Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:28 pm BST

PDB ID	:	2VIX
Title	:	Methylated Shigella flexneri MxiC
Authors	:	Deane, J.E.; Roversi, P.; King, C.; Johnson, S.; Lea, S.M.
Deposited on	:	2007-12-05
Resolution	:	2.85 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:

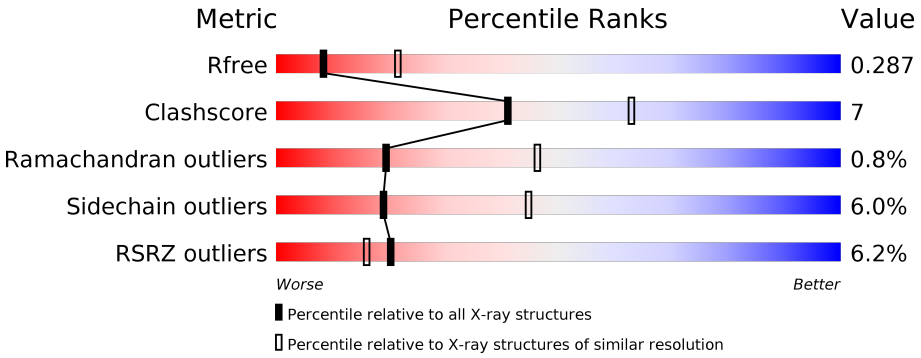
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	294	6% 83% 12%
1	B	294	3% 76% 18%
1	C	294	8% 72% 21%

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	132	-	-	-	X
1	MLY	B	132	-	-	-	X
1	MLY	B	98	-	-	-	X
1	MLY	C	132	-	-	-	X
1	MLY	C	269	-	-	-	X
1	MLY	C	329	-	-	-	X
1	MLY	C	350	-	-	-	X
1	MLY	C	351	-	-	-	X
2	ACT	A	1356	-	-	-	X
3	GOL	B	1356	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7117 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 PROTEIN MXIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2325	1489	381	447	8			
1	B	283	Total	C	N	O	S	0	0	0
			2325	1489	381	447	8			
1	C	281	Total	C	N	O	S	0	1	0
			2317	1487	378	444	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	HIS	-	expression tag	UNP Q04640
A	63	SER	-	expression tag	UNP Q04640
A	64	SER	-	expression tag	UNP Q04640
A	65	GLY	-	expression tag	UNP Q04640
A	66	LEU	-	expression tag	UNP Q04640
A	67	VAL	-	expression tag	UNP Q04640
A	68	PRO	-	expression tag	UNP Q04640
A	69	ARG	-	expression tag	UNP Q04640
A	70	GLY	-	expression tag	UNP Q04640
A	71	SER	-	expression tag	UNP Q04640
A	72	HIS	-	expression tag	UNP Q04640
A	73	MET	-	expression tag	UNP Q04640
B	62	HIS	-	expression tag	UNP Q04640
B	63	SER	-	expression tag	UNP Q04640
B	64	SER	-	expression tag	UNP Q04640
B	65	GLY	-	expression tag	UNP Q04640
B	66	LEU	-	expression tag	UNP Q04640
B	67	VAL	-	expression tag	UNP Q04640
B	68	PRO	-	expression tag	UNP Q04640
B	69	ARG	-	expression tag	UNP Q04640
B	70	GLY	-	expression tag	UNP Q04640
B	71	SER	-	expression tag	UNP Q04640
B	72	HIS	-	expression tag	UNP Q04640

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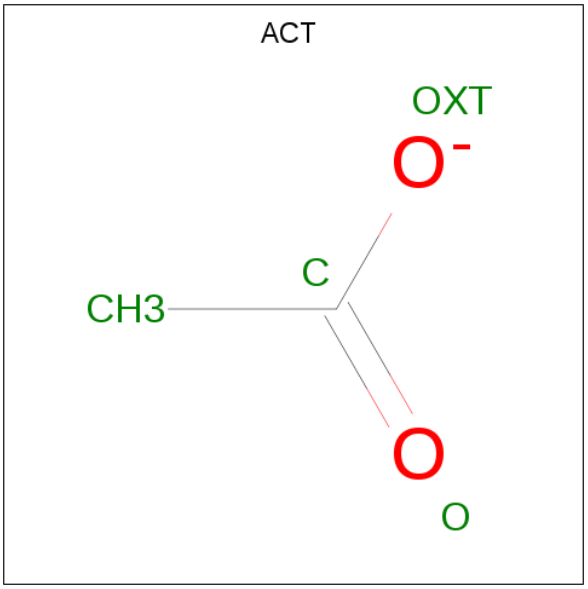
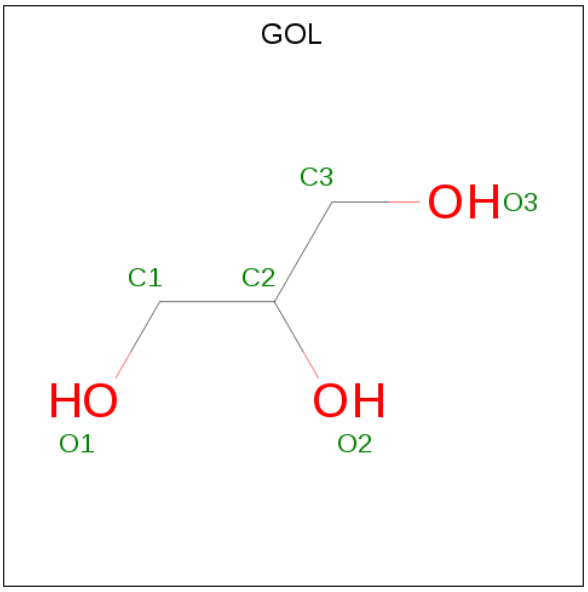
Chain	Residue	Modelled	Actual	Comment	Reference
B	73	MET	-	expression tag	UNP Q04640
C	62	HIS	-	expression tag	UNP Q04640
C	63	SER	-	expression tag	UNP Q04640
C	64	SER	-	expression tag	UNP Q04640
C	65	GLY	-	expression tag	UNP Q04640
C	66	LEU	-	expression tag	UNP Q04640
C	67	VAL	-	expression tag	UNP Q04640
C	68	PRO	-	expression tag	UNP Q04640
C	69	ARG	-	expression tag	UNP Q04640
C	70	GLY	-	expression tag	UNP Q04640
C	71	SER	-	expression tag	UNP Q04640
C	72	HIS	-	expression tag	UNP Q04640
C	73	MET	-	expression tag	UNP Q04640

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

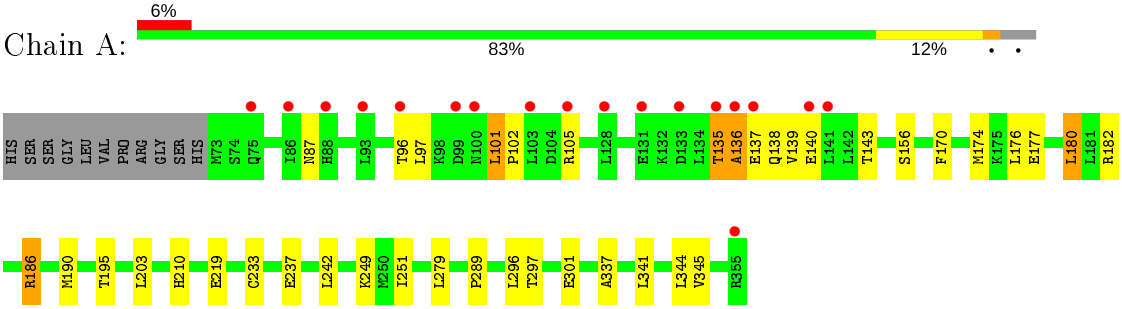
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	46	Total O 46 46	0	0
4	B	46	Total O 46 46	0	0
4	C	42	Total O 42 42	0	0

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.

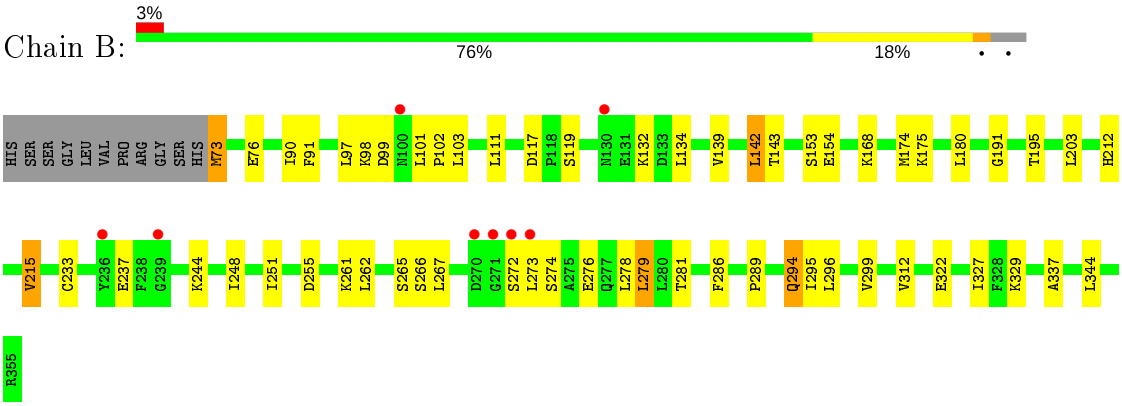
- Molecule 1: PROTEIN MXIC

Chain A:



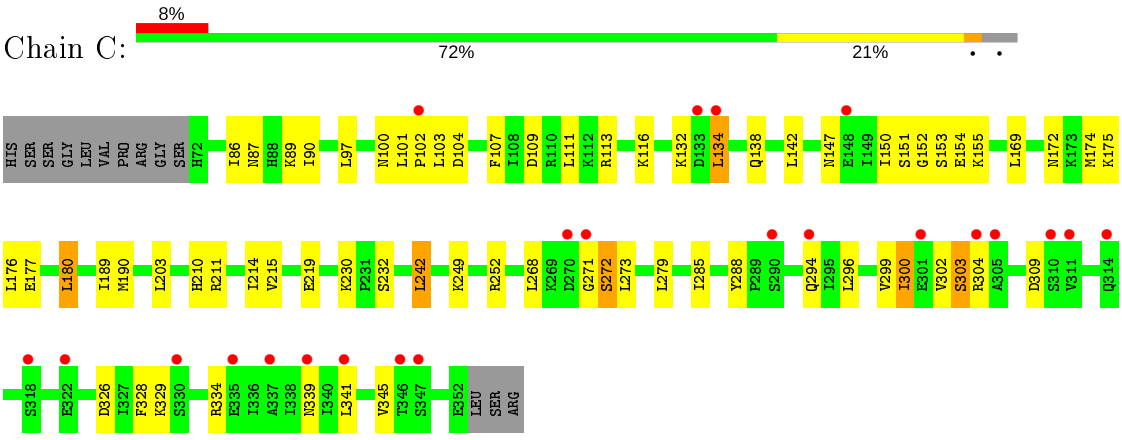
- Molecule 1: PROTEIN MXIC

Chain B:



- Molecule 1: PROTEIN MXIC

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.79Å 102.57Å 122.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.40 – 2.85 47.32 – 2.85	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.40-2.85) 91.9 (47.32-2.85)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.30 (at 2.86Å)	Xtriage
Refinement program	TNT 5.13.1.0	Depositor
R, R_{free}	0.244 , 0.273 0.255 , 0.287	Depositor DCC
R_{free} test set	1216 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	52.5	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 51.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	7117	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% 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, MLY, ACT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.25	0/2139	0.38	0/2901
1	B	0.26	0/2139	0.39	0/2901
1	C	0.25	0/2137	0.41	0/2901
All	All	0.25	0/6415	0.39	0/8703

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	2325	0	2362	19	0
1	B	2325	0	2363	38	0
1	C	2317	0	2345	44	0
2	A	4	0	3	0	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
4	A	46	0	0	0	0
4	B	46	0	0	0	0
4	C	42	0	0	0	0
All	All	7117	0	7089	100	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 7.

All (100) 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:132:MLY:HA	1:B:134:LEU:H	1.10	1.11
1:B:102:PRO:HA	1:B:103:LEU:HB2	1.29	1.08
1:B:132:MLY:HA	1:B:134:LEU:N	1.83	0.93
1:B:102:PRO:HA	1:B:103:LEU:CB	2.07	0.85
1:C:328:PHE:N	1:C:329:MLY:HA	1.92	0.84
1:C:97:LEU:HD21	1:C:134:LEU:HD13	1.60	0.83
1:C:89:MLY:HH21	1:C:116:MLY:HH13	1.65	0.78
1:C:172:ASN:O	1:C:175:MLY:HE3	1.87	0.74
1:C:328:PHE:H	1:C:329:MLY:HA	1.53	0.72
1:C:300:ILE:HG23	1:C:303:SER:HB2	1.72	0.71
1:A:101:LEU:N	1:A:102:PRO:HD3	2.06	0.71
1:C:134:LEU:HD23	1:C:134:LEU:H	1.53	0.71
1:B:255:ASP:OD2	1:B:279:LEU:HD11	1.92	0.69
1:B:273:LEU:H	1:B:273:LEU:HD23	1.60	0.67
1:B:281:THR:HG23	1:B:295:ILE:HG22	1.76	0.67
1:A:101:LEU:HD21	1:A:135:THR:HG21	1.77	0.67
1:B:139:VAL:O	1:B:143:THR:HG23	1.94	0.67
1:C:272:SER:HB2	1:C:302:VAL:HG11	1.81	0.63
1:C:296:LEU:O	1:C:299:VAL:HG12	1.98	0.63
1:C:177:GLU:HB2	1:C:180:LEU:HD22	1.81	0.61
1:A:156:SER:HA	1:A:190:MET:HE1	1.83	0.60
1:B:132:MLY:CA	1:B:134:LEU:H	2.01	0.59
1:C:189:ILE:HG13	1:C:190:MET:HG3	1.85	0.58
1:C:299:VAL:HG13	1:C:300:ILE:CD1	2.33	0.58
1:A:219:GLU:OE2	1:A:249:MLY:HH22	2.06	0.56
1:C:268:LEU:HD23	1:C:268:LEU:O	2.07	0.54
1:C:150:ILE:HG23	1:C:151:SER:N	2.23	0.53
1:C:150:ILE:HG12	1:C:154:GLU:HG3	1.89	0.53
1:B:195:THR:HG22	1:B:251:ILE:HD12	1.91	0.51
1:B:281:THR:CG2	1:B:295:ILE:HG22	2.39	0.51
1:B:296:LEU:O	1:B:299:VAL:HG12	2.09	0.51
1:A:182:ARG:O	1:A:186:ARG:HB2	2.11	0.50
1:B:286:PHE:CZ	1:B:327:ILE:HD12	2.47	0.50
1:B:289:PRO:HB3	1:B:337:ALA:HB2	1.93	0.50
1:C:104:ASP:HA	1:C:107:PHE:HB3	1.92	0.50
1:A:289:PRO:HB3	1:A:337:ALA:HB2	1.94	0.50
1:A:96:THR:HG23	1:A:102:PRO:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:PHE:HB3	1:A:174:MET:HE2	1.93	0.49
1:B:195:THR:HG23	1:B:248:ILE:HG13	1.95	0.49
1:A:174:MET:HB3	1:A:210:HIS:CE1	2.48	0.48
1:C:219:GLU:OE2	1:C:249:MLY:HH13	2.14	0.48
1:C:299:VAL:HG13	1:C:300:ILE:HD11	1.95	0.48
1:C:300:ILE:CG2	1:C:303:SER:HB2	2.42	0.48
1:C:328:PHE:N	1:C:329:MLY:CA	2.71	0.48
1:B:265:SER:O	1:B:266:SER:HB2	2.15	0.47
1:B:265:SER:OG	1:B:267:LEU:HD12	2.15	0.47
1:B:101:LEU:HB2	1:B:102:PRO:HD2	1.96	0.47
1:B:174:MET:O	1:B:175:MLY:HB3	2.13	0.47
1:B:73:MET:N	1:B:76:GLU:OE1	2.47	0.47
1:C:100:ASN:O	1:C:102:PRO:HD3	2.14	0.47
1:C:299:VAL:C	1:C:300:ILE:HG12	2.32	0.47
1:C:299:VAL:HG13	1:C:300:ILE:HG12	1.97	0.46
1:C:242:LEU:HD22	1:C:242:LEU:O	2.15	0.46
1:C:111:LEU:O	1:C:111:LEU:HD23	2.14	0.46
1:A:101:LEU:N	1:A:102:PRO:CD	2.78	0.46
1:B:99:ASP:HB2	1:B:101:LEU:HD22	1.97	0.46
1:C:174:MET:O	1:C:175:MLY:HB3	2.16	0.45
1:B:168:MLY:HH13	1:B:168:MLY:HD2	1.75	0.45
1:C:138:GLN:O	1:C:142:LEU:HB2	2.16	0.45
1:A:177:GLU:O	1:A:180:LEU:HB2	2.16	0.45
1:C:174:MET:HB3	1:C:210:HIS:CE1	2.52	0.45
1:B:132:MLY:HH13	1:B:132:MLY:HD3	1.59	0.45
1:C:151:SER:HA	1:C:154:GLU:CD	2.37	0.45
1:A:136:ALA:O	1:A:138:GLN:N	2.49	0.45
1:B:97:LEU:HD11	1:B:142:LEU:HD21	1.99	0.45
1:A:233:CYS:HB3	1:A:237:GLU:HB2	1.99	0.44
1:B:154:GLU:HB3	1:C:152:GLY:HA2	1.98	0.44
1:B:98:MLY:HH22	1:B:98:MLY:HD3	1.80	0.44
1:C:155:MLY:HG2	1:C:232:SER:O	2.18	0.43
1:C:150:ILE:CG2	1:C:151:SER:N	2.82	0.43
1:B:91:PHE:CE2	1:B:98:MLY:HH21	2.54	0.43
1:B:273:LEU:O	1:B:274:SER:HB2	2.18	0.43
1:C:147:ASN:HA	1:C:150:ILE:HG22	2.00	0.43
1:B:191:GLY:O	1:B:244:MLY:HH11	2.19	0.43
1:B:117:ASP:OD1	1:B:119:SER:HB2	2.19	0.42
1:C:132:MLY:HD2	1:C:132:MLY:HH13	1.73	0.42
1:C:211:ARG:O	1:C:214:ILE:HG22	2.18	0.42
1:B:294:GLN:HG3	1:B:295:ILE:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:ASP:O	1:C:113:ARG:HG3	2.20	0.42
1:A:139:VAL:O	1:A:143:THR:HG23	2.20	0.42
1:A:297:THR:O	1:A:301:GLU:HG2	2.19	0.42
1:C:300:ILE:HG23	1:C:303:SER:CB	2.47	0.42
1:C:302:VAL:C	1:C:304:ARG:H	2.23	0.42
1:C:86:ILE:O	1:C:90:ILE:HD13	2.20	0.42
1:A:219:GLU:OE2	1:A:249:MLY:HH13	2.20	0.42
1:A:341:LEU:O	1:A:345:VAL:HG23	2.20	0.41
1:B:262:LEU:HD21	1:B:278:LEU:HD23	2.01	0.41
1:B:274:SER:O	1:B:276:GLU:N	2.47	0.41
1:B:279:LEU:HD23	1:B:279:LEU:O	2.20	0.41
1:C:215:VAL:HG11	1:C:252:ARG:HD3	2.01	0.41
1:B:212:HIS:O	1:B:215:VAL:HG13	2.20	0.41
1:C:230:MLY:HD3	1:C:230:MLY:HH22	1.86	0.41
1:A:195:THR:HG22	1:A:251:ILE:HD12	2.03	0.41
1:C:285:ILE:HD11	1:C:296:LEU:HD21	2.03	0.41
1:C:341:LEU:O	1:C:345:VAL:HG23	2.20	0.41
1:A:96:THR:CG2	1:A:102:PRO:HG2	2.50	0.41
1:B:329:MLY:HD2	1:B:329:MLY:HH13	1.80	0.40
1:B:233:CYS:HB3	1:B:237:GLU:HB2	2.03	0.40
1:B:261:MLY:HH22	1:B:322:GLU:OE2	2.21	0.40
1:C:101:LEU:CD2	1:C:103:LEU:HB2	2.51	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	261/294 (89%)	249 (95%)	9 (3%)	3 (1%)	14 38
1	B	261/294 (89%)	252 (97%)	9 (3%)	0	100 100
1	C	260/294 (88%)	242 (93%)	15 (6%)	3 (1%)	13 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	782/882 (89%)	743 (95%)	33 (4%)	6 (1%)	19 46

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	GLU
1	A	97	LEU
1	C	271	GLY
1	A	136	ALA
1	C	303	SER
1	C	153	SER

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	241/250 (96%)	228 (95%)	13 (5%)	22 49
1	B	241/250 (96%)	228 (95%)	13 (5%)	22 49
1	C	240/250 (96%)	223 (93%)	17 (7%)	14 36
All	All	722/750 (96%)	679 (94%)	43 (6%)	19 45

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	101	LEU
1	A	105	ARG
1	A	135	THR
1	A	140	GLU
1	A	176	LEU
1	A	180	LEU
1	A	186	ARG
1	A	203	LEU
1	A	242	LEU

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Mol	Chain	Res	Type
1	A	279	LEU
1	A	296	LEU
1	A	344	LEU
1	B	73	MET
1	B	90	ILE
1	B	111	LEU
1	B	142	LEU
1	B	153	SER
1	B	180	LEU
1	B	203	LEU
1	B	215	VAL
1	B	272	SER
1	B	279	LEU
1	B	294	GLN
1	B	312	VAL
1	B	344	LEU
1	C	87	ASN
1	C	134	LEU
1	C	169	LEU
1	C	176	LEU
1	C	180	LEU
1	C	203	LEU
1	C	242	LEU
1	C	272	SER
1	C	273	LEU
1	C	279	LEU
1	C	288	TYR
1	C	294	GLN
1	C	300	ILE
1	C	309	ASP
1	C	326	ASP
1	C	334	ARG
1	C	339	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	100	ASN
1	C	294	GLN
1	C	339	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

60 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	350	1	9,10,11	0.58	0	6,11,13	0.73	0
1	MLY	C	89	1	9,10,11	0.55	0	6,11,13	0.72	0
1	MLY	B	155	1	9,10,11	0.53	0	6,11,13	0.72	0
1	MLY	C	175	1	9,10,11	0.56	0	6,11,13	0.80	0
1	MLY	A	269	1	9,10,11	0.50	0	6,11,13	0.72	0
1	MLY	B	173	1	9,10,11	0.54	0	6,11,13	0.81	0
1	MLY	B	175	1	9,10,11	0.55	0	6,11,13	0.72	0
1	MLY	C	112	1	9,10,11	0.58	0	6,11,13	0.72	0
1	MLY	C	98	1	9,10,11	0.55	0	6,11,13	0.75	0
1	MLY	A	351	1	9,10,11	0.59	0	6,11,13	0.74	0
1	MLY	B	89	1	9,10,11	0.59	0	6,11,13	0.72	0
1	MLY	C	116	1	9,10,11	0.56	0	6,11,13	0.72	0
1	MLY	A	94	1	9,10,11	0.56	0	6,11,13	0.76	0
1	MLY	A	249	1	9,10,11	0.62	0	6,11,13	0.72	0
1	MLY	A	112	1	9,10,11	0.58	0	6,11,13	0.75	0
1	MLY	C	249	1	9,10,11	0.56	0	6,11,13	0.79	0
1	MLY	B	329	1	9,10,11	0.52	0	6,11,13	0.79	0
1	MLY	A	173	1	9,10,11	0.53	0	6,11,13	0.79	0
1	MLY	B	261	1	9,10,11	0.61	0	6,11,13	0.77	0
1	MLY	C	132	1	9,10,11	0.45	0	6,11,13	0.90	0
1	MLY	B	132	1	9,10,11	0.53	0	6,11,13	0.77	0
1	MLY	B	116	1	9,10,11	0.56	0	6,11,13	0.75	0
1	MLY	C	261	1	9,10,11	0.64	0	6,11,13	0.73	0
1	MLY	A	261	1	9,10,11	0.50	0	6,11,13	0.96	0
1	MLY	A	244	1	9,10,11	0.52	0	6,11,13	0.93	0
1	MLY	A	89	1	9,10,11	0.60	0	6,11,13	0.75	0
1	MLY	C	155	1	9,10,11	0.49	0	6,11,13	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	MLY	B	144	1	9,10,11	0.49	0	6,11,13	0.73	0
1	MLY	A	132	1	9,10,11	0.50	0	6,11,13	0.92	0
1	MLY	A	116	1	9,10,11	0.55	0	6,11,13	0.74	0
1	MLY	B	112	1	9,10,11	0.53	0	6,11,13	0.85	0
1	MLY	B	249	1	9,10,11	0.58	0	6,11,13	0.78	0
1	MLY	C	260	1	9,10,11	0.56	0	6,11,13	0.82	0
1	MLY	A	144	1	9,10,11	0.51	0	6,11,13	0.84	0
1	MLY	C	168	1	9,10,11	0.53	0	6,11,13	0.80	0
1	MLY	A	230	1	9,10,11	0.56	0	6,11,13	0.72	0
1	MLY	C	269	1	9,10,11	0.60	0	6,11,13	0.72	0
1	MLY	A	175	1	9,10,11	0.58	0	6,11,13	0.69	0
1	MLY	B	269	1	9,10,11	0.55	0	6,11,13	0.76	0
1	MLY	A	329	1	9,10,11	0.56	0	6,11,13	0.71	0
1	MLY	C	173	1	9,10,11	0.58	0	6,11,13	0.74	0
1	MLY	C	351	1	9,10,11	0.56	0	6,11,13	0.71	0
1	MLY	B	94	1	9,10,11	0.54	0	6,11,13	0.78	0
1	MLY	B	260	1	9,10,11	0.54	0	6,11,13	0.78	0
1	MLY	A	260	1	9,10,11	0.47	0	6,11,13	0.78	0
1	MLY	B	351	1	9,10,11	0.52	0	6,11,13	0.73	0
1	MLY	B	350	1	9,10,11	0.46	0	6,11,13	0.78	0
1	MLY	C	230	1	9,10,11	0.54	0	6,11,13	0.77	0
1	MLY	C	144	1	9,10,11	0.50	0	6,11,13	0.81	0
1	MLY	C	329	1	9,10,11	0.56	0	6,11,13	0.70	0
1	MLY	A	168	1	9,10,11	0.56	0	6,11,13	0.78	0
1	MLY	C	94	1	9,10,11	0.54	0	6,11,13	0.72	0
1	MLY	C	244	1	9,10,11	0.59	0	6,11,13	0.78	0
1	MLY	B	98	1	9,10,11	0.54	0	6,11,13	0.88	0
1	MLY	B	244	1	9,10,11	0.57	0	6,11,13	0.74	0
1	MLY	A	98	1	9,10,11	0.53	0	6,11,13	0.78	0
1	MLY	B	230	1	9,10,11	0.56	0	6,11,13	0.69	0
1	MLY	C	350	1	9,10,11	0.49	0	6,11,13	0.73	0
1	MLY	A	155	1	9,10,11	0.52	0	6,11,13	0.84	0
1	MLY	B	168	1	9,10,11	0.52	0	6,11,13	0.78	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	350	1	-	5/8/9/11	-
1	MLY	C	89	1	-	2/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	B	155	1	-	4/8/9/11	-
1	MLY	C	175	1	-	2/8/9/11	-
1	MLY	A	269	1	-	3/8/9/11	-
1	MLY	B	173	1	-	3/8/9/11	-
1	MLY	B	175	1	-	5/8/9/11	-
1	MLY	C	112	1	-	3/8/9/11	-
1	MLY	C	98	1	-	5/8/9/11	-
1	MLY	A	351	1	-	6/8/9/11	-
1	MLY	B	89	1	-	0/8/9/11	-
1	MLY	C	116	1	-	8/8/9/11	-
1	MLY	A	94	1	-	3/8/9/11	-
1	MLY	A	249	1	-	4/8/9/11	-
1	MLY	A	112	1	-	5/8/9/11	-
1	MLY	C	249	1	-	5/8/9/11	-
1	MLY	B	329	1	-	3/8/9/11	-
1	MLY	A	173	1	-	6/8/9/11	-
1	MLY	B	261	1	-	3/8/9/11	-
1	MLY	C	132	1	-	4/8/9/11	-
1	MLY	B	132	1	-	6/8/9/11	-
1	MLY	B	116	1	-	4/8/9/11	-
1	MLY	C	261	1	-	3/8/9/11	-
1	MLY	A	261	1	-	1/8/9/11	-
1	MLY	A	244	1	-	2/8/9/11	-
1	MLY	A	89	1	-	3/8/9/11	-
1	MLY	C	155	1	-	6/8/9/11	-
1	MLY	B	144	1	-	3/8/9/11	-
1	MLY	A	132	1	-	4/8/9/11	-
1	MLY	A	116	1	-	6/8/9/11	-
1	MLY	B	112	1	-	1/8/9/11	-
1	MLY	B	249	1	-	2/8/9/11	-
1	MLY	C	260	1	-	3/8/9/11	-
1	MLY	A	144	1	-	3/8/9/11	-
1	MLY	C	168	1	-	4/8/9/11	-
1	MLY	A	230	1	-	3/8/9/11	-
1	MLY	C	269	1	-	6/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	175	1	-	3/8/9/11	-
1	MLY	B	269	1	-	5/8/9/11	-
1	MLY	A	329	1	-	4/8/9/11	-
1	MLY	C	173	1	-	3/8/9/11	-
1	MLY	C	351	1	-	7/8/9/11	-
1	MLY	B	94	1	-	4/8/9/11	-
1	MLY	B	260	1	-	3/8/9/11	-
1	MLY	A	260	1	-	1/8/9/11	-
1	MLY	B	351	1	-	6/8/9/11	-
1	MLY	B	350	1	-	0/8/9/11	-
1	MLY	C	230	1	-	4/8/9/11	-
1	MLY	C	144	1	-	4/8/9/11	-
1	MLY	C	329	1	-	6/8/9/11	-
1	MLY	A	168	1	-	3/8/9/11	-
1	MLY	C	94	1	-	5/8/9/11	-
1	MLY	C	244	1	-	4/8/9/11	-
1	MLY	B	98	1	-	2/8/9/11	-
1	MLY	B	244	1	-	4/8/9/11	-
1	MLY	A	98	1	-	4/8/9/11	-
1	MLY	B	230	1	-	5/8/9/11	-
1	MLY	C	350	1	-	4/8/9/11	-
1	MLY	A	155	1	-	4/8/9/11	-
1	MLY	B	168	1	-	3/8/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (227) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	350	MLY	N-CA-CB-CG
1	A	350	MLY	C-CA-CB-CG
1	C	98	MLY	N-CA-CB-CG
1	C	98	MLY	C-CA-CB-CG
1	A	351	MLY	N-CA-CB-CG
1	A	351	MLY	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	C	116	MLY	N-CA-CB-CG
1	C	116	MLY	C-CA-CB-CG
1	C	116	MLY	O-C-CA-CB
1	A	249	MLY	C-CA-CB-CG
1	A	112	MLY	O-C-CA-CB
1	C	249	MLY	O-C-CA-CB
1	B	329	MLY	N-CA-CB-CG
1	B	329	MLY	C-CA-CB-CG
1	A	173	MLY	C-CA-CB-CG
1	B	132	MLY	O-C-CA-CB
1	C	155	MLY	N-CA-CB-CG
1	C	155	MLY	C-CA-CB-CG
1	A	132	MLY	N-CA-CB-CG
1	A	132	MLY	C-CA-CB-CG
1	A	116	MLY	N-CA-CB-CG
1	A	116	MLY	C-CA-CB-CG
1	C	260	MLY	N-CA-CB-CG
1	C	260	MLY	C-CA-CB-CG
1	A	144	MLY	O-C-CA-CB
1	C	269	MLY	N-CA-CB-CG
1	C	269	MLY	C-CA-CB-CG
1	B	269	MLY	N-CA-CB-CG
1	B	269	MLY	C-CA-CB-CG
1	C	351	MLY	C-CA-CB-CG
1	C	351	MLY	O-C-CA-CB
1	B	94	MLY	C-CA-CB-CG
1	B	94	MLY	O-C-CA-CB
1	B	351	MLY	N-CA-CB-CG
1	B	351	MLY	C-CA-CB-CG
1	A	230	MLY	C-CA-CB-CG
1	C	230	MLY	N-CA-CB-CG
1	C	230	MLY	C-CA-CB-CG
1	C	329	MLY	N-CA-CB-CG
1	C	329	MLY	C-CA-CB-CG
1	C	94	MLY	N-CA-CB-CG
1	C	94	MLY	C-CA-CB-CG
1	C	269	MLY	CD-CE-NZ-CH2
1	A	175	MLY	CD-CE-NZ-CH1
1	B	94	MLY	CD-CE-NZ-CH2
1	B	351	MLY	CD-CE-NZ-CH1
1	A	350	MLY	CD-CE-NZ-CH1
1	A	350	MLY	CD-CE-NZ-CH2

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Mol	Chain	Res	Type	Atoms
1	B	173	MLY	CD-CE-NZ-CH1
1	B	173	MLY	CD-CE-NZ-CH2
1	B	175	MLY	CD-CE-NZ-CH1
1	B	175	MLY	CD-CE-NZ-CH2
1	C	112	MLY	CD-CE-NZ-CH1
1	C	98	MLY	CD-CE-NZ-CH1
1	A	351	MLY	CD-CE-NZ-CH1
1	A	351	MLY	CD-CE-NZ-CH2
1	A	94	MLY	CD-CE-NZ-CH1
1	A	94	MLY	CD-CE-NZ-CH2
1	A	112	MLY	CD-CE-NZ-CH1
1	A	112	MLY	CD-CE-NZ-CH2
1	A	173	MLY	CD-CE-NZ-CH2
1	B	116	MLY	CD-CE-NZ-CH1
1	B	116	MLY	CD-CE-NZ-CH2
1	A	89	MLY	CD-CE-NZ-CH1
1	A	116	MLY	CD-CE-NZ-CH1
1	C	168	MLY	CD-CE-NZ-CH1
1	C	168	MLY	CD-CE-NZ-CH2
1	C	269	MLY	CD-CE-NZ-CH1
1	B	269	MLY	CD-CE-NZ-CH2
1	A	329	MLY	CD-CE-NZ-CH2
1	C	351	MLY	CD-CE-NZ-CH1
1	B	94	MLY	CD-CE-NZ-CH1
1	B	260	MLY	CD-CE-NZ-CH1
1	B	260	MLY	CD-CE-NZ-CH2
1	B	351	MLY	CD-CE-NZ-CH2
1	C	144	MLY	CD-CE-NZ-CH2
1	C	329	MLY	CD-CE-NZ-CH1
1	A	98	MLY	CD-CE-NZ-CH1
1	C	351	MLY	CG-CD-CE-NZ
1	A	112	MLY	CG-CD-CE-NZ
1	C	269	MLY	CG-CD-CE-NZ
1	C	98	MLY	CG-CD-CE-NZ
1	A	351	MLY	CG-CD-CE-NZ
1	A	116	MLY	CG-CD-CE-NZ
1	A	249	MLY	CG-CD-CE-NZ
1	C	249	MLY	CG-CD-CE-NZ
1	B	132	MLY	CG-CD-CE-NZ
1	C	173	MLY	CG-CD-CE-NZ
1	B	144	MLY	CG-CD-CE-NZ
1	C	261	MLY	CG-CD-CE-NZ

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Mol	Chain	Res	Type	Atoms
1	A	261	MLY	CG-CD-CE-NZ
1	B	112	MLY	CG-CD-CE-NZ
1	A	98	MLY	CG-CD-CE-NZ
1	B	155	MLY	CD-CE-NZ-CH1
1	B	155	MLY	CD-CE-NZ-CH2
1	C	98	MLY	CD-CE-NZ-CH2
1	A	173	MLY	CD-CE-NZ-CH1
1	B	132	MLY	CD-CE-NZ-CH1
1	A	89	MLY	CD-CE-NZ-CH2
1	B	269	MLY	CD-CE-NZ-CH1
1	A	329	MLY	CD-CE-NZ-CH1
1	A	98	MLY	CD-CE-NZ-CH2
1	C	144	MLY	CG-CD-CE-NZ
1	B	329	MLY	CA-CB-CG-CD
1	A	175	MLY	CD-CE-NZ-CH2
1	A	155	MLY	CD-CE-NZ-CH1
1	B	249	MLY	CG-CD-CE-NZ
1	C	244	MLY	CG-CD-CE-NZ
1	A	269	MLY	CA-CB-CG-CD
1	C	116	MLY	CA-CB-CG-CD
1	C	351	MLY	CA-CB-CG-CD
1	B	230	MLY	CA-CB-CG-CD
1	C	230	MLY	CG-CD-CE-NZ
1	B	269	MLY	CG-CD-CE-NZ
1	C	112	MLY	CD-CE-NZ-CH2
1	C	116	MLY	CD-CE-NZ-CH2
1	B	261	MLY	CD-CE-NZ-CH1
1	B	144	MLY	CD-CE-NZ-CH1
1	A	116	MLY	CD-CE-NZ-CH2
1	C	351	MLY	CD-CE-NZ-CH2
1	C	144	MLY	CD-CE-NZ-CH1
1	C	329	MLY	CD-CE-NZ-CH2
1	A	249	MLY	CA-CB-CG-CD
1	C	261	MLY	CA-CB-CG-CD
1	C	269	MLY	CA-CB-CG-CD
1	B	168	MLY	CA-CB-CG-CD
1	C	116	MLY	CG-CD-CE-NZ
1	B	155	MLY	CG-CD-CE-NZ
1	C	132	MLY	CG-CD-CE-NZ
1	B	175	MLY	CA-CB-CG-CD
1	A	144	MLY	CA-CB-CG-CD
1	C	329	MLY	CA-CB-CG-CD

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Mol	Chain	Res	Type	Atoms
1	A	89	MLY	CG-CD-CE-NZ
1	B	244	MLY	CD-CE-NZ-CH1
1	B	98	MLY	CG-CD-CE-NZ
1	C	175	MLY	CE-CD-CG-CB
1	A	144	MLY	CE-CD-CG-CB
1	A	260	MLY	CG-CD-CE-NZ
1	C	94	MLY	CD-CE-NZ-CH1
1	C	244	MLY	CD-CE-NZ-CH1
1	C	173	MLY	CE-CD-CG-CB
1	A	112	MLY	CE-CD-CG-CB
1	C	94	MLY	CE-CD-CG-CB
1	A	351	MLY	CE-CD-CG-CB
1	C	155	MLY	CE-CD-CG-CB
1	C	350	MLY	CE-CD-CG-CB
1	A	116	MLY	CE-CD-CG-CB
1	A	155	MLY	CE-CD-CG-CB
1	A	132	MLY	CG-CD-CE-NZ
1	C	260	MLY	CE-CD-CG-CB
1	C	351	MLY	CE-CD-CG-CB
1	C	112	MLY	CE-CD-CG-CB
1	B	260	MLY	CE-CD-CG-CB
1	B	351	MLY	CA-CB-CG-CD
1	B	175	MLY	CE-CD-CG-CB
1	A	249	MLY	CE-CD-CG-CB
1	B	132	MLY	CE-CD-CG-CB
1	B	261	MLY	CD-CE-NZ-CH2
1	C	155	MLY	CD-CE-NZ-CH2
1	A	168	MLY	CE-CD-CG-CB
1	A	132	MLY	CA-CB-CG-CD
1	C	230	MLY	CA-CB-CG-CD
1	C	249	MLY	CE-CD-CG-CB
1	A	230	MLY	CE-CD-CG-CB
1	C	350	MLY	CG-CD-CE-NZ
1	A	269	MLY	CE-CD-CG-CB
1	C	116	MLY	CE-CD-CG-CB
1	A	98	MLY	CE-CD-CG-CB
1	C	249	MLY	CA-CB-CG-CD
1	B	230	MLY	CD-CE-NZ-CH2
1	C	350	MLY	CD-CE-NZ-CH1
1	C	175	MLY	CG-CD-CE-NZ
1	B	173	MLY	CE-CD-CG-CB
1	B	168	MLY	CE-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
1	B	116	MLY	CA-CB-CG-CD
1	C	89	MLY	C-CA-CB-CG
1	B	244	MLY	C-CA-CB-CG
1	B	244	MLY	CE-CD-CG-CB
1	C	116	MLY	CD-CE-NZ-CH1
1	A	244	MLY	CD-CE-NZ-CH2
1	B	144	MLY	CD-CE-NZ-CH2
1	B	244	MLY	CD-CE-NZ-CH2
1	A	173	MLY	CE-CD-CG-CB
1	B	249	MLY	CE-CD-CG-CB
1	B	116	MLY	CE-CD-CG-CB
1	B	261	MLY	CA-CB-CG-CD
1	A	350	MLY	CA-CB-CG-CD
1	A	269	MLY	CG-CD-CE-NZ
1	C	89	MLY	CG-CD-CE-NZ
1	C	244	MLY	CE-CD-CG-CB
1	B	230	MLY	CE-CD-CG-CB
1	B	98	MLY	CE-CD-CG-CB
1	B	351	MLY	CE-CD-CG-CB
1	A	168	MLY	CG-CD-CE-NZ
1	C	144	MLY	CE-CD-CG-CB
1	C	132	MLY	CE-CD-CG-CB
1	A	173	MLY	CG-CD-CE-NZ
1	C	94	MLY	CD-CE-NZ-CH2
1	C	132	MLY	CA-CB-CG-CD
1	C	329	MLY	CE-CD-CG-CB
1	C	155	MLY	CG-CD-CE-NZ
1	B	155	MLY	N-CA-CB-CG
1	A	155	MLY	N-CA-CB-CG
1	C	249	MLY	C-CA-CB-CG
1	B	230	MLY	C-CA-CB-CG
1	A	244	MLY	CG-CD-CE-NZ
1	A	329	MLY	CE-CD-CG-CB
1	B	132	MLY	CD-CE-NZ-CH2
1	C	155	MLY	CD-CE-NZ-CH1
1	C	168	MLY	CG-CD-CE-NZ
1	B	132	MLY	CA-CB-CG-CD
1	A	230	MLY	CA-CB-CG-CD
1	C	244	MLY	CD-CE-NZ-CH2
1	C	261	MLY	CD-CE-NZ-CH1
1	B	230	MLY	CD-CE-NZ-CH1
1	B	175	MLY	CG-CD-CE-NZ

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Mol	Chain	Res	Type	Atoms
1	A	155	MLY	CA-CB-CG-CD
1	A	94	MLY	C-CA-CB-CG
1	C	132	MLY	C-CA-CB-CG
1	A	168	MLY	C-CA-CB-CG
1	C	173	MLY	CA-CB-CG-CD
1	B	168	MLY	CD-CE-NZ-CH1
1	A	175	MLY	CA-CB-CG-CD
1	C	168	MLY	CE-CD-CG-CB
1	A	173	MLY	N-CA-CB-CG
1	A	329	MLY	N-CA-CB-CG
1	C	350	MLY	CD-CE-NZ-CH2

There are no ring outliers.

16 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	89	MLY	1	0
1	C	175	MLY	2	0
1	B	175	MLY	1	0
1	C	116	MLY	1	0
1	A	249	MLY	2	0
1	C	249	MLY	1	0
1	B	329	MLY	1	0
1	B	261	MLY	1	0
1	C	132	MLY	1	0
1	B	132	MLY	4	0
1	C	155	MLY	1	0
1	C	230	MLY	1	0
1	C	329	MLY	3	0
1	B	98	MLY	2	0
1	B	244	MLY	1	0
1	B	168	MLY	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

3 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	$\#\|Z\| > 2$
3	GOL	B	1356	-	5,5,5	0.46	0	5,5,5	1.66	2 (40%)
3	GOL	A	1357	-	5,5,5	0.31	0	5,5,5	1.60	1 (20%)
2	ACT	A	1356	-	1,3,3	4.02	1 (100%)	0,3,3	0.00	-

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	GOL	B	1356	-	-	1/4/4/4	-
3	GOL	A	1357	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1356	ACT	CH3-C	4.02	1.53	1.48

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1356	GOL	O1-C1-C2	-2.51	98.16	110.20
3	A	1357	GOL	O3-C3-C2	-2.18	99.76	110.20
3	B	1356	GOL	C3-C2-C1	-2.06	103.71	111.70

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1356	GOL	O1-C1-C2-C3
3	A	1357	GOL	C1-C2-C3-O3
3	A	1357	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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	263/294 (89%)	0.40	18 (6%) 17 13	32, 53, 96, 103	0
1	B	263/294 (89%)	0.22	8 (3%) 50 45	31, 50, 70, 83	0
1	C	261/294 (88%)	0.62	23 (8%) 10 6	32, 65, 121, 131	0
All	All	787/882 (89%)	0.42	49 (6%) 20 16	31, 53, 112, 131	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	346	THR	5.1
1	C	339	ASN	5.1
1	A	100	ASN	4.6
1	A	103	LEU	4.5
1	C	301	GLU	4.3
1	C	347	SER	4.3
1	A	355	ARG	4.3
1	A	137	GLU	4.2
1	C	304	ARG	4.0
1	C	270	ASP	3.9
1	A	141	LEU	3.9
1	A	135	THR	3.8
1	C	134	LEU	3.5
1	C	133	ASP	3.4
1	A	99	ASP	3.4
1	C	310	SER	3.3
1	C	305	ALA	3.3
1	C	271	GLY	3.3
1	C	322	GLU	3.3
1	C	294	GLN	3.2
1	C	314	GLN	3.1
1	B	273	LEU	3.1
1	C	341	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	271	GLY	2.9
1	A	93	LEU	2.9
1	A	140	GLU	2.8
1	A	88	HIS	2.8
1	A	133	ASP	2.8
1	C	337	ALA	2.7
1	A	136	ALA	2.6
1	A	131	GLU	2.5
1	B	236	TYR	2.4
1	A	96	THR	2.4
1	B	272	SER	2.4
1	A	75	GLN	2.4
1	C	102	PRO	2.3
1	A	105	ARG	2.3
1	C	290	SER	2.2
1	B	270	ASP	2.2
1	C	335	GLU	2.2
1	C	311	VAL	2.1
1	C	318	SER	2.1
1	C	330	SER	2.1
1	A	86	ILE	2.0
1	B	100	ASN	2.0
1	B	239	GLY	2.0
1	C	148	GLU	2.0
1	A	128	LEU	2.0
1	B	130	ASN	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, 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	C	132	11/12	0.67	0.46	75,85,93,104	0
1	MLY	C	269	11/12	0.69	0.51	81,85,93,99	0
1	MLY	A	132	11/12	0.74	0.57	81,92,106,107	0
1	MLY	B	132	11/12	0.75	0.56	54,62,84,98	0
1	MLY	C	351	11/12	0.75	0.48	121,124,126,130	0
1	MLY	A	98	11/12	0.77	0.31	83,96,102,106	0
1	MLY	B	98	11/12	0.78	0.46	56,66,77,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	MLY	C	329	11/12	0.79	0.47	112,115,124,130	0
1	MLY	C	350	11/12	0.79	0.46	119,124,125,126	0
1	MLY	C	144	11/12	0.82	0.39	64,72,85,85	0
1	MLY	A	269	11/12	0.82	0.27	64,68,87,89	0
1	MLY	B	269	11/12	0.84	0.44	73,78,83,83	0
1	MLY	C	98	11/12	0.84	0.49	80,85,97,98	0
1	MLY	A	89	11/12	0.86	0.28	64,80,91,92	0
1	MLY	C	112	11/12	0.86	0.19	51,68,80,91	0
1	MLY	C	230	11/12	0.87	0.26	39,49,74,82	0
1	MLY	C	94	11/12	0.88	0.30	53,69,75,76	0
1	MLY	A	116	11/12	0.88	0.38	60,81,99,104	0
1	MLY	A	350	11/12	0.88	0.34	63,76,82,85	0
1	MLY	A	144	11/12	0.89	0.30	75,78,93,93	0
1	MLY	B	351	11/12	0.89	0.27	49,62,81,90	0
1	MLY	B	261	11/12	0.89	0.22	53,58,70,81	0
1	MLY	C	261	11/12	0.89	0.30	59,64,76,80	0
1	MLY	A	261	11/12	0.90	0.22	36,49,67,67	0
1	MLY	A	351	11/12	0.90	0.21	62,73,87,87	0
1	MLY	A	94	11/12	0.90	0.24	77,92,98,98	0
1	MLY	B	155	11/12	0.90	0.31	40,43,57,57	0
1	MLY	B	260	11/12	0.91	0.30	48,55,73,80	0
1	MLY	C	116	11/12	0.91	0.19	49,52,83,83	0
1	MLY	B	112	11/12	0.91	0.24	31,43,58,58	0
1	MLY	A	112	11/12	0.91	0.34	70,72,83,92	0
1	MLY	B	168	11/12	0.91	0.23	37,46,57,59	0
1	MLY	B	350	11/12	0.92	0.22	14,46,65,65	0
1	MLY	B	144	11/12	0.92	0.22	35,42,64,64	0
1	MLY	A	230	11/12	0.92	0.26	18,48,76,85	0
1	MLY	A	173	11/12	0.92	0.22	38,45,63,69	0
1	MLY	C	168	11/12	0.92	0.20	20,37,50,64	0
1	MLY	A	260	11/12	0.93	0.15	29,43,74,75	0
1	MLY	B	329	11/12	0.93	0.25	48,58,79,81	0
1	MLY	B	230	11/12	0.93	0.26	34,47,70,71	0
1	MLY	B	175	11/12	0.93	0.28	44,52,79,79	0
1	MLY	A	168	11/12	0.93	0.22	18,34,56,59	0
1	MLY	C	173	11/12	0.94	0.21	26,39,63,66	0
1	MLY	C	155	11/12	0.94	0.23	44,47,62,62	0
1	MLY	B	94	11/12	0.94	0.21	50,52,67,69	0
1	MLY	B	89	11/12	0.94	0.15	14,41,52,59	0
1	MLY	C	249	11/12	0.94	0.20	14,36,42,54	0
1	MLY	B	249	11/12	0.94	0.19	24,45,50,68	0
1	MLY	C	260	11/12	0.94	0.18	40,56,65,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	MLY	A	329	11/12	0.94	0.31	48,59,79,79	0
1	MLY	B	244	11/12	0.95	0.19	33,41,45,45	0
1	MLY	B	116	11/12	0.95	0.20	30,39,66,73	0
1	MLY	A	175	11/12	0.95	0.20	15,40,53,53	0
1	MLY	A	249	11/12	0.95	0.23	16,35,46,46	0
1	MLY	A	155	11/12	0.95	0.24	34,44,51,53	0
1	MLY	B	173	11/12	0.95	0.20	23,54,58,58	0
1	MLY	C	175	11/12	0.96	0.16	20,35,42,42	0
1	MLY	A	244	11/12	0.96	0.23	21,33,62,62	0
1	MLY	C	89	11/12	0.96	0.23	41,62,63,66	0
1	MLY	C	244	11/12	0.97	0.21	33,40,76,76	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	GOL	A	1357	6/6	0.62	0.30	87,87,87,87	0
2	ACT	A	1356	4/4	0.64	0.51	95,95,95,95	0
3	GOL	B	1356	6/6	0.71	0.45	90,90,90,90	0

6.5 Other polymers (i)

There are no such residues in this entry.