A	C4-C5-N7	-13.20	104.10	110.70
2	J	2	A	C6-C5-N7	13.19	141.53	132.30
2	K	3	A	C5-C6-N1	13.17	124.29	117.70
2	J	3	A	C4-C5-N7	-13.03	104.19	110.70
2	I	2	A	C6-C5-N7	12.96	141.38	132.30
2	G	3	A	C4-C5-N7	-12.95	104.23	110.70
2	K	2	A	C2-N3-C4	12.85	117.03	110.60
2	J	1	A	N1-C2-N3	-12.76	122.92	129.30
2	G	1	A	N1-C2-N3	-12.72	122.94	129.30
2	G	3	A	C5-N7-C8	12.62	110.21	103.90
2	I	1	A	N1-C2-N3	-12.55	123.03	129.30
2	J	3	A	C5'-C4'-C3'	-12.44	96.10	116.00
2	K	1	A	N1-C2-N3	-12.43	123.09	129.30
2	H	1	A	N1-C2-N3	-12.40	123.10	129.30
2	H	3	A	N3-C4-C5	-12.37	118.14	126.80
2	K	1	A	C5-C6-N1	12.32	123.86	117.70
2	H	3	A	C4-C5-N7	-12.05	104.68	110.70
2	H	1	A	C5-C6-N1	11.90	123.65	117.70
2	I	1	A	N3-C4-N9	11.81	136.85	127.40
2	K	1	A	OP1-P-OP2	-11.52	102.33	119.60
2	G	1	A	N3-C4-N9	11.47	136.58	127.40
2	J	1	A	N3-C4-N9	11.43	136.54	127.40
2	I	3	A	C5-N7-C8	11.31	109.55	103.90
2	I	3	A	N9-C1'-C2'	-11.29	99.32	114.00
2	J	1	A	C4-C5-N7	-11.24	105.08	110.70
2	J	3	A	C5-N7-C8	11.17	109.49	103.90
2	K	1	A	C6-C5-N7	11.10	140.07	132.30
2	K	1	A	C4-C5-N7	-11.04	105.18	110.70
2	H	1	A	N3-C4-N9	11.00	136.20	127.40
2	K	1	A	N3-C4-N9	10.93	136.14	127.40
2	H	1	A	C4-C5-N7	-10.89	105.26	110.70
2	H	1	A	C6-C5-N7	10.83	139.88	132.30
2	G	1	A	C4-C5-N7	-10.82	105.29	110.70
2	I	1	A	C4-C5-N7	-10.79	105.30	110.70
2	H	3	A	C5-N7-C8	10.41	109.10	103.90
2	H	3	A	N1-C2-N3	-10.09	124.26	129.30
2	J	1	A	C5-N7-C8	9.97	108.88	103.90
2	H	3	A	C6-C5-N7	9.76	139.13	132.30
2	K	2	A	C5-N7-C8	9.72	108.76	103.90
2	H	2	A	C5-N7-C8	9.41	108.60	103.90
2	G	1	A	C5-N7-C8	9.38	108.59	103.90
2	J	3	A	N9-C1'-C2'	-9.36	101.71	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	3	A	C6-C5-N7	9.35	138.84	132.30
2	J	3	A	N9-C4-C5	-9.28	102.09	105.80
2	I	1	A	C5-N7-C8	9.24	108.52	103.90
2	H	3	A	C5-C6-N6	-9.22	116.33	123.70
2	G	3	A	C1'-O4'-C4'	-9.17	102.56	109.90
2	G	1	A	N9-C4-C5	-9.13	102.15	105.80
2	K	1	A	C5-N7-C8	9.12	108.46	103.90
2	H	1	A	C5-N7-C8	9.06	108.43	103.90
2	J	1	A	C3'-C2'-C1'	9.05	108.74	101.50
2	I	1	A	N9-C4-C5	-8.98	102.21	105.80
2	G	1	A	OP1-P-OP2	-8.97	106.15	119.60
2	G	3	A	N1-C2-N3	-8.96	124.82	129.30
2	I	1	A	C3'-C2'-C1'	8.94	108.65	101.50
2	J	1	A	N9-C4-C5	-8.90	102.24	105.80
2	J	1	A	C6-C5-N7	8.88	138.52	132.30
2	G	1	A	C3'-C2'-C1'	8.87	108.59	101.50
2	K	2	A	N1-C2-N3	-8.80	124.90	129.30
2	K	3	A	N1-C2-N3	-8.71	124.95	129.30
2	G	1	A	C6-C5-N7	8.65	138.35	132.30
2	H	1	A	N9-C4-C5	-8.65	102.34	105.80
2	H	2	A	N1-C2-N3	-8.49	125.05	129.30
2	I	3	A	N9-C4-C5	-8.40	102.44	105.80
2	I	1	A	N3-C4-C5	-8.37	120.94	126.80
2	I	1	A	C6-C5-N7	8.33	138.13	132.30
2	K	1	A	N9-C4-C5	-8.32	102.47	105.80
2	H	2	A	C5-C6-N6	-8.32	117.05	123.70
2	K	1	A	C5-C6-N6	-8.31	117.06	123.70
2	J	2	A	OP1-P-OP2	-8.25	107.22	119.60
2	I	2	A	C5-C6-N1	8.21	121.81	117.70
2	G	2	A	OP1-P-OP2	-8.17	107.34	119.60
2	H	1	A	C5-C6-N6	-8.16	117.17	123.70
2	K	2	A	C5-C6-N6	-8.15	117.18	123.70
2	H	1	A	OP1-P-OP2	-8.12	107.42	119.60
2	I	2	A	N3-C4-C5	-8.08	121.14	126.80
2	I	2	A	OP1-P-OP2	-8.07	107.49	119.60
2	I	2	A	C8-N9-C1'	-8.05	113.20	127.70
2	I	1	A	OP1-P-OP2	-8.03	107.55	119.60
2	G	2	A	C5-C6-N1	8.03	121.71	117.70
2	I	3	A	N1-C2-N3	-8.00	125.30	129.30
2	K	3	A	C5-C6-N6	-8.00	117.30	123.70
2	J	1	A	N3-C4-C5	-7.98	121.21	126.80
2	I	2	A	O3'-P-O5'	7.98	119.16	104.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	2	A	OP1-P-OP2	-7.96	107.67	119.60
2	J	2	A	C8-N9-C1'	-7.95	113.40	127.70
2	I	2	A	C5-N7-C8	7.94	107.87	103.90
2	I	3	A	OP1-P-OP2	-7.92	107.72	119.60
2	G	2	A	N1-C2-N3	-7.90	125.35	129.30
2	G	1	A	N3-C4-C5	-7.90	121.27	126.80
2	J	2	A	C5-C6-N1	7.87	121.63	117.70
2	J	2	A	N3-C4-C5	-7.82	121.32	126.80
2	G	2	A	C5-N7-C8	7.81	107.81	103.90
2	G	2	A	N3-C4-C5	-7.79	121.35	126.80
2	K	1	A	N3-C4-C5	-7.73	121.39	126.80
2	J	2	A	C5-N7-C8	7.72	107.76	103.90
2	J	1	A	C1'-O4'-C4'	-7.71	103.73	109.90
2	J	3	A	N1-C2-N3	-7.71	125.44	129.30
2	H	2	A	O3'-P-O5'	7.70	118.62	104.00
2	I	1	A	O3'-P-O5'	7.67	118.58	104.00
2	G	3	A	O4'-C4'-C3'	7.67	112.24	106.10
2	K	2	A	O3'-P-O5'	7.66	118.55	104.00
2	K	3	A	C3'-C2'-O2'	7.64	135.45	113.30
2	H	1	A	N3-C4-C5	-7.63	121.46	126.80
2	K	3	A	C4-N9-C1'	-7.62	112.58	126.30
2	H	2	A	N3-C4-C5	-7.62	121.47	126.80
2	K	2	A	O4'-C1'-N9	7.59	114.27	108.20
2	J	2	A	O3'-P-O5'	7.57	118.39	104.00
2	H	3	A	C4-N9-C1'	-7.55	112.70	126.30
2	H	1	A	C3'-C2'-C1'	7.49	107.49	101.50
2	K	2	A	N3-C4-C5	-7.48	121.56	126.80
2	H	3	A	C3'-C2'-O2'	7.46	134.95	113.30
2	G	3	A	OP1-P-OP2	-7.44	108.43	119.60
2	G	3	A	N9-C4-C5	-7.40	102.84	105.80
2	G	1	A	O3'-P-O5'	7.37	118.01	104.00
2	G	3	A	C5-C6-N1	7.37	121.38	117.70
2	G	2	A	O3'-P-O5'	7.34	117.94	104.00
2	J	1	A	O3'-P-O5'	7.28	117.82	104.00
2	G	2	A	C8-N9-C1'	-7.26	114.64	127.70
2	J	3	A	OP1-P-OP2	-7.19	108.81	119.60
2	I	1	A	C1'-O4'-C4'	-7.16	104.17	109.90
2	J	2	A	N1-C2-N3	-7.06	125.77	129.30
2	H	3	A	OP1-P-OP2	-6.99	109.11	119.60
2	K	3	A	OP1-P-OP2	-6.97	109.14	119.60
2	G	1	A	C1'-O4'-C4'	-6.90	104.38	109.90
2	K	1	A	C3'-C2'-C1'	6.86	106.99	101.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	1	A	OP1-P-OP2	-6.80	109.40	119.60
2	K	1	A	O3'-P-O5'	6.79	116.89	104.00
2	I	2	A	C5-C6-N6	-6.77	118.28	123.70
2	G	1	A	C5-C6-N6	-6.70	118.34	123.70
2	I	1	A	C5-C6-N6	-6.69	118.35	123.70
2	H	2	A	OP1-P-OP2	-6.67	109.60	119.60
2	I	2	A	N1-C2-N3	-6.66	125.97	129.30
2	H	1	A	O3'-P-O5'	6.61	116.55	104.00
2	H	3	A	C3'-C2'-C1'	-6.54	96.26	101.50
2	G	3	A	C6-C5-N7	6.50	136.85	132.30
2	G	3	A	N9-C1'-C2'	-6.49	104.86	112.00
2	J	3	A	O4'-C4'-C3'	6.44	111.25	106.10
2	J	2	A	C5-C6-N6	-6.42	118.56	123.70
2	H	3	A	C4'-C3'-C2'	6.38	108.98	102.60
2	G	3	A	C5-C6-N6	-6.38	118.60	123.70
2	I	3	A	C5-C6-N1	6.34	120.87	117.70
2	J	1	A	C5-C6-N6	-6.33	118.64	123.70
2	J	3	A	C5-C6-N1	6.32	120.86	117.70
2	K	1	A	C4'-C3'-C2'	6.32	108.92	102.60
2	G	3	A	C5'-C4'-C3'	-6.29	105.93	116.00
2	J	3	A	C5-C6-N6	-6.26	118.69	123.70
2	K	3	A	C5'-C4'-C3'	-6.21	106.06	116.00
2	K	2	A	C8-N9-C1'	-6.19	116.56	127.70
2	H	2	A	C8-N9-C1'	-6.16	116.62	127.70
2	G	3	A	O4'-C1'-C2'	6.13	113.12	107.60
2	I	2	A	C3'-C2'-C1'	6.13	106.41	101.50
2	K	2	A	C4-N9-C1'	-6.13	115.27	126.30
2	H	2	A	C4-N9-C1'	-6.11	115.31	126.30
2	G	2	A	C5-C6-N6	-6.08	118.84	123.70
2	I	2	A	O4'-C1'-N9	6.07	113.06	108.20
2	H	2	A	O4'-C1'-N9	6.06	113.05	108.20
2	I	3	A	C5-C6-N6	-5.97	118.92	123.70
2	H	1	A	C1'-O4'-C4'	-5.80	105.26	109.90
2	I	1	A	C5-C6-N1	5.69	120.55	117.70
2	K	1	A	C1'-O4'-C4'	-5.68	105.36	109.90
2	I	3	A	O4'-C4'-C3'	5.68	110.64	106.10
2	J	1	A	C5-C6-N1	5.67	120.54	117.70
2	H	3	A	C5'-C4'-C3'	-5.67	106.94	116.00
2	I	3	A	C6-C5-N7	5.60	136.22	132.30
2	J	3	A	C4-C5-C6	5.56	119.78	117.00
2	G	1	A	C5-C6-N1	5.55	120.48	117.70
2	G	3	A	C3'-C2'-O2'	5.55	129.39	113.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	3	A	N9-C4-C5	-5.54	103.58	105.80
2	G	3	A	C4'-C3'-C2'	5.50	108.10	102.60
2	J	3	A	C1'-O4'-C4'	-5.44	105.55	109.90
2	I	3	A	C4-C5-C6	5.36	119.68	117.00
2	H	1	A	C4'-C3'-C2'	5.34	107.94	102.60
2	J	3	A	C6-C5-N7	5.33	136.03	132.30
2	J	3	A	O4'-C1'-C2'	5.21	112.28	107.60
2	G	2	A	C3'-C2'-C1'	5.20	105.66	101.50
2	K	3	A	C4'-C3'-C2'	5.15	107.75	102.60
2	I	3	A	C1'-O4'-C4'	-5.14	105.79	109.90
2	H	3	A	C6-N1-C2	-5.13	115.52	118.60
2	K	3	A	C3'-C2'-C1'	-5.11	97.41	101.50
2	J	1	A	O5'-C5'-C4'	-5.01	102.19	111.70

There are no chirality outliers.

There are no planarity outliers.

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	3518	0	3466	27	0
1	B	3528	0	3474	29	0
1	C	3522	0	3469	23	0
1	D	3528	0	3474	23	0
1	E	3472	0	3424	47	0
1	F	3510	0	3454	38	0
2	G	66	0	33	0	0
2	H	66	33	33	1	0
2	I	66	0	33	3	0
2	J	66	0	33	1	0
2	K	66	33	33	13	0
3	A	5	0	0	0	0
3	B	5	0	0	3	0
3	C	10	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	10	0	0	0	0
4	A	237	0	0	10	0
4	B	277	0	0	13	0
4	C	242	0	0	2	0
4	D	272	0	0	12	0
4	E	229	0	0	11	0
4	F	220	0	0	14	0
4	G	7	0	0	0	0
4	H	3	0	0	0	0
4	J	3	0	0	0	0
All	All	22938	66	20926	190	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 4.

All (190) 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:E:160:ASP:OD1	4:E:601:HOH:O	1.83	0.96
1:E:427:PRO:HB3	2:K:2:A:N7	1.82	0.95
1:B:343:THR:OG1	4:B:602:HOH:O	1.90	0.90
1:B:227:GLU:O	4:B:601:HOH:O	1.90	0.89
1:E:72:SER:OG	4:E:602:HOH:O	1.92	0.88
1:E:427:PRO:HB3	2:K:2:A:C5	2.09	0.87
1:F:136:ASN:ND2	4:F:601:HOH:O	2.05	0.86
1:F:133:VAL:N	4:F:601:HOH:O	2.09	0.85
1:A:437:ARG:NH1	4:A:605:HOH:O	2.12	0.82
1:D:368:LYS:NZ	4:D:603:HOH:O	2.13	0.82
1:D:138:ARG:NH1	4:D:604:HOH:O	2.14	0.81
1:E:427:PRO:HB3	2:K:2:A:C8	2.16	0.81
1:D:291:ARG:NH1	4:D:601:HOH:O	1.81	0.79
1:E:422:LEU:O	4:E:604:HOH:O	2.00	0.79
1:E:186:ILE:O	4:E:603:HOH:O	2.00	0.78
3:B:501:SO4:O4	4:B:603:HOH:O	2.04	0.76
1:E:262:ASP:OD2	1:F:108:THR:OG1	2.02	0.75
1:C:15:ILE:O	4:C:601:HOH:O	2.05	0.74
1:C:344:LYS:HE3	1:C:383:LEU:HD11	1.68	0.74
1:A:462:LEU:O	4:A:603:HOH:O	2.05	0.74
1:F:382:ARG:HH11	1:F:384:ASN:HD21	1.34	0.73
1:B:186:ILE:O	4:B:605:HOH:O	2.07	0.73
1:B:261:PRO:O	4:B:604:HOH:O	2.06	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:501:SO4:S	4:B:603:HOH:O	2.46	0.72
1:F:174:SER:O	4:F:603:HOH:O	2.08	0.72
1:A:425:LYS:NZ	4:A:608:HOH:O	2.23	0.71
1:F:138:ARG:NH1	4:F:606:HOH:O	2.23	0.70
1:A:454:TYR:O	4:A:604:HOH:O	2.08	0.70
1:B:238:LYS:HE3	4:B:694:HOH:O	1.91	0.70
1:B:449:TRP:O	4:B:606:HOH:O	2.10	0.70
1:D:231:GLN:OE1	4:D:602:HOH:O	2.11	0.67
1:A:453:GLN:HG2	4:A:622:HOH:O	1.95	0.66
1:F:133:VAL:CA	4:F:601:HOH:O	2.43	0.66
1:A:263:ARG:NH1	4:A:602:HOH:O	2.04	0.66
1:C:331:THR:OG1	4:C:602:HOH:O	2.13	0.65
1:C:348:VAL:HB	1:C:381:PRO:HA	1.77	0.65
1:A:344:LYS:HD2	4:A:618:HOH:O	1.97	0.65
1:A:451:ASP:OD2	4:A:606:HOH:O	2.14	0.65
1:F:357:ILE:HD11	1:F:377:VAL:O	1.98	0.63
1:E:259:ASN:HB3	2:K:1:A:C2	2.33	0.63
1:A:358:VAL:HG11	1:A:408:LEU:HD21	1.81	0.62
1:D:382:ARG:HH11	1:D:384:ASN:HD21	1.47	0.62
1:D:240:ASN:HB3	4:D:803:HOH:O	1.99	0.62
1:A:346:GLU:HG2	1:A:346:GLU:O	1.98	0.62
1:D:439:ASN:ND2	4:D:607:HOH:O	2.33	0.61
1:E:335:LYS:HE3	1:E:395:GLU:HB2	1.83	0.60
1:C:358:VAL:HG11	1:C:408:LEU:HD21	1.83	0.60
1:B:382:ARG:HH11	1:B:384:ASN:HD21	1.50	0.59
1:E:382:ARG:HH11	1:E:384:ASN:HD21	1.49	0.59
1:D:437:ARG:HD3	4:D:820:HOH:O	2.01	0.59
1:F:321:GLU:HG2	1:F:330:ARG:HG2	1.83	0.59
1:E:29:ARG:NH1	1:E:179:GLU:OE1	2.37	0.58
1:D:323:GLU:HB3	4:D:826:HOH:O	2.03	0.58
1:B:392:ASP:OD1	1:B:392:ASP:N	2.38	0.57
1:C:347:ALA:HB3	1:C:382:ARG:HB2	1.84	0.57
1:C:382:ARG:HE	1:C:384:ASN:HD21	1.53	0.57
1:D:425:LYS:NZ	4:D:612:HOH:O	2.38	0.57
1:E:59:GLU:OE2	4:E:605:HOH:O	2.17	0.57
1:A:337:LYS:O	1:A:399:LEU:HD12	2.05	0.56
1:B:52:GLU:OE1	1:B:94:LYS:NZ	2.36	0.56
1:C:382:ARG:NH1	1:C:384:ASN:OD1	2.38	0.56
1:E:106:TYR:HB3	1:E:110:ILE:HD11	1.86	0.56
1:F:187:GLU:HA	4:F:602:HOH:O	2.06	0.56
1:C:375:ASN:OD1	1:C:375:ASN:N	2.38	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:SER:HB3	1:B:60:LYS:O	2.06	0.55
1:F:324:HIS:ND1	4:F:609:HOH:O	2.33	0.55
1:F:59:GLU:HG3	4:F:610:HOH:O	2.07	0.55
1:D:357:ILE:HD11	1:D:377:VAL:O	2.06	0.55
1:F:218:GLU:OE1	4:F:604:HOH:O	2.18	0.55
1:F:357:ILE:HB	1:F:382:ARG:HA	1.89	0.55
1:A:341:PHE:HB2	1:A:399:LEU:HD22	1.88	0.54
1:D:337:LYS:O	1:D:399:LEU:HD12	2.08	0.54
1:E:59:GLU:HG3	4:E:605:HOH:O	2.08	0.53
1:C:358:VAL:HG22	1:C:383:LEU:HB3	1.91	0.53
3:B:501:SO4:O3	4:B:603:HOH:O	2.18	0.53
1:E:426:ALA:HB1	1:E:427:PRO:HD2	1.90	0.53
1:F:52:GLU:OE1	1:F:94:LYS:NZ	2.33	0.52
1:F:29:ARG:NE	4:F:608:HOH:O	2.32	0.52
2:I:3:A:N3	2:I:3:A:H2'	2.19	0.52
1:C:374:ILE:HD12	1:C:374:ILE:H	1.74	0.52
1:C:355:GLU:HG2	1:C:419:LYS:HB3	1.92	0.52
1:F:227:GLU:O	4:F:605:HOH:O	2.19	0.51
1:D:439:ASN:CB	4:D:607:HOH:O	2.58	0.51
1:B:355:GLU:HG2	1:B:419:LYS:HB3	1.91	0.51
1:F:368:LYS:HD2	1:F:368:LYS:H	1.76	0.51
1:E:358:VAL:HG11	1:E:408:LEU:HD21	1.92	0.51
1:D:341:PHE:HB2	1:D:399:LEU:HD22	1.92	0.51
1:D:83:ARG:HG3	1:D:154:LEU:HD11	1.93	0.50
1:C:51:ILE:HB	1:C:66:TYR:HB2	1.93	0.50
1:F:448:ASP:HB2	1:F:457:THR:HG21	1.93	0.50
1:B:231:GLN:OE1	4:B:607:HOH:O	2.20	0.50
1:C:426:ALA:HB1	1:C:427:PRO:HD2	1.94	0.50
1:B:168:ASN:HB3	1:B:170:GLU:OE1	2.11	0.50
1:F:177:LEU:HD21	1:F:197:LYS:HD3	1.93	0.50
1:F:382:ARG:NH1	1:F:384:ASN:HD21	2.05	0.50
1:F:357:ILE:HG13	1:F:380:LEU:HB2	1.93	0.49
1:F:29:ARG:NH1	4:F:613:HOH:O	2.44	0.49
1:C:375:ASN:HA	1:C:378:LYS:HG2	1.94	0.49
1:E:321:GLU:OE1	4:E:606:HOH:O	2.20	0.49
1:E:51:ILE:HB	1:E:66:TYR:HB2	1.94	0.49
1:A:51:ILE:HB	1:A:66:TYR:HB2	1.95	0.49
1:D:358:VAL:HG11	1:D:408:LEU:HD21	1.94	0.49
1:E:107:ASN:HB3	1:E:110:ILE:HG13	1.95	0.48
1:D:355:GLU:HG2	1:D:419:LYS:HB3	1.94	0.48
1:F:358:VAL:HG11	1:F:408:LEU:HD21	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:383:LEU:HD22	1:F:411:PHE:CG	2.49	0.48
1:D:346:GLU:HB3	1:D:349:GLU:OE1	2.13	0.48
1:E:257:ASP:OD2	1:F:107:ASN:ND2	2.46	0.48
1:D:439:ASN:HB2	4:D:607:HOH:O	2.14	0.47
1:C:373:THR:HG22	1:C:454:TYR:HB2	1.96	0.47
1:E:335:LYS:HG3	1:E:395:GLU:HG3	1.96	0.47
1:E:373:THR:HG22	1:E:454:TYR:HB2	1.94	0.47
1:B:340:GLN:HG3	1:B:403:GLU:OE2	2.14	0.47
1:F:426:ALA:HB1	1:F:427:PRO:HD2	1.96	0.47
2:I:2:A:H8	2:I:2:A:H2'	1.56	0.47
1:B:262:ASP:HA	4:B:604:HOH:O	2.14	0.47
1:F:51:ILE:HB	1:F:66:TYR:HB2	1.97	0.47
1:C:106:TYR:HB3	1:C:110:ILE:HD11	1.96	0.47
1:B:426:ALA:HB1	1:B:427:PRO:HD2	1.97	0.47
1:E:427:PRO:CB	2:K:2:A:C5	2.90	0.47
1:A:189:LEU:O	1:A:193:VAL:HG23	2.15	0.47
1:E:337:LYS:N	1:E:395:GLU:HG2	2.30	0.47
1:B:106:TYR:HB3	1:B:110:ILE:HD11	1.97	0.46
1:A:14:ALA:N	4:A:614:HOH:O	2.47	0.46
1:A:188:LEU:HD21	1:A:225:LEU:HD23	1.97	0.46
1:E:391:ILE:HB	2:K:2:A:N6	2.31	0.46
1:E:454:TYR:OH	2:K:3:A:N7	2.39	0.46
1:A:426:ALA:HB1	1:A:427:PRO:HD2	1.98	0.46
1:E:441:ILE:HG13	1:E:442:CYS:N	2.31	0.46
1:B:393:ASN:OD1	1:B:396:THR:N	2.39	0.46
1:D:257:ASP:OD2	1:E:107:ASN:ND2	2.49	0.46
1:F:181:GLN:NE2	4:F:602:HOH:O	2.49	0.45
1:E:357:ILE:HD11	1:E:377:VAL:O	2.16	0.45
2:J:3:A:N3	2:J:3:A:H2'	2.28	0.45
1:E:391:ILE:HB	2:K:2:A:H61	1.81	0.45
1:E:427:PRO:HB3	2:K:2:A:C4	2.50	0.45
1:F:188:LEU:HD21	1:F:225:LEU:HD23	1.98	0.45
1:A:106:TYR:HB3	1:A:110:ILE:HD11	1.99	0.45
1:C:353:GLU:HG3	1:C:381:PRO:CG	2.47	0.45
1:F:29:ARG:NH1	4:F:612:HOH:O	2.37	0.45
1:A:316:ARG:HD3	4:A:619:HOH:O	2.17	0.45
1:E:370:ILE:HD12	1:E:382:ARG:CZ	2.47	0.45
1:F:355:GLU:HG2	1:F:419:LYS:HB3	1.98	0.44
1:B:402:ARG:NH2	4:B:617:HOH:O	2.50	0.44
1:E:337:LYS:O	1:E:399:LEU:HD12	2.17	0.44
1:E:301:ARG:HD3	2:K:1:A:O4'	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:GLU:OE1	1:A:94:LYS:NZ	2.41	0.44
1:F:350:PRO:HG2	1:F:415:ASN:OD1	2.18	0.44
1:A:333:ASP:O	1:A:334:HIS:HB2	2.18	0.44
1:F:370:ILE:HG13	1:F:382:ARG:CZ	2.47	0.44
1:A:382:ARG:HH11	1:A:384:ASN:HD21	1.65	0.43
1:B:348:VAL:HB	1:B:381:PRO:HA	2.00	0.43
1:C:412:LYS:HA	1:C:417:LEU:HD12	2.00	0.43
1:D:353:GLU:HG2	1:D:353:GLU:H	1.51	0.43
1:A:408:LEU:HD22	1:A:420:LEU:HD13	2.00	0.43
1:E:427:PRO:HG3	2:K:2:A:C6	2.53	0.43
1:B:291:ARG:NH1	4:B:614:HOH:O	2.45	0.43
1:E:316:ARG:HD3	4:E:618:HOH:O	2.19	0.43
1:E:341:PHE:HB2	1:E:399:LEU:HD22	2.01	0.43
1:E:427:PRO:HA	2:K:2:A:OP2	2.19	0.42
2:I:3:A:H5'	2:I:3:A:N3	2.34	0.42
1:E:423:PHE:HA	4:E:604:HOH:O	2.20	0.42
1:C:309:GLY:O	1:C:436:HIS:HA	2.19	0.42
1:B:408:LEU:HD22	1:B:420:LEU:HD13	2.02	0.42
1:A:358:VAL:HG21	1:A:408:LEU:CD2	2.50	0.42
1:E:189:LEU:O	1:E:193:VAL:HG23	2.19	0.42
1:B:344:LYS:HG3	1:B:383:LEU:HD11	2.02	0.42
1:F:285:ILE:HD13	1:F:294:LEU:HD21	2.01	0.42
1:E:52:GLU:OE1	1:E:94:LYS:NZ	2.43	0.41
1:B:434:LEU:O	1:B:438:LEU:HG	2.21	0.41
1:E:427:PRO:HD3	2:K:2:A:C4	2.55	0.41
1:B:397:LEU:HD21	1:B:433:VAL:HG21	2.02	0.41
1:E:262:ASP:HB2	4:E:637:HOH:O	2.20	0.41
1:A:382:ARG:NE	1:A:384:ASN:OD1	2.54	0.41
1:B:357:ILE:HD11	1:B:377:VAL:O	2.21	0.41
1:E:15:ILE:HA	4:E:726:HOH:O	2.20	0.41
1:A:373:THR:HG22	1:A:454:TYR:HB2	2.01	0.41
1:B:257:ASP:OD2	1:C:107:ASN:ND2	2.53	0.41
1:C:346:GLU:O	1:C:346:GLU:HG2	2.20	0.41
1:D:132:SER:N	4:D:626:HOH:O	2.54	0.41
1:F:336:GLN:HG2	1:F:398:ASN:HB3	2.03	0.41
1:B:390:ALA:HB1	2:H:2:A:N1	2.36	0.41
1:E:235:ASP:HA	1:E:236:PRO:HD3	1.92	0.40
1:E:336:GLN:HG2	1:E:398:ASN:HB3	2.02	0.40
1:F:106:TYR:HB3	1:F:110:ILE:HD11	2.04	0.40
1:A:77:GLU:O	1:A:81:GLU:HG2	2.22	0.40
1:B:235:ASP:HA	1:B:236:PRO:HD3	1.93	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:PHE:O	1:C:214:ARG:HD2	2.21	0.40
1:D:309:GLY:O	1:D:436:HIS:HA	2.21	0.40
1:F:227:GLU:H	1:F:227:GLU:CD	2.25	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%)	423 (98%)	11 (2%)	0	100	100
1	B	436/462 (94%)	427 (98%)	9 (2%)	0	100	100
1	C	435/462 (94%)	425 (98%)	10 (2%)	0	100	100
1	D	436/462 (94%)	429 (98%)	7 (2%)	0	100	100
1	E	426/462 (92%)	417 (98%)	9 (2%)	0	100	100
1	F	431/462 (93%)	421 (98%)	10 (2%)	0	100	100
All	All	2598/2772 (94%)	2542 (98%)	56 (2%)	0	100	100

There are no Ramachandran outliers to report.

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%)	388 (99%)	4 (1%)	76 82
1	B	393/411 (96%)	389 (99%)	4 (1%)	76 82
1	C	392/411 (95%)	387 (99%)	5 (1%)	69 75
1	D	393/411 (96%)	389 (99%)	4 (1%)	76 82
1	E	387/411 (94%)	385 (100%)	2 (0%)	88 92
1	F	391/411 (95%)	387 (99%)	4 (1%)	76 82
All	All	2348/2466 (95%)	2325 (99%)	23 (1%)	76 82

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ARG
1	A	113	LEU
1	A	353	GLU
1	A	439	ASN
1	B	84	ARG
1	B	113	LEU
1	B	338	GLU
1	B	353	GLU
1	C	84	ARG
1	C	113	LEU
1	C	375	ASN
1	C	412	LYS
1	C	439	ASN
1	D	57	SER
1	D	84	ARG
1	D	113	LEU
1	D	353	GLU
1	E	84	ARG
1	E	113	LEU
1	F	29	ARG
1	F	84	ARG
1	F	113	LEU
1	F	448	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	71	HIS
1	E	324	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	384	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	G	3/3 (100%)	1 (33%)	1 (33%)
2	H	3/3 (100%)	1 (33%)	1 (33%)
2	I	3/3 (100%)	1 (33%)	1 (33%)
2	J	2/3 (66%)	1 (50%)	0
2	K	2/3 (66%)	1 (50%)	0
All	All	13/15 (86%)	5 (38%)	3 (23%)

All (5) RNA backbone outliers are listed below:

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

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	G	1	A
2	H	1	A
2	I	1	A

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

8 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	0.05	0
3	SO4	A	501	-	4,4,4	0.12	0	6,6,6	0.15	0
3	SO4	D	501	-	4,4,4	0.14	0	6,6,6	0.17	0
3	SO4	B	501	-	4,4,4	0.16	0	6,6,6	0.13	0
3	SO4	F	502	-	4,4,4	0.14	0	6,6,6	0.14	0
3	SO4	C	501	-	4,4,4	0.15	0	6,6,6	0.15	0
3	SO4	E	501	-	4,4,4	0.18	0	6,6,6	0.11	0
3	SO4	C	502	-	4,4,4	0.14	0	6,6,6	0.05	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 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	SO4	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 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, 95^{th} 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%)	0.43	30 (6%) 17 21	28, 47, 77, 101	0
1	B	440/462 (95%)	0.33	19 (4%) 35 41	25, 45, 85, 111	0
1	C	439/462 (95%)	0.58	44 (10%) 7 9	28, 49, 99, 130	0
1	D	440/462 (95%)	0.35	17 (3%) 39 45	28, 45, 82, 110	0
1	E	432/462 (93%)	0.65	49 (11%) 5 6	28, 53, 108, 129	0
1	F	437/462 (94%)	0.85	80 (18%) 1 1	31, 54, 114, 148	0
2	G	3/3 (100%)	-0.69	0 100 100	50, 50, 55, 56	0
2	H	3/3 (100%)	0.99	0 100 100	66, 66, 68, 69	0
2	I	3/3 (100%)	0.84	0 100 100	95, 95, 95, 97	0
2	J	3/3 (100%)	-0.75	0 100 100	46, 46, 52, 53	0
2	K	3/3 (100%)	2.45	1 (33%) 0 0	76, 76, 77, 78	0
All	All	2641/2787 (94%)	0.53	240 (9%) 9 12	25, 49, 100, 148	0

All (240) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	133	VAL	8.4
1	C	347	ALA	7.6
1	C	133	VAL	7.4
1	C	345	ILE	6.9
1	F	413	SER	6.8
1	D	350	PRO	6.7
1	A	347	ALA	6.7
1	F	409	VAL	6.7
1	D	345	ILE	6.6
1	F	380	LEU	6.6
1	B	171	ASN	6.5
1	C	348	VAL	6.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	383	LEU	6.1
1	D	347	ALA	6.1
1	F	361	GLY	6.0
1	C	379	SER	5.7
1	F	350	PRO	5.6
1	F	373	THR	5.6
1	D	348	VAL	5.6
1	F	372	SER	5.5
1	F	411	PHE	5.5
1	E	374	ILE	5.5
1	C	350	PRO	5.4
1	F	410	SER	5.4
1	A	350	PRO	5.4
1	F	334	HIS	5.3
1	C	135	VAL	5.2
1	E	379	SER	5.1
1	F	135	VAL	5.0
1	A	348	VAL	5.0
1	E	418	SER	5.0
1	F	416	LYS	4.9
1	F	329	TYR	4.9
1	A	133	VAL	4.8
1	D	133	VAL	4.8
1	E	373	THR	4.8
1	B	371	ASP	4.8
1	C	385	LEU	4.7
1	F	345	ILE	4.6
1	F	383	LEU	4.6
1	E	338	GLU	4.6
1	C	134	SER	4.6
1	E	377	VAL	4.6
1	B	347	ALA	4.6
1	F	336	GLN	4.5
1	E	380	LEU	4.4
1	D	372	SER	4.4
1	C	340	GLN	4.3
1	A	346	GLU	4.3
1	E	376	GLU	4.3
1	C	351	GLN	4.3
1	F	379	SER	4.3
1	C	375	ASN	4.2
1	D	374	ILE	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	377	VAL	4.2
1	A	349	GLU	4.1
1	E	133	VAL	4.1
1	C	368	LYS	4.1
1	A	189	LEU	4.1
1	C	370	ILE	4.1
1	F	342	PHE	4.1
1	E	342	PHE	4.1
1	F	134	SER	4.0
1	E	411	PHE	4.0
1	E	416	LYS	4.0
1	A	351	GLN	4.0
1	F	338	GLU	4.0
1	F	346	GLU	4.0
1	F	354	THR	3.9
1	F	374	ILE	3.9
1	C	367	GLY	3.8
1	E	171	ASN	3.8
1	E	378	LYS	3.8
1	F	337	LYS	3.8
1	E	413	SER	3.8
1	F	351	GLN	3.8
1	E	375	ASN	3.8
2	K	2	A	3.7
1	F	368	LYS	3.7
1	F	396	THR	3.7
1	A	171	ASN	3.7
1	F	389	HIS	3.7
1	A	373	THR	3.6
1	F	340	GLN	3.6
1	F	399	LEU	3.6
1	E	462	LEU	3.6
1	D	352	GLY	3.6
1	F	392	ASP	3.5
1	F	395	GLU	3.5
1	E	385	LEU	3.5
1	F	376	GLU	3.5
1	F	171	ASN	3.5
1	F	367	GLY	3.5
1	A	190	ARG	3.5
1	F	170	GLU	3.5
1	F	377	VAL	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	379	SER	3.5
1	E	399	LEU	3.4
1	F	385	LEU	3.4
1	E	354	THR	3.4
1	B	338	GLU	3.4
1	B	399	LEU	3.4
1	C	359	ALA	3.4
1	A	135	VAL	3.4
1	E	409	VAL	3.4
1	E	334	HIS	3.4
1	F	366	ILE	3.4
1	C	378	LYS	3.4
1	C	386	GLU	3.4
1	A	345	ILE	3.3
1	C	376	GLU	3.3
1	E	396	THR	3.3
1	E	324	HIS	3.3
1	A	187	GLU	3.3
1	C	377	VAL	3.3
1	B	375	ASN	3.3
1	D	134	SER	3.3
1	F	341	PHE	3.2
1	C	349	GLU	3.1
1	C	383	LEU	3.1
1	E	440	GLY	3.1
1	F	412	LYS	3.1
1	D	375	ASN	3.1
1	F	418	SER	3.1
1	F	344	LYS	3.1
1	E	391	ILE	3.1
1	C	371	ASP	3.0
1	D	373	THR	3.0
1	E	336	GLN	3.0
1	E	325	ASN	3.0
1	F	325	ASN	3.0
1	F	362	PHE	3.0
1	F	405	LYS	3.0
1	C	336	GLN	3.0
1	C	334	HIS	2.9
1	F	378	LYS	2.9
1	C	372	SER	2.9
1	F	352	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	441	ILE	2.9
1	F	440	GLY	2.9
1	A	374	ILE	2.9
1	F	370	ILE	2.9
1	B	376	GLU	2.9
1	E	359	ALA	2.8
1	A	134	SER	2.8
1	A	372	SER	2.8
1	D	349	GLU	2.8
1	E	343	THR	2.8
1	C	171	ASN	2.8
1	C	384	ASN	2.8
1	F	408	LEU	2.8
1	F	349	GLU	2.8
1	C	364	THR	2.8
1	E	335	LYS	2.8
1	C	354	THR	2.7
1	C	389	HIS	2.7
1	D	462	LEU	2.7
1	A	136	ASN	2.7
1	E	337	LYS	2.7
1	C	365	ALA	2.7
1	D	13	GLY	2.7
1	A	416	LYS	2.7
1	F	335	LYS	2.7
1	F	324	HIS	2.6
1	A	352	GLY	2.6
1	C	366	ILE	2.6
1	F	391	ILE	2.6
1	F	390	ALA	2.6
1	E	392	ASP	2.6
1	E	414	GLU	2.6
1	F	406	SER	2.6
1	F	119	ARG	2.6
1	A	376	GLU	2.6
1	F	327	LEU	2.6
1	B	14	ALA	2.6
1	F	363	PRO	2.6
1	A	338	GLU	2.5
1	F	388	SER	2.5
1	E	369	ASP	2.5
1	E	327	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	103	CYS	2.5
1	F	375	ASN	2.5
1	F	382	ARG	2.5
1	B	351	GLN	2.4
1	F	172	SER	2.4
1	B	346	GLU	2.4
1	C	346	GLU	2.4
1	E	339	GLY	2.4
1	E	386	GLU	2.4
1	B	326	GLY	2.4
1	F	415	ASN	2.3
1	D	346	GLU	2.3
1	D	351	GLN	2.3
1	A	379	SER	2.3
1	B	349	GLU	2.3
1	E	341	PHE	2.3
1	C	358	VAL	2.3
1	F	394	MET	2.3
1	A	381	PRO	2.3
1	F	330	ARG	2.3
1	A	380	LEU	2.3
1	B	133	VAL	2.3
1	E	439	ASN	2.2
1	F	323	GLU	2.2
1	E	340	GLN	2.2
1	F	442	CYS	2.2
1	B	132	SER	2.2
1	B	348	VAL	2.2
1	C	454	TYR	2.2
1	F	403	GLU	2.2
1	F	438	LEU	2.2
1	F	333	ASP	2.2
1	F	314	ALA	2.1
1	B	327	LEU	2.1
1	C	409	VAL	2.1
1	E	361	GLY	2.1
1	F	331	THR	2.1
1	F	414	GLU	2.1
1	A	415	ASN	2.1
1	C	149	LYS	2.1
1	F	43	ILE	2.1
1	C	342	PHE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	356	ALA	2.1
1	E	368	LYS	2.1
1	D	371	ASP	2.1
1	C	13	GLY	2.1
1	F	328	ILE	2.1
1	A	119	ARG	2.1
1	F	402	ARG	2.1
1	C	363	PRO	2.0
1	E	353	GLU	2.0
1	F	13	GLY	2.0
1	C	369	ASP	2.0
1	E	449	TRP	2.0
1	C	353	GLU	2.0
1	A	370	ILE	2.0
1	E	119	ARG	2.0
1	A	194	LYS	2.0
1	B	339	GLY	2.0
1	C	440	GLY	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 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, 95^{th} 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	C	502	5/5	0.75	0.12	128,128,129,131	0
3	SO4	F	501	5/5	0.81	0.19	134,134,136,136	0
3	SO4	A	501	5/5	0.96	0.14	49,55,60,62	0
3	SO4	C	501	5/5	0.97	0.17	48,51,60,66	0
3	SO4	E	501	5/5	0.98	0.14	41,49,56,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	D	501	5/5	0.98	0.16	46,52,58,66	0
3	SO4	F	502	5/5	0.99	0.12	50,52,60,63	0
3	SO4	B	501	5/5	0.99	0.14	47,48,54,64	0

6.5 Other polymers (i)

There are no such residues in this entry.