Full wwPDB X-ray Structure Validation Report (i)

Jan 25, 2023 – 09:32 AM EST

PDB ID	:	3SBU
Title	:	Crystal structure of a ntf2-like protein (BF2862) from Bacteroides fragilis NCTC 9343 at 2.15 A resolution
Authors	:	Joint Center for Structural Genomics (JCSG)
Deposited on	:	2011-06-06
Resolution	:	2.15 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

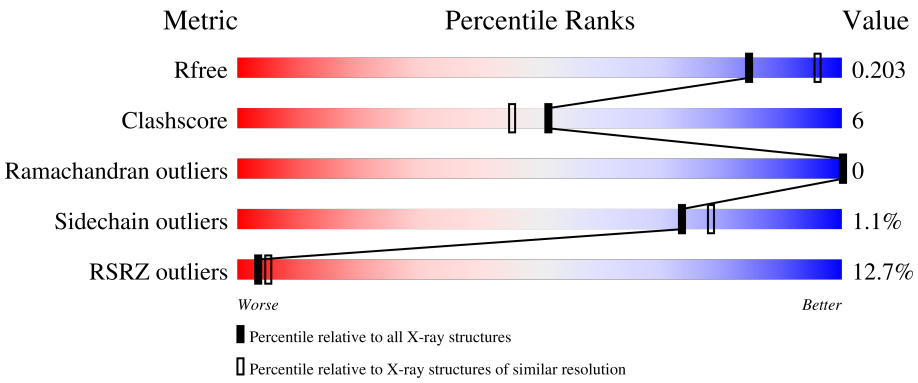
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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

Mol	Chain	Length	Quality of chain
1	A	261	10% 71% 15% • 12%
1	B	261	11% 76% 10% • 12%

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
2	GOL	A	285	-	-	-	X
2	GOL	A	289	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4167 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.

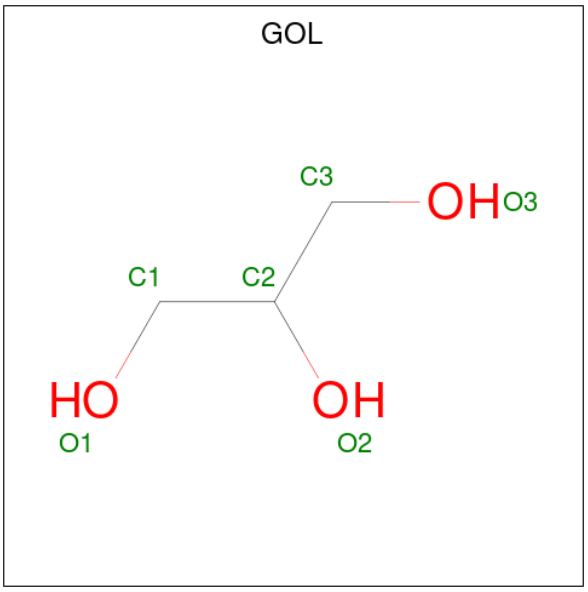
- Molecule 1 is a protein called Hypothetical ntf2-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	230	1947	1265	309	370	3	0	4	0
1	B	230	1986	1291	314	378	3	0	12	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q5LBG4
B	0	GLY	-	expression tag	UNP Q5LBG4

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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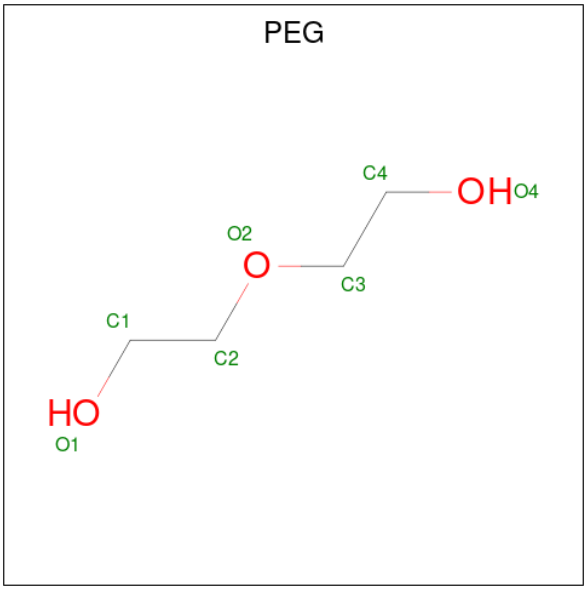
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
2	A	1	6	3	3		0	0
			Total	C	O			
2	A	1	6	3	3		0	0
			Total	C	O			
2	A	1	6	3	3		0	0
			Total	C	O			
2	A	1	6	3	3		0	0
			Total	C	O			
2	A	1	6	3	3		0	0
			Total	C	O			
2	A	1	6	3	3		0	0
			Total	C	O			
2	B	1	6	3	3		0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
3	A	1	7	4	3		0	0
			Total	C	O			
3	A	1	7	4	3		0	0
			Total	C	O			
3	A	1	7	4	3		0	0
			Total	C	O			
3	B	1	7	4	3		0	0

- Molecule 4 is water.

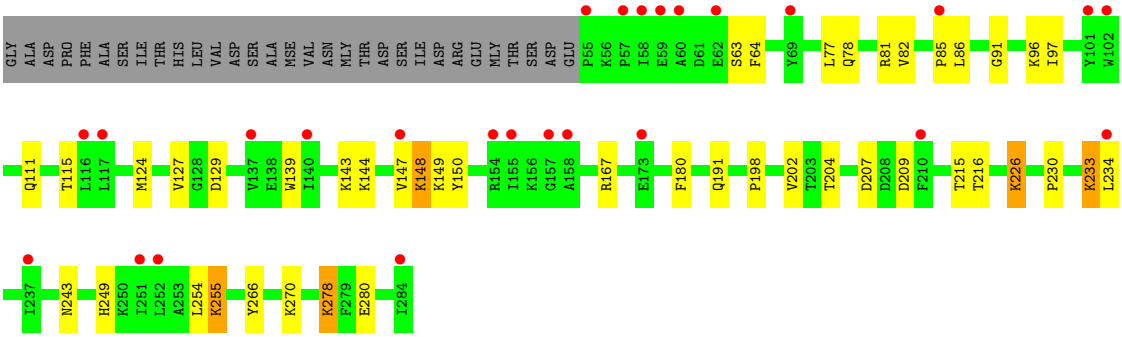
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	79	79	79	0	0
			Total	O		
4	B	79	79	79	0	1

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

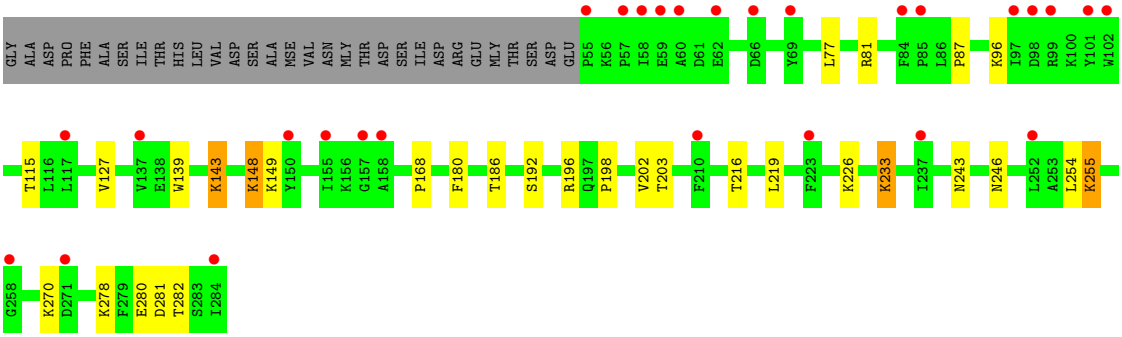
• Molecule 1: Hypothetical ntf2-like protein

Chain A:



• Molecule 1: Hypothetical ntf2-like protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	80.48Å 80.48Å 196.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.59 – 2.15 29.59 – 2.15	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.59-2.15) 99.9 (29.59-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 2.16Å)	Xtriage
Refinement program	BUSTER-TNT 2.8.0, BUSTER 2.8.0	Depositor
R, R_{free}	0.176 , 0.192 0.182 , 0.203	Depositor DCC
R_{free} test set	1951 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	46.0	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 60.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.064 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	4167	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MLY, GOL, PEG

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	0.52	1/1870 (0.1%)	0.61	0/2541
1	B	0.49	0/1936	0.63	0/2629
All	All	0.51	1/3806 (0.0%)	0.62	0/5170

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	124	MSE	SE-CE	-6.27	1.58	1.95

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1947	0	1824	30	0
1	B	1986	0	1864	16	0
2	A	42	0	56	9	0
2	B	6	0	8	0	0
3	A	21	0	30	2	0
3	B	7	0	10	0	0
4	A	79	0	0	1	0
4	B	79	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4167	0	3792	44	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 6.

All (44) 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:192:SER:HB2	1:B:219[B]:LEU:HD21	1.65	0.76
1:A:64:PHE:H	2:A:289:GOL:H12	1.55	0.71
1:A:85:PRO:HB2	1:A:96:MLY:HG3	1.73	0.69
1:A:115:THR:HG22	1:A:254:LEU:HD23	1.74	0.67
1:A:64:PHE:N	2:A:289:GOL:H12	2.14	0.62
1:B:115:THR:HG22	1:B:254:LEU:HD23	1.80	0.62
1:A:86:LEU:HB3	1:A:97:ILE:HG23	1.84	0.59
1:A:139:TRP:CE2	1:A:233:MLY:HH23	2.38	0.58
1:B:196:ARG:HH21	1:B:270:MLY:HH23	1.70	0.56
1:B:203:THR:HG22	1:B:281:ASP:HB3	1.86	0.55
1:B:280[B]:GLU:HG2	1:B:282:THR:HG23	1.88	0.54
1:B:77:LEU:O	1:B:81:ARG:HG2	2.09	0.53
1:A:167:ARG:HE	2:A:291:GOL:H12	1.74	0.53
1:B:143:MLY:HH23	1:B:186:THR:HG21	1.92	0.52
1:A:91:GLY:O	2:A:291:GOL:H2	2.11	0.51
1:B:87:PRO:HG3	1:B:96:MLY:HH11	1.92	0.51
1:A:198:PRO:HB2	1:A:216:THR:HB	1.93	0.50
1:B:198:PRO:HB2	1:B:216:THR:HB	1.92	0.50
1:A:147:VAL:HG21	2:A:285:GOL:H12	1.94	0.49
1:A:230:PRO:HB3	3:A:293:PEG:H22	1.96	0.48
1:A:249:HIS:HE1	4:A:338:HOH:O	1.97	0.47
1:A:127:VAL:HG11	1:A:255:MLY:HH11	1.96	0.46
1:A:204:THR:CG2	1:A:209:ASP:HA	2.45	0.46
1:A:202:VAL:HB	1:A:280[A]:GLU:HG2	1.96	0.45
1:A:78:GLN:O	1:A:82:VAL:HG23	2.17	0.45
1:A:129:ASP:O	2:A:289:GOL:H32	2.18	0.43
1:A:77:LEU:HD11	1:A:81:ARG:HH11	1.82	0.43
1:A:266:TYR:HB2	1:A:278:MLY:HB2	2.01	0.43
1:A:215:THR:HG21	1:B:168:PRO:HD3	2.01	0.42
1:A:230:PRO:HG2	1:A:234:LEU:HD23	2.02	0.42
1:A:148:MLY:HH13	1:A:150:TYR:OH	2.20	0.42
1:A:255:MLY:HH22	2:A:290:GOL:H2	2.02	0.42
1:A:77:LEU:O	1:A:81:ARG:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:VAL:HG11	1:B:255:MLY:HH11	2.01	0.42
1:B:139:TRP:CE2	1:B:233:MLY:HH23	2.55	0.42
1:A:191:GLN:OE1	1:A:226:MLY:HH12	2.20	0.41
1:A:63:SER:HB2	2:A:289:GOL:H11	2.02	0.41
1:A:111:GLN:HG2	3:A:293:PEG:H42	2.03	0.41
1:A:139:TRP:CE3	1:A:233:MLY:HD3	2.55	0.41
1:A:207:ASP:OD2	1:B:148:MLY:HH22	2.21	0.41
1:B:202:VAL:O	1:B:280[B]:GLU:HA	2.21	0.41
1:B:246[B]:ASN:ND2	4:B:335:HOH:O	2.54	0.41
1:A:167:ARG:NE	2:A:291:GOL:H12	2.35	0.40
1:B:96:MLY:HG3	1:B:96:MLY:HH12	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	217/261 (83%)	215 (99%)	2 (1%)	0	100	100
1	B	225/261 (86%)	222 (99%)	3 (1%)	0	100	100
All	All	442/522 (85%)	437 (99%)	5 (1%)	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	195/214 (91%)	193 (99%)	2 (1%)	76	81
1	B	201/214 (94%)	199 (99%)	2 (1%)	76	81
All	All	396/428 (92%)	392 (99%)	4 (1%)	73	81

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	180	PHE
1	A	243	ASN
1	B	180	PHE
1	B	243	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	243	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

30 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	B	226	1	9,10,11	1.17	1 (11%)	6,11,13	1.39	1 (16%)
1	MLY	A	156	1	7,8,11	0.56	0	3,8,13	0.70	0
1	MLY	B	96	1	9,10,11	0.79	0	6,11,13	0.91	0
1	MLY	B	149	1	9,10,11	0.84	0	6,11,13	2.62	4 (66%)
1	MLY	A	226	1	9,10,11	0.95	0	6,11,13	1.55	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	MLY	A	56	1	3,4,11	0.67	0	2,4,13	1.20	0
1	MLY	A	110	1	4,5,11	0.66	0	1,5,13	1.09	0
1	MLY	B	148	1	9,10,11	0.88	0	6,11,13	1.86	1 (16%)
1	MLY	A	144	1	9,10,11	1.16	1 (11%)	6,11,13	1.58	2 (33%)
1	MLY	A	148	1	9,10,11	0.93	1 (11%)	6,11,13	1.57	2 (33%)
1	MLY	A	255	1	9,10,11	0.83	0	6,11,13	1.31	1 (16%)
1	MLY	B	143	1	9,10,11	1.03	0	6,11,13	1.25	1 (16%)
1	MLY	A	278	1	9,10,11	0.96	0	6,11,13	1.46	1 (16%)
1	MLY	B	278	1	9,10,11	1.02	1 (11%)	6,11,13	1.30	1 (16%)
1	MLY	A	143	1	8,9,11	1.21	1 (12%)	4,9,13	0.99	0
1	MLY	B	100	1	3,4,11	0.75	0	2,4,13	1.35	0
1	MLY	A	233	1	9,10,11	1.10	1 (11%)	6,11,13	0.81	0
1	MLY	B	270	1	9,10,11	0.87	0	6,11,13	1.17	0
1	MLY	B	233	1	9,10,11	0.84	0	6,11,13	1.45	1 (16%)
1	MLY	A	270	1	9,10,11	0.75	0	6,11,13	1.72	2 (33%)
1	MLY	B	144	1	3,4,11	0.67	0	2,4,13	1.26	0
1	MLY	B	110	1	9,10,11	0.63	0	6,11,13	0.97	0
1	MLY	A	96	1	9,10,11	0.76	0	6,11,13	1.39	0
1	MLY	A	149	1	9,10,11	0.85	0	6,11,13	1.76	2 (33%)
1	MLY	B	156	1	3,4,11	0.80	0	2,4,13	1.06	0
1	MLY	B	103	1	3,4,11	0.82	0	2,4,13	1.23	0
1	MLY	B	255	1	9,10,11	0.92	0	6,11,13	1.38	1 (16%)
1	MLY	A	100	1	3,4,11	0.66	0	2,4,13	1.25	0
1	MLY	B	56	1	3,4,11	0.71	0	2,4,13	1.14	0
1	MLY	A	103	1	3,4,11	0.74	0	2,4,13	1.19	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
1	MLY	B	226	1	-	3/8/9/11	-
1	MLY	A	156	1	-	2/6/7/11	-
1	MLY	B	96	1	-	5/8/9/11	-
1	MLY	B	149	1	-	1/8/9/11	-
1	MLY	A	226	1	-	2/8/9/11	-
1	MLY	A	56	1	-	0/0/2/11	-
1	MLY	A	110	1	-	0/3/4/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	B	148	1	-	3/8/9/11	-
1	MLY	A	144	1	-	0/8/9/11	-
1	MLY	A	148	1	-	4/8/9/11	-
1	MLY	A	255	1	-	0/8/9/11	-
1	MLY	B	143	1	-	2/8/9/11	-
1	MLY	A	278	1	-	1/8/9/11	-
1	MLY	B	278	1	-	1/8/9/11	-
1	MLY	A	143	1	-	1/7/8/11	-
1	MLY	B	100	1	-	0/0/2/11	-
1	MLY	A	233	1	-	4/8/9/11	-
1	MLY	B	270	1	-	1/8/9/11	-
1	MLY	B	233	1	-	5/8/9/11	-
1	MLY	A	270	1	-	0/8/9/11	-
1	MLY	B	144	1	-	0/0/2/11	-
1	MLY	B	110	1	-	3/8/9/11	-
1	MLY	A	96	1	-	3/8/9/11	-
1	MLY	A	149	1	-	0/8/9/11	-
1	MLY	B	156	1	-	0/0/2/11	-
1	MLY	B	103	1	-	0/0/2/11	-
1	MLY	B	255	1	-	4/8/9/11	-
1	MLY	A	100	1	-	0/0/2/11	-
1	MLY	B	56	1	-	0/0/2/11	-
1	MLY	A	103	1	-	0/0/2/11	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	144	MLY	CH2-NZ	2.83	1.54	1.46
1	A	233	MLY	CB-CA	2.75	1.57	1.53
1	A	143	MLY	CB-CA	2.66	1.57	1.53
1	B	278	MLY	CH2-NZ	2.23	1.53	1.46
1	A	148	MLY	CB-CA	-2.10	1.50	1.53
1	B	226	MLY	CH2-NZ	2.07	1.52	1.46

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	149	MLY	CH1-NZ-CE	-4.30	93.72	110.74
1	B	148	MLY	CH2-NZ-CH1	-3.80	99.91	109.73
1	A	226	MLY	CH2-NZ-CH1	-3.41	100.91	109.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	149	MLY	CD-CG-CB	-3.01	102.99	113.62
1	A	255	MLY	CD-CE-NZ	-2.95	105.79	113.79
1	B	149	MLY	CD-CG-CB	-2.86	103.51	113.62
1	B	255	MLY	CD-CE-NZ	-2.76	106.33	113.79
1	A	270	MLY	CH2-NZ-CE	-2.71	99.98	110.74
1	B	226	MLY	CH2-NZ-CE	2.64	121.22	110.74
1	B	233	MLY	CD-CG-CB	-2.50	104.78	113.62
1	A	278	MLY	CD-CG-CB	-2.49	104.81	113.62
1	A	144	MLY	CH2-NZ-CH1	-2.48	103.32	109.73
1	A	270	MLY	CH2-NZ-CH1	-2.46	103.37	109.73
1	B	143	MLY	CH2-NZ-CH1	-2.41	103.50	109.73
1	A	148	MLY	CD-CG-CB	-2.40	105.14	113.62
1	A	148	MLY	CH1-NZ-CE	-2.38	101.33	110.74
1	B	149	MLY	CH2-NZ-CH1	-2.28	103.84	109.73
1	B	278	MLY	CD-CG-CB	-2.21	105.80	113.62
1	A	144	MLY	CD-CG-CB	-2.11	106.14	113.62
1	A	149	MLY	CH2-NZ-CH1	2.09	115.12	109.73
1	B	149	MLY	CD-CE-NZ	2.04	119.30	113.79

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	96	MLY	N-CA-CB-CG
1	A	96	MLY	C-CA-CB-CG
1	A	226	MLY	O-C-CA-CB
1	A	278	MLY	O-C-CA-CB
1	B	96	MLY	C-CA-CB-CG
1	B	233	MLY	C-CA-CB-CG
1	B	278	MLY	O-C-CA-CB
1	B	255	MLY	CE-CD-CG-CB
1	B	143	MLY	CD-CE-NZ-CH1
1	B	148	MLY	CD-CE-NZ-CH1
1	B	226	MLY	CD-CE-NZ-CH2
1	B	233	MLY	CD-CE-NZ-CH2
1	A	143	MLY	CD-CE-NZ-CH1
1	A	233	MLY	CD-CE-NZ-CH2
1	B	148	MLY	CD-CE-NZ-CH2
1	B	226	MLY	CD-CE-NZ-CH1
1	A	96	MLY	CA-CB-CG-CD
1	B	96	MLY	CA-CB-CG-CD
1	B	96	MLY	CD-CE-NZ-CH2

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Mol	Chain	Res	Type	Atoms
1	B	255	MLY	CA-CB-CG-CD
1	A	148	MLY	CG-CD-CE-NZ
1	B	143	MLY	CD-CE-NZ-CH2
1	B	233	MLY	CD-CE-NZ-CH1
1	B	149	MLY	CD-CE-NZ-CH2
1	A	148	MLY	CE-CD-CG-CB
1	A	233	MLY	CD-CE-NZ-CH1
1	A	226	MLY	CG-CD-CE-NZ
1	B	110	MLY	CA-CB-CG-CD
1	B	226	MLY	CG-CD-CE-NZ
1	A	156	MLY	CA-CB-CG-CD
1	B	270	MLY	CG-CD-CE-NZ
1	B	233	MLY	CE-CD-CG-CB
1	A	156	MLY	CE-CD-CG-CB
1	A	148	MLY	CD-CE-NZ-CH2
1	B	255	MLY	CG-CD-CE-NZ
1	B	233	MLY	N-CA-CB-CG
1	B	255	MLY	N-CA-CB-CG
1	A	233	MLY	CG-CD-CE-NZ
1	B	148	MLY	CE-CD-CG-CB
1	B	96	MLY	CD-CE-NZ-CH1
1	B	96	MLY	CE-CD-CG-CB
1	A	148	MLY	CA-CB-CG-CD
1	B	110	MLY	CG-CD-CE-NZ
1	A	233	MLY	CE-CD-CG-CB
1	B	110	MLY	CE-CD-CG-CB

There are no ring outliers.

12 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	96	MLY	2	0
1	A	226	MLY	1	0
1	B	148	MLY	1	0
1	A	148	MLY	1	0
1	A	255	MLY	2	0
1	B	143	MLY	1	0
1	A	278	MLY	1	0
1	A	233	MLY	2	0
1	B	270	MLY	1	0
1	B	233	MLY	1	0
1	A	96	MLY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	255	MLY	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 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	285	-	5,5,5	0.99	0	5,5,5	0.97	0
2	GOL	A	290	-	5,5,5	0.69	0	5,5,5	0.77	0
2	GOL	A	288	-	5,5,5	0.75	0	5,5,5	0.71	0
2	GOL	A	289	-	5,5,5	0.64	0	5,5,5	1.51	1 (20%)
2	GOL	B	286	-	5,5,5	0.59	0	5,5,5	0.83	0
2	GOL	A	291	-	5,5,5	0.60	0	5,5,5	1.12	0
3	PEG	B	296	-	6,6,6	0.67	0	5,5,5	0.53	0
3	PEG	A	293	-	6,6,6	0.35	0	5,5,5	0.39	0
2	GOL	A	292	-	5,5,5	0.56	0	5,5,5	0.77	0
2	GOL	A	287	-	5,5,5	0.76	0	5,5,5	0.66	0
3	PEG	A	294	-	6,6,6	0.58	0	5,5,5	0.48	0
3	PEG	A	295	-	6,6,6	0.16	0	5,5,5	0.18	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	285	-	-	2/4/4/4	-
2	GOL	A	290	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	288	-	-	2/4/4/4	-
2	GOL	A	289	-	-	2/4/4/4	-
2	GOL	B	286	-	-	2/4/4/4	-
2	GOL	A	291	-	-	3/4/4/4	-
3	PEG	B	296	-	-	3/4/4/4	-
3	PEG	A	293	-	-	2/4/4/4	-
2	GOL	A	292	-	-	2/4/4/4	-
2	GOL	A	287	-	-	0/4/4/4	-
3	PEG	A	294	-	-	2/4/4/4	-
3	PEG	A	295	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	289	GOL	O2-C2-C3	2.45	119.89	109.12

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	285	GOL	O1-C1-C2-O2
2	A	285	GOL	O1-C1-C2-C3
2	A	289	GOL	C1-C2-C3-O3
2	A	290	GOL	O1-C1-C2-C3
2	A	291	GOL	O1-C1-C2-C3
2	A	292	GOL	O1-C1-C2-C3
2	B	286	GOL	O1-C1-C2-C3
2	A	292	GOL	O1-C1-C2-O2
3	B	296	PEG	O2-C3-C4-O4
2	A	288	GOL	C1-C2-C3-O3
2	A	289	GOL	O2-C2-C3-O3
2	A	290	GOL	O1-C1-C2-O2
2	A	291	GOL	O1-C1-C2-O2
3	A	293	PEG	O2-C3-C4-O4
3	A	294	PEG	O1-C1-C2-O2
2	B	286	GOL	O1-C1-C2-O2
3	B	296	PEG	C4-C3-O2-C2
2	A	288	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	B	296	PEG	C1-C2-O2-C3
3	A	293	PEG	C4-C3-O2-C2
3	A	294	PEG	C4-C3-O2-C2
2	A	291	GOL	C1-C2-C3-O3
2	A	290	GOL	C1-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	285	GOL	1	0
2	A	290	GOL	1	0
2	A	289	GOL	4	0
2	A	291	GOL	3	0
3	A	293	PEG	2	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	212/261 (81%)	0.58	26 (12%)	4	5	33, 60, 101, 130	0
1	B	212/261 (81%)	0.71	28 (13%)	3	4	32, 61, 126, 155	0
All	All	424/522 (81%)	0.64	54 (12%)	3	5	32, 61, 115, 155	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	101	TYR	11.6
1	B	101	TYR	11.0
1	A	210	PHE	6.6
1	B	55	PRO	5.9
1	B	59	GLU	5.8
1	B	158	ALA	5.6
1	A	55	PRO	5.5
1	B	60	ALA	5.3
1	B	57	PRO	5.3
1	A	57	PRO	5.1
1	B	85	PRO	4.9
1	B	97	ILE	4.7
1	A	284	ILE	4.4
1	A	60	ALA	4.3
1	A	155	ILE	4.3
1	A	69	TYR	4.2
1	B	157	GLY	4.2
1	A	62[A]	GLU	3.7
1	A	102	TRP	3.7
1	B	98	ASP	3.5
1	B	155	ILE	3.5
1	B	137	VAL	3.4
1	B	271	ASP	3.4
1	A	58	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	252	LEU	3.2
1	B	284	ILE	3.2
1	B	69	TYR	3.1
1	B	84	PHE	3.0
1	B	252	LEU	2.9
1	A	234	LEU	2.8
1	B	258	GLY	2.8
1	B	62	GLU	2.8
1	A	140	ILE	2.8
1	A	147	VAL	2.7
1	B	99	ARG	2.7
1	A	237	ILE	2.6
1	A	116	LEU	2.6
1	B	210	PHE	2.6
1	A	117	LEU	2.6
1	A	85	PRO	2.5
1	B	58	ILE	2.4
1	A	137	VAL	2.4
1	B	66[A]	ASP	2.4
1	A	251	ILE	2.3
1	B	237	ILE	2.2
1	A	154	ARG	2.2
1	B	102	TRP	2.1
1	B	117[A]	LEU	2.1
1	A	173	GLU	2.1
1	A	157	GLY	2.1
1	A	158	ALA	2.1
1	B	150	TYR	2.1
1	A	59	GLU	2.0
1	B	223	PHE	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	MLY	B	270	11/12	0.85	0.41	58,70,79,81	0
1	MLY	A	100	5/12	0.86	0.38	119,122,125,126	0
1	MLY	B	56	5/12	0.86	0.33	153,156,158,162	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	MLY	A	56	5/12	0.86	0.35	128,130,131,135	0
1	MLY	A	96	11/12	0.87	0.26	95,105,108,109	0
1	MLY	B	143	11/12	0.88	0.28	65,74,86,89	0
1	MLY	B	100	5/12	0.89	0.43	127,129,130,133	0
1	MLY	B	96	11/12	0.90	0.28	101,108,111,113	0
1	MLY	B	156	5/12	0.91	0.30	105,109,114,115	0
1	MLY	B	110	11/12	0.91	0.35	81,87,104,107	0
1	MLY	A	149	11/12	0.92	0.21	55,60,66,67	0
1	MLY	A	156	9/12	0.92	0.36	93,100,112,115	0
1	MLY	A	143	10/12	0.92	0.14	49,56,72,72	0
1	MLY	A	110	6/12	0.93	0.27	81,83,85,89	0
1	MLY	A	226	11/12	0.94	0.13	52,53,67,69	0
1	MLY	B	148	11/12	0.94	0.22	52,57,69,71	0
1	MLY	A	270	11/12	0.94	0.15	45,54,69,70	0
1	MLY	B	226	11/12	0.94	0.12	49,51,65,68	0
1	MLY	A	103	5/12	0.94	0.13	91,94,96,96	0
1	MLY	A	144	11/12	0.95	0.09	46,47,52,55	0
1	MLY	A	233	11/12	0.95	0.12	51,54,62,62	0
1	MLY	B	103	5/12	0.95	0.13	100,104,105,106	0
1	MLY	B	149	11/12	0.96	0.18	56,59,63,63	0
1	MLY	B	255	11/12	0.96	0.11	45,51,65,65	0
1	MLY	A	255	11/12	0.96	0.10	47,52,63,64	0
1	MLY	A	148	11/12	0.97	0.20	48,55,69,71	0
1	MLY	A	278	11/12	0.97	0.12	34,35,38,39	0
1	MLY	B	144	5/12	0.97	0.09	66,66,67,69	0
1	MLY	B	233	11/12	0.98	0.12	54,59,66,67	0
1	MLY	B	278	11/12	0.98	0.16	35,36,36,38	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PEG	A	294	7/7	0.45	0.28	96,97,98,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PEG	A	293	7/7	0.52	0.39	95,97,98,99	0
2	GOL	B	286	6/6	0.55	0.24	90,91,91,92	0
2	GOL	A	290	6/6	0.62	0.28	83,85,86,87	0
2	GOL	A	291	6/6	0.74	0.32	94,95,95,96	0
2	GOL	A	287	6/6	0.76	0.19	73,76,77,77	0
2	GOL	A	285	6/6	0.76	0.44	81,83,84,84	0
2	GOL	A	288	6/6	0.79	0.20	96,96,97,97	0
3	PEG	A	295	7/7	0.79	0.34	101,102,105,105	0
3	PEG	B	296	7/7	0.81	0.19	83,85,86,86	0
2	GOL	A	292	6/6	0.85	0.37	90,92,93,93	0
2	GOL	A	289	6/6	0.91	0.23	76,76,77,78	0

6.5 Other polymers (i)

There are no such residues in this entry.