Full wwPDB X-ray Structure Validation Report (i)

Apr 17, 2017 – 05:03 PM EDT

PDB ID	:	5B55
Title	:	Crystal structure of hydrogen sulfide-producing enzyme (Fn1055) D232N mutant in complexed with alpha-aminoacrylate intermediate: lysine-dimethylated form
Authors	:	Kezuka, Y.; Yoshida, Y.; Nonaka, T.
Deposited on	:	2016-04-22
Resolution	:	2.14 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 (i) symbol.

The following versions of software and data (see references (i)) 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 (i)

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

The reported resolution of this entry is 2.14 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	Percentile Ranks	Value
Rfree		0.245
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		2.0%
RSRZ outliers		0.8%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
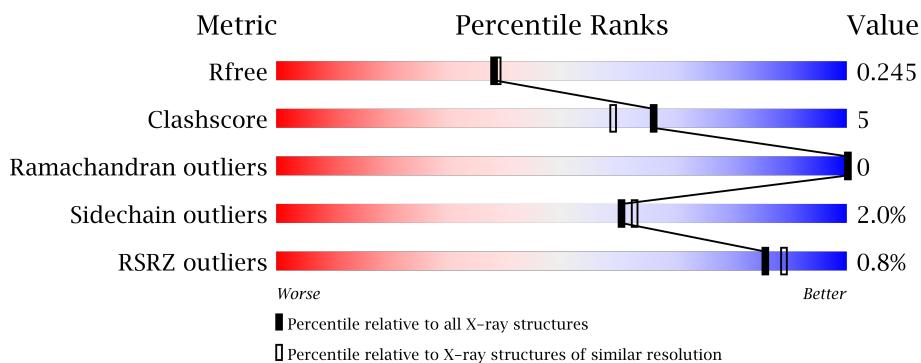
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1915 (2.16-2.12)
Clashscore	112137	2047 (2.16-2.12)
Ramachandran outliers	110173	2020 (2.16-2.12)
Sidechain outliers	110143	2019 (2.16-2.12)
RSRZ outliers	101464	1921 (2.16-2.12)

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 <=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	340	90% 8% ·
1	B	340	.% 89% 8% ··
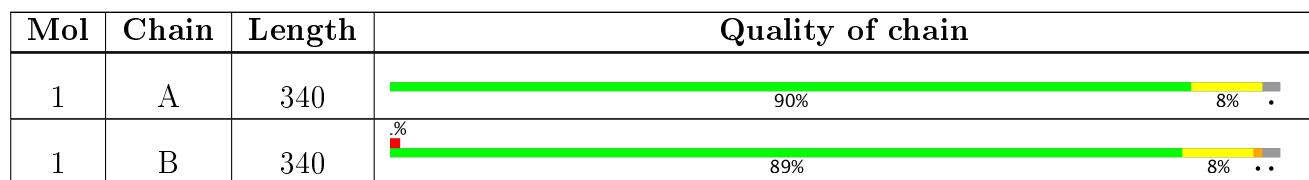
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	0JO	A	402[B]	-	-	-	X
3	0JO	B	402[B]	-	-	X	X
4	PEG	A	403	-	-	-	X
4	PEG	B	403	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5684 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 Cysteine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total 2643	C 1702	N 435	O 493	S 13	0	4	0
1	B	333	Total 2636	C 1700	N 434	O 489	S 13	0	2	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q8REP3
A	-2	PRO	-	expression tag	UNP Q8REP3
A	-1	LEU	-	expression tag	UNP Q8REP3
A	0	GLY	-	expression tag	UNP Q8REP3
A	1	SER	-	expression tag	UNP Q8REP3
A	232	ASN	ASP	engineered mutation	UNP Q8REP3
B	-3	GLY	-	expression tag	UNP Q8REP3
B	-2	PRO	-	expression tag	UNP Q8REP3
B	-1	LEU	-	expression tag	UNP Q8REP3
B	0	GLY	-	expression tag	UNP Q8REP3
B	1	SER	-	expression tag	UNP Q8REP3
B	232	ASN	ASP	engineered mutation	UNP Q8REP3

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).
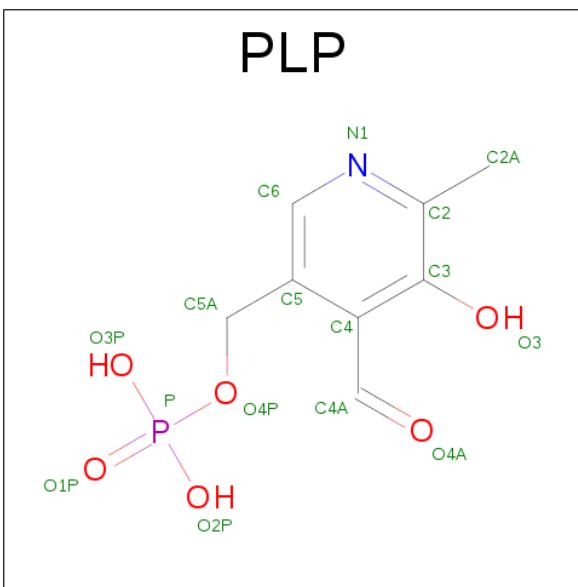
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	1
			15	8	1	5	1		

- Molecule 3 is 2-{[(E)-{3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridin-4-yl}methylid ene]amino}prop-2-enoic acid (three-letter code: 0JO) (formula: $C_{11}H_{13}N_2O_7P$).
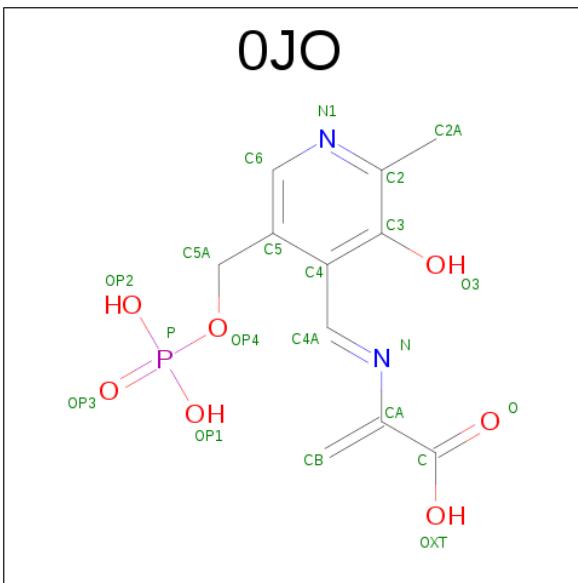
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	1
			21	11	2	7	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total 21	C 11	N 2	O 7	P 1	0	1

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).
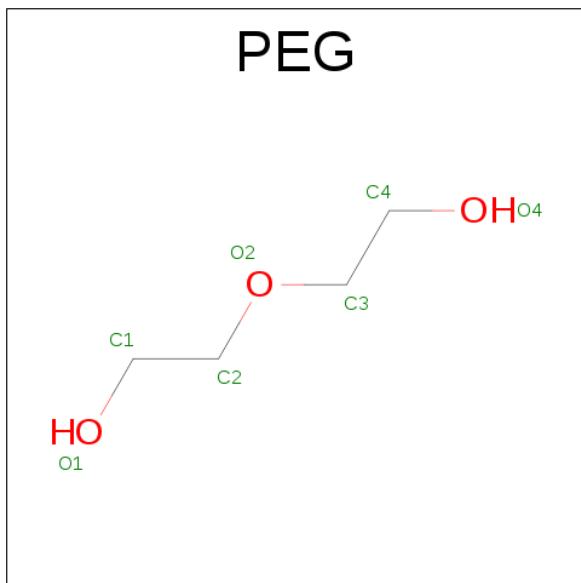
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 7	C 4	O 3	0	0
4	B	1	Total 7	C 4	O 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	169	Total 169	O 169	0	0
5	B	150	Total 150	O 150	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: Cysteine synthase
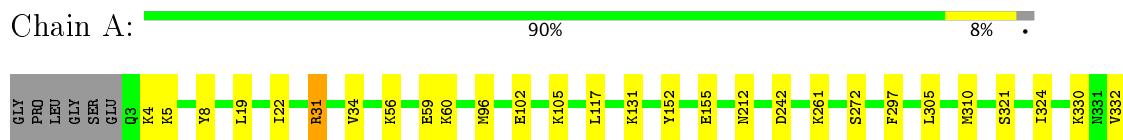
• Molecule 1: Cysteine synthase
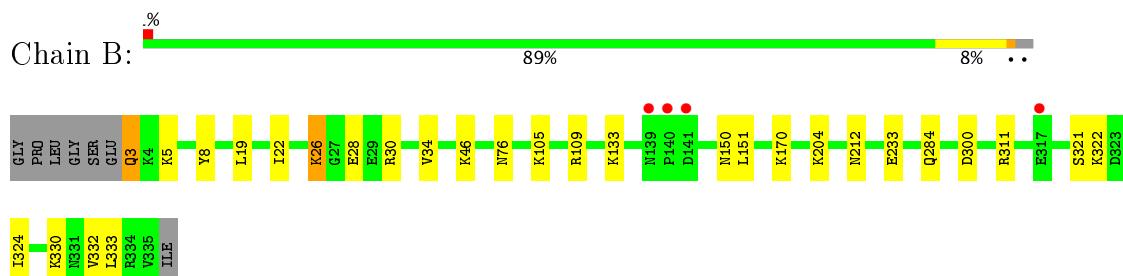
4   Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	191.05Å 57.13Å 94.29Å 90.00° 100.89° 90.00°	Depositor
Resolution (Å)	36.66 – 2.14 36.66 – 2.14	Depositor EDS
% Data completeness (in resolution range)	95.1 (36.66-2.14) 95.1 (36.66-2.14)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.90 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.201 , 0.237 0.208 , 0.245	Depositor DCC
R_{free} test set	2648 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	21.7	Xtriage
Anisotropy	0.709	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.3	EDS
L-test for twinning[2]	$< |L| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5684	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: 0JO, PEG, MLY, PLP

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	0.86	0/2341	0.87	0/3181
1	B	0.83	1/2317 (0.0%)	0.85	1/3151 (0.0%)
All	All	0.85	1/4658 (0.0%)	0.86	1/6332 (0.0%)

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
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	233	GLU	CD-OE1	5.36	1.31	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	300	ASP	CB-CG-OD1	5.65	123.39	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	26	MLY	Peptide

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	2643	0	2666	22	0
1	B	2636	0	2676	25	0
2	A	15	0	6	0	0
2	B	15	0	7	2	0
3	A	21	0	10	1	0
3	B	21	0	10	8	0
4	A	7	0	10	0	0
4	B	7	0	10	0	0
5	A	169	0	0	3	0
5	B	150	0	0	5	0
All	All	5684	0	5395	49	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 5.

All (49) 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:B:170:MLY:HH22	5:B:622:HOH:O	1.76	0.83
1:B:46[B]:LYS:NZ	3:B:402[B]:0JO:C4A	2.45	0.79
1:B:133:MLY:HH22	5:B:633:HOH:O	1.89	0.72
3:B:402[B]:0JO:OP3	3:B:402[B]:0JO:H4	1.90	0.72
1:B:204:MLY:HH22	5:B:638:HOH:O	1.92	0.69
1:B:46[B]:LYS:HZ1	3:B:402[B]:0JO:C4A	2.08	0.66
1:A:102:GLU:HA	1:A:105[B]:MLY:HE3	1.78	0.65
1:B:30:ARG:HH11	1:B:284:GLN:HE21	1.44	0.65
1:A:22:ILE:HD13	1:A:31:ARG:HB3	1.79	0.64
1:B:19:LEU:HD12	1:B:34:VAL:HG23	1.84	0.58
1:A:19:LEU:HD12	1:A:34[B]:VAL:HG23	1.84	0.58
1:A:22:ILE:HG12	1:A:330:MLY:HB3	1.88	0.56
1:B:76:ASN:ND2	2:B:401[A]:PLP:H2A1	2.22	0.54
1:A:105[B]:MLY:HD3	1:A:117:LEU:HD11	1.90	0.53
1:B:46[B]:LYS:CE	3:B:402[B]:0JO:N	2.72	0.52
1:B:3:GLN:HB2	5:B:629:HOH:O	2.08	0.52
1:B:46[B]:LYS:CE	3:B:402[B]:0JO:C4A	2.89	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:ILE:HG12	1:B:330:MLY:HB3	1.92	0.51
1:A:56:MLY:HH13	1:A:155:GLU:OE1	2.11	0.50
1:A:22:ILE:CD1	1:A:31:ARG:HB3	2.42	0.50
1:B:5:MLY:HA	1:B:8:TYR:CE2	2.47	0.49
1:B:46[B]:LYS:HZ1	3:B:402[B]:0JO:H4	1.78	0.49
1:B:46[B]:LYS:HZ3	3:B:402[B]:0JO:C4A	2.27	0.48
1:B:76:ASN:HD22	2:B:401[A]:PLP:H2A1	1.78	0.48
1:A:56:MLY:HD2	1:A:152:TYR:CE1	2.48	0.48
1:A:272:SER:HB2	5:A:619:HOH:O	2.15	0.46
1:A:4:MLY:H	1:A:4:MLY:CD	2.28	0.46
1:B:19:LEU:HD23	1:B:332:VAL:HG22	1.98	0.46
1:A:34[A]:VAL:HG11	1:A:297:PHE:CE1	2.51	0.46
1:A:19:LEU:HD23	1:A:332:VAL:HG22	1.97	0.46
1:B:26:MLY:HG2	1:B:26:MLY:O	2.16	0.46
1:B:322:MLY:CG	1:B:322:MLY:HH22	2.46	0.45
1:A:321:SER:HA	1:A:324:ILE:HD12	1.99	0.45
1:A:105[B]:MLY:CD	1:A:117:LEU:HD11	2.47	0.45
1:A:5:MLY:HA	1:A:8:TYR:CE2	2.53	0.44
1:B:46[B]:LYS:HE3	3:B:402[B]:0JO:N	2.33	0.44
1:A:261:MLY:HH23	1:A:324:ILE:O	2.18	0.44
1:A:59:GLU:HG3	5:A:525:HOH:O	2.17	0.43
3:A:402[B]:0JO:H4	3:A:402[B]:0JO:OP2	2.18	0.43
1:A:60:MLY:HE3	5:A:588:HOH:O	2.19	0.43
1:B:311:ARG:HD3	5:B:634:HOH:O	2.18	0.43
1:A:131:MLY:HD2	1:A:131:MLY:HH22	1.76	0.42
1:A:305:LEU:HD23	1:A:310:MET:HE3	2.02	0.42
1:B:321:SER:HA	1:B:324:ILE:HD12	2.02	0.42
1:A:96:MET:CE	1:A:105[B]:MLY:HG3	2.50	0.42
1:B:105:MLY:HE3	1:B:109:ARG:NH1	2.35	0.41
1:A:4:MLY:H	1:A:4:MLY:HD2	1.85	0.41
1:B:322:MLY:HH22	1:B:322:MLY:HG3	2.03	0.40
1:B:26:MLY:CG	1:B:26:MLY:O	2.68	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	299/340 (88%)	290 (97%)	9 (3%)	0	100	100
1	B	296/340 (87%)	288 (97%)	8 (3%)	0	100	100
All	All	595/680 (88%)	578 (97%)	17 (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	253/254 (100%)	249 (98%)	4 (2%)	68	71
1	B	250/254 (98%)	244 (98%)	6 (2%)	54	55
All	All	503/508 (99%)	493 (98%)	10 (2%)	60	63

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ARG
1	A	212	ASN
1	A	242	ASP
1	A	335	VAL
1	B	3	GLN
1	B	28	GLU
1	B	150	ASN
1	B	151	LEU
1	B	212	ASN
1	B	333	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	11	ASN
1	A	76	ASN
1	A	147	GLN
1	A	285	ASN
1	B	3	GLN
1	B	138	ASN
1	B	139	ASN
1	B	147	GLN
1	B	150	ASN
1	B	284	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)

74 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 Counts	Bond lengths RMSZ	Bond lengths $\#|Z| > 2$	Bond angles Counts	Bond angles RMSZ	Bond angles $\#|Z| > 2$
1	MLY	A	105[A]	-	10,10,11	1.42	2 (20%)	8,11,13	0.90	0
1	MLY	A	105[B]	-	10,10,11	1.65	2 (20%)	8,11,13	1.45	1 (12%)
1	MLY	A	114	1	8,8,11	0.69	0	5,8,13	0.83	0
1	MLY	A	121	1	8,8,11	1.53	1 (12%)	5,8,13	1.01	0
1	MLY	A	131	1	10,10,11	1.18	1 (10%)	8,11,13	0.96	1 (12%)
1	MLY	A	133	1	8,8,11	2.23	1 (12%)	5,8,13	1.02	0
1	MLY	A	137	1	8,8,11	1.41	1 (12%)	5,8,13	1.22	1 (20%)
1	MLY	A	15	1	10,10,11	1.75	2 (20%)	8,11,13	0.76	0
1	MLY	A	170	1	8,8,11	1.30	1 (12%)	5,8,13	0.91	1 (20%)
1	MLY	A	194	1	10,10,11	1.50	2 (20%)	8,11,13	1.93	1 (12%)
1	MLY	A	197	1	8,8,11	1.14	1 (12%)	5,8,13	1.32	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	MLY	A	204	1	10,10,11	1.55	2 (20%)	8,11,13	1.30	2 (25%)
1	MLY	A	221	1	10,10,11	0.97	0	8,11,13	1.00	0
1	MLY	A	224	1	8,8,11	0.59	0	5,8,13	1.05	0
1	MLY	A	240	1	10,10,11	1.21	1 (10%)	8,11,13	0.73	0
1	MLY	A	243	1	8,8,11	2.02	1 (12%)	5,8,13	1.04	0
1	MLY	A	26	1	10,10,11	1.55	3 (30%)	8,11,13	0.62	0
1	MLY	A	261	1	10,10,11	0.88	0	8,11,13	1.62	1 (12%)
1	MLY	A	264	1	8,8,11	1.34	1 (12%)	5,8,13	1.15	1 (20%)
1	MLY	A	286	1	8,8,11	0.80	0	5,8,13	1.52	2 (40%)
1	MLY	A	289	1	8,8,11	0.66	0	5,8,13	1.20	1 (20%)
1	MLY	A	302	1	8,8,11	0.59	0	5,8,13	1.01	0
1	MLY	A	303	1	8,8,11	1.44	1 (12%)	5,8,13	1.03	0
1	MLY	A	314	1	8,8,11	0.98	1 (12%)	5,8,13	1.21	1 (20%)
1	MLY	A	316	1	8,8,11	0.79	0	5,8,13	0.65	0
1	MLY	A	322	1	8,8,11	1.53	1 (12%)	5,8,13	1.23	1 (20%)
1	MLY	A	327	1	8,8,11	0.86	1 (12%)	5,8,13	1.13	0
1	MLY	A	330	1	8,8,11	0.64	0	5,8,13	1.28	1 (20%)
1	MLY	A	35	1	8,8,11	1.40	1 (12%)	5,8,13	0.70	0
1	MLY	A	4	1	8,8,11	2.29	2 (25%)	5,8,13	1.34	1 (20%)
1	MLY	A	5	1	8,8,11	1.13	1 (12%)	5,8,13	0.78	0
1	MLY	A	55	1	8,8,11	1.76	1 (12%)	5,8,13	1.07	0
1	MLY	A	56	1	10,10,11	1.30	1 (10%)	8,11,13	2.15	1 (12%)
1	MLY	A	60	1	8,8,11	0.83	1 (12%)	5,8,13	1.23	1 (20%)
1	MLY	A	64	1	8,8,11	0.79	0	5,8,13	1.52	1 (20%)
1	MLY	A	65	1	8,8,11	0.65	0	5,8,13	1.35	1 (20%)
1	MLY	A	7	1	8,8,11	1.48	1 (12%)	5,8,13	1.17	1 (20%)
1	MLY	B	105	1	8,8,11	1.02	1 (12%)	5,8,13	1.03	0
1	MLY	B	114	1	8,8,11	1.09	1 (12%)	5,8,13	0.94	0
1	MLY	B	121	1	8,8,11	1.66	1 (12%)	5,8,13	0.90	0
1	MLY	B	131[A]	-	10,10,11	1.50	1 (10%)	8,11,13	0.81	0
1	MLY	B	131[B]	-	10,10,11	1.25	1 (10%)	8,11,13	0.81	0
1	MLY	B	133	1	10,10,11	2.29	2 (20%)	8,11,13	1.62	1 (12%)
1	MLY	B	137	1	8,8,11	1.25	1 (12%)	5,8,13	0.91	0
1	MLY	B	15	1	10,10,11	1.59	3 (30%)	8,11,13	0.57	0
1	MLY	B	170	1	10,10,11	1.34	1 (10%)	8,11,13	0.94	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	MLY	B	194	1	10,10,11	1.46	2 (20%)	8,11,13	1.28	1 (12%)
1	MLY	B	197	1	8,8,11	0.74	0	5,8,13	1.35	1 (20%)
1	MLY	B	204	1	10,10,11	1.46	1 (10%)	8,11,13	1.23	1 (12%)
1	MLY	B	221	1	8,8,11	0.75	0	5,8,13	1.09	1 (20%)
1	MLY	B	224	1	10,10,11	1.29	1 (10%)	8,11,13	0.77	0
1	MLY	B	240	1	10,10,11	1.24	1 (10%)	8,11,13	0.87	1 (12%)
1	MLY	B	243	1	8,8,11	1.70	1 (12%)	5,8,13	1.07	1 (20%)
1	MLY	B	26	1	10,10,11	1.17	1 (10%)	8,11,13	0.81	0
1	MLY	B	261	1	10,10,11	0.95	0	8,11,13	1.64	1 (12%)
1	MLY	B	264	1	8,8,11	1.27	1 (12%)	5,8,13	1.26	1 (20%)
1	MLY	B	286	1	10,10,11	1.22	1 (10%)	8,11,13	1.02	1 (12%)
1	MLY	B	289	1	8,8,11	0.83	0	5,8,13	1.38	1 (20%)
1	MLY	B	302	1	8,8,11	1.22	1 (12%)	5,8,13	1.14	1 (20%)
1	MLY	B	303	1	8,8,11	1.38	1 (12%)	5,8,13	1.12	1 (20%)
1	MLY	B	314	1	8,8,11	1.10	1 (12%)	5,8,13	1.43	1 (20%)
1	MLY	B	316	1	10,10,11	0.94	0	8,11,13	0.99	1 (12%)
1	MLY	B	322	1	10,10,11	1.14	1 (10%)	8,11,13	1.45	2 (25%)
1	MLY	B	327	1	8,8,11	0.30	0	5,8,13	1.27	0
1	MLY	B	330	1	8,8,11	0.64	0	5,8,13	1.02	1 (20%)
1	MLY	B	35	1	8,8,11	1.07	1 (12%)	5,8,13	0.70	0
1	MLY	B	4	1	8,8,11	1.48	2 (25%)	5,8,13	1.27	1 (20%)
1	MLY	B	5	1	10,10,11	1.13	1 (10%)	8,11,13	0.85	0
1	MLY	B	55	1	10,10,11	1.89	1 (10%)	8,11,13	1.51	2 (25%)
1	MLY	B	56	1	10,10,11	1.14	1 (10%)	8,11,13	0.84	0
1	MLY	B	60	1	8,8,11	1.30	1 (12%)	5,8,13	1.33	2 (40%)
1	MLY	B	64	1	8,8,11	0.67	0	5,8,13	1.13	0
1	MLY	B	65	1	8,8,11	1.14	1 (12%)	5,8,13	0.74	0
1	MLY	B	7	1	8,8,11	1.51	1 (12%)	5,8,13	1.07	1 (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
1	MLY	A	105[A]	-	-	0/7/9/11	0/0/0/0
1	MLY	A	105[B]	-	-	0/7/9/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	114	1	-	0/5/7/11	0/0/0/0
1	MLY	A	121	1	-	0/5/7/11	0/0/0/0
1	MLY	A	131	1	-	0/7/9/11	0/0/0/0
1	MLY	A	133	1	-	0/5/7/11	0/0/0/0
1	MLY	A	137	1	-	0/5/7/11	0/0/0/0
1	MLY	A	15	1	-	0/7/9/11	0/0/0/0
1	MLY	A	170	1	-	0/5/7/11	0/0/0/0
1	MLY	A	194	1	-	0/7/9/11	0/0/0/0
1	MLY	A	197	1	-	0/5/7/11	0/0/0/0
1	MLY	A	204	1	-	0/7/9/11	0/0/0/0
1	MLY	A	221	1	-	0/7/9/11	0/0/0/0
1	MLY	A	224	1	-	0/5/7/11	0/0/0/0
1	MLY	A	240	1	-	0/7/9/11	0/0/0/0
1	MLY	A	243	1	-	0/5/7/11	0/0/0/0
1	MLY	A	26	1	-	0/7/9/11	0/0/0/0
1	MLY	A	261	1	-	0/7/9/11	0/0/0/0
1	MLY	A	264	1	-	0/5/7/11	0/0/0/0
1	MLY	A	286	1	-	0/5/7/11	0/0/0/0
1	MLY	A	289	1	-	0/5/7/11	0/0/0/0
1	MLY	A	302	1	-	0/5/7/11	0/0/0/0
1	MLY	A	303	1	-	0/5/7/11	0/0/0/0
1	MLY	A	314	1	-	0/5/7/11	0/0/0/0
1	MLY	A	316	1	-	0/5/7/11	0/0/0/0
1	MLY	A	322	1	-	0/5/7/11	0/0/0/0
1	MLY	A	327	1	-	0/5/7/11	0/0/0/0
1	MLY	A	330	1	-	0/5/7/11	0/0/0/0
1	MLY	A	35	1	-	0/5/7/11	0/0/0/0
1	MLY	A	4	1	-	0/5/7/11	0/0/0/0
1	MLY	A	5	1	-	0/5/7/11	0/0/0/0
1	MLY	A	55	1	-	0/5/7/11	0/0/0/0
1	MLY	A	56	1	-	0/7/9/11	0/0/0/0
1	MLY	A	60	1	-	0/5/7/11	0/0/0/0
1	MLY	A	64	1	-	0/5/7/11	0/0/0/0
1	MLY	A	65	1	-	0/5/7/11	0/0/0/0
1	MLY	A	7	1	-	0/5/7/11	0/0/0/0
1	MLY	B	105	1	-	0/5/7/11	0/0/0/0
1	MLY	B	114	1	-	0/5/7/11	0/0/0/0
1	MLY	B	121	1	-	0/5/7/11	0/0/0/0
1	MLY	B	131[A]	-	-	0/7/9/11	0/0/0/0
1	MLY	B	131[B]	-	-	0/7/9/11	0/0/0/0
1	MLY	B	133	1	-	0/7/9/11	0/0/0/0
1	MLY	B	137	1	-	0/5/7/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	B	15	1	-	0/7/9/11	0/0/0/0
1	MLY	B	170	1	-	0/7/9/11	0/0/0/0
1	MLY	B	194	1	-	0/7/9/11	0/0/0/0
1	MLY	B	197	1	-	0/5/7/11	0/0/0/0
1	MLY	B	204	1	-	0/7/9/11	0/0/0/0
1	MLY	B	221	1	-	0/5/7/11	0/0/0/0
1	MLY	B	224	1	-	0/7/9/11	0/0/0/0
1	MLY	B	240	1	-	0/7/9/11	0/0/0/0
1	MLY	B	243	1	-	0/5/7/11	0/0/0/0
1	MLY	B	26	1	-	0/7/9/11	0/0/0/0
1	MLY	B	261	1	-	0/7/9/11	0/0/0/0
1	MLY	B	264	1	-	0/5/7/11	0/0/0/0
1	MLY	B	286	1	-	0/7/9/11	0/0/0/0
1	MLY	B	289	1	-	0/5/7/11	0/0/0/0
1	MLY	B	302	1	-	0/5/7/11	0/0/0/0
1	MLY	B	303	1	-	0/5/7/11	0/0/0/0
1	MLY	B	314	1	-	0/5/7/11	0/0/0/0
1	MLY	B	316	1	-	0/7/9/11	0/0/0/0
1	MLY	B	322	1	-	0/7/9/11	0/0/0/0
1	MLY	B	327	1	-	0/5/7/11	0/0/0/0
1	MLY	B	330	1	-	0/5/7/11	0/0/0/0
1	MLY	B	35	1	-	0/5/7/11	0/0/0/0
1	MLY	B	4	1	-	0/5/7/11	0/0/0/0
1	MLY	B	5	1	-	0/7/9/11	0/0/0/0
1	MLY	B	55	1	-	0/7/9/11	0/0/0/0
1	MLY	B	56	1	-	0/7/9/11	0/0/0/0
1	MLY	B	60	1	-	0/5/7/11	0/0/0/0
1	MLY	B	64	1	-	0/5/7/11	0/0/0/0
1	MLY	B	65	1	-	0/5/7/11	0/0/0/0
1	MLY	B	7	1	-	0/5/7/11	0/0/0/0

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	327	MLY	CA-C	2.02	1.52	1.50
1	A	26	MLY	CE-NZ	2.07	1.54	1.46
1	B	4	MLY	CA-C	2.08	1.53	1.50
1	A	4	MLY	CB-CA	2.11	1.56	1.53
1	A	131	MLY	CA-C	2.11	1.53	1.50
1	A	60	MLY	CA-C	2.13	1.53	1.50
1	A	105[A]	MLY	CA-C	2.28	1.53	1.50
1	A	194	MLY	CE-NZ	2.29	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	314	MLY	CA-C	2.36	1.53	1.50
1	B	15	MLY	CB-CA	2.37	1.56	1.53
1	B	35	MLY	CA-C	2.39	1.53	1.50
1	B	302	MLY	CA-C	2.40	1.53	1.50
1	A	26	MLY	CB-CA	2.41	1.56	1.53
1	A	15	MLY	CE-NZ	2.43	1.55	1.46
1	B	105	MLY	CA-C	2.47	1.53	1.50
1	A	240	MLY	CE-NZ	2.51	1.55	1.46
1	A	105[A]	MLY	CE-NZ	2.57	1.55	1.46
1	B	194	MLY	CE-NZ	2.58	1.55	1.46
1	B	26	MLY	CE-NZ	2.60	1.56	1.46
1	B	194	MLY	CA-C	2.61	1.53	1.50
1	B	15	MLY	CE-NZ	2.61	1.56	1.46
1	B	5	MLY	CA-C	2.64	1.53	1.50
1	B	322	MLY	CE-NZ	2.72	1.56	1.46
1	B	114	MLY	CA-C	2.72	1.53	1.50
1	A	105[B]	MLY	CB-CA	2.73	1.57	1.53
1	B	15	MLY	CA-C	2.76	1.53	1.50
1	B	65	MLY	CA-C	2.78	1.53	1.50
1	B	56	MLY	CA-C	2.79	1.53	1.50
1	B	314	MLY	CA-C	2.80	1.53	1.50
1	A	26	MLY	CA-C	2.80	1.53	1.50
1	A	204	MLY	CE-NZ	2.83	1.56	1.46
1	A	197	MLY	CA-C	2.92	1.54	1.50
1	B	286	MLY	CA-C	2.92	1.54	1.50
1	B	240	MLY	CE-NZ	2.93	1.57	1.46
1	A	56	MLY	CA-C	2.99	1.54	1.50
1	A	5	MLY	CA-C	3.01	1.54	1.50
1	B	4	MLY	CB-CA	3.06	1.57	1.53
1	B	264	MLY	CA-C	3.16	1.54	1.50
1	A	170	MLY	CA-C	3.30	1.54	1.50
1	A	204	MLY	CA-C	3.32	1.54	1.50
1	B	170	MLY	CA-C	3.35	1.54	1.50
1	B	137	MLY	CA-C	3.39	1.54	1.50
1	B	224	MLY	CA-C	3.39	1.54	1.50
1	A	35	MLY	CA-C	3.42	1.54	1.50
1	B	133	MLY	CE-NZ	3.43	1.59	1.46
1	B	131[B]	MLY	CA-C	3.52	1.54	1.50
1	A	194	MLY	CA-C	3.52	1.54	1.50
1	B	60	MLY	CA-C	3.53	1.54	1.50
1	A	137	MLY	CA-C	3.53	1.54	1.50
1	A	264	MLY	CA-C	3.55	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	204	MLY	CA-C	3.59	1.55	1.50
1	B	131[A]	MLY	CE-NZ	3.64	1.59	1.46
1	A	303	MLY	CA-C	3.64	1.55	1.50
1	A	7	MLY	CA-C	3.75	1.55	1.50
1	B	303	MLY	CA-C	3.78	1.55	1.50
1	A	105[B]	MLY	CA-C	3.78	1.55	1.50
1	B	7	MLY	CA-C	3.96	1.55	1.50
1	A	15	MLY	CA-C	4.06	1.55	1.50
1	A	121	MLY	CA-C	4.08	1.55	1.50
1	A	322	MLY	CA-C	4.14	1.55	1.50
1	B	121	MLY	CA-C	4.38	1.56	1.50
1	B	243	MLY	CA-C	4.50	1.56	1.50
1	A	55	MLY	CA-C	4.72	1.56	1.50
1	A	243	MLY	CA-C	5.26	1.57	1.50
1	B	55	MLY	CA-C	5.43	1.57	1.50
1	A	4	MLY	CA-C	5.79	1.57	1.50
1	B	133	MLY	CA-C	5.95	1.58	1.50
1	A	133	MLY	CA-C	5.99	1.58	1.50

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	MLY	CD-CE-NZ	-2.92	105.83	113.77
1	B	197	MLY	O-C-CA	-2.85	117.16	125.02
1	A	197	MLY	O-C-CA	-2.82	117.23	125.02
1	A	64	MLY	CB-CA-C	-2.74	107.14	111.65
1	A	322	MLY	O-C-CA	-2.72	117.50	125.02
1	B	264	MLY	O-C-CA	-2.63	117.76	125.02
1	B	314	MLY	CB-CA-C	-2.60	107.36	111.65
1	A	286	MLY	O-C-CA	-2.52	118.05	125.02
1	A	7	MLY	O-C-CA	-2.52	118.06	125.02
1	A	289	MLY	O-C-CA	-2.45	118.26	125.02
1	B	289	MLY	O-C-CA	-2.44	118.27	125.02
1	A	60	MLY	O-C-CA	-2.39	118.41	125.02
1	B	322	MLY	O-C-CA	-2.39	118.43	125.02
1	A	264	MLY	O-C-CA	-2.39	118.43	125.02
1	B	4	MLY	CB-CA-C	-2.36	107.77	111.65
1	B	7	MLY	O-C-CA	-2.34	118.56	125.02
1	A	137	MLY	O-C-CA	-2.31	118.65	125.02
1	B	302	MLY	O-C-CA	-2.29	118.68	125.02
1	B	303	MLY	O-C-CA	-2.29	118.69	125.02
1	B	194	MLY	CD-CE-NZ	-2.29	107.55	113.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	314	MLY	CB-CA-C	-2.26	107.92	111.65
1	A	131	MLY	O-C-CA	-2.23	118.87	125.02
1	B	55	MLY	CB-CA-C	-2.22	107.99	111.65
1	A	65	MLY	CB-CA-C	-2.21	108.00	111.65
1	B	221	MLY	O-C-CA	-2.21	118.92	125.02
1	A	286	MLY	CB-CA-C	-2.18	108.06	111.65
1	B	286	MLY	O-C-CA	-2.12	119.16	125.02
1	B	330	MLY	O-C-CA	-2.10	119.23	125.02
1	B	243	MLY	O-C-CA	-2.09	119.25	125.02
1	B	60	MLY	O-C-CA	-2.08	119.26	125.02
1	B	60	MLY	CB-CA-C	-2.08	108.22	111.65
1	B	170	MLY	O-C-CA	-2.07	119.30	125.02
1	A	330	MLY	O-C-CA	-2.03	119.41	125.02
1	A	204	MLY	O-C-CA	-2.01	119.45	125.02
1	A	170	MLY	O-C-CA	-2.01	119.46	125.02
1	B	240	MLY	CD-CE-NZ	2.10	119.48	113.77
1	B	316	MLY	CD-CE-NZ	2.15	119.62	113.77
1	A	4	MLY	CD-CG-CB	2.55	122.69	113.63
1	B	204	MLY	CD-CE-NZ	2.83	121.46	113.77
1	B	322	MLY	CD-CE-NZ	3.22	122.53	113.77
1	B	55	MLY	CD-CE-NZ	3.25	122.61	113.77
1	B	261	MLY	CD-CE-NZ	3.44	123.13	113.77
1	A	261	MLY	CD-CE-NZ	3.69	123.81	113.77
1	A	105[B]	MLY	CD-CE-NZ	3.75	123.97	113.77
1	B	133	MLY	CD-CE-NZ	4.21	125.20	113.77
1	A	194	MLY	CD-CE-NZ	4.80	126.81	113.77
1	A	56	MLY	CD-CE-NZ	5.72	129.32	113.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	105[B]	MLY	4	0
1	A	131	MLY	1	0
1	A	261	MLY	1	0
1	A	330	MLY	1	0
1	A	4	MLY	2	0
1	A	5	MLY	1	0
1	A	56	MLY	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	60	MLY	1	0
1	B	105	MLY	1	0
1	B	133	MLY	1	0
1	B	170	MLY	1	0
1	B	204	MLY	1	0
1	B	26	MLY	2	0
1	B	322	MLY	2	0
1	B	330	MLY	1	0
1	B	5	MLY	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	PLP	A	401[A]	1	15,15,16	0.97	1 (6%)	20,22,23	1.96	5 (25%)
3	0JO	A	402[B]	-	18,21,21	1.85	5 (27%)	23,30,30	2.52	4 (17%)
4	PEG	A	403	-	6,6,6	0.68	0	5,5,5	0.70	0
2	PLP	B	401[A]	1	15,15,16	1.21	2 (13%)	20,22,23	1.86	6 (30%)
3	0JO	B	402[B]	-	18,21,21	2.23	5 (27%)	23,30,30	2.52	10 (43%)
4	PEG	B	403	-	6,6,6	0.96	0	5,5,5	0.57	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	A	401[A]	1	-	0/6/6/8	0/1/1/1
3	0JO	A	402[B]	-	-	0/8/15/15	0/1/1/1
4	PEG	A	403	-	-	0/4/4/4	0/0/0/0
2	PLP	B	401[A]	1	-	0/6/6/8	0/1/1/1
3	0JO	B	402[B]	-	-	0/8/15/15	0/1/1/1
4	PEG	B	403	-	-	0/4/4/4	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402[B]	0JO	C3-C2	-5.72	1.36	1.40
3	A	402[B]	0JO	P-OP1	-3.70	1.39	1.54
3	A	402[B]	0JO	C4-C5	-2.47	1.38	1.42
3	B	402[B]	0JO	P-OP1	-2.28	1.45	1.54
3	A	402[B]	0JO	P-OP3	-2.07	1.43	1.50
2	A	401[A]	PLP	C3-C2	2.12	1.42	1.40
2	B	401[A]	PLP	C6-N1	2.50	1.39	1.34
3	B	402[B]	0JO	CA-N	2.53	1.46	1.36
3	A	402[B]	0JO	CA-N	2.80	1.47	1.36
2	B	401[A]	PLP	C2-N1	2.89	1.39	1.33
3	B	402[B]	0JO	C4A-N	2.99	1.32	1.28
3	A	402[B]	0JO	C4-C4A	4.01	1.53	1.46
3	B	402[B]	0JO	C4-C4A	4.67	1.55	1.46

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402[B]	0JO	C5-C4-C4A	-5.96	112.45	121.36
3	B	402[B]	0JO	C5-C4-C4A	-5.15	113.66	121.36
3	B	402[B]	0JO	C2A-C2-C3	-4.79	115.25	120.96
2	A	401[A]	PLP	C4A-C4-C5	-4.06	116.75	120.86
3	A	402[B]	0JO	C4-C3-C2	-3.47	118.02	120.15
2	B	401[A]	PLP	C4A-C4-C5	-3.36	117.47	120.86
3	B	402[B]	0JO	C4-C4A-N	-3.13	115.60	123.41
2	B	401[A]	PLP	C5-C6-N1	-3.00	118.79	123.87
3	B	402[B]	0JO	O3-C3-C2	-2.83	111.84	117.78
3	B	402[B]	0JO	C3-C4-C5	-2.41	116.41	118.24
3	B	402[B]	0JO	OP2-P-OP1	2.02	115.78	107.61
2	B	401[A]	PLP	C6-C5-C4	2.03	119.87	118.18
2	A	401[A]	PLP	C4A-C4-C3	2.06	124.11	120.54
2	B	401[A]	PLP	C3-C4-C5	2.11	121.03	118.63
2	A	401[A]	PLP	O3P-P-O1P	2.33	119.61	110.50
3	B	402[B]	0JO	C2A-C2-N1	2.70	123.29	117.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401[A]	PLP	O3P-P-O2P	2.96	119.56	107.61
2	A	401[A]	PLP	C6-C5-C4	3.01	120.69	118.18
3	B	402[B]	0JO	O3-C3-C4	3.20	128.38	119.59
3	B	402[B]	0JO	C4A-N-CA	3.50	126.45	121.25
2	B	401[A]	PLP	O4P-C5A-C5	4.36	118.09	109.32
3	A	402[B]	0JO	C3-C4-C4A	4.60	129.31	120.52
3	B	402[B]	0JO	C3-C4-C4A	4.92	129.93	120.52
2	A	401[A]	PLP	O4P-C5A-C5	5.16	119.69	109.32
3	A	402[B]	0JO	C4A-N-CA	7.44	132.29	121.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402[B]	0JO	1	0
2	B	401[A]	PLP	2	0
3	B	402[B]	0JO	8	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	298/340 (87%)	-0.31	1 (0%)	93	95	11, 19, 36, 66	0
1	B	297/340 (87%)	-0.16	4 (1%)	77	81	12, 22, 42, 67	0
All	All	595/680 (87%)	-0.23	5 (0%)	86	89	11, 20, 41, 67	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	140	PRO	4.1
1	A	336	ILE	3.4
1	B	139	ASN	2.7
1	B	317	GLU	2.3
1	B	141	ASP	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. 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
1	MLY	A	316	9/12	0.90	0.12	-	35,42,47,49	0
1	MLY	A	286	9/12	0.88	0.19	-	21,24,45,47	0
1	MLY	B	4	9/12	0.78	0.27	-	40,53,66,67	0
1	MLY	A	60	9/12	0.91	0.13	-	22,24,38,44	0
1	MLY	A	330	9/12	0.95	0.10	-	19,22,39,40	0
1	MLY	B	131[B]	11/12	0.90	0.17	-	31,32,34,34	8
1	MLY	A	7	9/12	0.93	0.17	-	27,35,49,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	MLY	A	194	11/12	0.96	0.10	-	21,26,36,38	0
1	MLY	B	204	11/12	0.92	0.18	-	22,25,49,49	0
1	MLY	A	289	9/12	0.90	0.12	-	18,21,32,36	0
1	MLY	A	133	9/12	0.93	0.11	-	15,20,37,41	0
1	MLY	A	303	9/12	0.95	0.16	-	13,13,14,15	0
1	MLY	A	4	9/12	0.79	0.27	-	38,55,61,62	0
1	MLY	A	137	9/12	0.95	0.14	-	21,22,44,49	0
1	MLY	A	64	9/12	0.95	0.13	-	19,24,37,40	0
1	MLY	B	114	9/12	0.94	0.16	-	24,29,45,46	0
1	MLY	B	240	11/12	0.94	0.16	-	26,31,46,47	0
1	MLY	A	114	9/12	0.94	0.13	-	16,20,42,46	0
1	MLY	B	303	9/12	0.94	0.18	-	14,14,15,15	0
1	MLY	B	289	9/12	0.92	0.21	-	26,31,58,65	0
1	MLY	A	131	11/12	0.95	0.12	-	20,24,43,46	0
1	MLY	A	204	11/12	0.93	0.19	-	18,23,50,54	0
1	MLY	B	314	9/12	0.90	0.23	-	33,44,62,67	0
1	MLY	B	64	9/12	0.91	0.17	-	40,47,57,57	0
1	MLY	B	26	11/12	0.90	0.17	-	32,45,60,62	0
1	MLY	A	302	9/12	0.96	0.18	-	13,14,15,16	0
1	MLY	A	26	11/12	0.91	0.18	-	20,28,51,55	0
1	MLY	B	197	9/12	0.89	0.15	-	23,29,48,50	0
1	MLY	B	224	11/12	0.94	0.14	-	29,38,44,46	0
1	MLY	A	65	9/12	0.94	0.20	-	21,27,39,41	0
1	MLY	B	105	9/12	0.92	0.14	-	19,23,43,48	0
1	MLY	B	15	11/12	0.96	0.13	-	15,22,55,56	0
1	MLY	B	316	11/12	0.90	0.23	-	37,42,51,51	0
1	MLY	A	5	9/12	0.84	0.16	-	33,40,51,52	0
1	MLY	A	105[A]	11/12	0.92	0.20	-	15,19,29,30	8
1	MLY	A	170	9/12	0.93	0.17	-	22,30,47,50	0
1	MLY	A	221	11/12	0.93	0.14	-	23,29,47,49	0
1	MLY	B	327	9/12	0.94	0.18	-	22,26,45,48	0
1	MLY	B	56	11/12	0.94	0.18	-	25,29,32,32	0
1	MLY	A	105[B]	11/12	0.92	0.20	-	15,18,23,24	8
1	MLY	B	131[A]	11/12	0.90	0.17	-	31,33,36,37	8
1	MLY	B	5	11/12	0.92	0.14	-	33,39,53,59	0
1	MLY	B	137	9/12	0.89	0.28	-	45,51,74,76	0
1	MLY	B	7	9/12	0.86	0.19	-	28,32,52,53	0
1	MLY	B	60	9/12	0.88	0.19	-	39,40,56,57	0
1	MLY	A	264	9/12	0.94	0.12	-	21,24,40,45	0
1	MLY	A	240	11/12	0.96	0.12	-	18,25,37,39	0
1	MLY	B	286	11/12	0.93	0.13	-	30,36,47,48	0
1	MLY	B	221	9/12	0.90	0.21	-	26,33,58,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
1	MLY	B	261	11/12	0.95	0.10	-	14,19,34,34	0
1	MLY	A	56	11/12	0.94	0.11	-	16,21,40,41	0
1	MLY	B	121	9/12	0.87	0.20	-	38,44,60,65	0
1	MLY	A	327	9/12	0.90	0.15	-	22,25,46,50	0
1	MLY	B	65	9/12	0.92	0.30	-	35,50,71,74	0
1	MLY	A	121	9/12	0.83	0.24	-	42,51,62,62	0
1	MLY	A	224	9/12	0.91	0.19	-	25,29,52,56	0
1	MLY	A	261	11/12	0.95	0.12	-	15,21,36,36	0
1	MLY	B	330	9/12	0.96	0.16	-	21,23,42,51	0
1	MLY	A	15	11/12	0.94	0.14	-	13,20,43,44	0
1	MLY	B	322	11/12	0.95	0.13	-	26,30,47,48	0
1	MLY	A	243	9/12	0.95	0.20	-	29,35,61,64	0
1	MLY	A	197	9/12	0.94	0.14	-	24,27,45,52	0
1	MLY	B	243	9/12	0.87	0.24	-	30,33,54,55	0
1	MLY	B	264	9/12	0.94	0.14	-	18,21,44,51	0
1	MLY	B	133	11/12	0.90	0.15	-	30,38,49,52	0
1	MLY	B	302	9/12	0.97	0.13	-	12,13,14,16	0
1	MLY	A	322	9/12	0.93	0.16	-	26,29,53,56	0
1	MLY	B	35	9/12	0.98	0.11	-	13,14,16,16	0
1	MLY	B	194	11/12	0.93	0.11	-	17,21,31,31	0
1	MLY	A	35	9/12	0.97	0.13	-	13,13,14,15	0
1	MLY	B	170	11/12	0.94	0.12	-	19,23,33,34	0
1	MLY	A	314	9/12	0.89	0.32	-	45,51,71,75	0
1	MLY	A	55	9/12	0.95	0.08	-	17,18,31,36	0
1	MLY	B	55	11/12	0.93	0.14	-	20,25,42,46	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(Å²)	Q<0.9
4	PEG	A	403	7/7	0.57	0.30	12.71	58,69,77,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
4	PEG	B	403	7/7	0.75	0.32	6.53	43,53,54,55	0
3	0JO	B	402[B]	21/21	0.96	0.21	3.32	7,14,16,17	21
3	0JO	A	402[B]	21/21	0.95	0.16	2.00	7,14,16,16	21
2	PLP	B	401[A]	15/16	0.98	0.14	0.44	9,10,11,11	15
2	PLP	A	401[A]	15/16	0.98	0.11	-0.09	7,8,8,8	15

6.5 Other polymers (i)

There are no such residues in this entry.