Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 05:48 pm BST

PDB ID	:	5W1H
Title	:	Crystal structure of LbaCas13a (C2c2) bound to mature crRNA (24-nt spacer)
Authors	:	Knott, G.J.; Doudna, J.A.
Deposited on	:	2017-06-03
Resolution	:	1.99 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 following versions of software and data (see references ⓘ) were used in the production of this report:

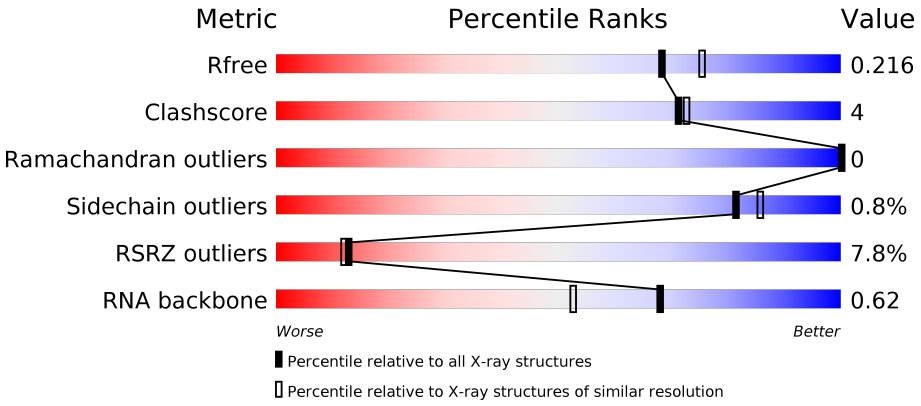
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)
RNA backbone	3102	1079 (2.50-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1440	7%, 82%, 8%, 10%
2	B	52	65%, 12%, •, 19%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	IOD	A	1515	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12499 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 LbaCas13a (C2c2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1301	10760	6847	1820	2052	41	0	0	0

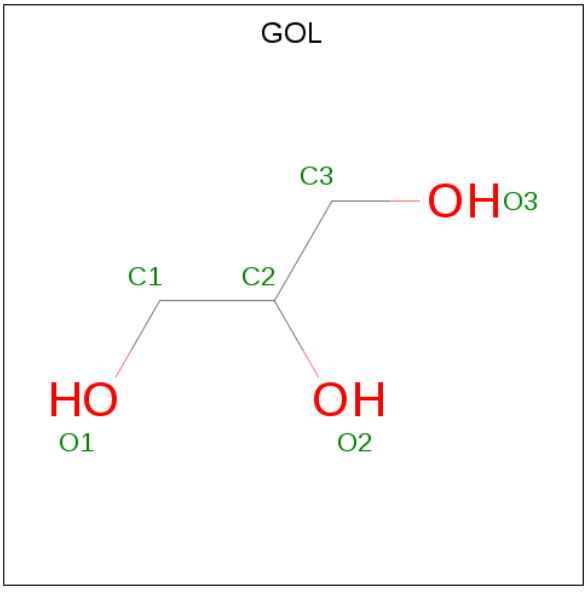
- Molecule 2 is a RNA chain called mature crRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	42	886	397	174	274	41	0	0	0

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	I		
3	A	23	23	23	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

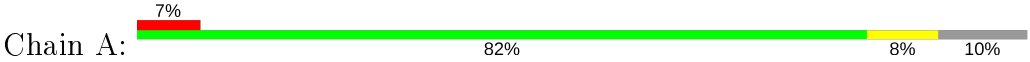
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	692	Total O 692 692	0	0
5	B	120	Total O 120 120	0	0

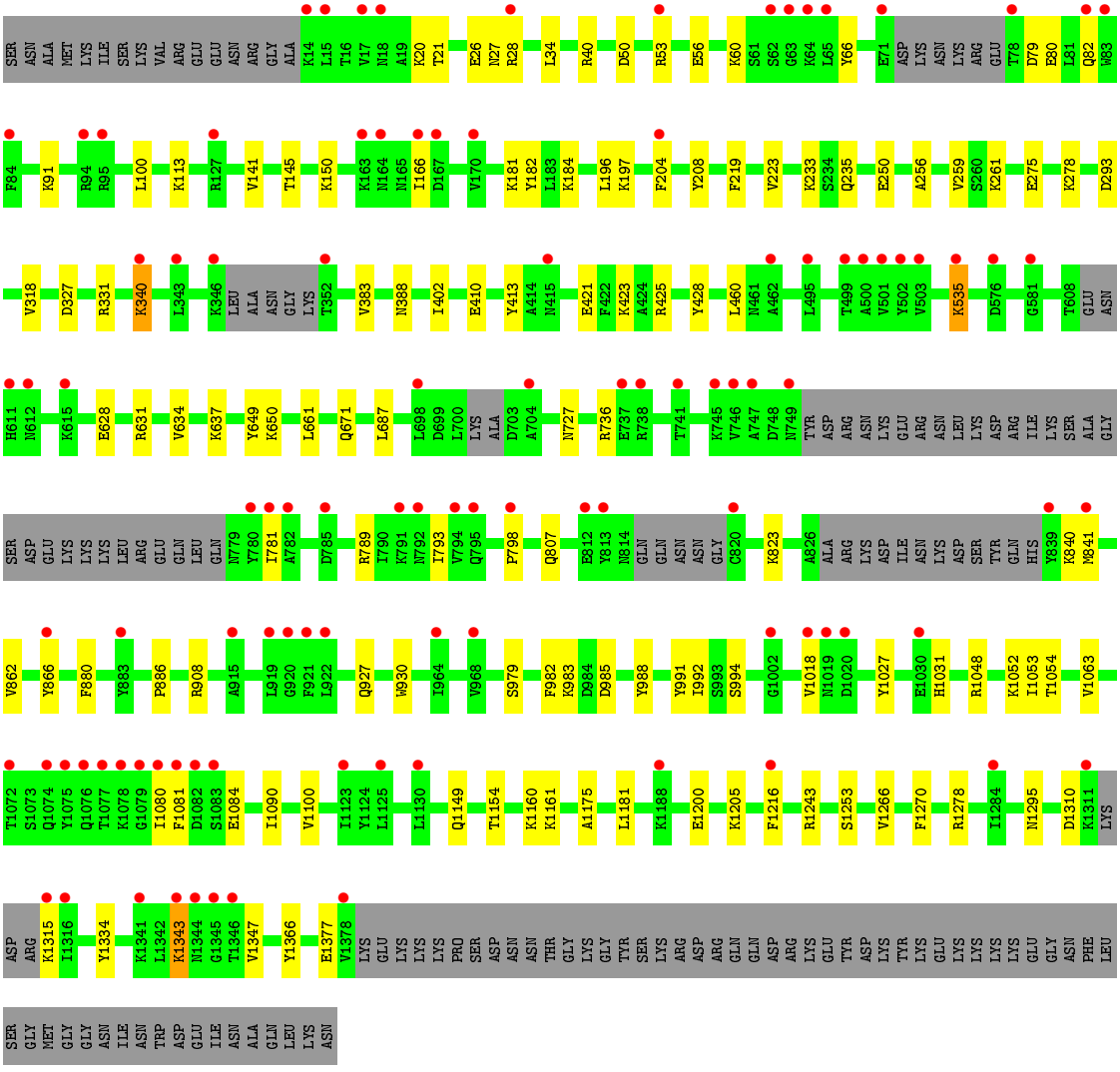
3 Residue-property plots (i)

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: LbaCas13a (C2c2)

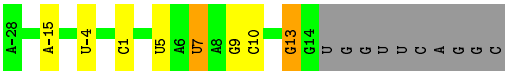
Chain A:





- Molecule 2: mature crRNA

Chain B:


A-28
A-15
U-4
C1
U5
A6
U7
A8
G9
C10
G13
G14
U
G
G
U
U
C
A
G
G
C

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	150.84Å 92.21Å 115.86Å 90.00° 92.42° 90.00°	Depositor
Resolution (Å)	47.12 – 1.99 47.12 – 1.99	Depositor EDS
% Data completeness (in resolution range)	98.6 (47.12-1.99) 94.1 (47.12-1.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.11.1-2575-000	Depositor
R, R_{free}	0.185 , 0.216 0.185 , 0.216	Depositor DCC
R_{free} test set	5242 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å^2)	30.1	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.008 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12499	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 3.59% 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: GOL, IOD

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	0.25	0/10962	0.40	0/14729
2	B	0.24	0/995	0.71	0/1550
All	All	0.25	0/11957	0.44	0/16279

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

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	10760	0	10599	78	0
2	B	886	0	447	5	0
3	A	23	0	0	4	0
4	A	18	0	24	2	0
5	A	692	0	0	12	0
5	B	120	0	0	0	0
All	All	12499	0	11070	80	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 (80) 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:1048:ARG:NH2	1:A:1253:SER:O	2.26	0.69
1:A:1278:ARG:NH1	5:A:1608:HOH:O	2.28	0.66
1:A:235:GLN:NE2	5:A:1606:HOH:O	2.26	0.66
1:A:789:ARG:NH1	5:A:1612:HOH:O	2.30	0.64
1:A:1278:ARG:NH2	5:A:1611:HOH:O	2.29	0.64
1:A:736:ARG:NH1	1:A:798:PRO:O	2.34	0.61
1:A:256:ALA:HB1	1:A:278:LYS:HD2	1.83	0.60
1:A:841:MET:HE3	2:B:13:G:H2'	1.84	0.59
1:A:26:GLU:HG2	1:A:27:ASN:H	1.68	0.59
1:A:460:LEU:HD22	1:A:1181:LEU:HD21	1.87	0.56
1:A:40:ARG:NH2	5:A:1627:HOH:O	2.38	0.55
1:A:421:GLU:OE1	1:A:425:ARG:NH1	2.41	0.54
1:A:141:VAL:HG13	1:A:145:THR:HB	1.89	0.54
1:A:637:LYS:NZ	5:A:1625:HOH:O	2.37	0.54
1:A:983:LYS:HD2	1:A:983:LYS:H	1.72	0.54
1:A:113:LYS:NZ	5:A:1624:HOH:O	2.37	0.53
1:A:259:VAL:HG11	1:A:275:GLU:HG2	1.92	0.52
1:A:1052:LYS:HD3	1:A:1366:TYR:CE1	2.45	0.51
1:A:983:LYS:HD2	1:A:983:LYS:N	2.25	0.50
1:A:927:GLN:HA	4:A:1526:GOL:H2	1.94	0.49
1:A:383:VAL:HG21	1:A:402:ILE:HD11	1.93	0.49
1:A:649:TYR:CE1	1:A:862:VAL:HA	2.48	0.49
1:A:634:VAL:HG22	3:A:1515:IOD:I	2.83	0.49
1:A:1200:GLU:HG2	1:A:1205:LYS:HG3	1.94	0.48
1:A:991:TYR:O	1:A:994:SER:OG	2.31	0.48
1:A:781:ILE:HD12	1:A:781:ILE:H	1.78	0.48
1:A:1266:VAL:HA	1:A:1270:PHE:HB2	1.96	0.48
1:A:56:GLU:HG2	1:A:233:LYS:HE3	1.96	0.48
2:B:7:U:P	2:B:9:G:H1	2.36	0.48
1:A:886:PRO:HD2	3:A:1503:IOD:I	2.86	0.46
1:A:1018:VAL:HG22	1:A:1063:VAL:HG13	1.97	0.46
1:A:840:LYS:HZ1	2:B:13:G:H1	1.63	0.46
1:A:650:LYS:HG2	1:A:866:TYR:OH	2.16	0.46
1:A:60:LYS:HG3	1:A:233:LYS:NZ	2.30	0.45
1:A:789:ARG:HH21	1:A:793:ILE:HD11	1.82	0.45
1:A:181:LYS:HD2	1:A:182:TYR:CZ	2.51	0.45
1:A:327:ASP:O	1:A:331:ARG:HG2	2.16	0.45
1:A:535:LYS:HD2	1:A:535:LYS:H	1.82	0.45
1:A:1149:GLN:OE1	1:A:1216:PHE:HA	2.17	0.44
1:A:1080:ILE:HB	1:A:1343:LYS:NZ	2.31	0.44
1:A:293:ASP:OD1	5:A:1603:HOH:O	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:LYS:NZ	5:A:1654:HOH:O	2.50	0.44
1:A:21:THR:HG22	1:A:34:LEU:HD23	2.00	0.44
1:A:671:GLN:HB2	1:A:807:GLN:HG2	1.98	0.44
1:A:410:GLU:HA	1:A:413:TYR:CE2	2.52	0.44
2:B:7:U:H5'	2:B:7:U:H6	1.83	0.44
1:A:100:LEU:HD23	1:A:100:LEU:HA	1.87	0.44
1:A:1310:ASP:HB3	1:A:1315:LYS:HD3	2.00	0.44
1:A:988:TYR:CZ	1:A:992:ILE:HD11	2.53	0.43
1:A:28:ARG:NE	1:A:250:GLU:O	2.51	0.43
1:A:66:TYR:CE2	1:A:184:LYS:HE2	2.54	0.43
1:A:1160:LYS:HE3	1:A:1161:LYS:HE2	1.99	0.43
1:A:1315:LYS:HB2	1:A:1315:LYS:HE2	1.72	0.43
1:A:100:LEU:HD11	1:A:223:VAL:HG12	2.00	0.43
1:A:661:LEU:HD22	1:A:727:ASN:HB2	2.01	0.43
1:A:979:SER:HA	1:A:982:PHE:O	2.19	0.43
1:A:318:VAL:HG11	1:A:388:ASN:O	2.19	0.43
1:A:880:PHE:HB3	3:A:1515:IOD:I	2.89	0.42
1:A:423:LYS:HG3	1:A:428:TYR:CE2	2.55	0.42
1:A:53:ARG:NH1	5:A:1641:HOH:O	2.46	0.42
1:A:196:LEU:HD13	1:A:219:PHE:CZ	2.55	0.42
1:A:1053:ILE:HG13	1:A:1054:THR:HG23	2.01	0.42
1:A:197:LYS:HE2	1:A:208:TYR:CE1	2.54	0.41
1:A:930:TRP:CG	4:A:1526:GOL:H32	2.54	0.41
1:A:985:ASP:OD2	1:A:1031:HIS:ND1	2.33	0.41
1:A:1334:TYR:HB3	1:A:1377:GLU:HB3	2.01	0.41
1:A:50:ASP:HA	1:A:53:ARG:HG2	2.02	0.41
1:A:1081:PHE:CZ	1:A:1090:ILE:HG13	2.55	0.41
1:A:1175:ALA:HA	1:A:1181:LEU:HD23	2.01	0.41
1:A:1154:THR:OG1	5:A:1602:HOH:O	2.21	0.41
1:A:1084:GLU:HG3	1:A:1347:VAL:HG21	2.02	0.41
1:A:261:LYS:HG3	1:A:261:LYS:H	1.73	0.41
1:A:79:ASP:OD1	1:A:80:GLU:N	2.53	0.41
1:A:82:GLN:HG3	1:A:181:LYS:NZ	2.36	0.41
1:A:340:LYS:HD3	3:A:1511:IOD:I	2.91	0.40
1:A:150:LYS:HE3	5:A:2263:HOH:O	2.20	0.40
1:A:166:ILE:HG21	1:A:204:PHE:HE1	1.86	0.40
1:A:823:LYS:HG3	2:B:1:C:OP1	2.21	0.40
1:A:91:LYS:HD3	1:A:166:ILE:HD13	2.03	0.40
1:A:628:GLU:O	1:A:631:ARG:HG2	2.22	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	1283/1440 (89%)	1246 (97%)	37 (3%)	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	1174/1296 (91%)	1165 (99%)	9 (1%)	81 86

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	340	LYS
1	A	535	LYS
1	A	687	LEU
1	A	908	ARG
1	A	1027	TYR
1	A	1100	VAL
1	A	1243	ARG
1	A	1295	ASN
1	A	1343	LYS

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

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	40/52 (76%)	5 (12%)	2 (5%)

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	-15	A
2	B	-4	U
2	B	5	U
2	B	7	U
2	B	10	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	7	U
2	B	13	G

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 26 ligands modelled in this entry, 23 are monoatomic - leaving 3 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	GOL	A	1524	-	5,5,5	0.36	0	5,5,5	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GOL	A	1525	-	5,5,5	0.38	0	5,5,5	0.24	0
4	GOL	A	1526	-	5,5,5	0.37	0	5,5,5	0.34	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	GOL	A	1524	-	-	2/4/4/4	-
4	GOL	A	1525	-	-	4/4/4/4	-
4	GOL	A	1526	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1525	GOL	O1-C1-C2-C3
4	A	1526	GOL	O1-C1-C2-C3
4	A	1524	GOL	O1-C1-C2-C3
4	A	1525	GOL	C1-C2-C3-O3
4	A	1525	GOL	O1-C1-C2-O2
4	A	1526	GOL	O1-C1-C2-O2
4	A	1525	GOL	O2-C2-C3-O3
4	A	1524	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1526	GOL	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	1301/1440 (90%)	0.54	105 (8%) 12 11	20, 35, 57, 77	0
2	B	42/52 (80%)	-0.10	0 100 100	23, 30, 48, 88	0
All	All	1343/1492 (90%)	0.52	105 (7%) 13 12	20, 35, 57, 88	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	780	TYR	7.3
1	A	167	ASP	7.1
1	A	1316	ILE	6.5
1	A	18	ASN	5.8
1	A	746	VAL	5.1
1	A	83	TRP	5.0
1	A	17	VAL	4.7
1	A	1019	ASN	4.6
1	A	62	SER	4.6
1	A	1346	THR	4.5
1	A	749	ASN	4.5
1	A	1081	PHE	4.4
1	A	1315	LYS	4.3
1	A	1080	ILE	4.2
1	A	795	GLN	4.2
1	A	1079	GLY	4.2
1	A	581	GLY	4.1
1	A	704	ALA	4.0
1	A	1378	VAL	4.0
1	A	1344	ASN	3.9
1	A	1345	GLY	3.9
1	A	95	ARG	3.8
1	A	78	THR	3.7
1	A	352	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	1083	SER	3.5
1	A	794	VAL	3.5
1	A	841	MET	3.5
1	A	71	GLU	3.5
1	A	883	TYR	3.4
1	A	1020	ASP	3.3
1	A	346	LYS	3.3
1	A	462	ALA	3.2
1	A	1082	ASP	3.2
1	A	820	CYS	3.2
1	A	1343	LYS	3.1
1	A	64	LYS	3.0
1	A	813	TYR	3.0
1	A	343	LEU	3.0
1	A	812	GLU	3.0
1	A	698	LEU	2.9
1	A	94	ARG	2.9
1	A	1076	GLN	2.9
1	A	745	LYS	2.9
1	A	166	ILE	2.8
1	A	747	ALA	2.8
1	A	1074	GLN	2.8
1	A	28	ARG	2.8
1	A	782	ALA	2.7
1	A	1077	THR	2.7
1	A	535	LYS	2.7
1	A	1078	LYS	2.7
1	A	1188	LYS	2.7
1	A	127	ARG	2.7
1	A	781	ILE	2.7
1	A	1072	THR	2.7
1	A	170	VAL	2.7
1	A	502	TYR	2.6
1	A	15	LEU	2.6
1	A	738	ARG	2.6
1	A	920	GLY	2.6
1	A	1002	GLY	2.6
1	A	53	ARG	2.5
1	A	495	LEU	2.5
1	A	922	LEU	2.5
1	A	501	VAL	2.5
1	A	791	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	612	ASN	2.5
1	A	1311	LYS	2.4
1	A	919	LEU	2.4
1	A	737	GLU	2.4
1	A	798	PRO	2.4
1	A	84	PHE	2.4
1	A	839	TYR	2.4
1	A	785	ASP	2.4
1	A	14	LYS	2.4
1	A	1075	TYR	2.3
1	A	1341	LYS	2.3
1	A	503	VAL	2.3
1	A	1125	LEU	2.3
1	A	792	ASN	2.3
1	A	204	PHE	2.3
1	A	576	ASP	2.3
1	A	615	LYS	2.2
1	A	1284	ILE	2.2
1	A	340	LYS	2.2
1	A	82	GLN	2.2
1	A	741	THR	2.2
1	A	866	TYR	2.2
1	A	164	ASN	2.2
1	A	1030	GLU	2.2
1	A	611	HIS	2.1
1	A	968	VAL	2.1
1	A	499	THR	2.1
1	A	65	LEU	2.1
1	A	915	ALA	2.1
1	A	1123	ILE	2.1
1	A	921	PHE	2.1
1	A	1018	VAL	2.1
1	A	500	ALA	2.1
1	A	415	ASN	2.0
1	A	964	ILE	2.0
1	A	1130	LEU	2.0
1	A	163	LYS	2.0
1	A	63	GLY	2.0
1	A	1216	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no 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. 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
4	GOL	A	1524	6/6	0.73	0.31	31,40,45,46	0
3	IOD	A	1511	1/1	0.74	0.12	82,82,82,82	1
4	GOL	A	1525	6/6	0.84	0.23	48,52,54,54	0
4	GOL	A	1526	6/6	0.94	0.14	34,36,40,43	0
3	IOD	A	1514	1/1	0.95	0.06	98,98,98,98	1
3	IOD	A	1518	1/1	0.95	0.07	74,74,74,74	1
3	IOD	A	1512	1/1	0.96	0.05	105,105,105,105	1
3	IOD	A	1523	1/1	0.96	0.05	63,63,63,63	1
3	IOD	A	1519	1/1	0.96	0.07	69,69,69,69	1
3	IOD	A	1520	1/1	0.97	0.04	74,74,74,74	1
3	IOD	A	1521	1/1	0.98	0.04	71,71,71,71	1
3	IOD	A	1507	1/1	0.98	0.04	70,70,70,70	1
3	IOD	A	1508	1/1	0.98	0.17	87,87,87,87	1
3	IOD	A	1517	1/1	0.99	0.04	70,70,70,70	1
3	IOD	A	1509	1/1	0.99	0.08	75,75,75,75	1
3	IOD	A	1516	1/1	0.99	0.16	70,70,70,70	1
3	IOD	A	1503	1/1	0.99	0.11	47,47,47,47	1
3	IOD	A	1510	1/1	0.99	0.09	84,84,84,84	1
3	IOD	A	1505	1/1	0.99	0.06	56,56,56,56	1
3	IOD	A	1506	1/1	0.99	0.07	45,45,45,45	1
3	IOD	A	1513	1/1	1.00	0.04	75,75,75,75	1
3	IOD	A	1504	1/1	1.00	0.10	37,37,37,37	1
3	IOD	A	1502	1/1	1.00	0.13	42,42,42,42	1
3	IOD	A	1515	1/1	1.00	0.07	48,48,48,48	1
3	IOD	A	1501	1/1	1.00	0.09	48,48,48,48	1
3	IOD	A	1522	1/1	1.00	0.05	43,43,43,43	1

6.5 Other polymers (i)

There are no such residues in this entry.