Full wwPDB X-ray Structure Validation Report (i)

Nov 20, 2023 – 04:46 PM JST

PDB ID	:	7CY6
Title	:	Crystal Structure of CMD1 in complex with 5mC-DNA
Authors	:	Li, W.; Zhang, T.; Sun, M.; Ding, J.
Deposited on	:	2020-09-03
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The 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:

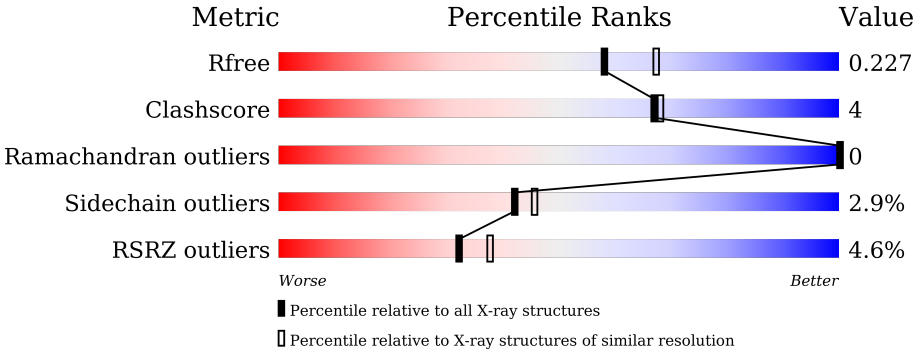
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	917	4%, 86%, 9%, 5%
2	C	14	29%, 29%, 29%, 7%, 36%
2	D	14	14%, 43%, 7%, 50%

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
4	EDO	A	612	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7502 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 Maltodextrin-binding protein,5-methylcytosine-modifying enzyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	872	6663	4240	1145	1251	27	0	6	0

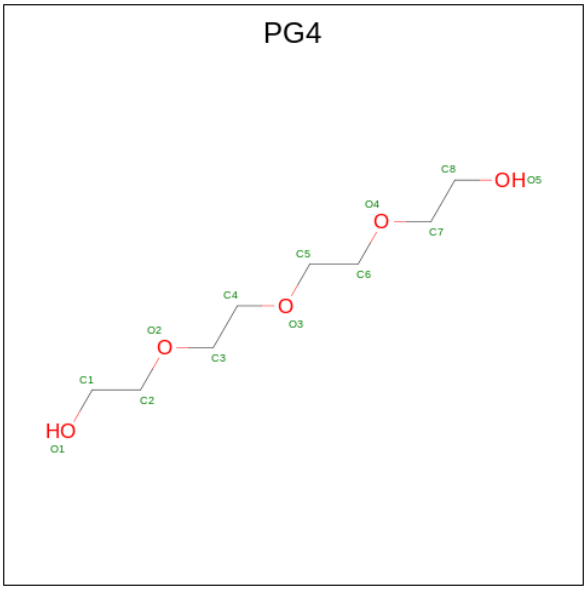
There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-373	MET	-	initiating methionine	UNP A0A376KDN7
A	-291	ALA	ASP	engineered mutation	UNP A0A376KDN7
A	-290	ALA	LYS	engineered mutation	UNP A0A376KDN7
A	-201	ALA	GLU	engineered mutation	UNP A0A376KDN7
A	-200	ALA	ASN	engineered mutation	UNP A0A376KDN7
A	-134	ALA	LYS	engineered mutation	UNP A0A376KDN7
A	-11	ALA	LYS	engineered mutation	UNP A0A376KDN7
A	-10	ALA	ASP	engineered mutation	UNP A0A376KDN7
A	-6	ASN	-	linker	UNP A0A376KDN7
A	-5	ALA	-	linker	UNP A0A376KDN7
A	-4	ALA	-	linker	UNP A0A376KDN7
A	-3	ARG	-	linker	UNP A0A376KDN7
A	-2	ALA	-	linker	UNP A0A376KDN7
A	-1	ALA	-	linker	UNP A0A376KDN7
A	0	ALA	-	linker	UNP A0A376KDN7
A	533	ALA	-	expression tag	UNP A0A2K3D5Z7
A	534	ALA	-	expression tag	UNP A0A2K3D5Z7
A	535	ALA	-	expression tag	UNP A0A2K3D5Z7
A	536	LEU	-	expression tag	UNP A0A2K3D5Z7
A	537	GLU	-	expression tag	UNP A0A2K3D5Z7
A	538	HIS	-	expression tag	UNP A0A2K3D5Z7
A	539	HIS	-	expression tag	UNP A0A2K3D5Z7
A	540	HIS	-	expression tag	UNP A0A2K3D5Z7
A	541	HIS	-	expression tag	UNP A0A2K3D5Z7
A	542	HIS	-	expression tag	UNP A0A2K3D5Z7
A	543	HIS	-	expression tag	UNP A0A2K3D5Z7

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

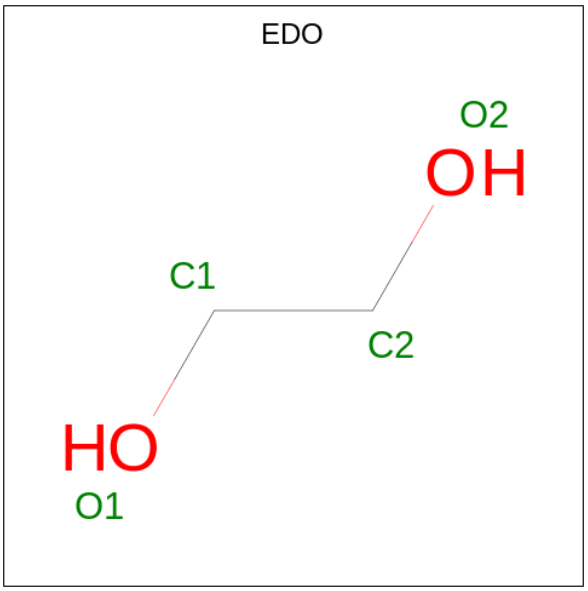
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	9	189	88	39	53	9	0	0	0
2	D	7	140	66	25	42	7	0	0	0

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	13	8	5	0	0
3	A	1	6	4	2	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is FE (II) ION (three-letter code: FE2) (formula: Fe) (labeled as "Ligand of

Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
5	A	1	1	1	0	0

- Molecule 6 is water.

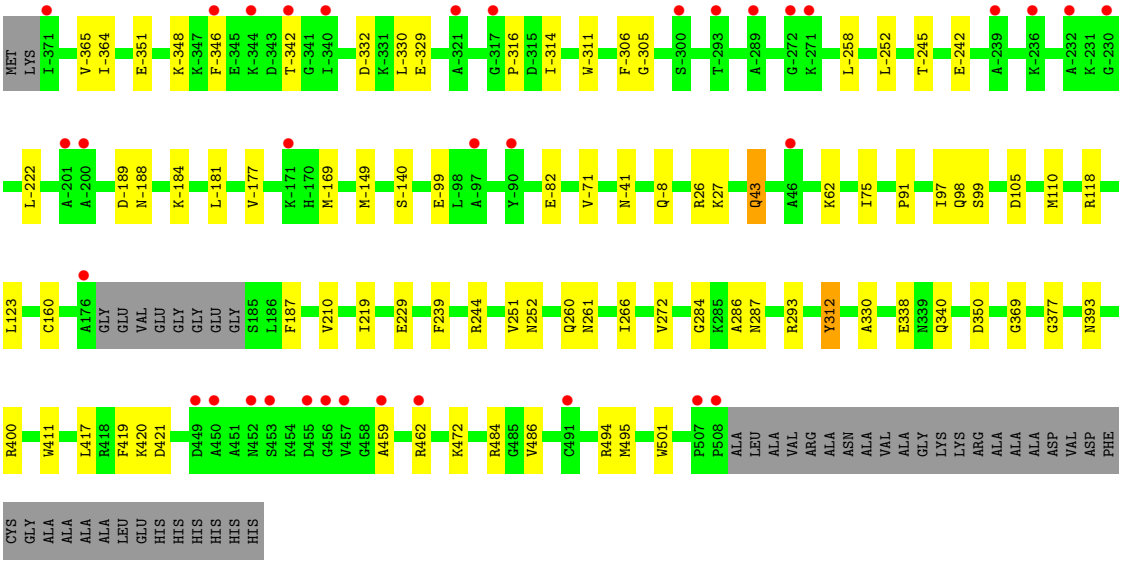
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	429	429	429	0	0
			Total	O		
6	C	5	5	5	0	0
			Total	O		
6	D	4	4	4	0	0

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.

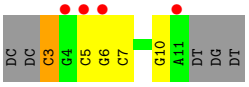
• Molecule 1: Maltodextrin-binding protein,5-methylcytosine-modifying enzyme 1

Chain A:



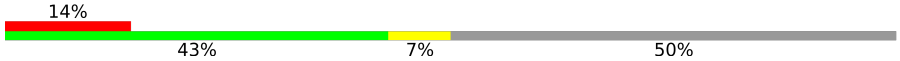
• Molecule 2: DNA (5'-D(P*(5CM)P*GP*CP*GP*CP*GP*GP*GP*A)-3')

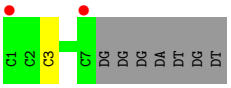
Chain C:



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

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	153.17Å 127.06Å 64.22Å 90.00° 102.74° 90.00°	Depositor
Resolution (Å)	50.01 – 2.10 48.39 – 2.09	Depositor EDS
% Data completeness (in resolution range)	89.0 (50.01-2.10) 88.6 (48.39-2.09)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.182 , 0.227 0.182 , 0.227	Depositor DCC
R_{free} test set	2999 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å^2)	28.6	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7502	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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: FE2, PG4, EDO, 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	0.40	0/6830	0.55	0/9285
2	C	0.44	0/190	0.76	0/292
2	D	0.42	0/132	0.88	0/198
All	All	0.41	0/7152	0.57	0/9775

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	6663	0	6632	48	0
2	C	189	0	102	6	0
2	D	140	0	80	0	0
3	A	19	0	24	6	0
4	A	52	0	78	8	0
5	A	1	0	0	0	0
6	A	429	0	0	0	0
6	C	5	0	0	0	0
6	D	4	0	0	0	0
All	All	7502	0	6916	54	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (54) 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:A:98:GLN:H	3:A:601:PG4:H71	1.18	1.09
1:A:287:ASN:H	4:A:612:EDO:C1	2.01	0.72
1:A:99:SER:HB2	3:A:601:PG4:H31	1.71	0.72
1:A:419:PHE:HB2	1:A:486:VAL:HG21	1.75	0.69
1:A:98:GLN:N	3:A:601:PG4:H71	2.02	0.66
1:A:287:ASN:ND2	4:A:612:EDO:H12	2.14	0.61
1:A:62:LYS:HG3	1:A:160:CYS:HB2	1.82	0.61
1:A:260:GLN:H	4:A:605:EDO:H21	1.65	0.60
1:A:-258:LEU:HD11	1:A:-149:MET:HE2	1.85	0.59
2:C:6:DG:H2"	2:C:7:DC:O5'	2.02	0.59
1:A:26:ARG:HG3	1:A:105:ASP:OD1	2.03	0.58
1:A:98:GLN:H	3:A:601:PG4:C7	2.06	0.57
1:A:-351:GLU:HA	1:A:-348:LYS:HE3	1.86	0.57
1:A:287:ASN:H	4:A:612:EDO:H11	1.69	0.56
1:A:-311:TRP:HB3	1:A:-306:PHE:HE1	1.73	0.54
1:A:75:ILE:HD11	1:A:219:ILE:HG21	1.90	0.54
1:A:330:ALA:HB3	4:A:610:EDO:H22	1.90	0.53
1:A:-245:THR:OG1	1:A:-242:GLU:HG3	2.09	0.53
1:A:239:PHE:HB3	1:A:252:ASN:HB3	1.91	0.53
1:A:459:ALA:HA	1:A:462:ARG:HD3	1.91	0.53
1:A:-305:GLY:HA3	1:A:-41:ASN:O	2.10	0.52
1:A:350:ASP:HA	1:A:417:LEU:O	2.10	0.51
1:A:286:ALA:N	4:A:612:EDO:H11	2.25	0.51
1:A:97:ILE:HA	3:A:601:PG4:H82	1.92	0.51
1:A:-188:ASN:O	1:A:-184:LYS:HG3	2.11	0.50
1:A:75:ILE:HD11	1:A:219:ILE:CG2	2.41	0.50
1:A:97:ILE:HD11	1:A:123:LEU:HG	1.92	0.50
1:A:-222:LEU:HD11	1:A:-169:MET:HE3	1.92	0.50
2:C:6:DG:H2'	2:C:7:DC:C6	2.48	0.49
1:A:312:TYR:HE2	4:A:610:EDO:H21	1.78	0.49
1:A:-258:LEU:HD21	1:A:-149:MET:HE3	1.96	0.48
1:A:-364:ILE:HD12	1:A:-314:ILE:HD12	1.96	0.48
1:A:-245:THR:HG1	1:A:-242:GLU:HG3	1.79	0.48
1:A:284:GLY:O	4:A:612:EDO:H22	2.14	0.47
1:A:229:GLU:OE2	1:A:293:ARG:HD2	2.14	0.47
1:A:-258:LEU:HD11	1:A:-149:MET:CE	2.43	0.47
3:A:601:PG4:H22	3:A:601:PG4:H62	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:PRO:HG3	1:A:377:GLY:HA3	1.98	0.46
1:A:420:LYS:HB2	1:A:420:LYS:HE2	1.57	0.46
1:A:-346:PHE:O	1:A:-342:THR:HG22	2.16	0.46
1:A:369:GLY:HA2	1:A:400:ARG:O	2.16	0.46
1:A:-329:GLU:HB3	1:A:-311:TRP:CZ2	2.51	0.45
1:A:-365:VAL:HG13	1:A:-316:PRO:HA	1.98	0.45
2:C:6:DG:H2"	2:C:7:DC:C5'	2.47	0.45
1:A:187:PHE:HB3	1:A:501:TRP:CZ2	2.52	0.44
2:C:3:5CM:H6	2:C:3:5CM:H2'	1.82	0.44
1:A:110:MET:HE2	1:A:210:VAL:HG23	1.99	0.43
1:A:472:LYS:HD2	2:C:10:DG:OP2	2.19	0.43
1:A:-189:ASP:HB2	1:A:-8:GLN:HB2	2.01	0.42
2:C:5:DC:H2"	2:C:6:DG:C8	2.55	0.42
1:A:338:GLU:HB2	1:A:411:TRP:CZ3	2.56	0.41
1:A:43:GLN:OE1	1:A:118:ARG:NH1	2.53	0.41
1:A:-181:LEU:O	1:A:-177:VAL:HG13	2.20	0.40
1:A:338:GLU:O	1:A:340:GLN:HG2	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	874/917 (95%)	852 (98%)	22 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	688/711 (97%)	668 (97%)	20 (3%)	42 46

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-332	ASP
1	A	-330	LEU
1	A	-252	LEU
1	A	-140	SER
1	A	-99	GLU
1	A	-82	GLU
1	A	-71	VAL
1	A	27	LYS
1	A	43	GLN
1	A	244	ARG
1	A	251	VAL
1	A	261	ASN
1	A	266	ILE
1	A	272	VAL
1	A	312	TYR
1	A	393	ASN
1	A	421	ASP
1	A	484	ARG
1	A	494	ARG
1	A	495	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 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	D	3	2	17,21,22	4.57	12 (70%)	24,30,33	1.64	7 (29%)
2	5CM	C	3	2	17,21,22	4.94	12 (70%)	24,30,33	1.13	2 (8%)

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	D	3	2	-	4/7/21/22	0/2/2/2
2	5CM	C	3	2	-	2/7/21/22	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	5CM	C6-C5	8.90	1.49	1.34
2	D	3	5CM	C6-C5	8.27	1.48	1.34
2	C	3	5CM	O4'-C1'	8.20	1.60	1.42
2	D	3	5CM	O4'-C1'	7.44	1.59	1.42
2	C	3	5CM	C2'-C1'	-7.19	1.32	1.52
2	C	3	5CM	C4-N3	6.69	1.45	1.34
2	D	3	5CM	C2'-C1'	-6.64	1.33	1.52
2	C	3	5CM	C2-N3	6.51	1.49	1.36
2	D	3	5CM	C4-N3	6.15	1.44	1.34
2	C	3	5CM	C3'-C4'	-5.85	1.36	1.53
2	D	3	5CM	C2-N3	5.55	1.47	1.36
2	D	3	5CM	C3'-C4'	-5.43	1.38	1.53
2	D	3	5CM	C6-N1	4.46	1.45	1.38
2	C	3	5CM	C4-N4	4.39	1.45	1.34
2	C	3	5CM	C6-N1	4.35	1.45	1.38
2	C	3	5CM	C2-N1	4.31	1.49	1.40
2	D	3	5CM	C2-N1	3.85	1.48	1.40
2	D	3	5CM	C4-N4	3.71	1.43	1.34
2	C	3	5CM	O4'-C4'	3.59	1.53	1.45
2	D	3	5CM	O4'-C4'	3.54	1.52	1.45
2	C	3	5CM	C2'-C3'	3.51	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	5CM	C2'-C3'	3.38	1.61	1.52
2	D	3	5CM	O2-C2	-3.33	1.17	1.23
2	C	3	5CM	O2-C2	-2.77	1.18	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	3	5CM	C1'-N1-C2	3.58	124.03	117.74
2	C	3	5CM	C5-C6-N1	-3.02	120.23	123.34
2	D	3	5CM	C3'-C2'-C1'	2.88	109.75	102.54
2	C	3	5CM	C5A-C5-C6	-2.59	119.39	122.85
2	D	3	5CM	C4-N3-C2	2.57	124.16	120.69
2	D	3	5CM	O2-C2-N1	2.48	124.01	118.89
2	D	3	5CM	O2-C2-N3	-2.35	118.51	122.33
2	D	3	5CM	C5-C4-N3	-2.34	119.15	121.67
2	D	3	5CM	C6-N1-C2	-2.17	117.87	120.87

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	3	5CM	C2'-C1'-N1-C2
2	D	3	5CM	C2'-C1'-N1-C6
2	D	3	5CM	O4'-C1'-N1-C6
2	D	3	5CM	O4'-C1'-N1-C2
2	C	3	5CM	C2'-C1'-N1-C6
2	C	3	5CM	O4'-C1'-N1-C6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	5CM	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 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	$\#\|Z\| > 2$
4	EDO	A	606	-	3,3,3	0.44	0	2,2,2	0.35	0
4	EDO	A	613	-	3,3,3	0.46	0	2,2,2	0.23	0
4	EDO	A	605	-	3,3,3	0.47	0	2,2,2	0.35	0
4	EDO	A	603	-	3,3,3	0.43	0	2,2,2	0.44	0
3	PG4	A	601	-	12,12,12	0.54	0	11,11,11	0.61	0
4	EDO	A	607	-	3,3,3	0.46	0	2,2,2	0.24	0
4	EDO	A	610	-	3,3,3	0.49	0	2,2,2	0.17	0
4	EDO	A	609	-	3,3,3	0.46	0	2,2,2	0.21	0
4	EDO	A	611	-	3,3,3	0.34	0	2,2,2	0.65	0
4	EDO	A	614	-	3,3,3	0.53	0	2,2,2	0.16	0
4	EDO	A	608	-	3,3,3	0.43	0	2,2,2	0.39	0
3	PG4	A	602	-	5,5,12	0.50	0	4,4,11	0.25	0
4	EDO	A	604	-	3,3,3	0.44	0	2,2,2	0.43	0
4	EDO	A	612	-	3,3,3	0.47	0	2,2,2	0.52	0
4	EDO	A	615	-	3,3,3	0.47	0	2,2,2	0.21	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
4	EDO	A	606	-	-	1/1/1/1	-
4	EDO	A	613	-	-	1/1/1/1	-
4	EDO	A	605	-	-	0/1/1/1	-
4	EDO	A	603	-	-	1/1/1/1	-
3	PG4	A	601	-	-	6/10/10/10	-
4	EDO	A	607	-	-	1/1/1/1	-
4	EDO	A	610	-	-	1/1/1/1	-
4	EDO	A	609	-	-	0/1/1/1	-
4	EDO	A	611	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	614	-	-	1/1/1/1	-
4	EDO	A	608	-	-	0/1/1/1	-
3	PG4	A	602	-	-	1/3/3/10	-
4	EDO	A	604	-	-	0/1/1/1	-
4	EDO	A	612	-	-	0/1/1/1	-
4	EDO	A	615	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	PG4	C4-C3-O2-C2
3	A	601	PG4	O2-C3-C4-O3
3	A	601	PG4	C5-C6-O4-C7
4	A	606	EDO	O1-C1-C2-O2
4	A	610	EDO	O1-C1-C2-O2
4	A	611	EDO	O1-C1-C2-O2
4	A	613	EDO	O1-C1-C2-O2
4	A	614	EDO	O1-C1-C2-O2
3	A	601	PG4	C6-C5-O3-C4
3	A	601	PG4	C8-C7-O4-C6
3	A	602	PG4	C4-C3-O2-C2
4	A	607	EDO	O1-C1-C2-O2
3	A	601	PG4	C3-C4-O3-C5
4	A	603	EDO	O1-C1-C2-O2
4	A	615	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	605	EDO	1	0
3	A	601	PG4	6	0
4	A	610	EDO	2	0
4	A	612	EDO	5	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	872/917 (95%)	0.11	35 (4%)	38	44	12, 30, 60, 87	0
2	C	8/14 (57%)	2.10	4 (50%)	0	0	67, 79, 110, 111	0
2	D	6/14 (42%)	1.65	2 (33%)	0	0	45, 68, 102, 117	0
All	All	886/945 (93%)	0.14	41 (4%)	32	38	12, 30, 63, 117	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-232	ALA	4.9
1	A	-321	ALA	4.8
1	A	176	ALA	4.2
1	A	457	VAL	3.9
2	C	4	DG	3.8
2	C	6	DG	3.5
1	A	-97	ALA	3.2
2	D	1	DC	3.1
1	A	-272	GLY	3.0
1	A	459	ALA	2.9
1	A	456	GLY	2.9
2	C	5	DC	2.8
1	A	-317	GLY	2.8
2	D	7	DC	2.8
1	A	-90	TYR	2.7
1	A	-346	PHE	2.7
1	A	508	PRO	2.7
1	A	453	SER	2.6
1	A	-300	SER	2.6
1	A	-236	LYS	2.6
1	A	507	PRO	2.5
1	A	462	ARG	2.4
1	A	455	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	-201	ALA	2.4
1	A	-342	THR	2.4
1	A	-200	ALA	2.3
1	A	46	ALA	2.3
1	A	-171	LYS	2.3
1	A	-289	ALA	2.3
1	A	-239	ALA	2.3
2	C	11	DA	2.2
1	A	-271	LYS	2.2
1	A	450	ALA	2.1
1	A	452	ASN	2.1
1	A	491	CYS	2.1
1	A	-371	ILE	2.0
1	A	-340	ILE	2.0
1	A	-293	THR	2.0
1	A	-230	GLY	2.0
1	A	449	ASP	2.0
1	A	-344	LYS	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, 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
2	5CM	C	3	20/21	0.68	0.37	112,123,140,142	0
2	5CM	D	3	20/21	0.94	0.13	39,43,62,65	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

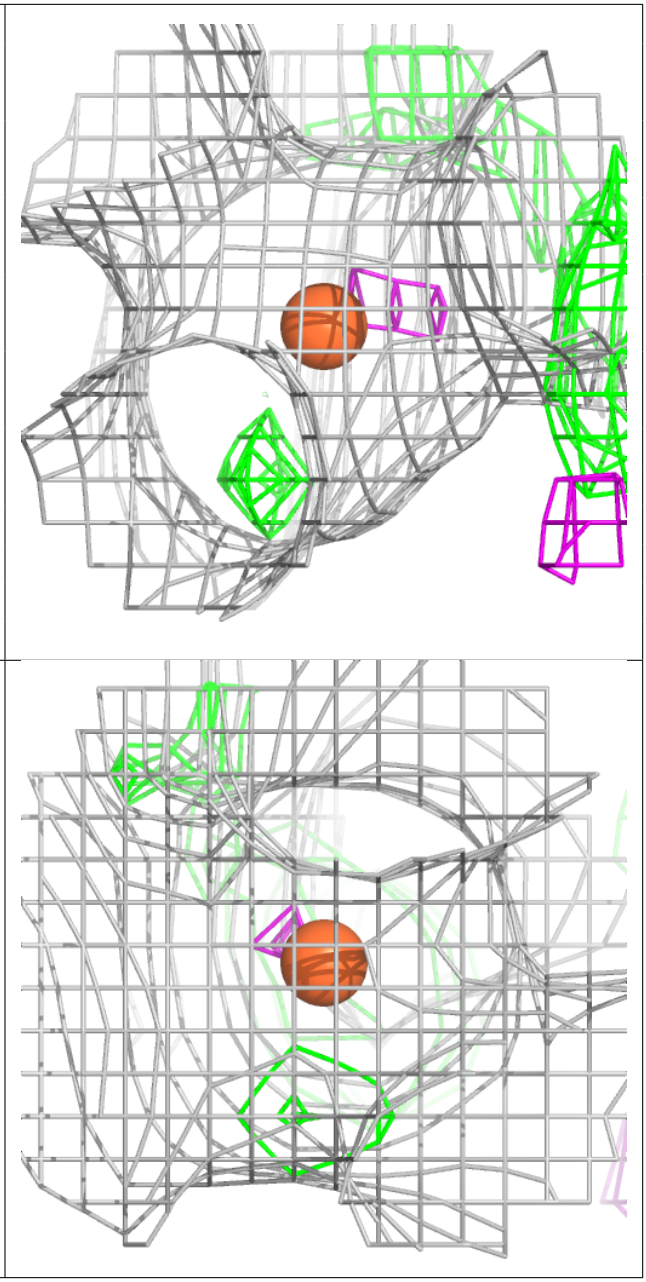
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	A	607	4/4	0.67	0.24	64,72,74,75	0
4	EDO	A	608	4/4	0.82	0.20	59,71,74,76	0
4	EDO	A	604	4/4	0.83	0.22	74,75,80,82	0
4	EDO	A	605	4/4	0.83	0.26	46,59,62,63	0
3	PG4	A	601	13/13	0.87	0.19	54,78,94,96	0
4	EDO	A	613	4/4	0.88	0.32	53,80,82,85	0
4	EDO	A	606	4/4	0.90	0.16	56,62,66,80	0
4	EDO	A	612	4/4	0.91	0.27	34,38,48,54	0
3	PG4	A	602	6/13	0.91	0.21	51,62,66,77	0
4	EDO	A	611	4/4	0.92	0.23	44,60,62,65	0
4	EDO	A	614	4/4	0.92	0.15	42,58,63,69	0
4	EDO	A	615	4/4	0.92	0.16	52,69,71,75	0
4	EDO	A	603	4/4	0.93	0.16	62,67,69,71	0
4	EDO	A	609	4/4	0.94	0.20	60,61,63,70	0
4	EDO	A	610	4/4	0.95	0.24	36,44,52,56	0
5	FE2	A	616	1/1	0.98	0.08	35,35,35,35	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FE2 A 616:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.