



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:48 am BST

PDB ID : 3I0N
Title : Structure of the *S. pombe* Nbs1 FHA/BRCT-repeat domain
Authors : Clapperton, J.A.; Lloyd, J.; Chapman, J.R.; Jackson, S.P.; Smerdon, S.J.
Deposited on : 2009-06-25
Resolution : 2.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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

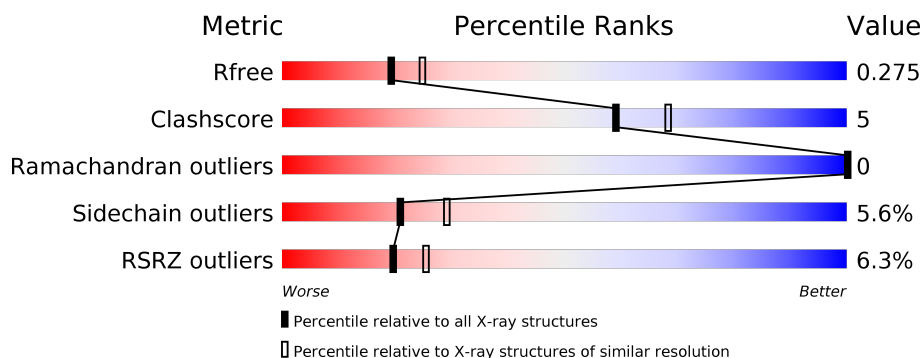
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. 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	324	<div> <div>6%</div> <div>85%</div> <div>12%</div> <div>..</div> </div>
1	B	324	<div> <div>5%</div> <div>84%</div> <div>13%</div> <div>..</div> </div>

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
1	MLY	A	282	-	-	-	X
1	MLY	B	282	-	-	-	X
1	MLY	B	318	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5384 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 repair and telomere maintenance protein nbs1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	0	0
			2584	1660	416	493	15			
1	B	319	Total	C	N	O	S	0	0	0
			2579	1657	415	492	15			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

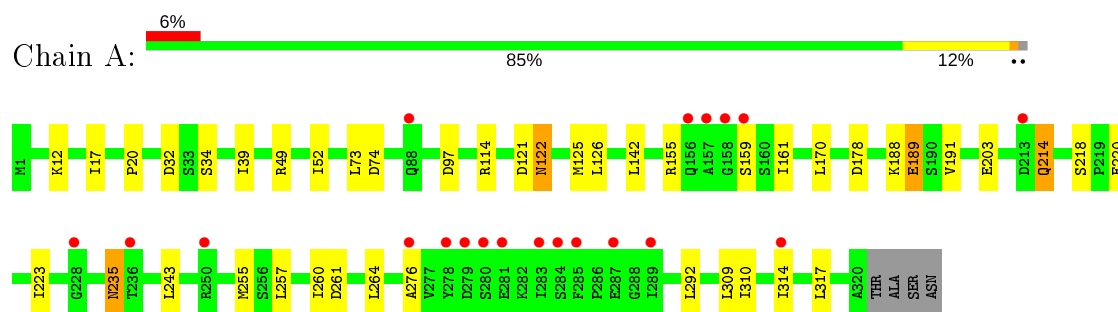
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	118	Total 118	O 118	0	0
3	B	91	Total 91	O 91	0	0

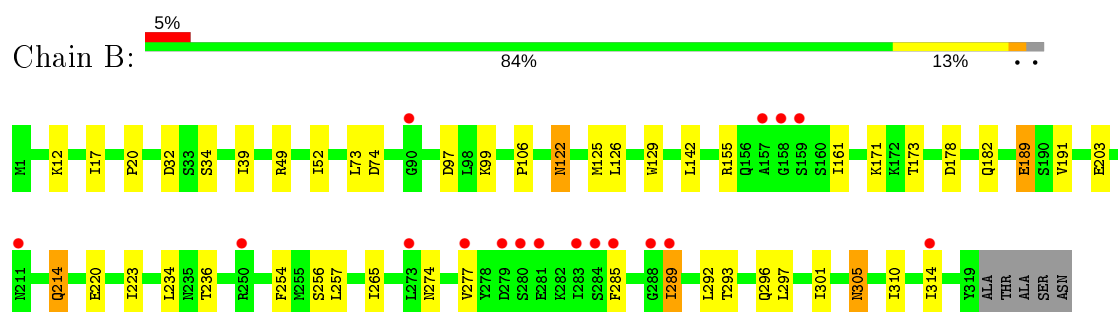
3 Residue-property plots [i](#)

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 repair and telomere maintenance protein nbs1



- Molecule 1: DNA repair and telomere maintenance protein nbs1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.19Å 64.90Å 106.36Å 90.00° 105.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.30 19.94 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.6 (15.00-2.30) 94.4 (19.94-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.215 , 0.263 0.227 , 0.275	Depositor DCC
R_{free} test set	1551 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	40.1	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.477 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5384	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.21% 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, MLY

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	0/2367	0.54	0/3222
1	B	0.41	0/2362	0.55	0/3215
All	All	0.41	0/4729	0.55	0/6437

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	2584	0	2596	23	0
1	B	2579	0	2592	27	0
2	A	6	0	8	1	0
2	B	6	0	8	0	0
3	A	118	0	0	6	0
3	B	91	0	0	2	0
All	All	5384	0	5204	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:A:161:ILE:HG23	1:A:214:GLN:HG2	1.63	0.80
1:B:305:ASN:HD22	1:B:305:ASN:H	1.24	0.80
1:B:161:ILE:HG23	1:B:214:GLN:HG2	1.66	0.77
1:B:155:ARG:HG2	3:B:372:HOH:O	1.94	0.67
1:B:12:MLY:HE2	1:B:39:ILE:HD11	1.81	0.61
1:B:305:ASN:HD22	1:B:305:ASN:N	1.94	0.61
1:A:12:MLY:HE2	1:A:39:ILE:HD11	1.82	0.61
1:A:235:ASN:HD21	1:A:255:MET:HA	1.67	0.60
1:B:310:ILE:O	1:B:314:ILE:HG12	2.05	0.57
1:A:188:MLY:HH11	3:A:400:HOH:O	2.05	0.56
1:B:293:THR:H	1:B:296:GLN:HE21	1.53	0.56
1:A:218:SER:HB2	3:A:444:HOH:O	2.06	0.56
1:A:114:ARG:HE	2:A:325:GOL:H32	1.73	0.54
1:A:155:ARG:HG2	3:A:388:HOH:O	2.08	0.54
1:A:310:ILE:O	1:A:314:ILE:HG12	2.08	0.53
1:B:234:LEU:HD12	1:B:254:PHE:CE1	2.44	0.53
1:B:305:ASN:H	1:B:305:ASN:ND2	2.02	0.52
1:B:155:ARG:HD3	1:B:178:ASP:HB2	1.92	0.51
1:A:155:ARG:HD3	1:A:178:ASP:HB2	1.93	0.51
1:B:122:ASN:ND2	1:B:125:MET:H	2.09	0.49
1:A:20:PRO:HA	1:A:52:ILE:HB	1.95	0.48
1:A:260:ILE:HA	1:A:264:LEU:HD23	1.94	0.48
1:B:305:ASN:N	1:B:305:ASN:ND2	2.62	0.47
1:A:17:ILE:HD12	1:A:191:VAL:CG1	2.44	0.47
1:B:20:PRO:HA	1:B:52:ILE:HB	1.97	0.47
1:A:122:ASN:ND2	1:A:125:MET:H	2.12	0.47
1:B:289:ILE:H	1:B:289:ILE:HD12	1.81	0.46
1:A:121:ASP:OD1	3:A:419:HOH:O	2.21	0.46
1:A:126:LEU:HD22	1:A:142:LEU:HG	1.97	0.45
1:B:155:ARG:O	1:B:155:ARG:HG3	2.16	0.45
1:A:220:GLU:HA	1:A:223:ILE:HD12	1.99	0.45
1:B:17:ILE:HD12	1:B:191:VAL:CG1	2.46	0.45
1:B:126:LEU:HD22	1:B:142:LEU:HG	1.98	0.45
1:A:32:ASP:HB3	1:A:34:SER:H	1.81	0.44
1:B:99:MLY:HE2	3:B:420:HOH:O	2.17	0.44
1:A:189:GLU:H	1:A:189:GLU:CD	2.20	0.44
1:B:189:GLU:H	1:B:189:GLU:CD	2.20	0.44
1:B:32:ASP:HB3	1:B:34:SER:H	1.82	0.44
1:B:220:GLU:HA	1:B:223:ILE:HD12	2.01	0.43
1:A:170:LEU:HD22	1:A:243:LEU:HD12	2.01	0.43
1:B:234:LEU:HD22	1:B:277:VAL:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:MLY:HH13	1:B:173:THR:OG1	2.20	0.42
1:B:265:ILE:HG12	1:B:289:ILE:HD11	2.02	0.42
1:B:297:LEU:O	1:B:301:ILE:HG12	2.20	0.42
1:A:276:ALA:HB3	3:A:424:HOH:O	2.20	0.41
1:B:129:TRP:CH2	1:B:182:GLN:HG3	2.56	0.41
1:A:155:ARG:HG3	1:A:155:ARG:O	2.20	0.41
1:A:159:SER:HB3	3:A:401:HOH:O	2.20	0.41
1:A:276:ALA:HA	1:B:106:PRO:HG2	2.03	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	294/324 (91%)	286 (97%)	8 (3%)	0	100	100
1	B	293/324 (90%)	286 (98%)	7 (2%)	0	100	100
All	All	587/648 (91%)	572 (97%)	15 (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	266/269 (99%)	252 (95%)	14 (5%)	22	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	266/269 (99%)	250 (94%)	16 (6%)	19	26
All	All	532/538 (99%)	502 (94%)	30 (6%)	21	29

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ARG
1	A	73	LEU
1	A	74	ASP
1	A	97	ASP
1	A	122	ASN
1	A	189	GLU
1	A	203	GLU
1	A	214	GLN
1	A	235	ASN
1	A	257	LEU
1	A	261	ASP
1	A	292	LEU
1	A	309	LEU
1	A	317	LEU
1	B	49	ARG
1	B	73	LEU
1	B	74	ASP
1	B	97	ASP
1	B	122	ASN
1	B	189	GLU
1	B	203	GLU
1	B	214	GLN
1	B	236	THR
1	B	256	SER
1	B	257	LEU
1	B	274	ASN
1	B	285	PHE
1	B	289	ILE
1	B	292	LEU
1	B	305	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN

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Mol	Chain	Res	Type
1	A	101	GLN
1	A	122	ASN
1	A	132	ASN
1	A	211	ASN
1	A	224	ASN
1	A	235	ASN
1	A	241	HIS
1	A	274	ASN
1	B	89	ASN
1	B	101	GLN
1	B	122	ASN
1	B	132	ASN
1	B	211	ASN
1	B	224	ASN
1	B	274	ASN
1	B	275	ASN
1	B	296	GLN
1	B	305	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

48 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	$\# Z > 2$
1	MLY	A	58	1	9,10,11	0.48	0	6,11,13	2.18	3 (50%)
1	MLY	A	99	1	9,10,11	0.47	0	6,11,13	2.23	3 (50%)
1	MLY	B	41	1	9,10,11	0.44	0	6,11,13	2.31	4 (66%)
1	MLY	B	14	1	9,10,11	0.45	0	6,11,13	2.33	4 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	B	206	1	9,10,11	0.37	0	6,11,13	2.28	4 (66%)
1	MLY	B	172	1	9,10,11	0.40	0	6,11,13	2.15	3 (50%)
1	MLY	B	188	1	9,10,11	0.38	0	6,11,13	2.11	2 (33%)
1	MLY	B	262	1	9,10,11	0.38	0	6,11,13	2.27	4 (66%)
1	MLY	B	84	1	9,10,11	0.42	0	6,11,13	2.27	4 (66%)
1	MLY	A	104	1	9,10,11	0.43	0	6,11,13	2.32	4 (66%)
1	MLY	B	12	1	9,10,11	0.42	0	6,11,13	2.19	3 (50%)
1	MLY	B	71	1	9,10,11	0.47	0	6,11,13	2.20	3 (50%)
1	MLY	A	267	1	9,10,11	0.37	0	6,11,13	2.27	4 (66%)
1	MLY	A	312	1	9,10,11	0.40	0	6,11,13	2.20	3 (50%)
1	MLY	B	210	1	9,10,11	0.49	0	6,11,13	2.16	3 (50%)
1	MLY	B	76	1	9,10,11	0.41	0	6,11,13	2.25	4 (66%)
1	MLY	A	96	1	9,10,11	0.40	0	6,11,13	2.24	4 (66%)
1	MLY	A	262	1	9,10,11	0.39	0	6,11,13	2.31	4 (66%)
1	MLY	A	12	1	9,10,11	0.44	0	6,11,13	2.19	3 (50%)
1	MLY	B	318	1	9,10,11	0.41	0	6,11,13	2.33	4 (66%)
1	MLY	B	312	1	9,10,11	0.43	0	6,11,13	2.29	4 (66%)
1	MLY	B	171	1	9,10,11	0.49	0	6,11,13	2.38	4 (66%)
1	MLY	A	71	1	9,10,11	0.42	0	6,11,13	2.21	3 (50%)
1	MLY	A	14	1	9,10,11	0.44	0	6,11,13	2.32	4 (66%)
1	MLY	A	84	1	9,10,11	0.41	0	6,11,13	2.30	4 (66%)
1	MLY	A	282	1	9,10,11	0.42	0	6,11,13	2.28	4 (66%)
1	MLY	B	94	1	9,10,11	0.50	0	6,11,13	2.50	4 (66%)
1	MLY	A	80	1	9,10,11	0.42	0	6,11,13	2.20	3 (50%)
1	MLY	A	318	1	9,10,11	0.42	0	6,11,13	2.28	4 (66%)
1	MLY	B	96	1	9,10,11	0.40	0	6,11,13	2.23	4 (66%)
1	MLY	B	104	1	9,10,11	0.42	0	6,11,13	2.36	4 (66%)
1	MLY	A	171	1	9,10,11	0.53	0	6,11,13	2.33	4 (66%)
1	MLY	A	206	1	9,10,11	0.35	0	6,11,13	2.30	4 (66%)
1	MLY	A	45	1	9,10,11	0.36	0	6,11,13	2.34	4 (66%)
1	MLY	B	267	1	9,10,11	0.39	0	6,11,13	2.23	4 (66%)
1	MLY	A	172	1	9,10,11	0.45	0	6,11,13	2.15	2 (33%)
1	MLY	A	210	1	9,10,11	0.49	0	6,11,13	2.16	3 (50%)
1	MLY	A	41	1	9,10,11	0.47	0	6,11,13	2.35	4 (66%)
1	MLY	B	282	1	9,10,11	0.41	0	6,11,13	2.26	4 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	B	45	1	9,10,11	0.39	0	6,11,13	2.35	4 (66%)
1	MLY	B	58	1	9,10,11	0.44	0	6,11,13	2.20	3 (50%)
1	MLY	A	299	1	9,10,11	0.38	0	6,11,13	2.27	4 (66%)
1	MLY	A	76	1	9,10,11	0.42	0	6,11,13	2.25	4 (66%)
1	MLY	B	299	1	9,10,11	0.40	0	6,11,13	2.18	3 (50%)
1	MLY	B	99	1	9,10,11	0.46	0	6,11,13	2.23	3 (50%)
1	MLY	A	94	1	9,10,11	0.48	0	6,11,13	2.47	4 (66%)
1	MLY	B	80	1	9,10,11	0.43	0	6,11,13	2.19	3 (50%)
1	MLY	A	188	1	9,10,11	0.39	0	6,11,13	2.11	2 (33%)

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	58	1	-	2/8/9/11	-
1	MLY	A	99	1	-	6/8/9/11	-
1	MLY	B	41	1	-	3/8/9/11	-
1	MLY	B	14	1	-	5/8/9/11	-
1	MLY	B	206	1	-	1/8/9/11	-
1	MLY	B	172	1	-	3/8/9/11	-
1	MLY	B	188	1	-	3/8/9/11	-
1	MLY	B	262	1	-	1/8/9/11	-
1	MLY	B	84	1	-	6/8/9/11	-
1	MLY	A	104	1	-	4/8/9/11	-
1	MLY	B	12	1	-	2/8/9/11	-
1	MLY	B	71	1	-	2/8/9/11	-
1	MLY	A	267	1	-	3/8/9/11	-
1	MLY	A	312	1	-	4/8/9/11	-
1	MLY	B	210	1	-	6/8/9/11	-
1	MLY	B	76	1	-	2/8/9/11	-
1	MLY	A	96	1	-	2/8/9/11	-
1	MLY	A	262	1	-	3/8/9/11	-
1	MLY	A	12	1	-	2/8/9/11	-
1	MLY	B	318	1	-	4/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	B	312	1	-	5/8/9/11	-
1	MLY	B	171	1	-	4/8/9/11	-
1	MLY	A	71	1	-	2/8/9/11	-
1	MLY	A	14	1	-	4/8/9/11	-
1	MLY	A	84	1	-	6/8/9/11	-
1	MLY	A	282	1	-	3/8/9/11	-
1	MLY	B	94	1	-	3/8/9/11	-
1	MLY	A	80	1	-	2/8/9/11	-
1	MLY	A	318	1	-	5/8/9/11	-
1	MLY	B	96	1	-	2/8/9/11	-
1	MLY	B	104	1	-	4/8/9/11	-
1	MLY	A	171	1	-	4/8/9/11	-
1	MLY	A	206	1	-	1/8/9/11	-
1	MLY	A	45	1	-	2/8/9/11	-
1	MLY	B	267	1	-	4/8/9/11	-
1	MLY	A	172	1	-	3/8/9/11	-
1	MLY	A	210	1	-	5/8/9/11	-
1	MLY	A	41	1	-	2/8/9/11	-
1	MLY	B	282	1	-	3/8/9/11	-
1	MLY	B	45	1	-	2/8/9/11	-
1	MLY	B	58	1	-	2/8/9/11	-
1	MLY	A	299	1	-	3/8/9/11	-
1	MLY	A	76	1	-	2/8/9/11	-
1	MLY	B	299	1	-	3/8/9/11	-
1	MLY	B	99	1	-	6/8/9/11	-
1	MLY	A	94	1	-	3/8/9/11	-
1	MLY	B	80	1	-	2/8/9/11	-
1	MLY	A	188	1	-	3/8/9/11	-

There are no bond length outliers.

All (171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	MLY	CH2-NZ-CH1	3.97	120.00	109.73
1	B	14	MLY	CH2-NZ-CH1	3.94	119.92	109.73
1	A	206	MLY	CH2-NZ-CH1	3.93	119.89	109.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	94	MLY	CH2-NZ-CH1	3.89	119.80	109.73
1	A	41	MLY	CH2-NZ-CH1	3.86	119.72	109.73
1	B	99	MLY	CH2-NZ-CH1	3.85	119.67	109.73
1	A	99	MLY	CH2-NZ-CH1	3.81	119.58	109.73
1	B	206	MLY	CH2-NZ-CH1	3.80	119.56	109.73
1	A	45	MLY	CH2-NZ-CH1	3.78	119.50	109.73
1	B	45	MLY	CH2-NZ-CH1	3.77	119.48	109.73
1	A	14	MLY	CH2-NZ-CH1	3.77	119.47	109.73
1	B	41	MLY	CH2-NZ-CH1	3.75	119.43	109.73
1	B	104	MLY	CH2-NZ-CH1	3.75	119.41	109.73
1	B	318	MLY	CH2-NZ-CH1	3.73	119.38	109.73
1	B	76	MLY	CH2-NZ-CH1	3.73	119.38	109.73
1	A	318	MLY	CH2-NZ-CH1	3.72	119.35	109.73
1	A	76	MLY	CH2-NZ-CH1	3.71	119.32	109.73
1	A	71	MLY	CH2-NZ-CH1	3.71	119.31	109.73
1	A	262	MLY	CH2-NZ-CH1	3.71	119.31	109.73
1	B	71	MLY	CH2-NZ-CH1	3.69	119.28	109.73
1	B	210	MLY	CH2-NZ-CH1	3.69	119.26	109.73
1	B	312	MLY	CH2-NZ-CH1	3.68	119.25	109.73
1	A	104	MLY	CH2-NZ-CH1	3.66	119.20	109.73
1	A	267	MLY	CH2-NZ-CH1	3.65	119.16	109.73
1	A	210	MLY	CH2-NZ-CH1	3.64	119.14	109.73
1	B	262	MLY	CH2-NZ-CH1	3.63	119.11	109.73
1	A	12	MLY	CH2-NZ-CH1	3.62	119.10	109.73
1	B	267	MLY	CH2-NZ-CH1	3.62	119.09	109.73
1	B	172	MLY	CH2-NZ-CH1	3.61	119.07	109.73
1	B	171	MLY	CH2-NZ-CH1	3.61	119.06	109.73
1	B	282	MLY	CH2-NZ-CH1	3.60	119.05	109.73
1	B	12	MLY	CH2-NZ-CH1	3.60	119.04	109.73
1	A	171	MLY	CH2-NZ-CH1	3.60	119.04	109.73
1	A	84	MLY	CH2-NZ-CH1	3.59	119.02	109.73
1	A	80	MLY	CH2-NZ-CH1	3.59	119.00	109.73
1	A	312	MLY	CH2-NZ-CH1	3.59	119.00	109.73
1	A	172	MLY	CH2-NZ-CH1	3.57	118.96	109.73
1	A	282	MLY	CH2-NZ-CH1	3.56	118.93	109.73
1	B	96	MLY	CH2-NZ-CH1	3.55	118.91	109.73
1	B	80	MLY	CH2-NZ-CH1	3.55	118.90	109.73
1	A	299	MLY	CH2-NZ-CH1	3.54	118.89	109.73
1	A	96	MLY	CH2-NZ-CH1	3.54	118.88	109.73
1	A	188	MLY	CH2-NZ-CH1	3.51	118.79	109.73
1	B	84	MLY	CH2-NZ-CH1	3.50	118.78	109.73
1	A	58	MLY	CH2-NZ-CH1	3.49	118.76	109.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	58	MLY	CH2-NZ-CH1	3.46	118.67	109.73
1	B	299	MLY	CH2-NZ-CH1	3.45	118.64	109.73
1	B	188	MLY	CH2-NZ-CH1	3.39	118.50	109.73
1	B	188	MLY	CH2-NZ-CE	3.18	123.34	110.74
1	A	188	MLY	CH2-NZ-CE	3.13	123.14	110.74
1	B	94	MLY	CD-CE-NZ	-3.06	105.51	113.79
1	A	172	MLY	CH2-NZ-CE	2.99	122.58	110.74
1	B	172	MLY	CH2-NZ-CE	2.88	122.15	110.74
1	A	94	MLY	CD-CE-NZ	-2.83	106.13	113.79
1	B	171	MLY	CH2-NZ-CE	2.75	121.64	110.74
1	B	99	MLY	CH1-NZ-CE	2.75	121.64	110.74
1	A	171	MLY	CH2-NZ-CE	2.73	121.53	110.74
1	B	84	MLY	CH2-NZ-CE	2.69	121.40	110.74
1	A	99	MLY	CH1-NZ-CE	2.69	121.39	110.74
1	A	84	MLY	CH2-NZ-CE	2.69	121.39	110.74
1	A	12	MLY	CH2-NZ-CE	2.68	121.37	110.74
1	B	12	MLY	CH2-NZ-CE	2.68	121.37	110.74
1	B	80	MLY	CH1-NZ-CE	2.67	121.30	110.74
1	B	104	MLY	CD-CE-NZ	-2.63	106.67	113.79
1	B	45	MLY	CD-CE-NZ	-2.61	106.72	113.79
1	A	312	MLY	CH2-NZ-CE	2.59	120.99	110.74
1	A	80	MLY	CH1-NZ-CE	2.59	120.99	110.74
1	B	96	MLY	CH1-NZ-CE	2.56	120.88	110.74
1	A	282	MLY	CH1-NZ-CE	2.55	120.85	110.74
1	A	104	MLY	CH2-NZ-CE	2.54	120.81	110.74
1	A	58	MLY	CH1-NZ-CE	2.54	120.80	110.74
1	A	206	MLY	CH2-NZ-CE	2.54	120.79	110.74
1	A	45	MLY	CD-CE-NZ	-2.53	106.93	113.79
1	B	58	MLY	CH1-NZ-CE	2.53	120.75	110.74
1	A	45	MLY	CH1-NZ-CE	2.53	120.75	110.74
1	A	71	MLY	CH2-NZ-CE	2.52	120.74	110.74
1	A	96	MLY	CH1-NZ-CE	2.52	120.74	110.74
1	A	318	MLY	CH2-NZ-CE	2.52	120.73	110.74
1	B	312	MLY	CH2-NZ-CE	2.52	120.72	110.74
1	B	45	MLY	CH1-NZ-CE	2.52	120.72	110.74
1	B	299	MLY	CH2-NZ-CE	2.52	120.72	110.74
1	B	206	MLY	CH2-NZ-CE	2.52	120.71	110.74
1	A	14	MLY	CH1-NZ-CE	2.51	120.69	110.74
1	B	104	MLY	CH2-NZ-CE	2.51	120.68	110.74
1	A	210	MLY	CH2-NZ-CE	2.50	120.64	110.74
1	B	299	MLY	CH1-NZ-CE	2.50	120.63	110.74
1	B	267	MLY	CH2-NZ-CE	2.49	120.60	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	14	MLY	CH1-NZ-CE	2.49	120.59	110.74
1	A	41	MLY	CD-CE-NZ	-2.48	107.06	113.79
1	B	71	MLY	CH2-NZ-CE	2.48	120.58	110.74
1	A	267	MLY	CH1-NZ-CE	2.48	120.57	110.74
1	A	299	MLY	CH2-NZ-CE	2.48	120.56	110.74
1	B	58	MLY	CH2-NZ-CE	2.48	120.56	110.74
1	A	299	MLY	CH1-NZ-CE	2.48	120.55	110.74
1	A	262	MLY	CH1-NZ-CE	2.48	120.55	110.74
1	A	104	MLY	CD-CE-NZ	-2.47	107.09	113.79
1	B	282	MLY	CH2-NZ-CE	2.47	120.52	110.74
1	B	41	MLY	CH1-NZ-CE	2.47	120.51	110.74
1	A	84	MLY	CD-CE-NZ	-2.45	107.14	113.79
1	B	262	MLY	CH1-NZ-CE	2.45	120.46	110.74
1	B	318	MLY	CD-CE-NZ	-2.45	107.15	113.79
1	B	171	MLY	CD-CE-NZ	-2.45	107.15	113.79
1	B	210	MLY	CH2-NZ-CE	2.45	120.45	110.74
1	A	76	MLY	CH2-NZ-CE	2.45	120.44	110.74
1	B	282	MLY	CH1-NZ-CE	2.45	120.43	110.74
1	B	262	MLY	CH2-NZ-CE	2.45	120.43	110.74
1	A	58	MLY	CH2-NZ-CE	2.44	120.42	110.74
1	B	76	MLY	CH2-NZ-CE	2.44	120.42	110.74
1	A	14	MLY	CD-CE-NZ	-2.44	107.18	113.79
1	A	96	MLY	CH2-NZ-CE	2.43	120.38	110.74
1	B	318	MLY	CH2-NZ-CE	2.43	120.37	110.74
1	A	41	MLY	CH1-NZ-CE	2.43	120.37	110.74
1	A	262	MLY	CD-CE-NZ	-2.43	107.22	113.79
1	B	94	MLY	CH2-NZ-CE	2.42	120.33	110.74
1	B	267	MLY	CH1-NZ-CE	2.42	120.31	110.74
1	B	210	MLY	CH1-NZ-CE	2.41	120.29	110.74
1	A	267	MLY	CH2-NZ-CE	2.40	120.27	110.74
1	A	94	MLY	CH2-NZ-CE	2.40	120.25	110.74
1	B	318	MLY	CH1-NZ-CE	2.40	120.24	110.74
1	A	76	MLY	CH1-NZ-CE	2.40	120.23	110.74
1	A	210	MLY	CH1-NZ-CE	2.39	120.22	110.74
1	B	96	MLY	CH2-NZ-CE	2.39	120.21	110.74
1	A	282	MLY	CH2-NZ-CE	2.39	120.21	110.74
1	B	76	MLY	CH1-NZ-CE	2.39	120.20	110.74
1	B	41	MLY	CD-CE-NZ	-2.39	107.33	113.79
1	B	84	MLY	CD-CE-NZ	-2.38	107.34	113.79
1	A	299	MLY	CD-CE-NZ	-2.38	107.35	113.79
1	A	262	MLY	CH2-NZ-CE	2.37	120.14	110.74
1	B	71	MLY	CH1-NZ-CE	2.37	120.14	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	MLY	CH2-NZ-CE	2.35	120.06	110.74
1	B	312	MLY	CH1-NZ-CE	2.35	120.03	110.74
1	A	80	MLY	CH2-NZ-CE	2.34	120.01	110.74
1	B	312	MLY	CD-CE-NZ	-2.34	107.46	113.79
1	A	312	MLY	CH1-NZ-CE	2.34	120.00	110.74
1	A	104	MLY	CH1-NZ-CE	2.34	119.99	110.74
1	A	282	MLY	CD-CE-NZ	-2.33	107.47	113.79
1	A	71	MLY	CH1-NZ-CE	2.32	119.94	110.74
1	A	318	MLY	CH1-NZ-CE	2.32	119.92	110.74
1	A	41	MLY	CH2-NZ-CE	2.32	119.91	110.74
1	B	104	MLY	CH1-NZ-CE	2.31	119.90	110.74
1	B	262	MLY	CD-CE-NZ	-2.31	107.53	113.79
1	B	94	MLY	CH1-NZ-CE	2.30	119.87	110.74
1	A	14	MLY	CH2-NZ-CE	2.30	119.84	110.74
1	B	84	MLY	CH1-NZ-CE	2.29	119.81	110.74
1	B	45	MLY	CH2-NZ-CE	2.29	119.80	110.74
1	B	80	MLY	CH2-NZ-CE	2.29	119.79	110.74
1	B	14	MLY	CD-CE-NZ	-2.28	107.61	113.79
1	A	94	MLY	CH1-NZ-CE	2.28	119.76	110.74
1	A	45	MLY	CH2-NZ-CE	2.28	119.75	110.74
1	B	206	MLY	CH1-NZ-CE	2.26	119.71	110.74
1	A	84	MLY	CH1-NZ-CE	2.24	119.59	110.74
1	A	267	MLY	CD-CE-NZ	-2.23	107.74	113.79
1	B	12	MLY	CH1-NZ-CE	2.23	119.59	110.74
1	B	282	MLY	CD-CE-NZ	-2.22	107.77	113.79
1	A	12	MLY	CH1-NZ-CE	2.22	119.53	110.74
1	B	14	MLY	CH2-NZ-CE	2.21	119.49	110.74
1	A	171	MLY	CD-CE-NZ	-2.19	107.85	113.79
1	A	171	MLY	CH1-NZ-CE	2.19	119.42	110.74
1	A	318	MLY	CD-CE-NZ	-2.18	107.88	113.79
1	A	206	MLY	CH1-NZ-CE	2.16	119.30	110.74
1	B	171	MLY	CH1-NZ-CE	2.16	119.28	110.74
1	A	96	MLY	CD-CE-NZ	-2.14	107.98	113.79
1	A	76	MLY	CD-CE-NZ	-2.10	108.10	113.79
1	B	76	MLY	CD-CE-NZ	-2.10	108.12	113.79
1	A	99	MLY	CH2-NZ-CE	2.09	119.03	110.74
1	B	96	MLY	CD-CE-NZ	-2.09	108.13	113.79
1	A	206	MLY	CD-CE-NZ	-2.06	108.21	113.79
1	B	267	MLY	CD-CE-NZ	-2.05	108.25	113.79
1	B	206	MLY	CD-CE-NZ	-2.04	108.26	113.79
1	B	172	MLY	CH1-NZ-CE	2.03	118.77	110.74
1	B	99	MLY	CH2-NZ-CE	2.01	118.68	110.74

There are no chirality outliers.

All (154) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	99	MLY	N-CA-CB-CG
1	A	99	MLY	C-CA-CB-CG
1	B	84	MLY	C-CA-CB-CG
1	A	104	MLY	C-CA-CB-CG
1	A	94	MLY	C-CA-CB-CG
1	A	94	MLY	O-C-CA-CB
1	B	210	MLY	C-CA-CB-CG
1	B	318	MLY	N-CA-CB-CG
1	B	318	MLY	C-CA-CB-CG
1	B	318	MLY	O-C-CA-CB
1	B	312	MLY	N-CA-CB-CG
1	B	312	MLY	C-CA-CB-CG
1	B	171	MLY	C-CA-CB-CG
1	B	267	MLY	C-CA-CB-CG
1	A	84	MLY	C-CA-CB-CG
1	B	94	MLY	C-CA-CB-CG
1	B	94	MLY	O-C-CA-CB
1	A	318	MLY	N-CA-CB-CG
1	A	318	MLY	C-CA-CB-CG
1	B	104	MLY	C-CA-CB-CG
1	A	171	MLY	C-CA-CB-CG
1	B	299	MLY	C-CA-CB-CG
1	B	299	MLY	O-C-CA-CB
1	A	210	MLY	C-CA-CB-CG
1	A	299	MLY	O-C-CA-CB
1	B	99	MLY	N-CA-CB-CG
1	B	99	MLY	C-CA-CB-CG
1	A	206	MLY	CD-CE-NZ-CH1
1	A	14	MLY	CD-CE-NZ-CH2
1	A	99	MLY	CD-CE-NZ-CH2
1	B	14	MLY	CD-CE-NZ-CH2
1	B	206	MLY	CD-CE-NZ-CH1
1	B	172	MLY	CD-CE-NZ-CH1
1	B	84	MLY	CD-CE-NZ-CH1
1	B	12	MLY	CD-CE-NZ-CH1
1	A	96	MLY	CD-CE-NZ-CH2
1	A	12	MLY	CD-CE-NZ-CH1
1	B	312	MLY	CD-CE-NZ-CH1
1	B	171	MLY	CD-CE-NZ-CH1
1	A	71	MLY	CD-CE-NZ-CH1

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Mol	Chain	Res	Type	Atoms
1	A	58	MLY	CD-CE-NZ-CH1
1	A	84	MLY	CD-CE-NZ-CH1
1	A	318	MLY	CD-CE-NZ-CH1
1	B	96	MLY	CD-CE-NZ-CH2
1	A	171	MLY	CD-CE-NZ-CH1
1	A	172	MLY	CD-CE-NZ-CH1
1	B	58	MLY	CD-CE-NZ-CH1
1	B	99	MLY	CD-CE-NZ-CH2
1	B	71	MLY	CD-CE-NZ-CH1
1	B	312	MLY	CG-CD-CE-NZ
1	A	282	MLY	CG-CD-CE-NZ
1	A	171	MLY	CG-CD-CE-NZ
1	B	99	MLY	CG-CD-CE-NZ
1	A	99	MLY	CG-CD-CE-NZ
1	B	210	MLY	CG-CD-CE-NZ
1	A	210	MLY	CG-CD-CE-NZ
1	B	282	MLY	CG-CD-CE-NZ
1	A	58	MLY	CG-CD-CE-NZ
1	A	84	MLY	CG-CD-CE-NZ
1	B	84	MLY	CG-CD-CE-NZ
1	B	171	MLY	CG-CD-CE-NZ
1	A	104	MLY	CG-CD-CE-NZ
1	B	104	MLY	CG-CD-CE-NZ
1	B	58	MLY	CG-CD-CE-NZ
1	B	188	MLY	CD-CE-NZ-CH2
1	A	104	MLY	CD-CE-NZ-CH1
1	A	80	MLY	CD-CE-NZ-CH2
1	B	104	MLY	CD-CE-NZ-CH1
1	A	299	MLY	CD-CE-NZ-CH1
1	B	80	MLY	CD-CE-NZ-CH2
1	A	312	MLY	CG-CD-CE-NZ
1	A	188	MLY	CD-CE-NZ-CH2
1	B	210	MLY	CA-CB-CG-CD
1	A	210	MLY	CA-CB-CG-CD
1	A	14	MLY	CG-CD-CE-NZ
1	B	14	MLY	CG-CD-CE-NZ
1	A	312	MLY	CD-CE-NZ-CH1
1	B	76	MLY	CD-CE-NZ-CH1
1	B	318	MLY	CD-CE-NZ-CH1
1	A	99	MLY	CA-CB-CG-CD
1	B	282	MLY	CA-CB-CG-CD
1	A	188	MLY	CG-CD-CE-NZ

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Mol	Chain	Res	Type	Atoms
1	A	282	MLY	CD-CE-NZ-CH2
1	A	45	MLY	CD-CE-NZ-CH2
1	B	299	MLY	CD-CE-NZ-CH1
1	A	172	MLY	CD-CE-NZ-CH2
1	B	45	MLY	CD-CE-NZ-CH2
1	A	76	MLY	CD-CE-NZ-CH1
1	B	188	MLY	CG-CD-CE-NZ
1	B	99	MLY	CA-CB-CG-CD
1	A	84	MLY	CE-CD-CG-CB
1	B	84	MLY	CE-CD-CG-CB
1	A	99	MLY	CE-CD-CG-CB
1	B	99	MLY	CE-CD-CG-CB
1	A	80	MLY	CE-CD-CG-CB
1	A	262	MLY	CD-CE-NZ-CH2
1	A	267	MLY	CE-CD-CG-CB
1	B	80	MLY	CE-CD-CG-CB
1	A	210	MLY	CD-CE-NZ-CH2
1	A	318	MLY	CG-CD-CE-NZ
1	A	267	MLY	CG-CD-CE-NZ
1	A	188	MLY	CE-CD-CG-CB
1	A	312	MLY	CE-CD-CG-CB
1	B	171	MLY	CE-CD-CG-CB
1	A	171	MLY	CE-CD-CG-CB
1	B	210	MLY	CD-CE-NZ-CH2
1	B	71	MLY	CE-CD-CG-CB
1	B	84	MLY	CA-CB-CG-CD
1	A	84	MLY	CA-CB-CG-CD
1	A	312	MLY	C-CA-CB-CG
1	B	312	MLY	CE-CD-CG-CB
1	B	188	MLY	CE-CD-CG-CB
1	A	71	MLY	CE-CD-CG-CB
1	B	172	MLY	CD-CE-NZ-CH2
1	A	282	MLY	CA-CB-CG-CD
1	A	267	MLY	CD-CE-NZ-CH2
1	B	267	MLY	CD-CE-NZ-CH2
1	A	96	MLY	CE-CD-CG-CB
1	B	104	MLY	CE-CD-CG-CB
1	B	96	MLY	CE-CD-CG-CB
1	B	94	MLY	CD-CE-NZ-CH2
1	A	104	MLY	CE-CD-CG-CB
1	B	262	MLY	CD-CE-NZ-CH1
1	A	94	MLY	CD-CE-NZ-CH2

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Mol	Chain	Res	Type	Atoms
1	A	76	MLY	CE-CD-CG-CB
1	B	76	MLY	CE-CD-CG-CB
1	B	12	MLY	CE-CD-CG-CB
1	A	12	MLY	CE-CD-CG-CB
1	B	172	MLY	CE-CD-CG-CB
1	A	172	MLY	CE-CD-CG-CB
1	A	262	MLY	CA-CB-CG-CD
1	B	210	MLY	CE-CD-CG-CB
1	A	210	MLY	CE-CD-CG-CB
1	A	318	MLY	CE-CD-CG-CB
1	A	14	MLY	CE-CD-CG-CB
1	B	282	MLY	CD-CE-NZ-CH1
1	B	14	MLY	CE-CD-CG-CB
1	B	84	MLY	N-CA-CB-CG
1	A	84	MLY	N-CA-CB-CG
1	A	14	MLY	C-CA-CB-CG
1	B	14	MLY	C-CA-CB-CG
1	A	41	MLY	CD-CE-NZ-CH1
1	A	41	MLY	CG-CD-CE-NZ
1	B	267	MLY	CG-CD-CE-NZ
1	B	41	MLY	CD-CE-NZ-CH1
1	B	41	MLY	CD-CE-NZ-CH2
1	B	41	MLY	CG-CD-CE-NZ
1	A	299	MLY	C-CA-CB-CG
1	B	267	MLY	CE-CD-CG-CB
1	B	45	MLY	CG-CD-CE-NZ
1	A	45	MLY	CG-CD-CE-NZ
1	B	14	MLY	CA-CB-CG-CD
1	B	210	MLY	N-CA-CB-CG
1	A	262	MLY	N-CA-CB-CG

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	12	MLY	1	0
1	A	12	MLY	1	0
1	B	171	MLY	1	0
1	B	99	MLY	1	0
1	A	188	MLY	1	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 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	GOL	A	325	-	5,5,5	0.40	0	5,5,5	0.42	0
2	GOL	B	325	-	5,5,5	0.42	0	5,5,5	0.44	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	GOL	A	325	-	-	0/4/4/4	-
2	GOL	B	325	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	325	GOL	1	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, 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	296/324 (91%)	0.35	20 (6%) 17 22	26, 37, 48, 57	0
1	B	295/324 (91%)	0.40	17 (5%) 23 29	26, 37, 48, 53	0
All	All	591/648 (91%)	0.37	37 (6%) 20 25	26, 37, 48, 57	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	283	ILE	13.1
1	A	283	ILE	9.8
1	A	157	ALA	8.2
1	B	157	ALA	5.4
1	B	280	SER	5.3
1	A	280	SER	4.7
1	A	276	ALA	4.7
1	B	279	ASP	4.4
1	B	285	PHE	4.2
1	A	284	SER	4.0
1	A	281	GLU	3.9
1	B	158	GLY	3.8
1	A	236	THR	3.7
1	A	158	GLY	3.7
1	B	281	GLU	3.7
1	B	159	SER	3.5
1	A	279	ASP	3.2
1	A	285	PHE	3.1
1	B	284	SER	3.0
1	A	159	SER	3.0
1	B	289	ILE	2.8
1	A	314	ILE	2.6
1	A	88	GLN	2.5
1	B	273	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	288	GLY	2.5
1	B	250	ARG	2.4
1	B	314	ILE	2.3
1	A	278	TYR	2.3
1	A	250	ARG	2.3
1	A	228	GLY	2.2
1	A	289	ILE	2.2
1	A	156	GLN	2.1
1	A	213	ASP	2.1
1	A	287	GLU	2.0
1	B	90	GLY	2.0
1	B	277	VAL	2.0
1	B	211	ASN	2.0

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

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
1	MLY	A	282	11/12	0.32	0.57	52,52,52,52	0
1	MLY	B	282	11/12	0.46	0.55	51,52,52,52	0
1	MLY	B	210	11/12	0.67	0.37	42,43,51,51	0
1	MLY	A	210	11/12	0.70	0.31	42,43,51,51	0
1	MLY	B	318	11/12	0.77	0.41	50,51,52,52	0
1	MLY	A	318	11/12	0.79	0.38	51,52,52,52	0
1	MLY	A	299	11/12	0.81	0.27	32,34,41,42	0
1	MLY	B	41	11/12	0.84	0.29	38,38,44,44	0
1	MLY	A	41	11/12	0.84	0.32	38,38,44,44	0
1	MLY	A	171	11/12	0.85	0.21	35,37,52,52	0
1	MLY	B	262	11/12	0.86	0.43	43,43,44,44	0
1	MLY	A	267	11/12	0.87	0.23	40,40,40,40	0
1	MLY	B	299	11/12	0.87	0.25	33,35,41,42	0
1	MLY	A	58	11/12	0.87	0.24	31,33,43,43	0
1	MLY	B	99	11/12	0.87	0.21	36,38,44,44	0
1	MLY	A	99	11/12	0.88	0.22	36,38,44,44	0
1	MLY	B	58	11/12	0.88	0.25	31,33,43,43	0
1	MLY	B	267	11/12	0.88	0.20	40,40,40,41	0
1	MLY	A	76	11/12	0.88	0.31	36,36,40,41	0
1	MLY	A	262	11/12	0.88	0.32	43,43,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	MLY	B	104	11/12	0.89	0.30	36,36,41,41	0
1	MLY	B	84	11/12	0.89	0.22	40,40,46,46	0
1	MLY	B	71	11/12	0.89	0.24	35,35,42,43	0
1	MLY	A	84	11/12	0.90	0.18	40,40,46,46	0
1	MLY	B	171	11/12	0.90	0.15	35,37,52,52	0
1	MLY	A	312	11/12	0.91	0.29	44,45,46,46	0
1	MLY	A	12	11/12	0.91	0.21	34,35,43,44	0
1	MLY	A	71	11/12	0.92	0.19	35,35,42,43	0
1	MLY	B	12	11/12	0.93	0.19	34,35,43,44	0
1	MLY	B	188	11/12	0.93	0.19	37,38,41,41	0
1	MLY	B	14	11/12	0.93	0.19	34,34,40,40	0
1	MLY	B	206	11/12	0.93	0.17	38,39,44,44	0
1	MLY	B	76	11/12	0.93	0.30	36,36,40,41	0
1	MLY	A	206	11/12	0.93	0.17	38,39,44,44	0
1	MLY	A	45	11/12	0.93	0.20	33,34,39,39	0
1	MLY	A	104	11/12	0.93	0.33	36,36,41,41	0
1	MLY	B	80	11/12	0.93	0.16	35,36,38,38	0
1	MLY	A	188	11/12	0.93	0.17	37,38,41,41	0
1	MLY	A	14	11/12	0.94	0.20	34,34,40,41	0
1	MLY	B	172	11/12	0.94	0.16	35,36,40,41	0
1	MLY	B	312	11/12	0.94	0.23	44,45,46,46	0
1	MLY	B	94	11/12	0.94	0.18	39,40,43,43	0
1	MLY	B	45	11/12	0.94	0.18	33,34,39,39	0
1	MLY	A	80	11/12	0.94	0.18	35,36,38,38	0
1	MLY	A	172	11/12	0.95	0.14	35,36,40,41	0
1	MLY	B	96	11/12	0.95	0.13	39,40,44,44	0
1	MLY	A	96	11/12	0.95	0.15	39,40,44,44	0
1	MLY	A	94	11/12	0.96	0.16	39,40,42,43	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. 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(\AA^2)	Q<0.9
2	GOL	A	325	6/6	0.97	0.15	60,61,62,63	0
2	GOL	B	325	6/6	0.97	0.15	55,57,58,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.