Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2023 – 07:04 AM EST

PDB ID	:	1WWJ
Title	:	crystal structure of KaiB from Synechocystis sp.
Authors	:	Hitomi, K.; Oyama, T.; Han, S.; Arvai, A.S.; Tainer, J.A.; Getzoff, E.D.
Deposited on	:	2005-01-06
Resolution	:	1.90 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

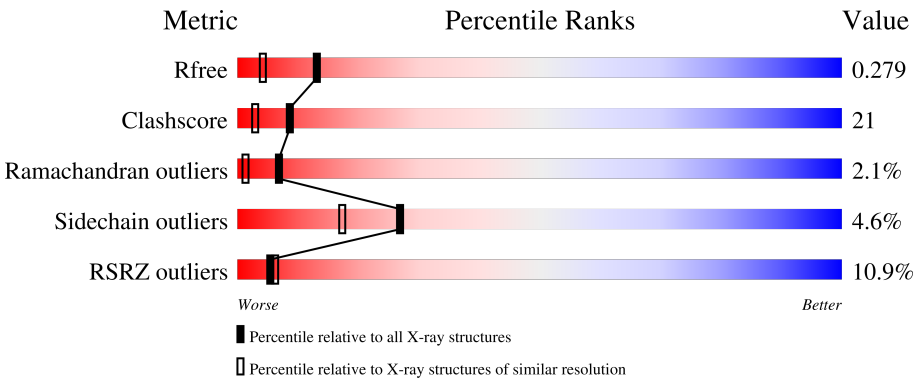
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	105	5% 62% 29% • 6%
1	B	105	12% 57% 29% • 13%
1	C	105	10% 53% 33% 7% 7%
1	D	105	12% 60% 30% • • 7%

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
2	MLT	A	6001	X	-	-	-
2	MLT	B	6002	X	-	-	-
2	MLT	B	6003	X	-	X	-
2	MLT	B	6004	X	-	-	-
2	MLT	B	6005	X	-	-	-
2	MLT	C	6006	X	-	-	-
2	MLT	C	6007	X	-	-	-
2	MLT	D	6008	X	-	-	X
3	BET	B	5002	-	X	-	X
3	BET	D	5001	-	X	-	-
4	IMD	B	7002	-	-	-	X

2 Entry composition (i)

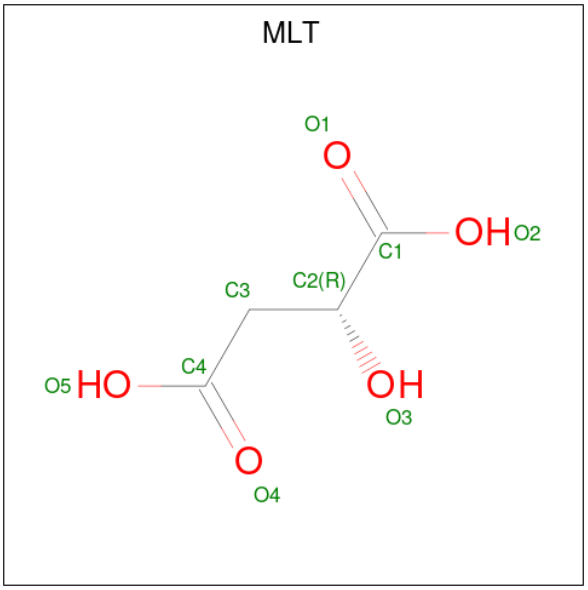
There are 5 unique types of molecules in this entry. The entry contains 3429 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Circadian clock protein kaiB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	99	788	514	129	143	2	0	0	0
1	B	91	719	469	117	132	1	0	0	0
1	C	98	779	509	128	140	2	0	0	0
1	D	98	779	509	128	140	2	0	0	0

- Molecule 2 is D-MALATE (three-letter code: MLT) (formula: $C_4H_6O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	9	4	5	0	0
2	B	1	9	4	5	0	0

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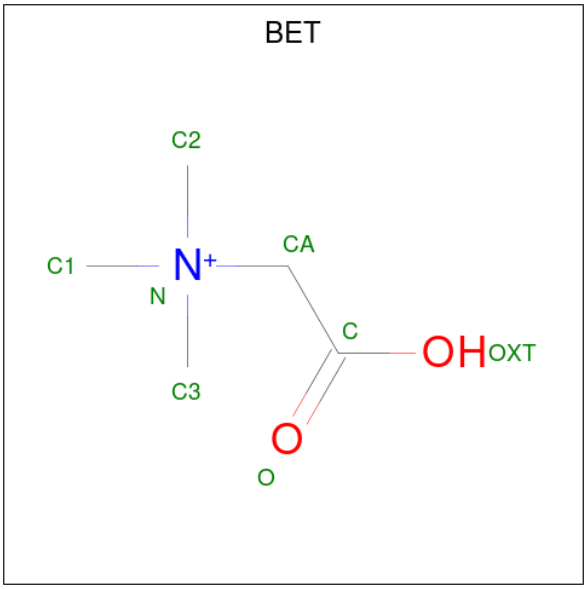
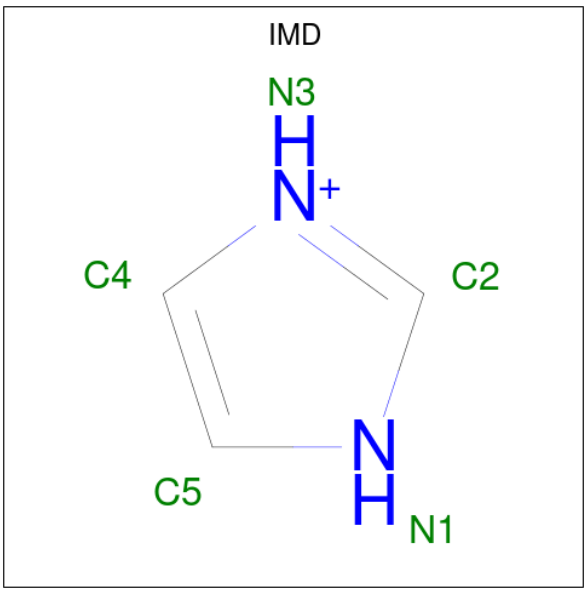
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
2	B	1	9	4	5		0	0
			Total	C	O			
2	B	1	9	4	5		0	0
			Total	C	O			
2	B	1	9	4	5		0	0
			Total	C	O			
2	C	1	9	4	5		0	0
			Total	C	O			
2	C	1	9	4	5		0	0
			Total	C	O			
2	D	1	9	4	5		0	0

- Molecule 3 is TRIMETHYL GLYCINE (three-letter code: BET) (formula: $C_5H_{12}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	8	5	1	2	0	0
			Total	C	N	O		
3	B	1	8	5	1	2	0	0
			Total	C	N	O		
3	B	1	8	5	1	2	0	0
			Total	C	N	O		
3	C	1	8	5	1	2	0	0
			Total	C	N	O		
3	D	1	8	5	1	2	0	0

- Molecule 4 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
4	B	1	5	3	2	0	0
			Total	C	N		
4	B	1	5	3	2	0	0
			Total	C	N		
4	D	1	5	3	2	0	0

- Molecule 5 is water.

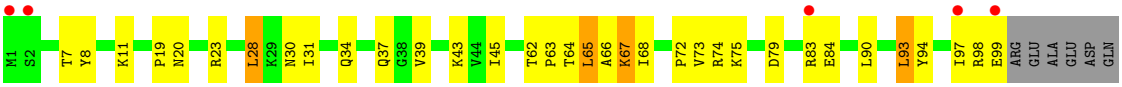
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	73	73	73	0	0
			Total	O		
5	B	58	58	58	0	0
			Total	O		
5	C	59	59	59	0	0
			Total	O		
5	D	47	47	47	0	0

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.

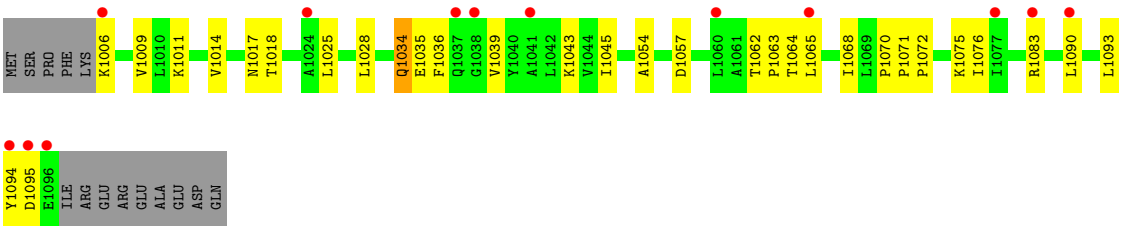
• Molecule 1: Circadian clock protein kaiB

Chain A:



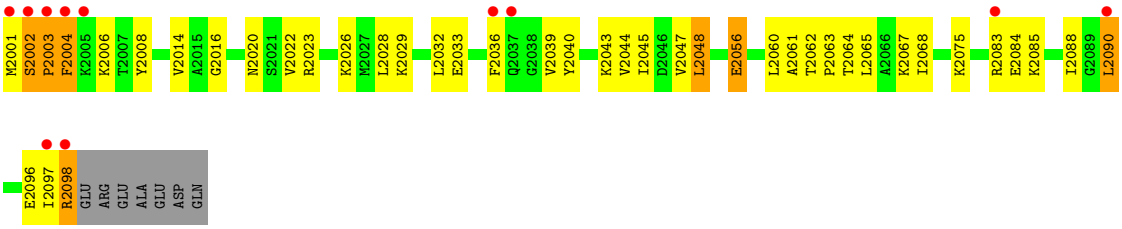
• Molecule 1: Circadian clock protein kaiB

Chain B:



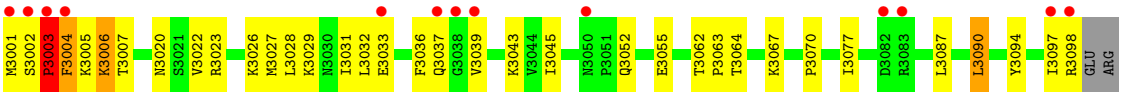
• Molecule 1: Circadian clock protein kaiB

Chain C:



• Molecule 1: Circadian clock protein kaiB

Chain D:



GLU
ALA
GLU
ASP
GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	52.77Å 66.04Å 114.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.04 – 1.90 28.04 – 1.90	Depositor EDS
% Data completeness (in resolution range)	90.7 (28.04-1.90) 90.7 (28.04-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.84 (at 1.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.250 , 0.284 0.240 , 0.279	Depositor DCC
R_{free} test set	1521 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	26.1	Xtriage
Anisotropy	0.731	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 64.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3429	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.20% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BET, MLT, IMD

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	0.35	0/800	0.64	0/1082
1	B	0.30	0/729	0.61	0/988
1	C	0.33	0/791	0.65	0/1070
1	D	0.32	0/791	0.63	0/1070
All	All	0.33	0/3111	0.63	0/4210

There are no bond length outliers.

There are no bond angle outliers.

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	788	0	853	34	0
1	B	719	0	777	27	0
1	C	779	0	844	51	0
1	D	779	0	844	37	0
2	A	9	0	4	0	0
2	B	36	0	16	6	0
2	C	18	0	8	1	0
2	D	9	0	4	0	0
3	A	8	0	11	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	16	0	22	0	0
3	C	8	0	11	0	0
3	D	8	0	11	0	0
4	B	10	0	10	2	0
4	D	5	0	5	0	0
5	A	73	0	0	4	0
5	B	58	0	0	2	0
5	C	59	0	0	4	0
5	D	47	0	0	1	0
All	All	3429	0	3420	136	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 21.

All (136) 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:D:3002:SER:HB3	1:D:3003:PRO:HD2	1.43	1.01
1:C:2061:ALA:O	1:C:2064:THR:HG22	1.58	1.00
1:A:34:GLN:OE1	1:D:3002:SER:HB2	1.63	0.98
1:B:1011:LYS:HE3	1:B:1093:LEU:HD11	1.48	0.95
1:B:1017:ASN:HB3	2:B:6003:MLT:H31	1.46	0.94
1:C:2098:ARG:HE	1:C:2098:ARG:N	1.72	0.87
1:B:1011:LYS:HE2	1:B:1043:LYS:HD3	1.56	0.86
1:C:2097:ILE:HA	1:C:2098:ARG:HH21	1.42	0.85
1:C:2002:SER:HA	1:C:2004:PHE:N	1.99	0.78
1:C:2065:LEU:HB2	1:C:2090:LEU:CD1	2.17	0.74
1:D:3029:LYS:HE2	1:D:3033:GLU:OE1	1.88	0.74
1:B:1064:THR:HB	5:B:4226:HOH:O	1.87	0.73
1:B:1017:ASN:CB	2:B:6003:MLT:H31	2.18	0.73
1:D:3002:SER:HB3	1:D:3003:PRO:CD	2.19	0.72
1:B:1093:LEU:HD22	2:B:6005:MLT:H31	1.72	0.72
1:C:2002:SER:HA	1:C:2004:PHE:H	1.54	0.72
1:A:11:LYS:HE3	1:A:93:LEU:HD21	1.73	0.71
1:C:2065:LEU:HB2	1:C:2090:LEU:HD11	1.74	0.70
1:C:2044:VAL:O	2:C:6007:MLT:H2	1.91	0.69
1:A:28:LEU:HD23	1:A:31:ILE:HD11	1.76	0.68
1:D:3036:PHE:O	1:D:3039:VAL:HG23	1.93	0.68
1:A:23:ARG:HD3	5:A:4176:HOH:O	1.94	0.67
1:C:2022:VAL:O	1:C:2026:LYS:HG3	1.95	0.66
1:A:67:LYS:HE3	1:D:3055:GLU:HG3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3003:PRO:HB2	1:D:3006:LYS:NZ	2.13	0.64
1:C:2098:ARG:HE	1:C:2098:ARG:H	1.41	0.64
1:C:2096:GLU:O	1:C:2097:ILE:HD13	1.99	0.63
1:C:2097:ILE:HA	1:C:2098:ARG:NH2	2.12	0.63
1:B:1009:VAL:HB	1:B:1093:LEU:HB2	1.80	0.63
1:D:3006:LYS:N	1:D:3006:LYS:HD2	2.15	0.61
1:B:1054:ALA:HB3	1:B:1057:ASP:OD2	2.01	0.61
1:C:2075:LYS:HE3	5:C:4149:HOH:O	2.00	0.61
1:A:43:LYS:HG2	1:A:45:ILE:HD11	1.83	0.60
1:D:3043:LYS:HG2	1:D:3045:ILE:HD11	1.81	0.60
1:C:2006:LYS:HG2	1:C:2096:GLU:HG2	1.83	0.60
1:D:3027:MET:O	1:D:3027:MET:HE2	2.02	0.60
1:B:1062:THR:HB	1:B:1063:PRO:HD3	1.83	0.59
1:C:2002:SER:HB2	1:C:2003:PRO:HA	1.84	0.59
1:D:3062:THR:HA	1:D:3090:LEU:HD11	1.84	0.58
1:C:2083:ARG:HG2	1:C:2083:ARG:HH11	1.68	0.58
1:A:11:LYS:HE3	1:A:93:LEU:CD2	2.34	0.58
1:A:8:TYR:CE1	1:D:3064:THR:HG21	2.40	0.57
1:A:34:GLN:HA	3:A:5003:BET:H32	1.86	0.57
1:A:62:THR:HA	1:A:90:LEU:HD21	1.85	0.57
1:D:3064:THR:O	1:D:3067:LYS:HE2	2.05	0.56
1:B:1011:LYS:CE	1:B:1093:LEU:HD11	2.30	0.56
1:C:2060:LEU:HB3	1:C:2064:THR:HG21	1.87	0.56
1:B:1094:TYR:HB2	1:C:2036:PHE:HZ	1.71	0.56
1:D:3002:SER:O	1:D:3003:PRO:O	2.24	0.56
1:C:2065:LEU:O	1:C:2068:ILE:HG12	2.07	0.55
1:C:2043:LYS:HD2	1:C:2045:ILE:HD11	1.88	0.55
1:A:45:ILE:HD12	1:A:45:ILE:N	2.22	0.55
1:B:1045:ILE:HD12	1:B:1045:ILE:N	2.21	0.55
1:D:3005:LYS:HG3	1:D:3097:ILE:HB	1.89	0.55
1:D:3003:PRO:HB2	1:D:3006:LYS:HZ1	1.72	0.54
1:A:31:ILE:HG22	1:D:3002:SER:HB3	1.89	0.54
1:C:2023:ARG:HG2	5:C:4203:HOH:O	2.07	0.54
1:C:2097:ILE:HG23	1:C:2098:ARG:HH21	1.73	0.54
1:A:90:LEU:HD23	1:A:90:LEU:N	2.23	0.53
1:A:64:THR:O	1:A:67:LYS:HD3	2.09	0.53
1:A:67:LYS:HE3	1:D:3055:GLU:CG	2.37	0.53
1:A:67:LYS:HD2	5:A:4197:HOH:O	2.08	0.53
1:D:3020:ASN:ND2	1:D:3023:ARG:HE	2.06	0.53
1:D:3027:MET:HE2	1:D:3031:ILE:HG13	1.91	0.53
1:A:19:PRO:HD2	5:A:4087:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:THR:HG21	1:A:97:ILE:HD11	1.91	0.52
1:A:28:LEU:HD21	1:A:73:VAL:HG13	1.90	0.52
1:C:2098:ARG:N	1:C:2098:ARG:NE	2.52	0.52
1:C:2065:LEU:HB2	1:C:2090:LEU:HD13	1.91	0.52
1:D:3022:VAL:O	1:D:3026:LYS:HG3	2.10	0.52
1:B:1064:THR:HG21	1:C:2008:TYR:CE1	2.45	0.51
1:B:1068:ILE:HD12	1:B:1068:ILE:O	2.11	0.50
1:D:3020:ASN:HD21	1:D:3023:ARG:HH21	1.60	0.50
1:A:99:GLU:O	1:A:99:GLU:HG2	2.12	0.49
1:B:1006:LYS:HD2	1:B:1094:TYR:CE2	2.47	0.49
1:C:2016:GLY:CA	1:C:2048:LEU:HD22	2.42	0.49
1:B:1065:LEU:HD11	1:C:2039:VAL:HG13	1.94	0.48
1:B:1075:LYS:O	4:B:7002:IMD:H4	2.12	0.48
1:C:2065:LEU:HD12	1:C:2090:LEU:CD1	2.44	0.48
1:C:2097:ILE:HG22	1:C:2098:ARG:N	2.28	0.48
1:D:3062:THR:HB	1:D:3063:PRO:HD3	1.94	0.48
1:C:2032:LEU:HD22	1:C:2040:TYR:HB2	1.95	0.47
1:A:20:ASN:HB2	1:A:84:GLU:CD	2.33	0.47
1:A:62:THR:HA	1:A:90:LEU:CD2	2.44	0.47
1:B:1036:PHE:HB3	1:B:1039:VAL:HB	1.97	0.47
1:C:2065:LEU:HD12	1:C:2090:LEU:HD13	1.96	0.47
1:C:2001:MET:O	1:C:2002:SER:CB	2.61	0.47
1:A:39:VAL:HG13	1:D:3064:THR:HG22	1.97	0.47
1:D:3045:ILE:HG12	5:D:4242:HOH:O	2.14	0.47
1:C:2062:THR:N	1:C:2063:PRO:HD2	2.29	0.47
1:B:1018:THR:HG22	2:B:6002:MLT:O2	2.15	0.46
1:C:2097:ILE:HG23	1:C:2098:ARG:NH2	2.30	0.46
1:D:3045:ILE:N	1:D:3045:ILE:HD12	2.30	0.46
1:A:72:PRO:HG2	1:D:3094:TYR:CZ	2.51	0.46
1:B:1025:LEU:HD11	2:B:6003:MLT:O4	2.16	0.46
1:A:64:THR:O	1:A:67:LYS:NZ	2.45	0.46
1:C:2014:VAL:O	1:C:2047:VAL:HG22	2.15	0.46
1:B:1028:LEU:HB2	1:B:1076:ILE:HG21	1.97	0.46
1:C:2098:ARG:H	1:C:2098:ARG:NE	2.10	0.46
1:D:3022:VAL:CG1	1:D:3026:LYS:HE3	2.46	0.46
1:C:2020:ASN:HB2	1:C:2084:GLU:OE1	2.16	0.45
1:C:2083:ARG:HG2	1:C:2083:ARG:NH1	2.30	0.45
1:C:2047:VAL:HG21	1:C:2088:ILE:HD11	1.97	0.45
1:C:2045:ILE:N	1:C:2045:ILE:HD12	2.32	0.45
1:B:1014:VAL:HG21	2:B:6003:MLT:H2	1.98	0.45
1:D:3022:VAL:HG12	1:D:3026:LYS:HE3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3028:LEU:O	1:D:3032:LEU:HG	2.16	0.45
1:B:1083:ARG:HD2	4:B:7002:IMD:H2	1.99	0.45
1:A:65:LEU:HD13	1:A:65:LEU:O	2.18	0.44
1:B:1034:GLN:HE21	1:B:1034:GLN:HB3	1.58	0.44
1:C:2033:GLU:HG2	5:C:4150:HOH:O	2.17	0.44
1:A:62:THR:N	1:A:63:PRO:HD2	2.33	0.44
1:C:2047:VAL:HG21	1:C:2088:ILE:CD1	2.47	0.44
1:D:3007:THR:OG1	1:D:3097:ILE:HD11	2.18	0.43
1:A:97:ILE:HG23	5:A:4183:HOH:O	2.19	0.43
1:C:2085:LYS:NZ	1:D:3052:GLN:HE22	2.16	0.43
1:A:65:LEU:O	1:A:68:ILE:HG12	2.19	0.43
1:C:2043:LYS:HD2	1:C:2045:ILE:CD1	2.49	0.42
1:C:2063:PRO:O	1:C:2067:LYS:HG3	2.19	0.42
1:D:3036:PHE:CZ	1:D:3070:PRO:HB3	2.53	0.42
1:A:11:LYS:CE	1:A:93:LEU:HD21	2.47	0.42
1:B:1071:PRO:N	1:B:1072:PRO:HD2	2.34	0.42
1:B:1035:GLU:HB3	5:B:4129:HOH:O	2.20	0.42
1:A:66:ALA:O	1:A:74:ARG:HG2	2.20	0.41
1:A:79:ASP:O	1:A:83:ARG:HB2	2.19	0.41
1:D:3004:PHE:O	1:D:3005:LYS:HB3	2.20	0.41
1:D:3097:ILE:O	1:D:3098:ARG:HB2	2.20	0.41
1:C:2002:SER:CA	1:C:2004:PHE:H	2.27	0.41
1:C:2097:ILE:CA	1:C:2098:ARG:HH21	2.24	0.41
1:A:30:ASN:HB3	1:D:3001:MET:HG2	2.02	0.41
1:C:2002:SER:CB	1:C:2003:PRO:HA	2.50	0.41
1:A:94:TYR:CD2	1:C:2056:GLU:HB3	2.56	0.40
1:B:1070:PRO:HA	1:B:1071:PRO:HD3	1.95	0.40
1:C:2064:THR:HB	5:C:4038:HOH:O	2.21	0.40
1:D:3077:ILE:HG23	1:D:3087:LEU:CD2	2.51	0.40
1:C:2029:LYS:O	1:C:2033:GLU:HG3	2.21	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	97/105 (92%)	93 (96%)	2 (2%)	2 (2%)	7	1
1	B	89/105 (85%)	83 (93%)	5 (6%)	1 (1%)	14	5
1	C	96/105 (91%)	89 (93%)	4 (4%)	3 (3%)	4	0
1	D	96/105 (91%)	87 (91%)	7 (7%)	2 (2%)	7	1
All	All	378/420 (90%)	352 (93%)	18 (5%)	8 (2%)	7	1

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	3003	PRO
1	A	98	ARG
1	D	3037	GLN
1	A	37	GLN
1	B	1095	ASP
1	C	2002	SER
1	C	2003	PRO
1	C	2004	PHE

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	89/94 (95%)	84 (94%)	5 (6%)	21	11
1	B	81/94 (86%)	79 (98%)	2 (2%)	47	41
1	C	88/94 (94%)	83 (94%)	5 (6%)	20	11
1	D	88/94 (94%)	84 (96%)	4 (4%)	27	18
All	All	346/376 (92%)	330 (95%)	16 (5%)	27	17

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	65	LEU
1	A	67	LYS
1	A	75	LYS
1	A	93	LEU
1	B	1034	GLN
1	B	1090	LEU
1	C	2028	LEU
1	C	2048	LEU
1	C	2056	GLU
1	C	2090	LEU
1	C	2098	ARG
1	D	3003	PRO
1	D	3004	PHE
1	D	3006	LYS
1	D	3090	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	B	1030	ASN
1	B	1034	GLN
1	C	2020	ASN
1	C	2034	GLN
1	C	2050	ASN
1	D	3020	ASN
1	D	3034	GLN
1	D	3052	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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)

16 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	$\#\|Z\| > 2$
2	MLT	B	6005	-	8,8,8	1.62	3 (37%)	10,10,10	1.79	4 (40%)
3	BET	B	5004	-	7,7,7	3.32	5 (71%)	10,10,10	0.76	0
3	BET	D	5001	-	7,7,7	3.39	5 (71%)	10,10,10	0.72	0
2	MLT	B	6004	-	8,8,8	1.63	2 (25%)	10,10,10	1.92	3 (30%)
2	MLT	C	6007	-	8,8,8	1.59	2 (25%)	10,10,10	2.15	4 (40%)
3	BET	C	5005	-	7,7,7	3.27	5 (71%)	10,10,10	0.82	0
3	BET	B	5002	-	7,7,7	3.33	5 (71%)	10,10,10	0.90	0
2	MLT	C	6006	-	8,8,8	1.89	2 (25%)	10,10,10	1.77	4 (40%)
2	MLT	A	6001	-	8,8,8	1.80	3 (37%)	10,10,10	1.86	4 (40%)
2	MLT	B	6002	-	8,8,8	1.95	2 (25%)	10,10,10	1.91	4 (40%)
3	BET	A	5003	-	7,7,7	3.34	5 (71%)	10,10,10	0.72	0
4	IMD	B	7001	-	3,5,5	0.65	0	4,5,5	0.49	0
2	MLT	D	6008	-	8,8,8	1.63	2 (25%)	10,10,10	2.05	4 (40%)
2	MLT	B	6003	-	8,8,8	1.67	2 (25%)	10,10,10	2.28	4 (40%)
4	IMD	D	7003	-	3,5,5	0.52	0	4,5,5	0.49	0
4	IMD	B	7002	-	3,5,5	0.58	0	4,5,5	0.44	0

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
2	MLT	B	6005	-	1/1/3/3	2/8/8/8	-
3	BET	B	5004	-	-	2/5/5/5	-
3	BET	D	5001	-	-	5/5/5/5	-
2	MLT	B	6004	-	1/1/3/3	1/8/8/8	-
2	MLT	C	6007	-	1/1/3/3	2/8/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BET	C	5005	-	-	2/5/5/5	-
3	BET	B	5002	-	-	5/5/5/5	-
2	MLT	C	6006	-	1/1/3/3	3/8/8/8	-
2	MLT	A	6001	-	1/1/3/3	0/8/8/8	-
2	MLT	B	6002	-	1/1/3/3	0/8/8/8	-
3	BET	A	5003	-	-	2/5/5/5	-
4	IMD	B	7001	-	-	-	0/1/1/1
2	MLT	D	6008	-	1/1/3/3	0/8/8/8	-
2	MLT	B	6003	-	1/1/3/3	2/8/8/8	-
4	IMD	D	7003	-	-	-	0/1/1/1
4	IMD	B	7002	-	-	-	0/1/1/1

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	5001	BET	C3-N	-4.57	1.36	1.50
3	A	5003	BET	C3-N	-4.50	1.36	1.50
3	B	5002	BET	C3-N	-4.35	1.37	1.50
3	B	5004	BET	C3-N	-4.35	1.37	1.50
3	D	5001	BET	CA-N	-4.35	1.42	1.50
2	B	6002	MLT	O1-C1	4.32	1.35	1.22
3	C	5005	BET	C3-N	-4.29	1.37	1.50
3	B	5004	BET	CA-N	-4.21	1.42	1.50
3	B	5002	BET	CA-N	-4.16	1.42	1.50
3	A	5003	BET	CA-N	-4.15	1.42	1.50
3	C	5005	BET	CA-N	-4.05	1.43	1.50
3	B	5004	BET	C2-N	-4.03	1.38	1.50
3	D	5001	BET	C2-N	-4.02	1.38	1.50
3	B	5002	BET	C2-N	-4.00	1.38	1.50
3	A	5003	BET	C2-N	-4.00	1.38	1.50
3	A	5003	BET	C1-N	-3.97	1.38	1.50
3	C	5005	BET	C1-N	-3.90	1.38	1.50
3	D	5001	BET	C1-N	-3.89	1.38	1.50
3	B	5002	BET	C1-N	-3.89	1.38	1.50
3	C	5005	BET	C2-N	-3.86	1.38	1.50
3	B	5004	BET	C1-N	-3.85	1.38	1.50
2	A	6001	MLT	O4-C4	3.51	1.33	1.22
2	C	6006	MLT	O1-C1	3.51	1.32	1.22
2	B	6003	MLT	O1-C1	3.41	1.32	1.22
2	C	6007	MLT	O1-C1	3.40	1.32	1.22
2	D	6008	MLT	O1-C1	3.39	1.32	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6004	MLT	O4-C4	3.37	1.33	1.22
2	C	6006	MLT	O4-C4	3.35	1.33	1.22
2	B	6002	MLT	O4-C4	3.15	1.32	1.22
2	B	6004	MLT	O1-C1	3.04	1.31	1.22
2	B	6005	MLT	O4-C4	2.99	1.32	1.22
2	B	6003	MLT	O4-C4	2.96	1.32	1.22
2	D	6008	MLT	O4-C4	2.92	1.31	1.22
2	A	6001	MLT	O1-C1	2.85	1.30	1.22
3	B	5002	BET	CA-C	2.63	1.56	1.52
2	B	6005	MLT	O1-C1	2.54	1.29	1.22
3	C	5005	BET	CA-C	2.50	1.56	1.52
2	C	6007	MLT	O4-C4	2.41	1.30	1.22
3	D	5001	BET	CA-C	2.40	1.56	1.52
3	B	5004	BET	CA-C	2.38	1.56	1.52
3	A	5003	BET	CA-C	2.32	1.56	1.52
2	A	6001	MLT	C2-C1	-2.15	1.49	1.52
2	B	6005	MLT	C2-C1	-2.11	1.49	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	6003	MLT	O2-C1-O1	-4.18	114.59	124.09
2	D	6008	MLT	O2-C1-O1	-3.86	115.31	124.09
2	C	6007	MLT	O2-C1-O1	-3.80	115.46	124.09
2	B	6004	MLT	O2-C1-O1	-3.67	115.75	124.09
2	B	6002	MLT	O2-C1-O1	-3.56	116.01	124.09
2	A	6001	MLT	O2-C1-O1	-3.47	116.20	124.09
2	B	6005	MLT	O2-C1-O1	-3.44	116.29	124.09
2	B	6003	MLT	O2-C1-C2	3.32	120.02	112.72
2	C	6007	MLT	O5-C4-O4	-3.25	115.19	123.30
2	A	6001	MLT	O2-C1-C2	3.16	119.66	112.72
2	B	6003	MLT	O5-C4-O4	-3.05	115.69	123.30
2	C	6007	MLT	O2-C1-C2	3.04	119.40	112.72
2	D	6008	MLT	O2-C1-C2	3.01	119.33	112.72
2	D	6008	MLT	O5-C4-O4	-2.91	116.04	123.30
2	C	6006	MLT	O2-C1-O1	-2.86	117.59	124.09
2	B	6005	MLT	O2-C1-C2	2.84	118.96	112.72
2	B	6002	MLT	O5-C4-O4	-2.65	116.70	123.30
2	B	6004	MLT	O2-C1-C2	2.60	118.43	112.72
2	B	6004	MLT	O5-C4-O4	-2.53	117.00	123.30
2	C	6007	MLT	O5-C4-C3	2.52	122.13	114.07
2	C	6006	MLT	O2-C1-C2	2.46	118.12	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	6001	MLT	O5-C4-O4	-2.37	117.39	123.30
2	C	6006	MLT	O5-C4-O4	-2.36	117.41	123.30
2	C	6006	MLT	O5-C4-C3	2.34	121.58	114.07
2	B	6003	MLT	O5-C4-C3	2.22	121.18	114.07
2	B	6005	MLT	O5-C4-O4	-2.20	117.82	123.30
2	D	6008	MLT	O5-C4-C3	2.17	121.03	114.07
2	B	6002	MLT	O2-C1-C2	2.14	117.41	112.72
2	A	6001	MLT	O5-C4-C3	2.12	120.87	114.07
2	B	6002	MLT	O1-C1-C2	2.06	126.58	122.54
2	B	6005	MLT	O5-C4-C3	2.05	120.63	114.07

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	6001	MLT	C2
2	B	6002	MLT	C2
2	B	6003	MLT	C2
2	B	6004	MLT	C2
2	B	6005	MLT	C2
2	C	6006	MLT	C2
2	C	6007	MLT	C2
2	D	6008	MLT	C2

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	6003	MLT	C1-C2-C3-C4
2	B	6003	MLT	O3-C2-C3-C4
2	B	6005	MLT	C1-C2-C3-C4
2	B	6005	MLT	O3-C2-C3-C4
2	C	6006	MLT	C1-C2-C3-C4
2	C	6006	MLT	O3-C2-C3-C4
2	C	6007	MLT	C1-C2-C3-C4
2	C	6007	MLT	O3-C2-C3-C4
3	A	5003	BET	O-C-CA-N
3	A	5003	BET	OXT-C-CA-N
3	B	5002	BET	O-C-CA-N
3	B	5002	BET	OXT-C-CA-N
3	B	5004	BET	O-C-CA-N
3	B	5004	BET	OXT-C-CA-N
3	C	5005	BET	O-C-CA-N
3	C	5005	BET	OXT-C-CA-N

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Mol	Chain	Res	Type	Atoms
3	D	5001	BET	O-C-CA-N
3	D	5001	BET	OXT-C-CA-N
3	B	5002	BET	C-CA-N-C1
3	D	5001	BET	C-CA-N-C1
3	D	5001	BET	C-CA-N-C2
2	B	6004	MLT	C1-C2-C3-C4
3	B	5002	BET	C-CA-N-C2
2	C	6006	MLT	C2-C3-C4-O5
3	D	5001	BET	C-CA-N-C3
3	B	5002	BET	C-CA-N-C3

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	6005	MLT	1	0
2	C	6007	MLT	1	0
2	B	6002	MLT	1	0
3	A	5003	BET	1	0
2	B	6003	MLT	4	0
4	B	7002	IMD	2	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 (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	99/105 (94%)	0.48	5 (5%)	28	31	20, 30, 50, 71	0
1	B	91/105 (86%)	0.92	13 (14%)	2	2	21, 38, 55, 81	0
1	C	98/105 (93%)	0.92	11 (11%)	5	6	19, 34, 61, 83	0
1	D	98/105 (93%)	0.81	13 (13%)	3	3	20, 37, 58, 82	0
All	All	386/420 (91%)	0.78	42 (10%)	5	6	19, 35, 58, 83	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2001	MET	11.6
1	C	2003	PRO	10.7
1	C	2002	SER	7.0
1	B	1096	GLU	5.4
1	D	3098	ARG	5.1
1	A	1	MET	4.7
1	C	2098	ARG	4.6
1	A	99	GLU	4.5
1	C	2004	PHE	4.3
1	C	2097	ILE	4.1
1	D	3001	MET	3.9
1	D	3003	PRO	3.9
1	B	1037	GLN	3.7
1	D	3004	PHE	3.6
1	D	3002	SER	3.4
1	C	2005	LYS	3.3
1	D	3037	GLN	3.3
1	A	97	ILE	3.3
1	B	1083	ARG	3.2
1	D	3083	ARG	3.1
1	D	3097	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	1006	LYS	3.1
1	D	3033	GLU	3.0
1	A	2	SER	3.0
1	C	2037	GLN	2.8
1	B	1038	GLY	2.8
1	D	3038	GLY	2.8
1	A	83	ARG	2.8
1	D	3082	ASP	2.7
1	D	3039	VAL	2.7
1	B	1065	LEU	2.5
1	B	1095	ASP	2.5
1	C	2083	ARG	2.5
1	C	2090	LEU	2.3
1	B	1060	LEU	2.2
1	D	3050	ASN	2.2
1	C	2036	PHE	2.2
1	B	1041	ALA	2.1
1	B	1094	TYR	2.0
1	B	1024	ALA	2.0
1	B	1077	ILE	2.0
1	B	1090	LEU	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, 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	BET	B	5002	8/8	0.45	0.46	76,76,77,77	0
3	BET	C	5005	8/8	0.48	0.39	75,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MLT	B	6002	9/9	0.55	0.28	57,58,59,59	0
3	BET	A	5003	8/8	0.56	0.39	67,67,68,68	0
2	MLT	C	6006	9/9	0.58	0.32	57,59,61,61	0
2	MLT	B	6004	9/9	0.60	0.30	62,63,64,65	0
2	MLT	D	6008	9/9	0.68	0.41	63,63,64,64	0
2	MLT	C	6007	9/9	0.72	0.27	50,55,57,58	0
2	MLT	A	6001	9/9	0.75	0.31	53,57,58,60	0
4	IMD	B	7001	5/5	0.75	0.26	61,61,62,62	0
4	IMD	B	7002	5/5	0.75	0.47	58,58,59,59	0
2	MLT	B	6003	9/9	0.77	0.34	45,50,53,53	0
3	BET	B	5004	8/8	0.80	0.22	64,65,66,66	0
4	IMD	D	7003	5/5	0.83	0.22	48,48,49,49	0
2	MLT	B	6005	9/9	0.88	0.14	47,49,50,50	0
3	BET	D	5001	8/8	0.91	0.16	48,49,49,51	0

6.5 Other polymers (i)

There are no such residues in this entry.