Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 11:51 am BST

PDB ID	:	5JMF
Title	:	Heparinase III-BT4657 gene product
Authors	:	Ulaganathan, T.S.; Shi, R.; Yao, D.; Garron, M.-L.; Cherney, M.; Cygler, M.
Deposited on	:	2016-04-28
Resolution	:	1.85 Å(reported)

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

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

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

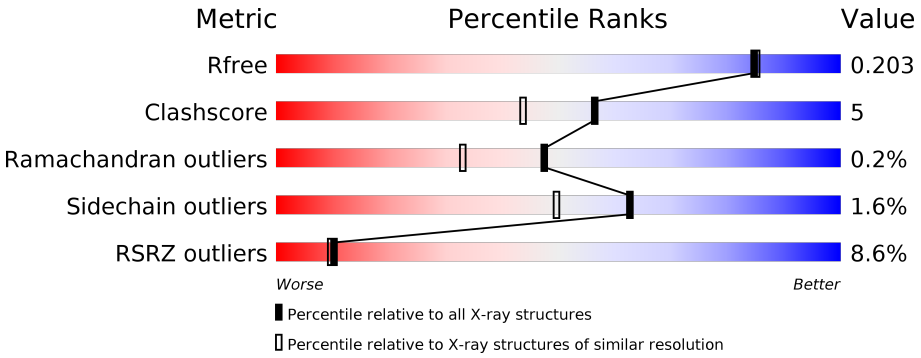
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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

Mol	Chain	Length	Quality of chain
1	A	655	8% 89% 8% .

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5829 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.

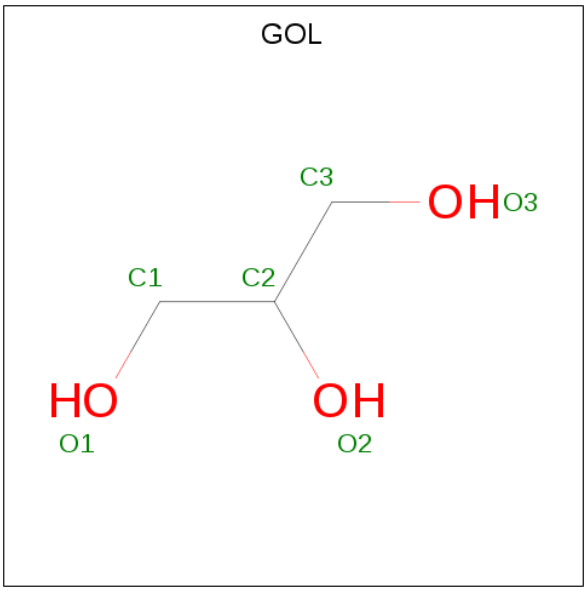
- Molecule 1 is a protein called Heparinase III protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	638	Total	C	N	O	S	15	9	0
			5278	3402	882	969	25			

There are 11 discrepancies between the modelled and reference sequences:

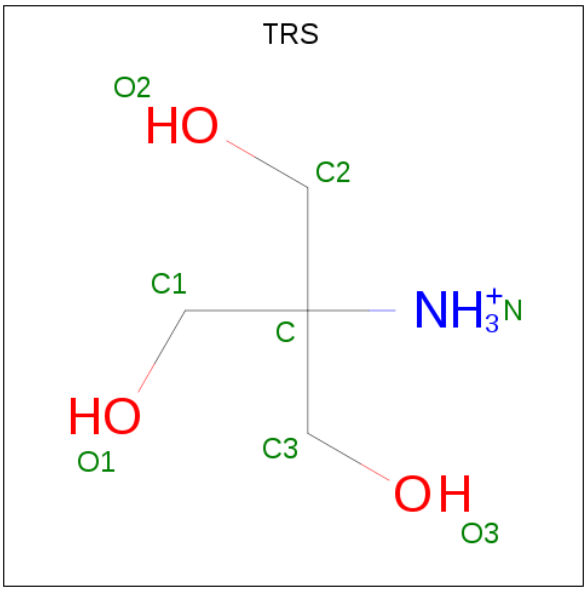
Chain	Residue	Modelled	Actual	Comment	Reference
A	12	SER	-	expression tag	UNP Q89YS4
A	13	ASP	-	expression tag	UNP Q89YS4
A	14	SER	-	expression tag	UNP Q89YS4
A	15	GLU	-	expression tag	UNP Q89YS4
A	16	ASN	-	expression tag	UNP Q89YS4
A	17	LEU	-	expression tag	UNP Q89YS4
A	18	TYR	-	expression tag	UNP Q89YS4
A	19	PHE	-	expression tag	UNP Q89YS4
A	20	GLN	-	expression tag	UNP Q89YS4
A	21	GLY	-	expression tag	UNP Q89YS4
A	22	SER	-	expression tag	UNP Q89YS4

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



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

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0

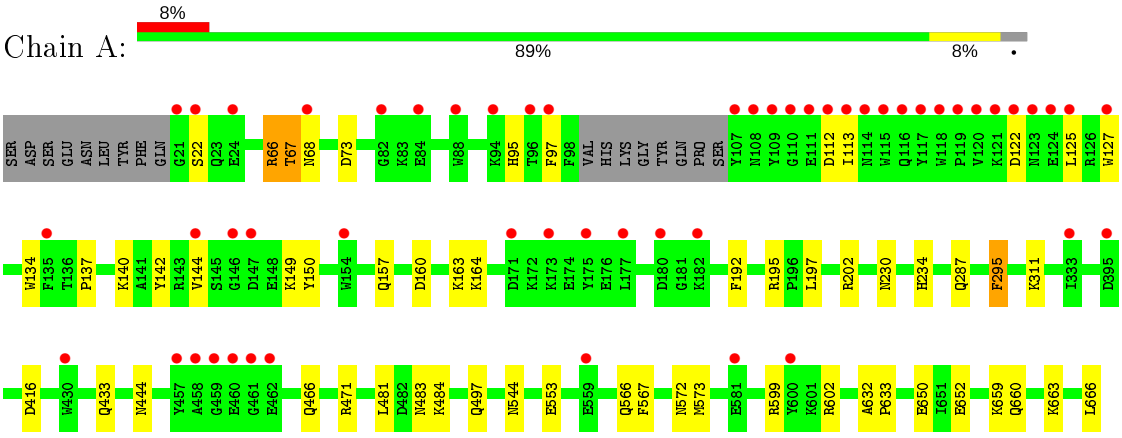
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	536	Total O 536 536	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: Heparinase III protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	186.69Å 45.74Å 80.51Å 90.00° 94.05° 90.00°	Depositor
Resolution (Å)	20.50 – 1.85 20.50 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.50-1.85) 92.3 (20.50-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.75 (at 1.85Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.165 , 0.203 0.165 , 0.203	Depositor DCC
R_{free} test set	2904 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	26.3	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 59.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5829	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.50	0/5157	0.58	1/7001 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	66	ARG	C-N-CA	6.13	137.01	121.70

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	5278	0	5049	51	0
2	A	6	0	8	0	0
3	A	8	0	12	1	0
4	A	1	0	0	0	0
5	A	536	0	0	4	1
All	All	5829	0	5069	52	1

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 (52) 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:202:ARG:HE	1:A:234:HIS:HE1	1.16	0.89
1:A:567:PHE:H	1:A:572:ASN:HD21	1.32	0.78
1:A:134:TRP:HE1	1:A:157:GLN:HE22	1.36	0.74
1:A:202:ARG:HE	1:A:234:HIS:CE1	2.05	0.73
1:A:287:GLN:HG2	1:A:295:PHE:HE1	1.54	0.73
1:A:67:THR:HG23	1:A:68:ASN:H	1.53	0.71
1:A:287:GLN:HG2	1:A:295:PHE:CE1	2.25	0.71
1:A:66:ARG:HG3	1:A:67:THR:HG22	1.75	0.68
1:A:466:GLN:HE21	1:A:599:ARG:HH12	1.43	0.66
1:A:666:LEU:O	5:A:801:HOH:O	2.15	0.65
1:A:67:THR:HG23	1:A:68:ASN:N	2.12	0.64
1:A:66:ARG:HA	1:A:67:THR:HB	1.79	0.63
1:A:230:ASN:O	1:A:234:HIS:HD2	1.84	0.61
1:A:202:ARG:NE	1:A:234:HIS:HE1	1.96	0.59
1:A:67:THR:HG21	5:A:1249:HOH:O	2.03	0.58
1:A:112:ASP:OD1	1:A:164:LYS:NZ	2.37	0.57
1:A:160:ASP:OD2	1:A:164:LYS:HE2	2.03	0.57
1:A:466:GLN:NE2	1:A:599:ARG:HH12	2.02	0.57
1:A:134:TRP:HE1	1:A:157:GLN:NE2	2.03	0.56
1:A:22:SER:HB3	1:A:163:LYS:NZ	2.21	0.56
1:A:567:PHE:H	1:A:572:ASN:ND2	2.04	0.54
1:A:66:ARG:CG	1:A:67:THR:HG22	2.38	0.54
1:A:466:GLN:HE21	1:A:599:ARG:NH1	2.04	0.53
1:A:650:GLU:HG3	1:A:663:MLY:HB2	1.91	0.52
3:A:702:TRS:H12	5:A:904:HOH:O	2.10	0.52
1:A:67:THR:CG2	1:A:68:ASN:H	2.20	0.52
1:A:66:ARG:HA	1:A:67:THR:CB	2.40	0.51
1:A:416:ASP:HA	1:A:444:ASN:HD22	1.76	0.51
1:A:483:ASN:ND2	5:A:814:HOH:O	2.45	0.49
1:A:140:MLY:O	1:A:144:VAL:HG22	2.14	0.48
1:A:142:TYR:HB2	1:A:150:TYR:HB2	1.95	0.48
1:A:481:LEU:HD23	1:A:484:MLY:HH22	1.94	0.48
1:A:202:ARG:HH21	1:A:234:HIS:CE1	2.32	0.47
1:A:466:GLN:NE2	1:A:599:ARG:HH22	2.13	0.47
1:A:97:PHE:HB3	1:A:134:TRP:CZ3	2.50	0.47
1:A:433:GLN:HG2	1:A:471:ARG:HG2	1.97	0.46
1:A:311:MLY:HD2	1:A:311:MLY:HH12	1.81	0.46
1:A:553:GLU:HG2	1:A:566:GLN:HB2	1.99	0.45
1:A:67:THR:CG2	1:A:68:ASN:N	2.78	0.44
1:A:95:HIS:HA	1:A:97:PHE:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ILE:HD11	1:A:157:GLN:HG2	2.00	0.43
1:A:295:PHE:HD1	1:A:295:PHE:H	1.68	0.42
1:A:134:TRP:HA	1:A:137:PRO:HG2	2.02	0.42
1:A:632:ALA:HA	1:A:633:PRO:HD3	1.80	0.42
1:A:67:THR:HG23	1:A:68:ASN:OD1	2.20	0.41
1:A:195:ARG:NH2	1:A:197:LEU:HD23	2.35	0.41
1:A:567:PHE:N	1:A:572:ASN:HD21	2.08	0.41
1:A:66:ARG:HA	1:A:67:THR:HG22	2.01	0.41
1:A:127:TRP:CD1	1:A:192:PHE:HA	2.56	0.41
1:A:122:ASP:HB3	1:A:125:LEU:HB3	2.02	0.40
1:A:663:MLY:HH23	1:A:663:MLY:HD2	1.83	0.40
1:A:652:GLU:OE2	1:A:659:LYS:HD3	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1099:HOH:O	5:A:1108:HOH:O[4_546]	2.12	0.08

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	618/655 (94%)	598 (97%)	19 (3%)	1 (0%)	47 33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	THR

5.3.2 Protein sidechains

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	525/554 (95%)	516 (98%)	9 (2%)	60 47

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

Mol	Chain	Res	Type
1	A	73	ASP
1	A	149	LYS
1	A	295	PHE
1	A	497	GLN
1	A	544	ASN
1	A	573	MET
1	A	602	ARG
1	A	660[A]	GLN
1	A	660[B]	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	123	ASN
1	A	157	GLN
1	A	234	HIS
1	A	444	ASN
1	A	466	GLN
1	A	572	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

25 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	26	1	9,10,11	0.70	0	6,11,13	0.73	0
1	MLY	A	274	1	9,10,11	0.77	0	6,11,13	0.64	0
1	MLY	A	610	1	9,10,11	0.76	0	6,11,13	0.75	0
1	MLY	A	587	1	9,10,11	0.62	0	6,11,13	0.73	0
1	MLY	A	361	1	9,10,11	0.67	0	6,11,13	0.79	0
1	MLY	A	399	1	9,10,11	0.71	0	6,11,13	0.60	0
1	MLY	A	663	1	9,10,11	0.74	0	6,11,13	0.87	0
1	MLY	A	335	1	9,10,11	0.74	0	6,11,13	0.78	0
1	MLY	A	658	1,2	9,10,11	0.72	0	6,11,13	0.71	0
1	MLY	A	57	1	9,10,11	0.60	0	6,11,13	0.74	0
1	MLY	A	628	1	9,10,11	0.66	0	6,11,13	0.75	0
1	MLY	A	627	1	9,10,11	0.78	0	6,11,13	0.74	0
1	MLY	A	484	1	9,10,11	0.58	0	6,11,13	0.81	0
1	MLY	A	267	1	9,10,11	0.63	0	6,11,13	0.90	0
1	MLY	A	311	1	9,10,11	0.69	0	6,11,13	0.61	0
1	MLY	A	389	1	9,10,11	0.95	0	6,11,13	0.99	0
1	MLY	A	140	1	9,10,11	0.75	0	6,11,13	0.81	0
1	MLY	A	540	1	9,10,11	0.63	0	6,11,13	0.63	0
1	MLY	A	377	1	9,10,11	0.55	0	6,11,13	1.10	0
1	MLY	A	574	1	9,10,11	0.88	0	6,11,13	1.23	1 (16%)
1	MLY	A	654	1	9,10,11	1.09	1 (11%)	6,11,13	0.76	0
1	MLY	A	44	1	9,10,11	0.75	0	6,11,13	0.83	0
1	MLY	A	382	1	9,10,11	0.83	0	6,11,13	0.95	0
1	MLY	A	494	1	9,10,11	0.65	0	6,11,13	0.95	0
1	MLY	A	634	1	9,10,11	0.67	0	6,11,13	0.59	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	A	26	1	-	2/8/9/11	-
1	MLY	A	274	1	-	0/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	610	1	-	0/8/9/11	-
1	MLY	A	587	1	-	2/8/9/11	-
1	MLY	A	361	1	-	1/8/9/11	-
1	MLY	A	399	1	-	1/8/9/11	-
1	MLY	A	663	1	-	0/8/9/11	-
1	MLY	A	335	1	-	1/8/9/11	-
1	MLY	A	658	1,2	-	3/8/9/11	-
1	MLY	A	57	1	-	1/8/9/11	-
1	MLY	A	628	1	-	0/8/9/11	-
1	MLY	A	627	1	-	2/8/9/11	-
1	MLY	A	484	1	-	2/8/9/11	-
1	MLY	A	267	1	-	1/8/9/11	-
1	MLY	A	311	1	-	2/8/9/11	-
1	MLY	A	389	1	-	2/8/9/11	-
1	MLY	A	140	1	-	0/8/9/11	-
1	MLY	A	540	1	-	0/8/9/11	-
1	MLY	A	377	1	-	1/8/9/11	-
1	MLY	A	574	1	-	0/8/9/11	-
1	MLY	A	654	1	-	0/8/9/11	-
1	MLY	A	44	1	-	0/8/9/11	-
1	MLY	A	382	1	-	0/8/9/11	-
1	MLY	A	494	1	-	0/8/9/11	-
1	MLY	A	634	1	-	0/8/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	654	MLY	CE-NZ	2.29	1.54	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	574	MLY	CH2-NZ-CH1	-2.20	104.04	109.73

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	484	MLY	O-C-CA-CB
1	A	389	MLY	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
1	A	627	MLY	CD-CE-NZ-CH1
1	A	658	MLY	CD-CE-NZ-CH1
1	A	658	MLY	CD-CE-NZ-CH2
1	A	311	MLY	CG-CD-CE-NZ
1	A	26	MLY	CG-CD-CE-NZ
1	A	658	MLY	CA-CB-CG-CD
1	A	627	MLY	CD-CE-NZ-CH2
1	A	389	MLY	CD-CE-NZ-CH1
1	A	587	MLY	CG-CD-CE-NZ
1	A	361	MLY	CD-CE-NZ-CH1
1	A	399	MLY	CD-CE-NZ-CH1
1	A	267	MLY	CD-CE-NZ-CH1
1	A	377	MLY	CD-CE-NZ-CH1
1	A	57	MLY	CA-CB-CG-CD
1	A	311	MLY	CD-CE-NZ-CH1
1	A	484	MLY	CD-CE-NZ-CH1
1	A	26	MLY	CD-CE-NZ-CH2
1	A	587	MLY	CE-CD-CG-CB
1	A	335	MLY	C-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	663	MLY	2	0
1	A	484	MLY	1	0
1	A	311	MLY	1	0
1	A	140	MLY	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	TRS	A	702	-	7,7,7	0.21	0	9,9,9	0.62	0
2	GOL	A	701	1	5,5,5	0.37	0	5,5,5	0.50	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
3	TRS	A	702	-	-	6/9/9/9	-
2	GOL	A	701	1	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	TRS	C2-C-C3-O3
3	A	702	TRS	N-C-C3-O3
2	A	701	GOL	O1-C1-C2-O2
2	A	701	GOL	O1-C1-C2-C3
3	A	702	TRS	C1-C-C3-O3
3	A	702	TRS	C1-C-C2-O2
3	A	702	TRS	C3-C-C2-O2
3	A	702	TRS	N-C-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	TRS	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	613/655 (93%)	0.21	53 (8%)	10	10	20, 35, 85, 141	6 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	120	VAL	12.0
1	A	118	TRP	10.8
1	A	121	LYS	6.9
1	A	109	TYR	6.8
1	A	119	PRO	6.7
1	A	108	ASN	6.6
1	A	112	ASP	6.2
1	A	107	TYR	6.0
1	A	111	GLU	5.8
1	A	116	GLN	5.8
1	A	96	THR	5.5
1	A	113	ILE	5.2
1	A	117	TYR	4.8
1	A	115	TRP	4.0
1	A	110	GLY	3.9
1	A	97	PHE	3.8
1	A	68	ASN	3.7
1	A	171	ASP	3.5
1	A	459	GLY	3.5
1	A	180	ASP	3.4
1	A	430	TRP	3.4
1	A	21	GLY	3.3
1	A	146	GLY	3.3
1	A	144	VAL	3.3
1	A	177	LEU	3.1
1	A	559	GLU	3.0
1	A	600[A]	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	457	TYR	2.9
1	A	461	GLY	2.9
1	A	24	GLU	2.8
1	A	88	TRP	2.8
1	A	458	ALA	2.6
1	A	84	GLU	2.6
1	A	182	LYS	2.5
1	A	114	ASN	2.5
1	A	460	GLU	2.5
1	A	82	GLY	2.5
1	A	135	PHE	2.5
1	A	175	TYR	2.4
1	A	123	ASN	2.4
1	A	124	GLU	2.4
1	A	462	GLU	2.4
1	A	122	ASP	2.4
1	A	125	LEU	2.4
1	A	147	ASP	2.4
1	A	127	TRP	2.3
1	A	154	TRP	2.3
1	A	94	LYS	2.3
1	A	173	LYS	2.2
1	A	581	GLU	2.2
1	A	22	SER	2.1
1	A	395[A]	ASP	2.1
1	A	333	ILE	2.1

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	MLY	A	140	11/12	0.85	0.15	49,53,58,61	0
1	MLY	A	57	11/12	0.88	0.18	30,36,59,61	0
1	MLY	A	610	11/12	0.89	0.16	34,47,63,65	0
1	MLY	A	540	11/12	0.89	0.15	46,50,64,67	0
1	MLY	A	627	11/12	0.91	0.17	24,31,51,52	0
1	MLY	A	311	11/12	0.91	0.14	26,31,61,62	0
1	MLY	A	587	11/12	0.91	0.14	39,44,53,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	MLY	A	26	11/12	0.91	0.15	34,41,60,61	0
1	MLY	A	335	11/12	0.92	0.12	22,29,53,53	0
1	MLY	A	663	11/12	0.92	0.14	35,38,60,61	0
1	MLY	A	658	11/12	0.93	0.14	33,44,79,91	0
1	MLY	A	628	11/12	0.93	0.12	28,32,54,55	0
1	MLY	A	274	11/12	0.94	0.12	24,27,41,42	0
1	MLY	A	389	11/12	0.94	0.13	28,31,50,51	0
1	MLY	A	377	11/12	0.94	0.15	26,37,62,64	0
1	MLY	A	574	11/12	0.94	0.16	21,24,44,51	0
1	MLY	A	654	11/12	0.94	0.13	29,32,49,52	0
1	MLY	A	382	11/12	0.94	0.12	22,28,58,58	0
1	MLY	A	267	11/12	0.96	0.09	20,23,42,43	0
1	MLY	A	361	11/12	0.96	0.08	27,32,46,46	0
1	MLY	A	484	11/12	0.96	0.09	34,37,52,52	0
1	MLY	A	634	11/12	0.96	0.07	28,31,40,42	0
1	MLY	A	494	11/12	0.97	0.09	25,28,53,55	0
1	MLY	A	399	11/12	0.97	0.08	19,22,39,42	0
1	MLY	A	44	11/12	0.98	0.12	21,24,30,33	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(Å^2)	Q<0.9
3	TRS	A	702	8/8	0.72	0.18	59,62,65,66	0
2	GOL	A	701	6/6	0.75	0.33	58,63,63,64	0
4	MG	A	703	1/1	1.00	0.04	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.