



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2017 – 01:43 PM EDT

PDB ID : 4AQX
Title : Crystal structure of I-CreI complexed with its target methylated at position plus 2 (in the b strand) in the presence of magnesium
Authors : Valton, J.; Daboussi, F.; Leduc, S.; Redondo, P.; Macmaster, R.; Molina, R.; Montoya, G.; Duchateau, P.
Deposited on : 2012-04-19
Resolution : 2.20 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029077
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029077

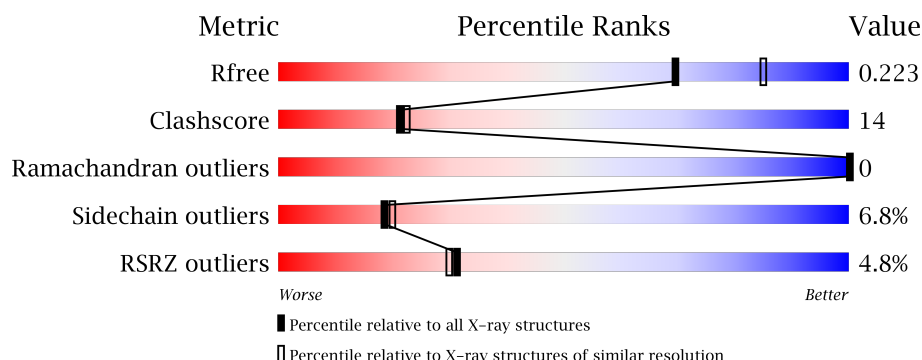
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	152	<div> <div>8%</div> <div> <div></div> <div>74%</div> <div>21%</div> <div>5%</div> </div> </div>
1	B	152	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>24%</div> <div>.</div> </div> </div>
2	C	14	<div> <div></div> <div> <div>50%</div> <div>36%</div> <div>14%</div> </div> </div>
3	D	10	<div> <div></div> <div> <div>30%</div> <div>60%</div> <div>10%</div> </div> </div>
4	E	14	<div> <div></div> <div> <div>57%</div> <div>36%</div> <div>7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	F	10	

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
6	GOL	A	1154	-	-	X	X
6	GOL	A	1155	-	-	X	X
6	GOL	B	1354	-	-	X	-
6	GOL	B	1355	-	-	X	X
6	GOL	C	1515	-	-	X	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 3619 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 DNA ENDONUCLEASE I-CREI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	152	Total	C	N	O	S	0	0	0
			1236	796	210	229	1			
1	B	152	Total	C	N	O	S	0	0	0
			1236	796	210	229	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	14	Total	C	N	O	P	0	0	0
			285	137	55	80	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	10	Total	C	N	O	P	0	0	0
			210	99	39	62	10			

- Molecule 4 is a DNA chain called 5'-D(*CP*CP*AP*AP*AP*CP*TP*GP*TP*CP*TP*CP*AP*5CM)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	14	Total	C	N	O	P	0	0	0
			278	135	49	81	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	10	Total	C	N	O	P	0	0	0
			208	99	36	63	10			

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	2	Total	Mg	0	0
			2	2		
7	F	1	Total	Mg	0	0
			1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	56	Total	O	0	0
			56	56		
8	B	42	Total	O	0	0
			42	42		

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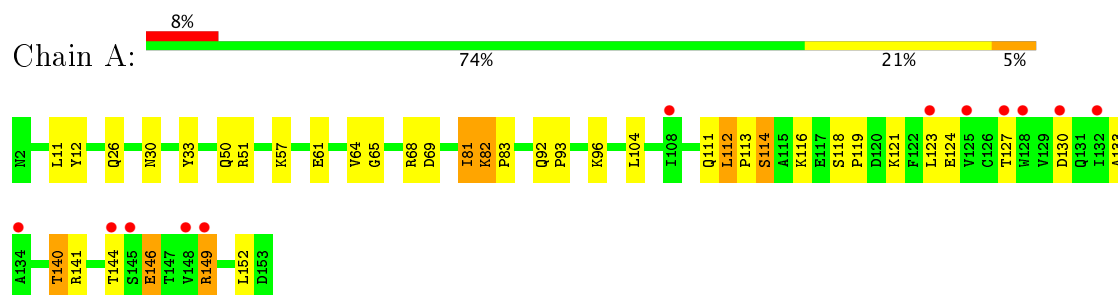
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	19	Total 19	O 19	0	0
8	D	9	Total 9	O 9	0	0
8	E	5	Total 5	O 5	0	0
8	F	2	Total 2	O 2	0	0

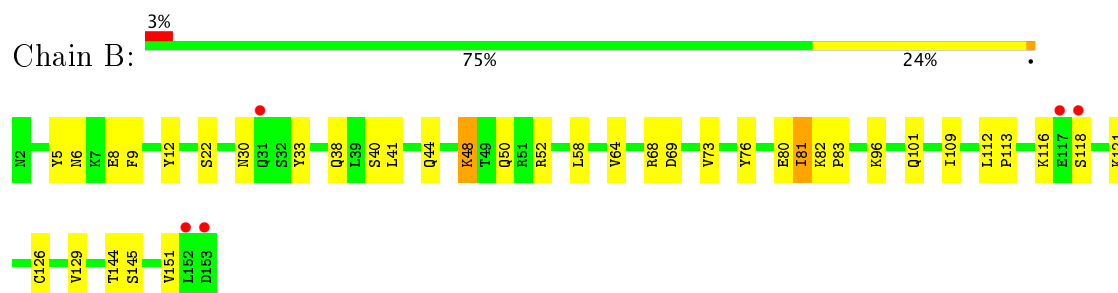
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: DNA ENDONUCLEASE I-CREI



- Molecule 1: DNA ENDONUCLEASE I-CREI



- Molecule 2: 5'-D(*TP*CP*AP*AP*AP*AP*CP*GP*TP*CP*GP*TP*GP*AP)-3'

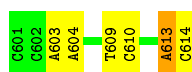


- Molecule 3: 5'-D(*GP*AP*CP*AP*GP*TP*TP*TP*GP*GP)-3'



- Molecule 4: 5'-D(*CP*CP*AP*AP*AP*CP*TP*GP*TP*CP*TP*CP*AP*5CM)-3'





- Molecule 5: 5'-D(*GP*AP*CP*GP*TP*TP*TP*TP*GP*AP)-3'

Chain F:  30% 40% 20% 10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	45.84Å 71.40Å 179.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.79 – 2.20 45.79 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.79-2.20) 99.8 (45.79-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 2.20Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.202 , 0.242 0.181 , 0.223	Depositor DCC
R_{free} test set	1998 reflections (6.51%)	DCC
Wilson B-factor (Å ²)	49.9	Xtriage
Anisotropy	0.529	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3619	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, 5CM

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	0.41	0/1259	0.54	0/1700
1	B	0.37	0/1259	0.53	0/1700
2	C	0.75	0/320	1.36	2/492 (0.4%)
3	D	0.89	1/235 (0.4%)	1.50	3/360 (0.8%)
4	E	0.70	0/288	1.40	3/441 (0.7%)
5	F	6.98	2/232 (0.9%)	4.81	4/355 (1.1%)
All	All	1.84	3/3593 (0.1%)	1.53	12/5048 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	F	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	624	DA	C1'-N9	105.55	2.95	1.47
3	D	515	DG	OP3-P	-9.25	1.50	1.61
5	F	615	DG	OP3-P	-8.80	1.50	1.61

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	624	DA	O4'-C1'-N9	-85.91	47.87	108.00
5	F	624	DA	N9-C1'-C2'	13.05	137.39	112.60
4	E	613	DA	O4'-C1'-N9	-8.64	101.95	108.00
2	C	513	DG	O4'-C1'-N9	-7.69	102.62	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	522	DT	O4'-C1'-N1	-7.13	103.01	108.00
3	D	516	DA	O4'-C1'-N9	6.37	112.46	108.00
4	E	609	DT	O4'-C1'-N1	-6.07	103.75	108.00
2	C	514	DA	N9-C1'-C2'	5.99	123.97	112.60
5	F	622	DT	O4'-C1'-N1	-5.82	103.93	108.00
4	E	610	DC	O4'-C1'-N1	-5.67	104.03	108.00
3	D	524	DG	O4'-C1'-N9	5.33	111.73	108.00
5	F	616	DA	O4'-C1'-N9	5.01	111.50	108.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	F	624	DA	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1236	0	1270	37	0
1	B	1236	0	1270	33	0
2	C	285	0	158	8	0
3	D	210	0	114	12	0
4	E	278	0	160	4	0
5	F	208	0	115	5	0
6	A	12	0	16	18	0
6	B	12	0	16	9	0
6	C	6	0	8	6	0
7	D	2	0	0	0	0
7	F	1	0	0	0	0
8	A	56	0	0	3	0
8	B	42	0	0	3	0
8	C	19	0	0	1	0
8	D	9	0	0	0	0
8	E	5	0	0	1	0
8	F	2	0	0	0	0
All	All	3619	0	3127	90	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 14.

All (90) 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)
6:A:1155:GOL:H12	3:D:518:DA:P	1.81	1.20
8:B:2016:HOH:O	6:C:1515:GOL:H31	1.63	0.97
6:A:1155:GOL:H12	3:D:518:DA:OP2	1.66	0.94
1:A:144:THR:HG23	1:A:146:GLU:H	1.33	0.93
2:C:509:DT:OP2	8:C:2009:HOH:O	1.97	0.82
1:A:141:ARG:NH1	6:A:1155:GOL:O3	2.14	0.81
6:A:1155:GOL:C1	3:D:518:DA:P	2.68	0.79
6:B:1355:GOL:O1	8:B:2031:HOH:O	2.00	0.78
1:A:26:GLN:HG2	6:A:1155:GOL:H2	1.65	0.76
6:A:1155:GOL:C1	3:D:518:DA:OP2	2.33	0.76
1:B:5:TYR:HD1	6:B:1354:GOL:H31	1.51	0.73
1:A:144:THR:HG23	1:A:146:GLU:N	2.04	0.71
1:A:61:GLU:OE1	6:A:1154:GOL:H2	1.89	0.71
1:B:38:GLN:NE2	6:C:1515:GOL:H11	2.07	0.70
5:F:624:DA:O4'	5:F:624:DA:N9	2.25	0.69
5:F:618:DG:H2''	5:F:619:DT:H5'	1.76	0.67
6:A:1154:GOL:H31	1:B:96:LYS:HD3	1.79	0.64
1:B:6:ASN:N	6:B:1354:GOL:O3	2.18	0.64
1:B:101:GLN:HE22	6:B:1355:GOL:H31	1.63	0.63
1:A:149:ARG:HB2	1:A:149:ARG:HH11	1.65	0.61
1:B:113:PRO:HG2	8:B:2033:HOH:O	1.99	0.60
1:A:82:LYS:HB3	1:A:83:PRO:HD3	1.85	0.59
6:A:1155:GOL:H32	3:D:517:DC:H5'	1.86	0.58
2:C:504:DA:OP2	6:C:1515:GOL:H32	2.04	0.57
1:A:96:LYS:HD2	1:B:12:TYR:CZ	2.40	0.56
1:B:82:LYS:HB3	1:B:83:PRO:HD3	1.88	0.56
1:B:81:ILE:HD12	6:C:1515:GOL:O3	2.06	0.56
1:B:64:VAL:HG11	1:B:83:PRO:HB3	1.88	0.55
1:A:133:ALA:HB2	1:A:141:ARG:HH11	1.71	0.55
1:A:26:GLN:HA	6:A:1155:GOL:H2	1.89	0.55
1:A:12:TYR:CZ	1:B:96:LYS:HD2	2.43	0.54
1:A:51:ARG:CZ	6:B:1355:GOL:H12	2.39	0.53
1:A:113:PRO:HG2	8:A:2045:HOH:O	2.08	0.53
1:B:118:SER:HB3	1:B:121:LYS:HB3	1.91	0.53
1:B:81:ILE:HG12	1:B:109:ILE:HG12	1.91	0.53
1:A:140:THR:CG2	3:D:517:DC:H2''	2.39	0.53
1:A:30:ASN:HB3	1:A:33:TYR:CD1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LEU:HD11	1:B:8:GLU:HG2	1.92	0.52
1:B:101:GLN:NE2	6:B:1355:GOL:H31	2.25	0.52
1:B:52:ARG:NH1	1:B:69:ASP:OD1	2.39	0.51
1:B:40:SER:HA	6:C:1515:GOL:H12	1.92	0.51
1:A:33:TYR:OH	4:E:603:DA:N7	2.43	0.51
1:B:33:TYR:OH	2:C:503:DA:N7	2.40	0.51
8:E:2005:HOH:O	5:F:615:DG:OP3	2.20	0.50
1:B:73:VAL:HG21	4:E:614:5CM:H5A1	1.94	0.50
1:A:26:GLN:HA	6:A:1155:GOL:C2	2.42	0.50
1:A:111:GLN:OE1	1:A:121:LYS:NZ	2.31	0.49
1:A:141:ARG:HH21	1:A:144:THR:HA	1.79	0.48
6:B:1355:GOL:O2	5:F:616:DA:OP1	2.30	0.48
1:A:112:LEU:N	1:A:113:PRO:HD2	2.28	0.48
2:C:504:DA:H2''	2:C:505:DA:O5'	2.13	0.48
1:A:141:ARG:HD2	6:A:1155:GOL:H31	1.95	0.47
1:A:57:LYS:HB3	6:A:1154:GOL:O1	2.15	0.47
1:A:133:ALA:HB2	1:A:141:ARG:NH1	2.30	0.47
1:A:119:PRO:HB3	1:A:152:LEU:HD13	1.96	0.47
1:B:116:LYS:HE3	2:C:502:DC:H5''	1.96	0.47
1:A:123:LEU:HD13	1:A:149:ARG:HH12	1.80	0.46
3:D:518:DA:H2''	3:D:519:DG:H5'	1.98	0.46
1:A:30:ASN:HB3	1:A:33:TYR:HD1	1.80	0.46
1:B:5:TYR:CD1	6:B:1354:GOL:H31	2.41	0.46
1:B:22:SER:HB3	1:B:44:GLN:HG2	1.97	0.46
1:A:140:THR:O	1:A:140:THR:HG23	2.15	0.45
1:B:9:PHE:CD2	6:B:1354:GOL:H32	2.51	0.45
8:A:2008:HOH:O	3:D:517:DC:OP2	2.21	0.45
1:A:127:THR:O	1:A:130:ASP:HB2	2.17	0.45
1:B:126:CYS:HA	1:B:129:VAL:HG13	1.99	0.44
1:A:114:SER:HB3	8:A:2045:HOH:O	2.17	0.44
6:A:1155:GOL:C3	3:D:517:DC:H5'	2.48	0.44
1:B:44:GLN:HA	1:B:76:TYR:O	2.18	0.44
6:A:1154:GOL:H31	1:B:96:LYS:CD	2.46	0.44
1:B:112:LEU:N	1:B:113:PRO:HD2	2.32	0.43
4:E:613:DA:H1'	4:E:614:5CM:O4'	2.17	0.43
1:A:26:GLN:CG	6:A:1155:GOL:H2	2.43	0.43
1:B:58:LEU:HD23	1:B:58:LEU:HA	1.85	0.43
2:C:514:DA:C6	3:D:515:DG:C6	3.07	0.43
1:B:48:LYS:HE3	1:B:48:LYS:HB3	1.82	0.42
2:C:513:DG:H1'	2:C:514:DA:O4'	2.19	0.42
1:A:64:VAL:HG22	1:A:65:GLY:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:623:DG:H2''	5:F:624:DA:H5''	1.99	0.42
1:B:30:ASN:HB3	1:B:33:TYR:CD1	2.55	0.42
2:C:504:DA:H8	6:C:1515:GOL:O2	2.03	0.41
1:B:80:GLU:HB3	1:B:83:PRO:HG2	2.02	0.41
1:A:140:THR:HG23	3:D:517:DC:H2''	2.01	0.41
1:A:92:GLN:N	1:A:93:PRO:HD2	2.36	0.41
1:A:81:ILE:HD12	4:E:604:DA:OP2	2.20	0.41
1:A:64:VAL:HG11	1:A:83:PRO:HB3	2.03	0.41
1:B:144:THR:OG1	1:B:145:SER:N	2.53	0.41
1:A:61:GLU:OE2	6:A:1154:GOL:O3	2.28	0.40
6:A:1155:GOL:H12	3:D:517:DC:O3'	2.20	0.40
1:B:41:LEU:N	1:B:41:LEU:HD22	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	150/152 (99%)	144 (96%)	6 (4%)	0	100	100
1	B	150/152 (99%)	146 (97%)	4 (3%)	0	100	100
All	All	300/304 (99%)	290 (97%)	10 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	139/139 (100%)	125 (90%)	14 (10%)	9	8
1	B	139/139 (100%)	134 (96%)	5 (4%)	40	50
All	All	278/278 (100%)	259 (93%)	19 (7%)	18	20

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	68	ARG
1	A	69	ASP
1	A	81	ILE
1	A	82	LYS
1	A	104	LEU
1	A	112	LEU
1	A	114	SER
1	A	116	LYS
1	A	118	SER
1	A	124	GLU
1	A	140	THR
1	A	146	GLU
1	A	149	ARG
1	B	48	LYS
1	B	50	GLN
1	B	68	ARG
1	B	81	ILE
1	B	151	VAL

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

Mol	Chain	Res	Type
1	A	26	GLN
1	A	37	HIS
1	A	44	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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$
4	5CM	E	614	2,4,7	14,21,22	2.71	6 (42%)	18,30,33	1.90	7 (38%)

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
4	5CM	E	614	2,4,7	-	0/3/21/22	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	614	5CM	O5'-C5'	-2.98	1.40	1.44
4	E	614	5CM	C6-C5	2.67	1.47	1.40
4	E	614	5CM	C2-N3	3.65	1.45	1.38
4	E	614	5CM	C4-N4	3.95	1.44	1.34
4	E	614	5CM	C5-C4	4.26	1.47	1.41
4	E	614	5CM	C4-N3	5.17	1.42	1.35

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	614	5CM	C5-C6-N1	-3.40	118.47	122.15
4	E	614	5CM	C4'-O4'-C1'	-2.25	103.91	109.42
4	E	614	5CM	C5A-C5-C4	-2.13	119.46	121.65
4	E	614	5CM	C3'-C2'-C1'	-2.12	97.05	102.48
4	E	614	5CM	O5'-C5'-C4'	2.39	117.41	109.01
4	E	614	5CM	O4'-C1'-N1	3.53	113.73	107.78
4	E	614	5CM	C2'-C1'-N1	3.73	123.04	114.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	614	5CM	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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	$\# Z > 2$
6	GOL	A	1154	-	5,5,5	0.33	0	5,5,5	0.48	0
6	GOL	A	1155	-	5,5,5	0.37	0	5,5,5	1.83	3 (60%)
6	GOL	B	1354	-	5,5,5	0.28	0	5,5,5	0.23	0
6	GOL	B	1355	-	5,5,5	0.41	0	5,5,5	0.37	0
6	GOL	C	1515	-	5,5,5	0.78	0	5,5,5	1.05	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
6	GOL	A	1154	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1155	-	-	0/4/4/4	0/0/0/0
6	GOL	B	1354	-	-	0/4/4/4	0/0/0/0
6	GOL	B	1355	-	-	0/4/4/4	0/0/0/0
6	GOL	C	1515	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
6	A	1155	GOL	O1-C1-C2	-2.73	96.30	110.07
6	A	1155	GOL	O2-C2-C1	-2.07	99.05	108.84
6	A	1155	GOL	O3-C3-C2	-2.04	99.81	110.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1154	GOL	5	0
6	A	1155	GOL	13	0
6	B	1354	GOL	4	0
6	B	1355	GOL	5	0
6	C	1515	GOL	6	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, 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	152/152 (100%)	0.52	12 (7%) 13 12	30, 57, 104, 120	0
1	B	152/152 (100%)	0.24	5 (3%) 47 44	29, 54, 87, 103	0
2	C	14/14 (100%)	0.04	0 100 100	36, 52, 63, 68	0
3	D	10/10 (100%)	-0.06	0 100 100	35, 59, 63, 65	1 (10%)
4	E	13/14 (92%)	-0.10	0 100 100	41, 53, 64, 68	3 (23%)
5	F	10/10 (100%)	-0.08	0 100 100	37, 59, 61, 72	0
All	All	351/352 (99%)	0.32	17 (4%) 31 30	29, 54, 93, 120	4 (1%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	118	SER	4.0
1	A	128	TRP	3.3
1	A	149	ARG	3.3
1	A	134	ALA	3.3
1	A	148	VAL	2.8
1	A	123	LEU	2.8
1	A	125	VAL	2.7
1	B	152	LEU	2.7
1	A	145	SER	2.5
1	A	130	ASP	2.5
1	B	117	GLU	2.5
1	A	127	THR	2.3
1	A	144	THR	2.2
1	A	132	ILE	2.2
1	B	31	GLN	2.2
1	B	153	ASP	2.2
1	A	108	ILE	2.1

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	5CM	E	614	20/21	0.92	0.16	-	31,39,48,50	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
6	GOL	C	1515	6/6	0.60	0.56	23.12	66,81,85,86	0
6	GOL	A	1154	6/6	0.84	0.38	11.10	50,71,73,82	0
6	GOL	A	1155	6/6	0.89	0.60	7.61	58,74,76,78	0
6	GOL	B	1355	6/6	0.93	0.30	7.30	52,64,72,79	0
7	MG	F	1625	1/1	0.94	0.14	-1.57	40,40,40,40	0
7	MG	D	1525	1/1	0.99	0.10	-3.77	31,31,31,31	0
7	MG	D	1526	1/1	0.98	0.07	-4.14	30,30,30,30	0
6	GOL	B	1354	6/6	0.94	0.20	-	60,74,82,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.