Full wwPDB X-ray Structure Validation Report ⓘ

Feb 29, 2024 – 02:12 PM JST

PDB ID	:	8JKK
Title	:	Crystal Structure of the dioxygenase CcTet from Coprinopsis cinerea bound to 12bp 5-methylcytosine (5mC) containing duplex DNA
Authors	:	Zhang, L.; Zhang, L.
Deposited on	:	2023-06-01
Resolution	:	2.30 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:

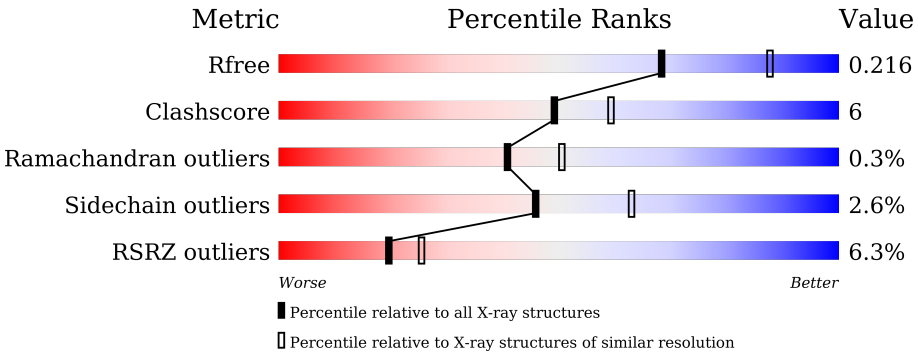
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	415	7% 78% 10% • 9%
1	D	415	2% 78% 13% • 8%
1	G	415	3% 76% 13% • 9%
1	J	415	10% 76% 14% • 8%
2	B	12	8% 50% 25% 25%
2	E	12	8% 33% 42% 25%

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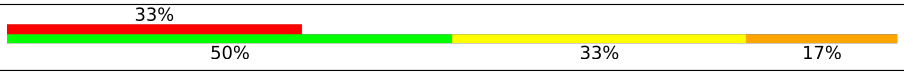
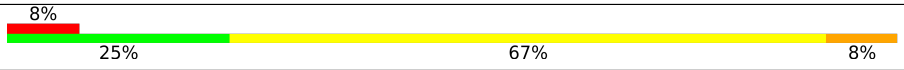
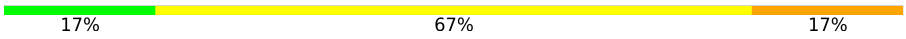
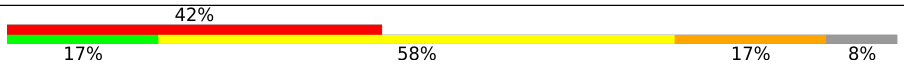
Mol	Chain	Length	Quality of chain
2	H	12	
2	K	12	
3	C	12	
3	F	12	
3	I	12	
3	L	12	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 14841 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 2OGFeDO JBP1/TET oxygenase domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	0	0	0
			2955	1889	523	529	14			
1	D	383	Total	C	N	O	S	0	0	0
			3007	1921	535	536	15			
1	G	376	Total	C	N	O	S	0	0	0
			2947	1886	520	527	14			
1	J	383	Total	C	N	O	S	0	0	0
			3007	1921	533	538	15			

- Molecule 2 is a DNA chain called DNA (5'-D(P*CP*GP*AP*TP*CP*(5CM)P*GP*CP*TP*AP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	12	Total	C	N	O	P	0	0	0
			244	116	44	72	12			
2	E	12	Total	C	N	O	P	0	0	0
			244	116	44	72	12			
2	H	12	Total	C	N	O	P	0	0	0
			244	116	44	72	12			
2	K	12	Total	C	N	O	P	0	0	0
			244	116	44	72	12			

- Molecule 3 is a DNA chain called DNA (5'-D(P*CP*GP*TP*AP*GP*CP*TP*GP*AP*TP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	12	Total	C	N	O	P	0	0	0
			247	117	45	73	12			
3	F	12	Total	C	N	O	P	0	0	0
			247	117	45	73	12			
3	I	12	Total	C	N	O	P	0	0	0
			247	117	45	73	12			

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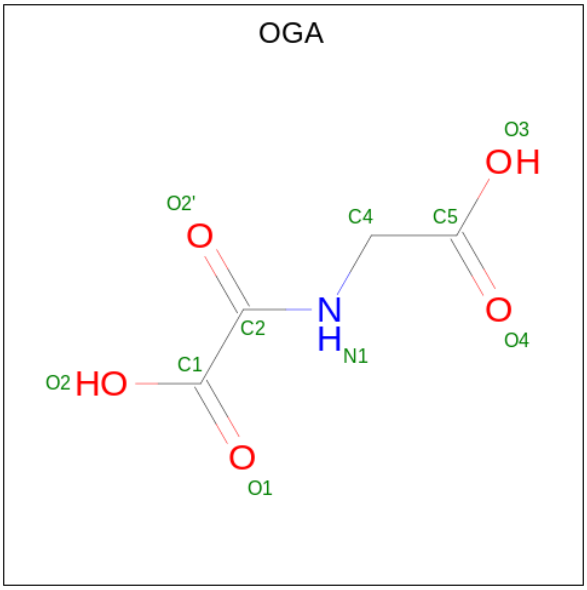
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	11	Total	C	N	O	P	0	0	0
			228	108	42	67	11			

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mn	0	0
			1	1		
4	D	1	Total	Mn	0	0
			1	1		
4	G	1	Total	Mn	0	0
			1	1		
4	J	1	Total	Mn	0	0
			1	1		

- Molecule 5 is N-OXALYLGLYCINE (three-letter code: OGA) (formula: $C_4H_5NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			10	4	1	5		
5	D	1	Total	C	N	O	0	0
			10	4	1	5		
5	G	1	Total	C	N	O	0	0
			10	4	1	5		
5	J	1	Total	C	N	O	0	0
			10	4	1	5		

- Molecule 6 is water.

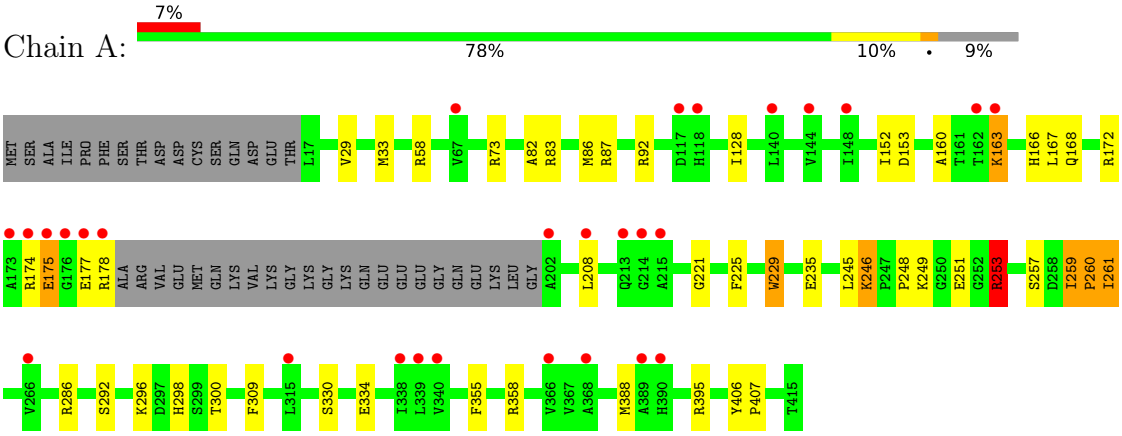
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	298	Total O 298 298	0	0
6	B	16	Total O 16 16	0	0
6	C	9	Total O 9 9	0	0
6	D	275	Total O 275 275	0	0
6	E	21	Total O 21 21	0	0
6	F	23	Total O 23 23	0	0
6	G	188	Total O 188 188	0	0
6	H	22	Total O 22 22	0	0
6	I	10	Total O 10 10	0	0
6	J	70	Total O 70 70	0	0
6	K	3	Total O 3 3	0	0
6	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.

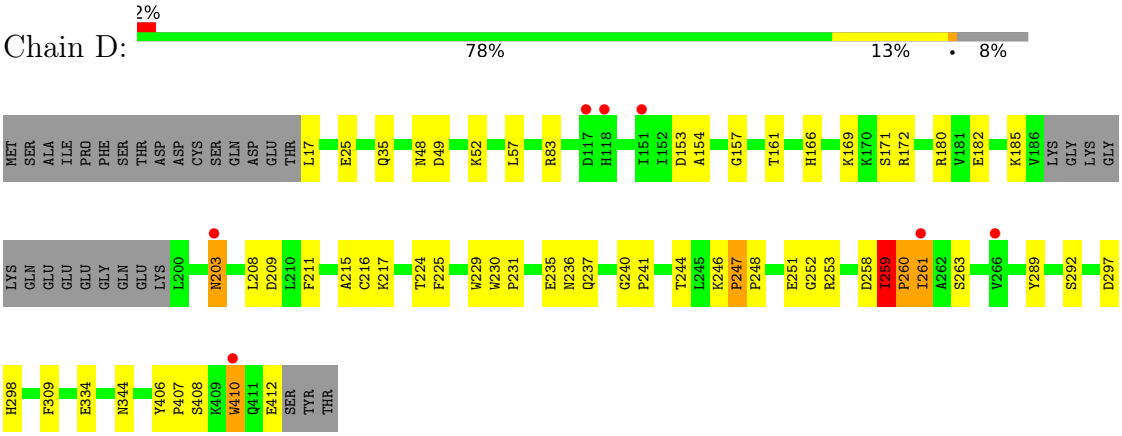
• Molecule 1: 2OGFeDO JBP1/TET oxygenase domain-containing protein

Chain A:



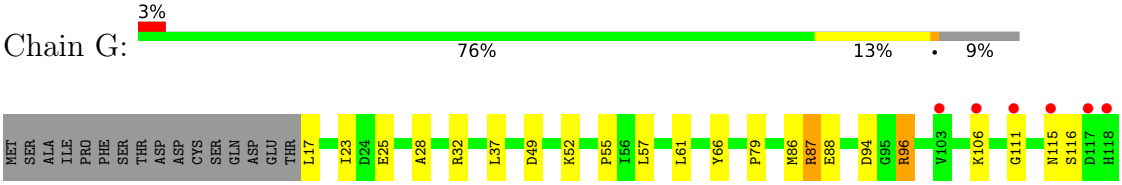
• Molecule 1: 2OGFeDO JBP1/TET oxygenase domain-containing protein

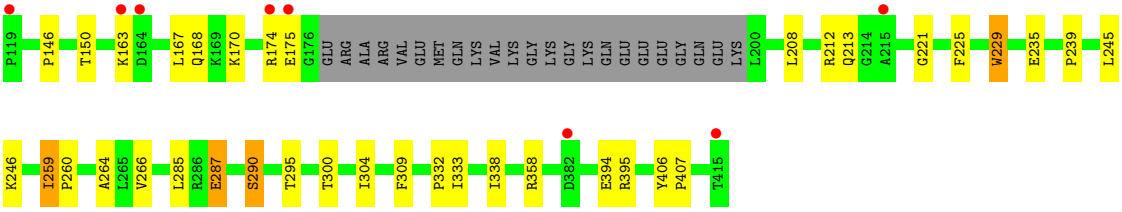
Chain D:



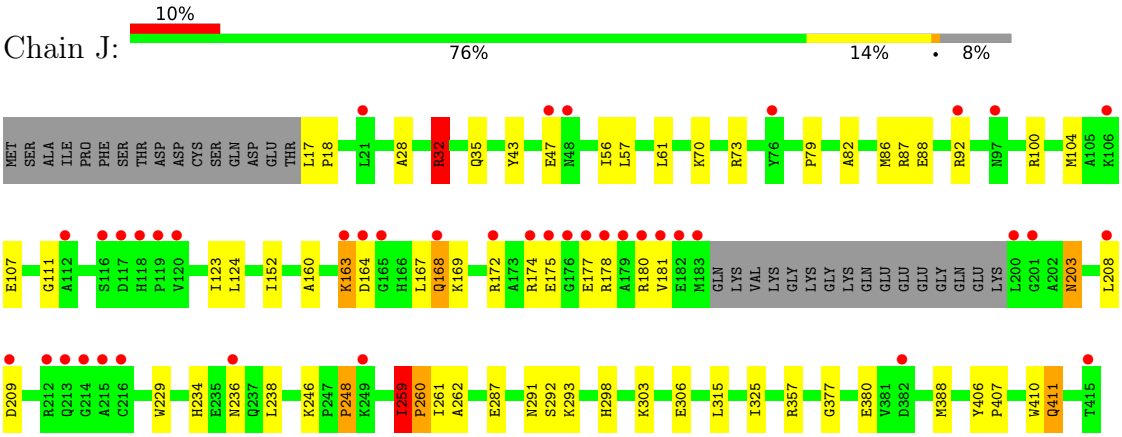
• Molecule 1: 2OGFeDO JBP1/TET oxygenase domain-containing protein

Chain G:

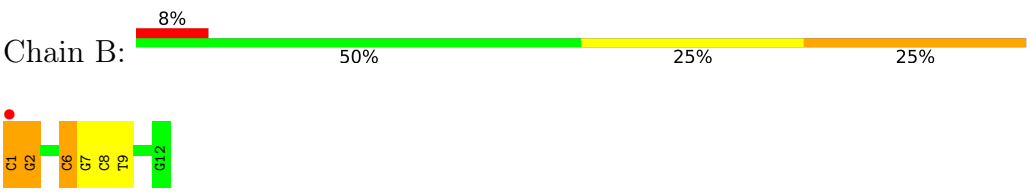




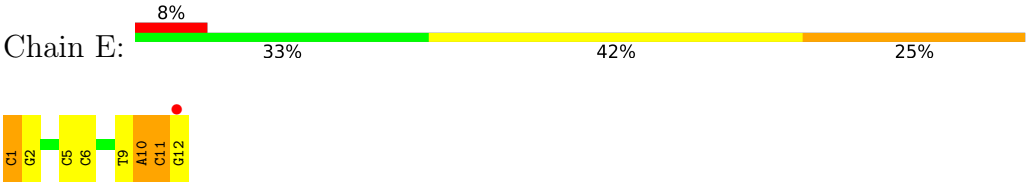
• Molecule 1: 2OGFeDO JBP1/TET oxygenase domain-containing protein



• Molecule 2: DNA (5'-D(P*CP*GP*AP*TP*CP*(5CM)P*GP*CP*TP*AP*CP*G)-3')

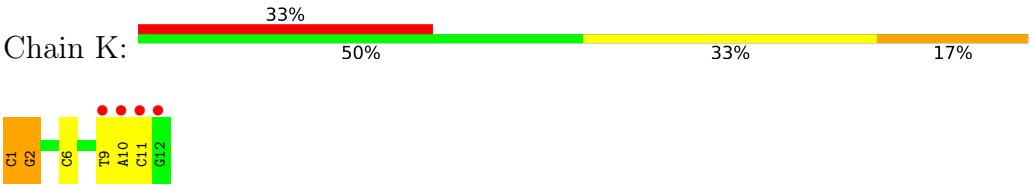


• Molecule 2: DNA (5'-D(P*CP*GP*AP*TP*CP*(5CM)P*GP*CP*TP*AP*CP*G)-3')



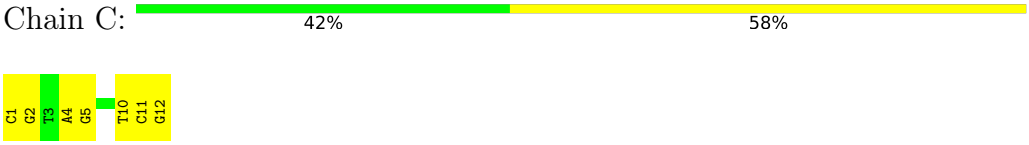
• Molecule 2: DNA (5'-D(P*CP*GP*AP*TP*CP*(5CM)P*GP*CP*TP*AP*CP*G)-3')

• Molecule 2: DNA (5'-D(P*CP*GP*AP*TP*CP*(5CM)P*GP*CP*TP*AP*CP*G)-3')



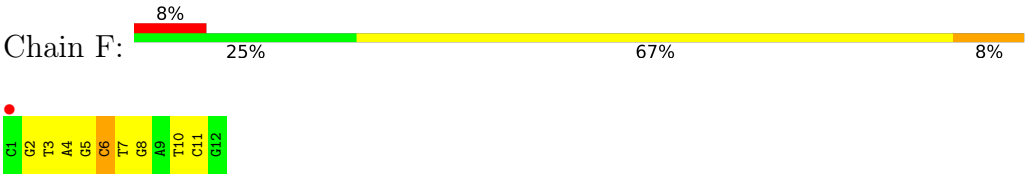
• Molecule 3: DNA (5'-D(P*CP*GP*TP*AP*GP*CP*TP*GP*AP*TP*CP*G)-3')

Chain C:



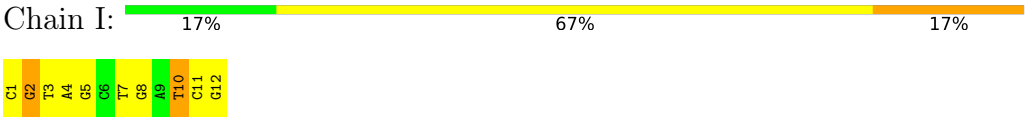
• Molecule 3: DNA (5'-D(P*CP*GP*TP*AP*GP*CP*TP*GP*AP*TP*CP*G)-3')

Chain F:



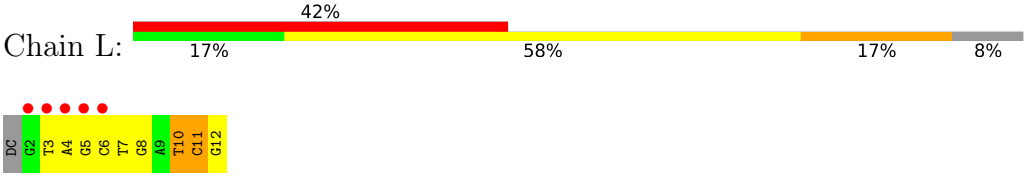
• Molecule 3: DNA (5'-D(P*CP*GP*TP*AP*GP*CP*TP*GP*AP*TP*CP*G)-3')

Chain I:



• Molecule 3: DNA (5'-D(P*CP*GP*TP*AP*GP*CP*TP*GP*AP*TP*CP*G)-3')

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	86.57Å 127.63Å 212.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.98 – 2.30 49.93 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.5 (21.98-2.30) 90.5 (49.93-2.30)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.98 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.187 , 0.216 0.189 , 0.216	Depositor DCC
R_{free} test set	4770 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	31.5	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.0	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	0.94	EDS
Total number of atoms	14841	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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: OGA, 5CM, MN

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	0.63	6/3033 (0.2%)	0.76	7/4128 (0.2%)
1	D	1.13	38/3084 (1.2%)	0.84	3/4194 (0.1%)
1	G	0.63	6/3025 (0.2%)	0.77	6/4118 (0.1%)
1	J	0.69	7/3085 (0.2%)	0.92	19/4197 (0.5%)
2	B	0.90	0/249	1.38	3/379 (0.8%)
2	E	1.75	5/249 (2.0%)	1.51	4/379 (1.1%)
2	H	0.92	0/249	1.19	0/379
2	K	0.87	0/249	1.39	4/379 (1.1%)
3	C	0.98	0/276	1.07	0/424
3	F	1.09	0/276	1.21	1/424 (0.2%)
3	I	1.26	3/276 (1.1%)	1.31	2/424 (0.5%)
3	L	1.02	1/255 (0.4%)	1.19	3/392 (0.8%)
All	All	0.86	66/14306 (0.5%)	0.91	52/19817 (0.3%)

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	5	DC	P-OP2	-11.96	1.28	1.49
1	J	248	PRO	N-CA	11.47	1.66	1.47
1	D	251	GLU	CD-OE1	-9.46	1.15	1.25
1	G	395	ARG	CZ-NH1	8.79	1.44	1.33
1	D	251	GLU	CD-OE2	-8.60	1.16	1.25
1	D	182	GLU	CD-OE2	-8.37	1.16	1.25
2	E	5	DC	P-OP1	-8.30	1.34	1.49
1	D	247	PRO	C-O	-8.19	1.06	1.23
1	D	235	GLU	CD-OE2	-7.89	1.17	1.25
1	J	246	LYS	C-N	7.63	1.48	1.34
1	J	238	LEU	C-N	7.54	1.48	1.34
1	D	260	PRO	C-O	-7.53	1.08	1.23
1	D	182	GLU	CD-OE1	-7.31	1.17	1.25
3	I	12	DG	P-OP2	-7.29	1.36	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	235	GLU	CD-OE1	-7.18	1.17	1.25
1	G	246	LYS	C-N	7.14	1.47	1.34
2	E	10	DA	O3'-P	-6.95	1.52	1.61
1	A	259	ILE	C-O	-6.84	1.10	1.23
3	I	12	DG	P-OP1	-6.70	1.37	1.49
1	D	412	GLU	CD-OE1	-6.50	1.18	1.25
1	D	231	PRO	C-O	-6.49	1.10	1.23
1	D	258	ASP	C-O	-6.44	1.11	1.23
1	D	154	ALA	C-O	-6.43	1.11	1.23
1	D	412	GLU	CD-OE2	-6.28	1.18	1.25
1	D	240	GLY	C-O	-6.27	1.13	1.23
1	D	241	PRO	C-O	-6.19	1.10	1.23
1	D	230	TRP	C-O	-6.16	1.11	1.23
2	E	1	DC	P-O5'	6.14	1.65	1.59
1	D	180	ARG	C-O	-6.08	1.11	1.23
1	J	260	PRO	C-O	-6.05	1.11	1.23
1	D	215	ALA	C-O	-6.05	1.11	1.23
1	D	209	ASP	C-O	-5.93	1.12	1.23
1	D	171	SER	CA-CB	-5.92	1.44	1.52
3	L	10	DT	C3'-O3'	5.90	1.51	1.44
1	D	153	ASP	CG-OD2	-5.87	1.11	1.25
1	D	217	LYS	C-O	-5.78	1.12	1.23
1	D	259	ILE	C-O	-5.76	1.12	1.23
1	D	408	SER	CA-CB	-5.75	1.44	1.52
1	A	257	SER	C-O	-5.62	1.12	1.23
1	D	172	ARG	C-O	-5.62	1.12	1.23
1	J	32	ARG	CZ-NH2	5.62	1.40	1.33
1	D	157	GLY	C-O	-5.61	1.14	1.23
1	A	257	SER	CB-OG	-5.60	1.34	1.42
1	G	290	SER	CA-CB	-5.55	1.44	1.52
1	D	252	GLY	C-O	-5.51	1.14	1.23
1	J	47	GLU	CD-OE1	5.50	1.31	1.25
1	D	263	SER	CA-CB	-5.50	1.44	1.52
1	D	208	LEU	C-O	-5.46	1.12	1.23
1	D	251	GLU	C-O	-5.43	1.13	1.23
1	G	259	ILE	C-O	-5.36	1.13	1.23
1	A	261	ILE	C-O	-5.26	1.13	1.23
1	A	260	PRO	C-O	-5.23	1.12	1.23
1	D	224	THR	C-O	-5.21	1.13	1.23
2	E	11	DC	O3'-P	-5.21	1.54	1.61
3	I	2	DG	C3'-O3'	-5.19	1.37	1.44
1	D	161	THR	C-O	-5.17	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	153	ASP	CG-OD1	-5.13	1.13	1.25
1	D	166	HIS	C-O	-5.12	1.13	1.23
1	D	253	ARG	C-O	-5.10	1.13	1.23
1	D	216	CYS	C-O	-5.10	1.13	1.23
1	J	259	ILE	C-O	-5.05	1.13	1.23
1	A	249	LYS	C-O	-5.04	1.13	1.23
1	D	211	PHE	C-O	-5.03	1.13	1.23
1	G	287	GLU	CD-OE1	-5.03	1.20	1.25
1	G	88	GLU	CD-OE2	-5.01	1.20	1.25
1	D	244	THR	C-O	-5.00	1.13	1.23

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	106	LYS	CD-CE-NZ	15.62	147.62	111.70
1	J	32	ARG	NE-CZ-NH1	-11.84	114.38	120.30
2	B	1	DC	OP1-P-O3'	-11.02	80.95	105.20
2	K	1	DC	OP1-P-O3'	-10.78	81.49	105.20
1	J	32	ARG	CA-CB-CG	10.49	136.49	113.40
1	J	87	ARG	NE-CZ-NH1	-9.61	115.50	120.30
2	K	1	DC	OP2-P-O3'	-9.36	84.62	105.20
1	J	163	LYS	CD-CE-NZ	-9.32	90.26	111.70
2	E	5	DC	O5'-P-OP2	-9.30	97.33	105.70
2	B	1	DC	OP2-P-O3'	-8.82	85.79	105.20
1	J	92	ARG	NE-CZ-NH2	-8.58	116.01	120.30
2	K	2	DG	OP1-P-OP2	8.37	132.15	119.60
2	K	11	DC	O4'-C4'-C3'	-8.26	101.04	106.00
1	J	293	LYS	CD-CE-NZ	7.98	130.05	111.70
2	B	2	DG	OP1-P-OP2	7.60	130.99	119.60
3	I	10	DT	P-O3'-C3'	7.51	128.71	119.70
1	G	106	LYS	CG-CD-CE	-7.47	89.49	111.90
1	J	92	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	D	203	ASN	CB-CA-C	7.18	124.75	110.40
1	J	87	ARG	CB-CG-CD	-7.00	93.40	111.60
2	E	10	DA	C4'-C3'-O3'	-6.81	92.68	109.70
1	J	87	ARG	CG-CD-NE	6.58	125.62	111.80
1	J	248	PRO	CA-N-CD	-6.42	102.52	111.50
1	J	203	ASN	CB-CA-C	6.39	123.19	110.40
3	L	3	DT	C3'-C2'-C1'	6.36	110.13	102.50
1	A	172	ARG	CB-CA-C	-6.34	97.71	110.40
1	J	47	GLU	CG-CD-OE2	-6.07	106.17	118.30
1	A	246	LYS	CA-CB-CG	-5.96	100.28	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	3	DT	C2'-C3'-O3'	-5.91	93.09	112.60
3	F	6	DC	O4'-C1'-N1	-5.89	103.87	108.00
1	J	73	ARG	CG-CD-NE	-5.89	99.43	111.80
1	J	92	ARG	CD-NE-CZ	5.89	131.84	123.60
1	J	87	ARG	CA-CB-CG	5.66	125.86	113.40
2	E	5	DC	O5'-P-OP1	5.58	117.40	110.70
1	G	87	ARG	CD-NE-CZ	-5.45	115.97	123.60
1	A	153	ASP	CB-CG-OD1	5.41	123.17	118.30
1	G	87	ARG	NE-CZ-NH1	-5.41	117.59	120.30
3	I	12	DG	O5'-P-OP2	-5.39	100.85	105.70
1	J	236	ASN	CB-CA-C	-5.39	99.63	110.40
1	J	32	ARG	N-CA-CB	-5.35	100.97	110.60
1	A	296	LYS	CB-CA-C	-5.32	99.77	110.40
1	A	87	ARG	NE-CZ-NH1	-5.31	117.65	120.30
3	L	11	DC	O5'-P-OP2	-5.28	100.95	105.70
1	D	410	TRP	CA-CB-CG	-5.27	103.68	113.70
1	D	83	ARG	CA-CB-CG	5.24	124.94	113.40
1	A	87	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	G	395	ARG	CG-CD-NE	5.20	122.72	111.80
1	J	47	GLU	CG-CD-OE1	5.15	128.60	118.30
1	G	208	LEU	CB-CG-CD2	-5.15	102.25	111.00
1	J	168	GLN	CA-CB-CG	5.08	124.58	113.40
1	A	253	ARG	CG-CD-NE	-5.07	101.16	111.80
2	E	11	DC	P-O5'-C5'	-5.04	112.83	120.90

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	2955	0	2964	28	0
1	D	3007	0	3029	27	0
1	G	2947	0	2959	33	0
1	J	3007	0	3020	34	0
2	B	244	0	137	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	244	0	137	5	0
2	H	244	0	137	3	0
2	K	244	0	137	5	0
3	C	247	0	136	6	0
3	F	247	0	136	6	0
3	I	247	0	136	7	0
3	L	228	0	125	5	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0
5	A	10	0	3	0	0
5	D	10	0	3	0	0
5	G	10	0	3	0	0
5	J	10	0	3	0	0
6	A	298	0	0	6	0
6	B	16	0	0	2	0
6	C	9	0	0	0	0
6	D	275	0	0	2	0
6	E	21	0	0	0	0
6	F	23	0	0	0	0
6	G	188	0	0	7	0
6	H	22	0	0	0	0
6	I	10	0	0	0	0
6	J	70	0	0	1	0
6	K	3	0	0	1	0
6	L	1	0	0	0	0
All	All	14841	0	13065	159	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 6.

All (159) 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:57:LEU:HB2	1:D:261:ILE:HD11	1.31	1.06
1:D:57:LEU:CB	1:D:261:ILE:HD11	2.01	0.90
1:A:178:ARG:HG2	1:A:208:LEU:HD21	1.61	0.80
1:D:57:LEU:HB2	1:D:261:ILE:CD1	2.14	0.75
1:J:123:ILE:HG13	1:J:124:LEU:HD22	1.76	0.68
1:D:246:LYS:NZ	1:D:297:ASP:OD2	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:GLU:O	1:A:175:GLU:HG3	1.95	0.66
3:L:11:DC:H2"	3:L:12:DG:C8	2.30	0.66
1:D:57:LEU:CA	1:D:261:ILE:HD11	2.25	0.66
3:I:10:DT:H2'	3:I:11:DC:C6	2.31	0.66
1:J:303:LYS:NZ	1:J:306:GLU:OE2	2.29	0.65
1:G:285:LEU:CD2	6:G:647:HOH:O	2.44	0.65
3:L:10:DT:H2"	3:L:11:DC:H5"	1.78	0.65
2:B:1:DC:H2'	2:B:2:DG:C8	2.31	0.65
1:A:246:LYS:HE3	6:A:642:HOH:O	1.97	0.63
1:J:292:SER:HA	1:J:298:HIS:CD2	2.34	0.63
3:I:10:DT:H2"	3:I:11:DC:O5'	1.99	0.63
1:G:94:ASP:OD1	1:G:96:ARG:HG2	1.98	0.62
1:J:57:LEU:HB2	1:J:261:ILE:HG23	1.83	0.61
1:G:86:MET:HG2	1:G:333:ILE:CD1	2.30	0.60
3:L:7:DT:H2'	3:L:8:DG:C8	2.36	0.60
1:G:86:MET:HG2	1:G:333:ILE:HD13	1.83	0.59
2:K:1:DC:H2'	2:K:2:DG:C8	2.38	0.59
1:J:325:ILE:HD13	1:J:377:GLY:HA3	1.85	0.59
1:J:32:ARG:HG3	1:J:43:TYR:CE1	2.39	0.58
1:J:56:ILE:HD12	1:J:56:ILE:H	1.68	0.58
1:D:406:TYR:CG	1:D:407:PRO:HD2	2.38	0.58
1:A:246:LYS:HG3	1:A:300:THR:HG21	1.85	0.57
1:G:167:LEU:HD22	1:G:221:GLY:HA3	1.85	0.57
1:J:175:GLU:OE2	1:J:175:GLU:HA	2.02	0.57
1:J:160:ALA:HA	1:J:167:LEU:HD12	1.85	0.56
2:B:6:5CM:H3'	6:B:101:HOH:O	2.04	0.56
1:D:52:LYS:HB2	1:D:52:LYS:NZ	2.21	0.56
1:D:292:SER:HA	1:D:298:HIS:CD2	2.41	0.56
2:H:9:DT:H2"	2:H:10:DA:C8	2.40	0.56
3:I:2:DG:H2'	3:I:3:DT:H72	1.88	0.56
3:I:7:DT:H2'	3:I:8:DG:C8	2.42	0.56
2:K:9:DT:H2"	2:K:10:DA:C8	2.41	0.55
3:C:1:DC:H2'	3:C:2:DG:C8	2.41	0.55
1:A:334:GLU:HB3	1:A:407:PRO:HD3	1.88	0.55
1:J:259:ILE:N	1:J:260:PRO:HD3	2.21	0.55
1:G:23:ILE:HG22	1:G:264:ALA:HA	1.88	0.54
1:D:344:ASN:O	1:D:344:ASN:OD1	2.25	0.54
3:I:3:DT:H2"	3:I:4:DA:C8	2.43	0.54
1:G:225:PHE:HB3	1:G:245:LEU:HD11	1.90	0.53
1:A:235:GLU:HB2	1:A:395:ARG:NH1	2.24	0.53
1:D:260:PRO:HB3	1:D:309:PHE:CD1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ALA:O	1:A:86:MET:HG2	2.08	0.53
1:A:128:ILE:HD13	1:A:355:PHE:CD2	2.44	0.53
1:A:260:PRO:HB3	1:A:309:PHE:CD1	2.44	0.52
2:E:10:DA:H2"	2:E:11:DC:H5"	1.91	0.52
1:J:82:ALA:O	1:J:86:MET:HG3	2.08	0.52
2:E:1:DC:H2'	2:E:2:DG:C8	2.44	0.52
1:A:261:ILE:HG22	6:A:720:HOH:O	2.08	0.52
3:F:7:DT:H2'	3:F:8:DG:C8	2.45	0.51
2:K:2:DG:N7	6:K:102:HOH:O	2.33	0.51
1:J:164:ASP:H	1:J:168:GLN:HG3	1.75	0.51
1:D:410:TRP:O	1:D:410:TRP:CD2	2.64	0.51
1:D:410:TRP:HD1	6:D:807:HOH:O	1.94	0.51
1:A:358:ARG:NH1	6:A:607:HOH:O	2.37	0.51
1:G:163:LYS:HA	1:G:168:GLN:NE2	2.27	0.50
1:G:239:PRO:HG2	1:G:295:THR:HG22	1.93	0.50
1:J:88:GLU:HG3	1:J:104:MET:SD	2.52	0.50
1:J:28:ALA:O	1:J:32:ARG:HB2	2.11	0.50
3:C:12:DG:H2"	2:K:1:DC:H5"	1.94	0.49
1:D:410:TRP:CD2	1:D:410:TRP:C	2.85	0.49
2:E:10:DA:H2"	2:E:11:DC:C5'	2.42	0.49
3:I:4:DA:H2"	3:I:5:DG:O5'	2.12	0.49
1:D:410:TRP:HB3	6:D:807:HOH:O	2.13	0.49
2:B:1:DC:H5"	2:B:1:DC:H6	1.76	0.49
1:A:330:SER:OG	2:B:6:5CM:OP1	2.25	0.49
3:C:1:DC:H3'	3:C:1:DC:OP1	2.12	0.48
1:D:259:ILE:N	1:D:260:PRO:HD3	2.29	0.48
3:F:5:DG:H2"	3:F:6:DC:C6	2.48	0.48
2:E:9:DT:H2"	2:E:10:DA:C8	2.48	0.48
1:G:260:PRO:HB3	1:G:309:PHE:CD1	2.49	0.48
1:J:380:GLU:O	6:J:601:HOH:O	2.20	0.48
1:J:410:TRP:CE2	1:J:411:GLN:OE1	2.67	0.48
1:D:25:GLU:OE1	1:D:49:ASP:HB2	2.13	0.48
3:F:3:DT:H2"	3:F:4:DA:C8	2.48	0.48
1:J:410:TRP:CZ3	1:J:411:GLN:HG3	2.50	0.47
1:A:168:GLN:HB2	6:A:608:HOH:O	2.13	0.47
1:A:166:HIS:ND1	1:A:251:GLU:OE1	2.46	0.47
1:G:358:ARG:NE	6:G:601:HOH:O	2.22	0.47
1:G:79:PRO:HD3	1:G:111:GLY:HA3	1.97	0.47
1:D:17:LEU:HD11	1:D:289:TYR:CZ	2.50	0.46
2:K:1:DC:H5"	2:K:1:DC:H6	1.81	0.46
1:J:152:ILE:HD11	1:J:262:ALA:HB1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:229:TRP:CH2	2:H:7:DG:H5"	2.50	0.46
1:A:406:TYR:CG	1:A:407:PRO:HD2	2.51	0.46
2:B:7:DG:O5'	6:B:101:HOH:O	2.21	0.46
1:D:410:TRP:O	1:D:410:TRP:CE3	2.69	0.46
1:D:169:LYS:HG2	3:F:2:DG:OP1	2.17	0.45
1:G:332:PRO:HB3	1:G:394:GLU:HB2	1.98	0.45
1:J:315:LEU:HD11	1:J:388:MET:HB3	1.97	0.45
1:G:37:LEU:HD21	1:G:66:TYR:CE1	2.52	0.45
2:H:8:DC:C6	2:H:9:DT:H72	2.52	0.45
1:A:225:PHE:HB3	1:A:245:LEU:HD11	1.97	0.45
1:J:406:TYR:CG	1:J:407:PRO:HD2	2.51	0.45
1:A:286:ARG:HD2	6:A:601:HOH:O	2.16	0.45
1:A:229:TRP:CH2	2:B:7:DG:H5"	2.52	0.45
1:G:55:PRO:HD2	6:G:748:HOH:O	2.16	0.45
1:J:79:PRO:HD3	1:J:111:GLY:HA3	1.98	0.45
1:D:25:GLU:CD	1:D:49:ASP:HB2	2.37	0.45
3:C:4:DA:H2"	3:C:5:DG:O5'	2.17	0.44
1:J:169:LYS:HA	1:J:172:ARG:HD3	1.98	0.44
1:A:160:ALA:HA	1:A:167:LEU:HD12	1.98	0.44
1:J:234:HIS:HE1	3:L:6:DC:O2	2.00	0.44
1:G:57:LEU:O	1:G:61:LEU:HG	2.18	0.44
1:A:29:VAL:O	1:A:33:MET:HG3	2.18	0.44
2:E:11:DC:H2'	2:E:12:DG:C8	2.52	0.44
3:F:4:DA:H2"	3:F:5:DG:O5'	2.17	0.44
1:G:87:ARG:HH11	1:G:87:ARG:HD3	1.49	0.44
1:D:406:TYR:CD2	1:D:407:PRO:HD2	2.52	0.44
1:G:115:ASN:O	1:G:115:ASN:OD1	2.36	0.44
1:A:248:PRO:HA	1:A:253:ARG:CZ	2.48	0.44
1:G:17:LEU:HA	1:G:17:LEU:HD23	1.62	0.43
1:G:170:LYS:O	1:G:174:ARG:HG3	2.17	0.43
1:A:92:ARG:HD3	3:C:10:DT:H4'	2.00	0.43
1:D:17:LEU:HD11	1:D:289:TYR:CE2	2.52	0.43
1:J:100:ARG:O	1:J:104:MET:HG2	2.18	0.43
1:J:178:ARG:HH21	1:J:208:LEU:HD22	1.81	0.43
3:I:1:DC:P	3:I:1:DC:H3'	2.58	0.43
1:A:73:ARG:HH11	1:A:73:ARG:HD2	1.71	0.43
1:D:52:LYS:HB2	1:D:52:LYS:HZ2	1.81	0.43
1:G:260:PRO:HB3	1:G:309:PHE:CG	2.54	0.43
1:J:410:TRP:CE3	1:J:411:GLN:HG3	2.52	0.43
1:A:167:LEU:HD22	1:A:221:GLY:HA3	2.00	0.43
1:G:94:ASP:OD1	1:G:96:ARG:CG	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:212:ARG:NH1	6:G:602:HOH:O	2.47	0.43
1:J:287:GLU:OE2	1:J:291:ASN:HB2	2.19	0.43
1:D:406:TYR:CD1	1:D:407:PRO:HD2	2.54	0.43
1:G:406:TYR:CG	1:G:407:PRO:HD2	2.54	0.42
1:J:174:ARG:HH21	1:J:174:ARG:HD2	1.68	0.42
1:D:334:GLU:HB3	1:D:407:PRO:HD3	2.01	0.42
1:G:52:LYS:NZ	6:G:609:HOH:O	2.50	0.42
3:L:4:DA:H2"	3:L:5:DG:O5'	2.18	0.42
1:J:410:TRP:CD2	1:J:411:GLN:OE1	2.73	0.42
1:G:146:PRO:O	1:G:150:THR:HG23	2.18	0.42
2:B:8:DC:C6	2:B:9:DT:H72	2.55	0.42
3:F:10:DT:H2"	3:F:11:DC:O5'	2.19	0.42
1:G:28:ALA:O	1:G:32:ARG:HG3	2.19	0.42
1:G:212:ARG:NE	6:G:602:HOH:O	2.28	0.42
1:J:177:GLU:HG3	1:J:181:VAL:HG23	2.02	0.42
1:A:292:SER:HA	1:A:298:HIS:CD2	2.55	0.42
1:J:57:LEU:O	1:J:61:LEU:HG	2.20	0.42
1:A:58:ARG:NH1	6:A:620:HOH:O	2.52	0.41
1:G:116:SER:HB2	6:G:714:HOH:O	2.19	0.41
1:G:300:THR:O	1:G:304:ILE:HG13	2.20	0.41
3:C:10:DT:H2"	3:C:11:DC:H5'	2.02	0.41
1:D:247:PRO:HA	1:D:248:PRO:HD3	1.83	0.41
1:J:357:ARG:HD3	1:J:357:ARG:HA	1.92	0.41
1:D:57:LEU:HB2	1:D:261:ILE:CG1	2.49	0.41
1:G:266:VAL:HG13	1:G:338:ILE:HG21	2.02	0.41
1:J:17:LEU:HA	1:J:18:PRO:HD3	1.94	0.41
1:A:152:ILE:HD13	1:A:388:MET:HE1	2.03	0.41
1:A:163:LYS:H	1:A:163:LYS:HG2	1.41	0.41
1:J:209:ASP:OD1	1:J:209:ASP:N	2.51	0.41
1:G:25:GLU:OE1	1:G:49:ASP:HB2	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	372/415 (90%)	360 (97%)	11 (3%)	1 (0%)	41	50
1	D	379/415 (91%)	368 (97%)	10 (3%)	1 (0%)	41	50
1	G	372/415 (90%)	361 (97%)	10 (3%)	1 (0%)	41	50
1	J	379/415 (91%)	367 (97%)	11 (3%)	1 (0%)	41	50
All	All	1502/1660 (90%)	1456 (97%)	42 (3%)	4 (0%)	41	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	259	ILE
1	G	259	ILE
1	D	259	ILE
1	J	259	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	315/348 (90%)	308 (98%)	7 (2%)	52	69
1	D	320/348 (92%)	311 (97%)	9 (3%)	43	60
1	G	314/348 (90%)	307 (98%)	7 (2%)	52	69
1	J	320/348 (92%)	310 (97%)	10 (3%)	40	55
All	All	1269/1392 (91%)	1236 (97%)	33 (3%)	46	63

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ARG
1	A	163	LYS
1	A	174	ARG
1	A	175	GLU

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Mol	Chain	Res	Type
1	A	177	GLU
1	A	229	TRP
1	A	253	ARG
1	D	35	GLN
1	D	48	ASN
1	D	185	LYS
1	D	203	ASN
1	D	225	PHE
1	D	229	TRP
1	D	236	ASN
1	D	237	GLN
1	D	261	ILE
1	G	96	ARG
1	G	175	GLU
1	G	213	GLN
1	G	229	TRP
1	G	235	GLU
1	G	287	GLU
1	G	290	SER
1	J	32	ARG
1	J	35	GLN
1	J	70	LYS
1	J	107	GLU
1	J	163	LYS
1	J	180	ARG
1	J	203	ASN
1	J	229	TRP
1	J	248	PRO
1	J	411	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	D	237	GLN
1	D	344	ASN
1	G	115	ASN
1	G	168	GLN
1	J	35	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)

4 non-standard protein/DNA/RNA residues 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	5CM	B	6	2	17,21,22	2.12	8 (47%)	24,30,33	2.42	11 (45%)
2	5CM	E	6	2	17,21,22	3.03	8 (47%)	24,30,33	2.50	10 (41%)
2	5CM	H	6	2	17,21,22	1.90	6 (35%)	24,30,33	2.36	11 (45%)
2	5CM	K	6	2	17,21,22	2.09	7 (41%)	24,30,33	2.39	10 (41%)

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	5CM	B	6	2	-	6/7/21/22	0/2/2/2
2	5CM	E	6	2	-	6/7/21/22	0/2/2/2
2	5CM	H	6	2	-	6/7/21/22	0/2/2/2
2	5CM	K	6	2	-	6/7/21/22	0/2/2/2

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	6	5CM	C6-N1	-6.27	1.27	1.38
2	E	6	5CM	O2-C2	-5.83	1.12	1.23
2	B	6	5CM	C4-N3	-4.05	1.27	1.34
2	E	6	5CM	C2-N3	-3.94	1.28	1.36
2	E	6	5CM	C4-N3	-3.82	1.27	1.34
2	E	6	5CM	O4'-C1'	-3.81	1.33	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	6	5CM	C4-N3	-3.74	1.28	1.34
2	B	6	5CM	O3'-C3'	-3.62	1.35	1.43
2	H	6	5CM	C6-N1	-3.48	1.32	1.38
2	E	6	5CM	O5'-C5'	-3.35	1.36	1.44
2	K	6	5CM	O3'-C3'	-3.31	1.36	1.43
2	K	6	5CM	C6-N1	-3.31	1.32	1.38
2	H	6	5CM	C4-N3	-3.21	1.28	1.34
2	B	6	5CM	C6-C5	2.83	1.39	1.34
2	H	6	5CM	O3'-C3'	-2.77	1.37	1.43
2	B	6	5CM	C6-N1	-2.75	1.33	1.38
2	K	6	5CM	C2-N3	-2.73	1.30	1.36
2	E	6	5CM	O4'-C4'	-2.66	1.39	1.45
2	B	6	5CM	O4'-C1'	-2.66	1.36	1.42
2	K	6	5CM	O2-C2	-2.59	1.18	1.23
2	H	6	5CM	O4'-C1'	-2.57	1.36	1.42
2	K	6	5CM	O5'-C5'	-2.55	1.38	1.44
2	H	6	5CM	C6-C5	2.53	1.38	1.34
2	B	6	5CM	C2-N3	-2.51	1.31	1.36
2	K	6	5CM	O4'-C1'	-2.41	1.36	1.42
2	B	6	5CM	O5'-C5'	-2.26	1.39	1.44
2	E	6	5CM	C1'-N1	-2.25	1.42	1.48
2	B	6	5CM	O2-C2	-2.25	1.19	1.23
2	H	6	5CM	O5'-C5'	-2.22	1.39	1.44

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	6	5CM	C1'-N1-C2	5.38	127.18	117.74
2	B	6	5CM	O3'-C3'-C2'	-5.35	91.76	110.90
2	K	6	5CM	O2-C2-N3	-5.10	114.03	122.33
2	B	6	5CM	O2-C2-N3	-5.05	114.12	122.33
2	K	6	5CM	O3'-C3'-C2'	-5.01	92.98	110.90
2	H	6	5CM	O3'-C3'-C2'	-4.45	94.99	110.90
2	K	6	5CM	C1'-N1-C2	4.28	125.24	117.74
2	H	6	5CM	C1'-N1-C2	4.19	125.09	117.74
2	H	6	5CM	O2-C2-N3	-4.13	115.61	122.33
2	E	6	5CM	O3'-C3'-C2'	-4.07	96.34	110.90
2	E	6	5CM	O2-C2-N3	-4.00	115.82	122.33
2	H	6	5CM	C5-C4-N3	-3.85	117.52	121.67
2	E	6	5CM	C5-C4-N3	-3.84	117.54	121.67
2	E	6	5CM	C2'-C1'-N1	3.51	121.86	113.77
2	B	6	5CM	C5-C4-N3	-3.46	117.94	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	6	5CM	O5'-C5'-C4'	3.33	120.33	108.99
2	B	6	5CM	C1'-N1-C2	3.25	123.45	117.74
2	K	6	5CM	C5-C4-N3	-3.08	118.35	121.67
2	B	6	5CM	C6-N1-C2	-3.06	116.64	120.87
2	K	6	5CM	C2'-C1'-N1	3.05	120.79	113.77
2	B	6	5CM	O5'-C5'-C4'	2.96	119.06	108.99
2	K	6	5CM	C5-C6-N1	-2.95	120.30	123.34
2	K	6	5CM	N1-C2-N3	2.93	124.14	118.81
2	E	6	5CM	C1'-N1-C6	-2.87	115.83	120.77
2	E	6	5CM	C3'-C2'-C1'	2.86	109.70	102.54
2	B	6	5CM	O4'-C4'-C3'	2.83	112.27	105.67
2	E	6	5CM	N4-C4-N3	2.82	123.62	118.48
2	B	6	5CM	N1-C2-N3	2.82	123.94	118.81
2	E	6	5CM	C6-N1-C2	-2.80	116.99	120.87
2	H	6	5CM	C6-N1-C2	-2.78	117.03	120.87
2	K	6	5CM	C6-N1-C2	-2.65	117.20	120.87
2	B	6	5CM	C5-C6-N1	-2.64	120.63	123.34
2	H	6	5CM	O4'-C4'-C3'	2.58	111.69	105.67
2	H	6	5CM	O4'-C1'-N1	-2.46	103.45	107.86
2	E	6	5CM	N1-C2-N3	2.45	123.27	118.81
2	K	6	5CM	O3'-C3'-C4'	-2.42	100.84	110.10
2	H	6	5CM	N1-C2-N3	2.35	123.09	118.81
2	H	6	5CM	C5-C6-N1	-2.25	121.03	123.34
2	B	6	5CM	O4'-C1'-N1	-2.14	104.03	107.86
2	H	6	5CM	C2'-C1'-N1	2.12	118.66	113.77
2	B	6	5CM	C3'-C2'-C1'	2.10	107.78	102.54
2	K	6	5CM	O4'-C1'-N1	-2.06	104.17	107.86

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	6	5CM	C3'-C4'-C5'-O5'
2	H	6	5CM	O4'-C4'-C5'-O5'
2	B	6	5CM	C3'-C4'-C5'-O5'
2	B	6	5CM	O4'-C4'-C5'-O5'
2	E	6	5CM	C3'-C4'-C5'-O5'
2	E	6	5CM	C2'-C1'-N1-C2
2	K	6	5CM	C2'-C1'-N1-C2
2	K	6	5CM	C2'-C1'-N1-C6
2	B	6	5CM	C2'-C1'-N1-C2
2	K	6	5CM	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	E	6	5CM	C2'-C1'-N1-C6
2	H	6	5CM	C2'-C1'-N1-C2
2	B	6	5CM	O4'-C1'-N1-C6
2	H	6	5CM	C2'-C1'-N1-C6
2	H	6	5CM	O4'-C1'-N1-C6
2	E	6	5CM	O4'-C4'-C5'-O5'
2	E	6	5CM	O4'-C1'-N1-C6
2	B	6	5CM	C2'-C1'-N1-C6
2	K	6	5CM	O4'-C1'-N1-C6
2	H	6	5CM	O4'-C1'-N1-C2
2	B	6	5CM	O4'-C1'-N1-C2
2	K	6	5CM	O4'-C1'-N1-C2
2	E	6	5CM	O4'-C1'-N1-C2
2	K	6	5CM	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	6	5CM	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	OGA	G	502	4	9,9,9	1.14	1 (11%)	10,11,11	1.61	2 (20%)
5	OGA	D	502	4	9,9,9	1.11	0	10,11,11	1.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	OGA	J	502	4	9,9,9	1.22	0	10,11,11	1.50	1 (10%)
5	OGA	A	502	4	9,9,9	1.26	0	10,11,11	1.47	2 (20%)

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
5	OGA	G	502	4	-	0/8/9/9	-
5	OGA	D	502	4	-	1/8/9/9	-
5	OGA	J	502	4	-	1/8/9/9	-
5	OGA	A	502	4	-	0/8/9/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	502	OGA	O3-C5	-2.14	1.23	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	502	OGA	O2-C1-C2	3.10	122.29	113.15
5	J	502	OGA	O2-C1-C2	2.63	120.89	113.15
5	A	502	OGA	O2-C1-C2	2.28	119.88	113.15
5	A	502	OGA	O2'-C2-C1	-2.21	118.20	121.32
5	G	502	OGA	O1-C1-C2	-2.03	117.66	122.18

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	502	OGA	N1-C4-C5-O4
5	J	502	OGA	N1-C4-C5-O4

There are no ring outliers.

No monomer is involved in short contacts.

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	376/415 (90%)	0.38	28 (7%) 14 19	18, 28, 51, 89	0
1	D	383/415 (92%)	0.12	7 (1%) 68 74	19, 29, 50, 79	0
1	G	376/415 (90%)	0.11	14 (3%) 41 48	24, 38, 56, 94	0
1	J	383/415 (92%)	0.54	41 (10%) 6 8	36, 51, 76, 105	0
2	B	11/12 (91%)	0.09	1 (9%) 9 12	34, 42, 50, 64	0
2	E	11/12 (91%)	0.33	1 (9%) 9 12	30, 33, 65, 73	0
2	H	11/12 (91%)	-0.22	0 100 100	33, 37, 53, 59	0
2	K	11/12 (91%)	2.01	4 (36%) 0 0	54, 61, 108, 111	0
3	C	12/12 (100%)	0.05	0 100 100	39, 46, 49, 50	0
3	F	12/12 (100%)	0.18	1 (8%) 11 15	28, 45, 70, 81	0
3	I	12/12 (100%)	-0.09	0 100 100	44, 47, 49, 51	0
3	L	11/12 (91%)	1.72	5 (45%) 0 0	57, 62, 119, 123	0
All	All	1609/1756 (91%)	0.30	102 (6%) 20 25	18, 38, 65, 123	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	118	HIS	6.5
1	A	178	ARG	6.4
1	J	181	VAL	5.7
1	J	117	ASP	5.5
1	J	172	ARG	5.5
1	A	215	ALA	5.4
1	A	173	ALA	5.3
1	G	117	ASP	5.3
1	G	118	HIS	5.1
1	J	180	ARG	4.9
1	J	178	ARG	4.9

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Mol	Chain	Res	Type	RSRZ
1	D	118	HIS	4.7
1	J	209	ASP	4.7
1	J	168	GLN	4.7
1	J	214	GLY	4.6
2	K	12	DG	4.5
3	L	5	DG	4.5
1	A	118	HIS	4.4
1	G	415	THR	4.3
1	J	200	LEU	4.3
2	K	9	DT	4.1
1	J	183	MET	4.1
1	J	215	ALA	4.1
2	K	11	DC	4.0
1	J	164	ASP	4.0
1	A	176	GLY	4.0
1	J	163	LYS	4.0
1	J	208	LEU	4.0
3	L	4	DA	3.9
1	G	115	ASN	3.9
1	J	177	GLU	3.8
1	A	202	ALA	3.6
1	A	117	ASP	3.6
1	G	119	PRO	3.5
1	A	177	GLU	3.5
1	A	174	ARG	3.5
1	J	179	ALA	3.5
2	K	10	DA	3.5
1	D	117	ASP	3.5
1	A	214	GLY	3.4
3	L	2	DG	3.4
3	L	3	DT	3.3
1	J	213	GLN	3.3
1	J	176	GLY	3.2
1	J	92	ARG	3.2
1	J	165	GLY	3.2
1	D	410	TRP	3.2
1	A	175	GLU	3.2
1	G	111	GLY	3.2
1	J	106	LYS	3.1
1	J	119	PRO	3.0
1	G	106	LYS	3.0
1	J	116	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	J	21	LEU	2.9
1	J	175	GLU	2.9
1	J	415	THR	2.8
1	A	208	LEU	2.8
1	A	366	VAL	2.8
1	A	340	VAL	2.8
3	F	1	DC	2.8
1	A	338	ILE	2.7
1	A	389	ALA	2.7
2	E	12	DG	2.7
1	A	315	LEU	2.7
1	J	112	ALA	2.6
1	A	162	THR	2.6
1	G	382	ASP	2.6
1	D	203	ASN	2.6
1	J	47	GLU	2.6
1	D	151	ILE	2.6
1	J	182	GLU	2.6
1	G	163	LYS	2.6
1	J	120	VAL	2.6
1	J	201	GLY	2.5
1	G	175	GLU	2.5
1	A	213	GLN	2.5
1	J	216	CYS	2.4
1	J	174	ARG	2.4
1	D	261	ILE	2.4
1	J	249	LYS	2.3
1	A	266	VAL	2.3
1	G	164	ASP	2.3
1	A	67	VAL	2.3
1	J	97	ASN	2.3
1	G	215	ALA	2.3
1	A	163	LYS	2.2
1	A	144	VAL	2.2
1	A	368	ALA	2.2
1	A	140	LEU	2.2
1	D	266	VAL	2.2
1	J	48	ASN	2.2
1	J	236	ASN	2.2
1	J	76	TYR	2.2
1	G	103	VAL	2.2
1	G	174	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	339	LEU	2.1
1	J	382	ASP	2.1
2	B	1	DC	2.1
1	A	148	ILE	2.1
1	A	390	HIS	2.1
3	L	6	DC	2.1
1	J	212	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
2	5CM	B	6	20/21	0.91	0.17	25,32,50,52	0
2	5CM	H	6	20/21	0.91	0.15	29,37,48,54	0
2	5CM	K	6	20/21	0.92	0.12	39,45,57,63	0
2	5CM	E	6	20/21	0.96	0.12	20,28,36,39	0

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
5	OGA	J	502	10/10	0.94	0.13	36,41,44,44	0
5	OGA	D	502	10/10	0.98	0.10	17,20,26,38	0
5	OGA	A	502	10/10	0.98	0.13	20,23,25,26	0
5	OGA	G	502	10/10	0.99	0.10	28,30,32,33	0
4	MN	J	501	1/1	0.99	0.11	37,37,37,37	0
4	MN	G	501	1/1	1.00	0.10	33,33,33,33	0
4	MN	A	501	1/1	1.00	0.11	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MN	D	501	1/1	1.00	0.14	21,21,21,21	0

6.5 Other polymers (i)

There are no such residues in this entry.