



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:56 pm BST

PDB ID : 3ZCJ
Title : Crystal structure of Helicobacter pylori T4SS protein CagL in a tetragonal crystal form with a helical RGD-motif (6 Mol per ASU)
Authors : Barden, S.; Niemann, H.H.
Deposited on : 2012-11-20
Resolution : 3.25 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

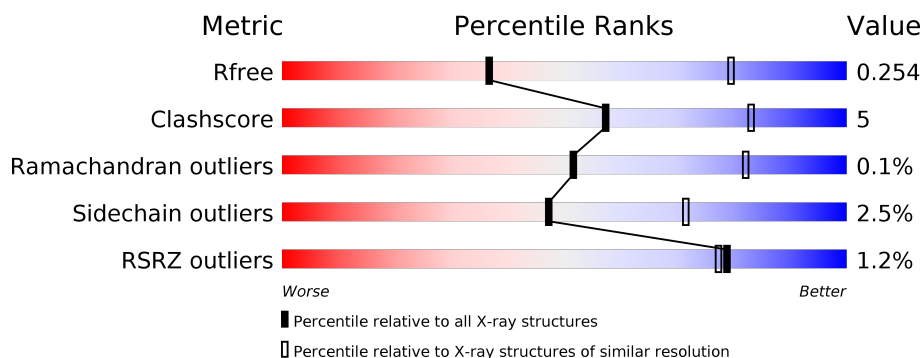
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	220	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>13%</div> <div>7%</div> </div> </div>
1	B	220	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>8%</div> <div>10%</div> </div> </div>
1	C	220	<div> <div></div> <div> <div>71%</div> <div>12%</div> <div>•</div> <div>16%</div> </div> </div>
1	D	220	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>13%</div> <div>•</div> <div>12%</div> </div> </div>
1	E	220	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>9%</div> <div>12%</div> </div> </div>
1	F	220	<div> <div></div> <div> <div>65%</div> <div>10%</div> <div>25%</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	E	70	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9442 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 CAGL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1679	1069	275	329	6			
1	B	199	Total	C	N	O	S	0	0	0
			1631	1043	267	315	6			
1	C	185	Total	C	N	O	S	0	0	0
			1522	984	245	288	5			
1	D	194	Total	C	N	O	S	0	0	0
			1586	1016	259	305	6			
1	E	193	Total	C	N	O	S	0	0	0
			1585	1015	262	303	5			
1	F	166	Total	C	N	O	S	0	0	0
			1367	882	225	256	4			

There are 18 discrepancies between the modelled and reference sequences:

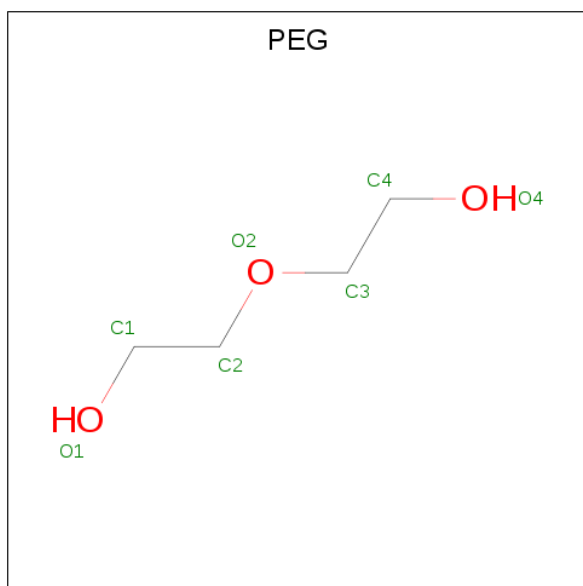
Chain	Residue	Modelled	Actual	Comment	Reference
A	18	GLY	-	expression tag	UNP O25272
A	19	ALA	-	expression tag	UNP O25272
A	20	MET	-	expression tag	UNP O25272
B	18	GLY	-	expression tag	UNP O25272
B	19	ALA	-	expression tag	UNP O25272
B	20	MET	-	expression tag	UNP O25272
C	18	GLY	-	expression tag	UNP O25272
C	19	ALA	-	expression tag	UNP O25272
C	20	MET	-	expression tag	UNP O25272
D	18	GLY	-	expression tag	UNP O25272
D	19	ALA	-	expression tag	UNP O25272
D	20	MET	-	expression tag	UNP O25272
E	18	GLY	-	expression tag	UNP O25272
E	19	ALA	-	expression tag	UNP O25272
E	20	MET	-	expression tag	UNP O25272
F	18	GLY	-	expression tag	UNP O25272
F	19	ALA	-	expression tag	UNP O25272

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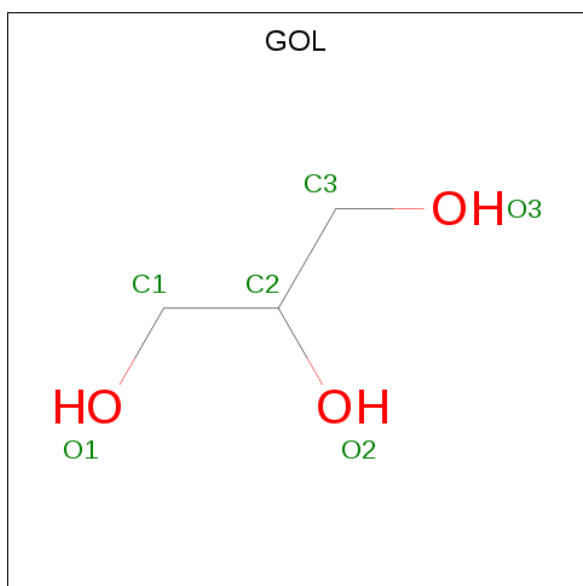
Chain	Residue	Modelled	Actual	Comment	Reference
F	20	MET	-	expression tag	UNP O25272

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



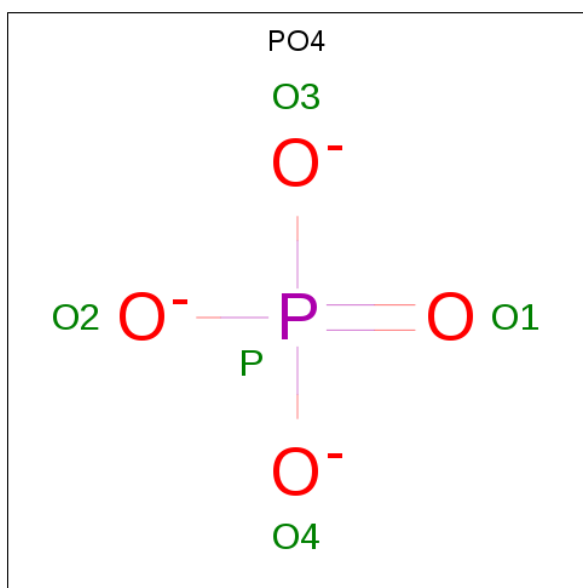
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		

- 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	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O P 5 4 1	0	0
4	F	1	Total O P 5 4 1	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total K 1 1	0	0

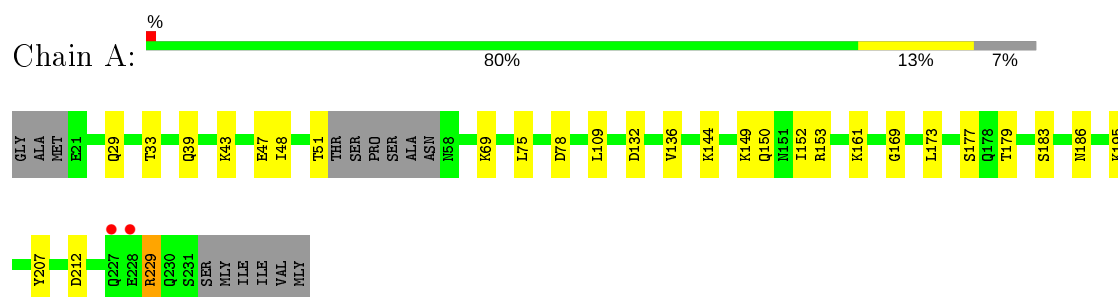
- Molecule 6 is water.

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

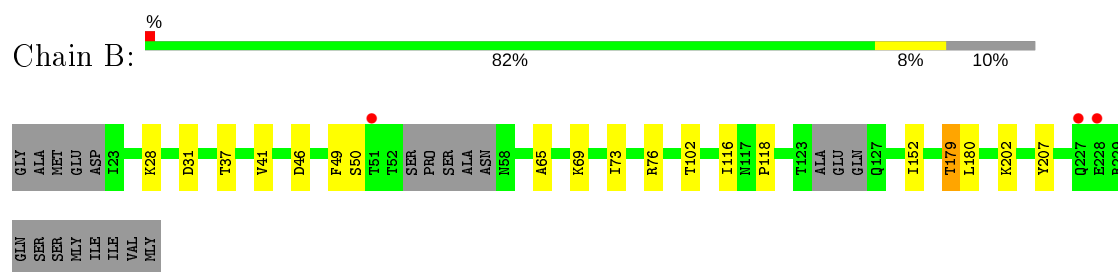
3 Residue-property plots [i](#)

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.

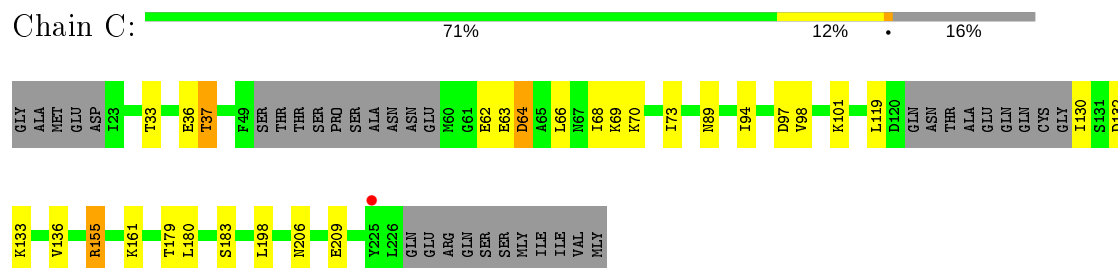
• Molecule 1: CAGL



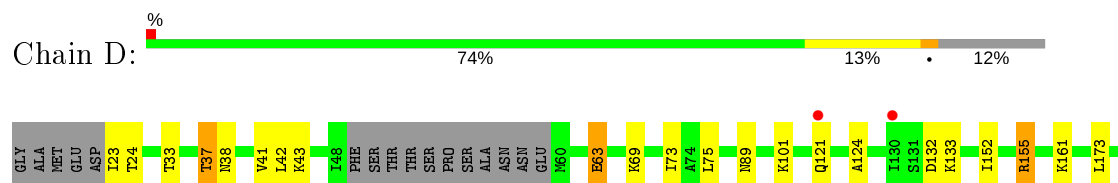
• Molecule 1: CAGL



• Molecule 1: CAGL

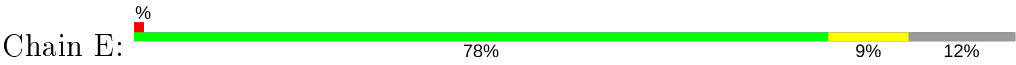


• Molecule 1: CAGL

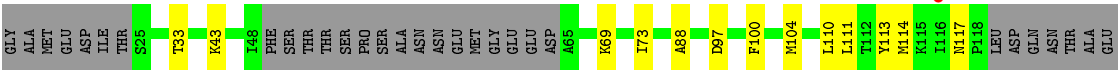




• Molecule 1: CAGL



• Molecule 1: CAGL



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	197.12Å 197.12Å 106.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.97 – 3.25 55.97 – 3.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (55.97-3.25) 100.0 (55.97-3.25)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 3.26Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.205 , 0.251 0.205 , 0.254	Depositor DCC
R_{free} test set	1706 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	70.0	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 79.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9442	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, GOL, K, MLY, PO4

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	0.37	0/1496	0.56	0/2027
1	B	0.35	0/1447	0.50	0/1960
1	C	0.34	0/1338	0.52	0/1813
1	D	0.34	0/1402	0.50	0/1901
1	E	0.33	0/1401	0.51	0/1900
1	F	0.33	0/1192	0.50	0/1614
All	All	0.34	0/8276	0.52	0/11215

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 [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	1679	0	1718	19	0
1	B	1631	0	1683	13	0
1	C	1522	0	1589	17	0
1	D	1586	0	1644	22	0
1	E	1585	0	1646	12	0
1	F	1367	0	1435	15	0
2	A	7	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	12	0	16	1	0
3	B	12	0	16	0	0
3	C	6	0	8	1	0
3	D	6	0	8	0	0
3	E	6	0	8	1	0
3	F	6	0	8	1	0
4	B	5	0	0	0	0
4	F	5	0	0	0	0
5	D	1	0	0	0	0
6	A	4	0	0	0	0
6	B	1	0	0	0	0
6	E	1	0	0	1	0
All	All	9442	0	9789	94	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 (94) 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:109:LEU:HD21	1:B:73:ILE:HD12	1.53	0.91
1:A:132:ASP:OD2	1:A:229:ARG:NH2	2.19	0.75
1:C:89:ASN:OD1	1:C:155:ARG:NH1	2.23	0.71
1:C:180:LEU:HB2	1:F:157:GLU:HG3	1.73	0.69
1:C:132:ASP:OD1	1:C:133:MLY:N	2.27	0.67
1:E:97:ASP:OD2	3:E:1231:GOL:O2	2.11	0.66
1:B:46:ASP:OD1	1:B:76:ARG:NH2	2.22	0.65
1:E:178:GLN:NE2	6:E:2001:HOH:O	2.28	0.65
1:D:132:ASP:OD1	1:D:133:MLY:N	2.34	0.60
1:D:219:GLU:HG3	1:D:222:MLY:HH22	1.83	0.60
1:D:184:LEU:O	1:D:188:ASN:ND2	2.25	0.59
1:F:186:ASN:ND2	3:F:1225:GOL:O2	2.35	0.59
1:E:191:MLY:HG2	1:E:194:ARG:HH21	1.66	0.59
1:A:109:LEU:HD21	1:B:73:ILE:CD1	2.28	0.59
1:C:130:ILE:HD12	1:C:136:VAL:HA	1.85	0.58
1:A:186:ASN:OD1	3:A:1233:GOL:O1	2.17	0.58
1:A:43:MLY:O	1:A:47:GLU:HG2	2.06	0.56
1:B:69:MLY:O	1:B:73:ILE:HG12	2.07	0.55
1:C:97:ASP:OD2	3:C:1227:GOL:O2	2.19	0.55
1:C:66:LEU:HG	1:C:70:MLY:HE2	1.89	0.55
1:A:149:MLY:HH13	1:A:212:ASP:OD1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:THR:OG1	1:B:180:LEU:N	2.42	0.53
1:D:121:GLN:HA	1:D:124:ALA:HB3	1.90	0.53
1:D:69:MLY:O	1:D:73:ILE:HG12	2.08	0.53
1:D:179:THR:HG1	1:D:182:GLU:H	1.57	0.52
1:D:63:GLU:H	1:D:63:GLU:CD	2.10	0.52
1:A:29:GLN:O	1:A:33:THR:HG23	2.10	0.52
1:B:152:ILE:HD13	1:B:207:TYR:HB3	1.91	0.52
1:D:23:ILE:HG23	1:D:24:THR:H	1.75	0.51
1:D:75:LEU:HD21	1:D:173:LEU:HD13	1.91	0.51
1:B:49:PHE:CE1	1:B:73:ILE:HD11	2.46	0.51
1:E:26:GLY:O	1:E:30:LEU:HG	2.11	0.50
1:F:111:LEU:HD11	1:F:138:TYR:CE1	2.47	0.50
1:F:69:MLY:O	1:F:73:ILE:HG12	2.12	0.50
1:C:206:ASN:HA	1:C:209:GLU:HG2	1.94	0.49
1:E:66:LEU:HD13	1:E:70:MLY:HG2	1.94	0.49
1:E:120:ASP:OD2	1:E:122:ASN:HB3	2.13	0.49
1:F:155:ARG:HD3	1:F:155:ARG:O	2.12	0.49
1:D:33:THR:O	1:D:37:THR:OG1	2.31	0.49
1:C:63:GLU:H	1:C:63:GLU:CD	2.15	0.48
1:C:63:GLU:N	1:C:63:GLU:OE1	2.33	0.48
1:D:219:GLU:HG2	1:D:223:ARG:NH1	2.29	0.48
1:E:132:ASP:OD1	1:E:133:MLY:N	2.47	0.47
1:E:224:GLN:O	1:E:227:GLN:HG2	2.15	0.46
1:C:69:MLY:O	1:C:73:ILE:HG12	2.16	0.46
1:D:173:LEU:O	1:D:186:ASN:ND2	2.48	0.46
1:D:63:GLU:OE1	1:D:63:GLU:N	2.46	0.45
1:C:33:THR:O	1:C:37:THR:OG1	2.33	0.45
1:E:119:LEU:HD12	1:E:140:GLU:HG2	1.99	0.44
1:A:144:MLY:HD3	1:A:144:MLY:HH23	1.68	0.44
1:F:88:ALA:CB	1:F:155:ARG:HH21	2.31	0.44
1:B:202:MLY:HH22	1:B:202:MLY:HD3	1.78	0.43
1:D:89:ASN:OD1	1:D:155:ARG:NH1	2.49	0.43
1:F:198:LEU:HD23	1:F:198:LEU:HA	1.76	0.43
1:F:97:ASP:OD1	1:F:207:TYR:OH	2.23	0.43
1:B:65:ALA:O	1:B:69:MLY:HG2	2.19	0.43
1:D:198:LEU:HA	1:D:198:LEU:HD23	1.90	0.43
1:D:37:THR:O	1:D:41:VAL:HG23	2.19	0.43
1:C:64:ASP:O	1:C:68:ILE:HG12	2.19	0.42
1:F:205:LEU:O	1:F:209:GLU:HG2	2.19	0.42
1:B:116:ILE:O	1:B:118:PRO:HD3	2.20	0.42
1:B:37:THR:O	1:B:41:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:LEU:HA	1:A:109:LEU:HD23	1.66	0.42
1:A:132:ASP:O	1:A:136:VAL:HG23	2.19	0.42
1:B:28:MLY:HH23	1:B:28:MLY:HD2	1.81	0.42
1:A:195:MLY:HH23	1:A:195:MLY:HD2	1.82	0.42
1:E:133:MLY:HH23	1:E:133:MLY:HD3	1.74	0.42
1:F:110:LEU:O	1:F:114:MET:HG2	2.18	0.42
1:F:177:SER:OG	1:F:186:ASN:OD1	2.37	0.42
1:F:100:PHE:HA	1:F:104:MET:HB2	2.01	0.42
1:A:152:ILE:HD13	1:A:207:TYR:HB3	2.01	0.42
1:E:45:LEU:HA	1:E:48:ILE:HD12	2.02	0.42
1:F:113:TYR:O	1:F:117:ASN:N	2.38	0.42
1:A:78:ASP:OD2	1:A:169:GLY:HA3	2.20	0.41
1:D:101:MLY:HE2	1:D:101:MLY:HB3	1.84	0.41
1:C:161:MLY:HH22	1:C:161:MLY:HD2	1.69	0.41
1:C:94:ILE:O	1:C:98:VAL:HG23	2.20	0.41
1:A:75:LEU:HD21	1:A:173:LEU:HD13	2.00	0.41
1:D:38:ASN:O	1:D:42:LEU:HG	2.21	0.41
1:A:144:MLY:HA	1:A:144:MLY:HD2	1.87	0.41
1:A:150:GLN:OE1	1:A:153:ARG:NH2	2.53	0.41
1:D:173:LEU:HA	1:D:173:LEU:HD12	1.90	0.41
1:F:43:MLY:HH12	1:F:43:MLY:HD3	1.85	0.41
1:C:62:GLU:H	1:C:62:GLU:CD	2.25	0.41
1:A:39:GLN:HG2	1:B:102:THR:HG21	2.02	0.41
1:A:69:MLY:HH12	1:A:69:MLY:HD3	1.83	0.41
1:E:177:SER:HB2	1:E:182:GLU:HB3	2.03	0.41
1:D:152:ILE:HD13	1:D:207:TYR:HB3	2.03	0.41
1:C:101:MLY:HD2	1:C:101:MLY:HH13	1.86	0.40
1:D:43:MLY:HH12	1:D:43:MLY:HD3	1.80	0.40
1:D:161:MLY:HH22	1:D:161:MLY:HD3	1.92	0.40
1:C:198:LEU:HD23	1:C:198:LEU:HA	1.85	0.40
1:F:111:LEU:HD11	1:F:138:TYR:CZ	2.56	0.40
1:A:161:MLY:HH23	1:A:161:MLY:HD2	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	183/220 (83%)	175 (96%)	8 (4%)	0	100	100
1	B	175/220 (80%)	168 (96%)	7 (4%)	0	100	100
1	C	161/220 (73%)	157 (98%)	3 (2%)	1 (1%)	25	59
1	D	172/220 (78%)	164 (95%)	8 (5%)	0	100	100
1	E	171/220 (78%)	163 (95%)	8 (5%)	0	100	100
1	F	143/220 (65%)	142 (99%)	1 (1%)	0	100	100
All	All	1005/1320 (76%)	969 (96%)	35 (4%)	1 (0%)	51	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	119	LEU

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	166/176 (94%)	160 (96%)	6 (4%)	35	63
1	B	161/176 (92%)	158 (98%)	3 (2%)	57	76
1	C	148/176 (84%)	142 (96%)	6 (4%)	30	60
1	D	155/176 (88%)	151 (97%)	4 (3%)	46	71
1	E	155/176 (88%)	153 (99%)	2 (1%)	69	82
1	F	131/176 (74%)	129 (98%)	2 (2%)	65	80
All	All	916/1056 (87%)	893 (98%)	23 (2%)	47	71

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ILE
1	A	51	THR
1	A	177	SER
1	A	179	THR
1	A	183	SER
1	A	229	ARG
1	B	31	ASP
1	B	50	SER
1	B	179	THR
1	C	36	GLU
1	C	37	THR
1	C	64	ASP
1	C	155	ARG
1	C	179	THR
1	C	183	SER
1	D	37	THR
1	D	63	GLU
1	D	155	ARG
1	D	179	THR
1	E	179	THR
1	E	224	GLN
1	F	33	THR
1	F	155	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	40	GLN
1	F	186	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

107 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	D	144	1	9,10,11	0.54	0	6,11,13	0.87	0
1	MLY	B	83	1	9,10,11	0.52	0	6,11,13	0.82	0
1	MLY	B	195	1	9,10,11	0.62	0	6,11,13	0.83	0
1	MLY	A	195	1	9,10,11	0.59	0	6,11,13	0.98	0
1	MLY	D	101	1	9,10,11	0.62	0	6,11,13	0.64	0
1	MLY	A	149	1	9,10,11	0.54	0	6,11,13	1.14	0
1	MLY	C	115	1	9,10,11	0.66	0	6,11,13	0.60	0
1	MLY	F	185	1	9,10,11	0.60	0	6,11,13	0.82	0
1	MLY	A	185	1	9,10,11	0.57	0	6,11,13	0.85	0
1	MLY	D	202	1	9,10,11	0.58	0	6,11,13	0.87	0
1	MLY	D	133	1	9,10,11	0.49	0	6,11,13	0.89	0
1	MLY	E	161	1	9,10,11	0.54	0	6,11,13	0.85	0
1	MLY	B	191	1	9,10,11	0.54	0	6,11,13	0.84	0
1	MLY	A	28	1	9,10,11	0.60	0	6,11,13	0.81	0
1	MLY	D	43	1	9,10,11	0.53	0	6,11,13	0.86	0
1	MLY	C	222	1	9,10,11	0.57	0	6,11,13	0.81	0
1	MLY	E	83	1	9,10,11	0.54	0	6,11,13	0.74	0
1	MLY	A	144	1	9,10,11	0.63	0	6,11,13	0.86	0
1	MLY	E	142	1	9,10,11	0.54	0	6,11,13	1.01	0
1	MLY	C	101	1	9,10,11	0.62	0	6,11,13	0.58	0
1	MLY	C	191	1	9,10,11	0.62	0	6,11,13	0.65	0
1	MLY	D	83	1	9,10,11	0.66	0	6,11,13	0.72	0
1	MLY	F	195	1	9,10,11	0.64	0	6,11,13	0.75	0
1	MLY	A	191	1	9,10,11	0.52	0	6,11,13	0.77	0
1	MLY	F	149	1	9,10,11	0.54	0	6,11,13	0.85	0
1	MLY	C	28	1	9,10,11	0.59	0	6,11,13	0.91	0
1	MLY	E	202	1	9,10,11	0.65	0	6,11,13	0.79	0
1	MLY	C	69	1	9,10,11	0.60	0	6,11,13	1.03	0
1	MLY	C	144	1	9,10,11	0.55	0	6,11,13	0.80	0
1	MLY	F	69	1	9,10,11	0.58	0	6,11,13	0.90	0
1	MLY	F	28	1	9,10,11	0.64	0	6,11,13	0.71	0
1	MLY	F	222	1	9,10,11	0.60	0	6,11,13	0.82	0
1	MLY	A	187	1	9,10,11	0.55	0	6,11,13	0.97	0
1	MLY	F	43	1	9,10,11	0.58	0	6,11,13	0.77	0
1	MLY	B	222	1	9,10,11	0.57	0	6,11,13	0.75	0
1	MLY	E	43	1	9,10,11	0.59	0	6,11,13	0.75	0
1	MLY	F	191	1	9,10,11	0.60	0	6,11,13	0.77	0
1	MLY	D	187	1	9,10,11	0.56	0	6,11,13	0.83	0
1	MLY	C	195	1	9,10,11	0.60	0	6,11,13	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	E	149	1	9,10,11	0.62	0	6,11,13	0.87	0
1	MLY	F	101	1	9,10,11	0.66	0	6,11,13	0.73	0
1	MLY	E	69	1	9,10,11	0.58	0	6,11,13	0.88	0
1	MLY	C	149	1	9,10,11	0.53	0	6,11,13	0.81	0
1	MLY	B	185	1	9,10,11	0.66	0	6,11,13	0.73	0
1	MLY	B	144	1	9,10,11	0.56	0	6,11,13	0.77	0
1	MLY	C	43	1	9,10,11	0.50	0	6,11,13	0.89	0
1	MLY	B	28	1	9,10,11	0.53	0	6,11,13	0.87	0
1	MLY	A	69	1	9,10,11	0.58	0	6,11,13	0.85	0
1	MLY	A	161	1	9,10,11	0.58	0	6,11,13	0.82	0
1	MLY	E	185	1	9,10,11	0.55	0	6,11,13	0.86	0
1	MLY	E	101	1	9,10,11	0.57	0	6,11,13	0.76	0
1	MLY	B	149	1	9,10,11	0.58	0	6,11,13	0.73	0
1	MLY	B	202	1	9,10,11	0.53	0	6,11,13	0.90	0
1	MLY	D	191	1	9,10,11	0.62	0	6,11,13	0.76	0
1	MLY	B	101	1	9,10,11	0.61	0	6,11,13	0.87	0
1	MLY	E	70	1	9,10,11	0.58	0	6,11,13	0.76	0
1	MLY	F	83	1	9,10,11	0.55	0	6,11,13	1.02	0
1	MLY	C	185	1	9,10,11	0.58	0	6,11,13	0.78	0
1	MLY	A	115	1	9,10,11	0.56	0	6,11,13	0.81	0
1	MLY	C	70	1	9,10,11	0.64	0	6,11,13	0.80	0
1	MLY	A	222	1	9,10,11	0.60	0	6,11,13	0.70	0
1	MLY	E	222	1	9,10,11	0.66	0	6,11,13	0.67	0
1	MLY	F	115	1	9,10,11	0.58	0	6,11,13	0.82	0
1	MLY	A	43	1	9,10,11	0.71	0	6,11,13	0.57	0
1	MLY	E	28	1	9,10,11	0.64	0	6,11,13	0.59	0
1	MLY	B	43	1	9,10,11	0.48	0	6,11,13	0.97	0
1	MLY	C	187	1	9,10,11	0.60	0	6,11,13	0.79	0
1	MLY	F	202	1	9,10,11	0.63	0	6,11,13	1.00	0
1	MLY	A	83	1	9,10,11	0.62	0	6,11,13	0.65	0
1	MLY	E	133	1	9,10,11	0.63	0	6,11,13	0.67	0
1	MLY	B	142	1	9,10,11	0.56	0	6,11,13	0.63	0
1	MLY	D	70	1	9,10,11	0.65	0	6,11,13	0.69	0
1	MLY	B	115	1	9,10,11	0.60	0	6,11,13	0.62	0
1	MLY	D	222	1	9,10,11	0.53	0	6,11,13	0.84	0
1	MLY	F	144	1	9,10,11	0.57	0	6,11,13	0.85	0
1	MLY	F	161	1	9,10,11	0.63	0	6,11,13	0.83	0
1	MLY	E	195	1	9,10,11	0.58	0	6,11,13	0.78	0
1	MLY	F	70	1	9,10,11	0.59	0	6,11,13	0.70	0
1	MLY	A	70	1	9,10,11	0.65	0	6,11,13	0.85	0
1	MLY	D	185	1	9,10,11	0.66	0	6,11,13	0.62	0
1	MLY	A	101	1	9,10,11	0.53	0	6,11,13	0.94	0
1	MLY	B	69	1	9,10,11	0.49	0	6,11,13	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	C	202	1	9,10,11	0.66	0	6,11,13	0.68	0
1	MLY	A	133	1	9,10,11	0.54	0	6,11,13	0.78	0
1	MLY	C	133	1	9,10,11	0.58	0	6,11,13	0.77	0
1	MLY	D	115	1	9,10,11	0.68	0	6,11,13	0.80	0
1	MLY	A	202	1	9,10,11	0.61	0	6,11,13	0.67	0
1	MLY	E	191	1	9,10,11	0.57	0	6,11,13	0.77	0
1	MLY	F	187	1	9,10,11	0.72	0	6,11,13	0.84	0
1	MLY	A	142	1	9,10,11	0.49	0	6,11,13	0.86	0
1	MLY	C	142	1	9,10,11	0.63	0	6,11,13	0.80	0
1	MLY	D	69	1	9,10,11	0.53	0	6,11,13	0.80	0
1	MLY	D	28	1	9,10,11	0.56	0	6,11,13	0.79	0
1	MLY	F	142	1	9,10,11	0.54	0	6,11,13	0.85	0
1	MLY	E	115	1	9,10,11	0.54	0	6,11,13	0.87	0
1	MLY	C	161	1	9,10,11	0.56	0	6,11,13	0.63	0
1	MLY	B	70	1	9,10,11	0.59	0	6,11,13	1.27	0
1	MLY	B	133	1	9,10,11	0.54	0	6,11,13	0.82	0
1	MLY	D	161	1	9,10,11	0.56	0	6,11,13	0.76	0
1	MLY	B	187	1	9,10,11	0.57	0	6,11,13	0.98	0
1	MLY	D	149	1	9,10,11	0.61	0	6,11,13	0.57	0
1	MLY	E	187	1	9,10,11	0.58	0	6,11,13	0.78	0
1	MLY	E	144	1	9,10,11	0.51	0	6,11,13	0.97	0
1	MLY	D	195	1	9,10,11	0.67	0	6,11,13	0.65	0
1	MLY	C	83	1	9,10,11	0.58	0	6,11,13	0.89	0
1	MLY	B	161	1	9,10,11	0.60	0	6,11,13	0.68	0
1	MLY	D	142	1	9,10,11	0.51	0	6,11,13	0.97	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	D	144	1	-	0/8/9/11	-
1	MLY	B	83	1	-	0/8/9/11	-
1	MLY	B	195	1	-	2/8/9/11	-
1	MLY	A	195	1	-	0/8/9/11	-
1	MLY	D	101	1	-	1/8/9/11	-
1	MLY	A	149	1	-	0/8/9/11	-
1	MLY	C	115	1	-	0/8/9/11	-
1	MLY	F	185	1	-	1/8/9/11	-
1	MLY	A	185	1	-	4/8/9/11	-
1	MLY	D	202	1	-	1/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	D	133	1	-	1/8/9/11	-
1	MLY	E	161	1	-	0/8/9/11	-
1	MLY	B	191	1	-	2/8/9/11	-
1	MLY	A	28	1	-	1/8/9/11	-
1	MLY	D	43	1	-	2/8/9/11	-
1	MLY	C	222	1	-	2/8/9/11	-
1	MLY	E	83	1	-	1/8/9/11	-
1	MLY	A	144	1	-	4/8/9/11	-
1	MLY	E	142	1	-	0/8/9/11	-
1	MLY	C	101	1	-	0/8/9/11	-
1	MLY	C	191	1	-	1/8/9/11	-
1	MLY	D	83	1	-	0/8/9/11	-
1	MLY	F	195	1	-	2/8/9/11	-
1	MLY	A	191	1	-	2/8/9/11	-
1	MLY	F	149	1	-	3/8/9/11	-
1	MLY	C	28	1	-	2/8/9/11	-
1	MLY	E	202	1	-	2/8/9/11	-
1	MLY	C	69	1	-	2/8/9/11	-
1	MLY	C	144	1	-	1/8/9/11	-
1	MLY	F	69	1	-	4/8/9/11	-
1	MLY	F	28	1	-	2/8/9/11	-
1	MLY	F	222	1	-	5/8/9/11	-
1	MLY	A	187	1	-	2/8/9/11	-
1	MLY	F	43	1	-	0/8/9/11	-
1	MLY	B	222	1	-	4/8/9/11	-
1	MLY	E	43	1	-	1/8/9/11	-
1	MLY	F	191	1	-	1/8/9/11	-
1	MLY	D	187	1	-	0/8/9/11	-
1	MLY	C	195	1	-	1/8/9/11	-
1	MLY	E	149	1	-	3/8/9/11	-
1	MLY	F	101	1	-	3/8/9/11	-
1	MLY	E	69	1	-	3/8/9/11	-
1	MLY	C	149	1	-	1/8/9/11	-
1	MLY	B	185	1	-	2/8/9/11	-
1	MLY	B	144	1	-	0/8/9/11	-
1	MLY	C	43	1	-	2/8/9/11	-
1	MLY	B	28	1	-	0/8/9/11	-
1	MLY	A	69	1	-	0/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	161	1	-	0/8/9/11	-
1	MLY	E	185	1	-	1/8/9/11	-
1	MLY	E	101	1	-	2/8/9/11	-
1	MLY	B	149	1	-	1/8/9/11	-
1	MLY	B	202	1	-	0/8/9/11	-
1	MLY	D	191	1	-	1/8/9/11	-
1	MLY	B	101	1	-	1/8/9/11	-
1	MLY	E	70	1	-	2/8/9/11	-
1	MLY	F	83	1	-	0/8/9/11	-
1	MLY	C	185	1	-	2/8/9/11	-
1	MLY	A	115	1	-	2/8/9/11	-
1	MLY	C	70	1	-	1/8/9/11	-
1	MLY	A	222	1	-	1/8/9/11	-
1	MLY	E	222	1	-	2/8/9/11	-
1	MLY	F	115	1	-	1/8/9/11	-
1	MLY	A	43	1	-	4/8/9/11	-
1	MLY	E	28	1	-	0/8/9/11	-
1	MLY	B	43	1	-	1/8/9/11	-
1	MLY	C	187	1	-	2/8/9/11	-
1	MLY	F	202	1	-	2/8/9/11	-
1	MLY	A	83	1	-	2/8/9/11	-
1	MLY	E	133	1	-	5/8/9/11	-
1	MLY	B	142	1	-	0/8/9/11	-
1	MLY	D	70	1	-	1/8/9/11	-
1	MLY	B	115	1	-	1/8/9/11	-
1	MLY	D	222	1	-	0/8/9/11	-
1	MLY	F	144	1	-	2/8/9/11	-
1	MLY	F	161	1	-	2/8/9/11	-
1	MLY	E	195	1	-	3/8/9/11	-
1	MLY	F	70	1	-	2/8/9/11	-
1	MLY	A	70	1	-	2/8/9/11	-
1	MLY	D	185	1	-	0/8/9/11	-
1	MLY	A	101	1	-	2/8/9/11	-
1	MLY	B	69	1	-	0/8/9/11	-
1	MLY	C	202	1	-	1/8/9/11	-
1	MLY	A	133	1	-	1/8/9/11	-
1	MLY	C	133	1	-	2/8/9/11	-
1	MLY	D	115	1	-	3/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	202	1	-	1/8/9/11	-
1	MLY	E	191	1	-	0/8/9/11	-
1	MLY	F	187	1	-	3/8/9/11	-
1	MLY	A	142	1	-	1/8/9/11	-
1	MLY	C	142	1	-	0/8/9/11	-
1	MLY	D	69	1	-	4/8/9/11	-
1	MLY	D	28	1	-	1/8/9/11	-
1	MLY	F	142	1	-	3/8/9/11	-
1	MLY	E	115	1	-	3/8/9/11	-
1	MLY	C	161	1	-	4/8/9/11	-
1	MLY	B	70	1	-	1/8/9/11	-
1	MLY	B	133	1	-	3/8/9/11	-
1	MLY	D	161	1	-	2/8/9/11	-
1	MLY	B	187	1	-	0/8/9/11	-
1	MLY	D	149	1	-	1/8/9/11	-
1	MLY	E	187	1	-	2/8/9/11	-
1	MLY	E	144	1	-	0/8/9/11	-
1	MLY	D	195	1	-	4/8/9/11	-
1	MLY	C	83	1	-	0/8/9/11	-
1	MLY	B	161	1	-	2/8/9/11	-
1	MLY	D	142	1	-	2/8/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (163) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	F	185	MLY	O-C-CA-CB
1	D	43	MLY	C-CA-CB-CG
1	D	142	MLY	C-CA-CB-CG
1	F	69	MLY	O-C-CA-CB
1	F	222	MLY	N-CA-CB-CG
1	F	222	MLY	O-C-CA-CB
1	E	149	MLY	C-CA-CB-CG
1	F	101	MLY	N-CA-CB-CG
1	F	101	MLY	C-CA-CB-CG
1	E	101	MLY	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	E	101	MLY	C-CA-CB-CG
1	E	70	MLY	C-CA-CB-CG
1	A	83	MLY	N-CA-CB-CG
1	A	83	MLY	C-CA-CB-CG
1	E	133	MLY	O-C-CA-CB
1	B	222	MLY	C-CA-CB-CG
1	A	101	MLY	C-CA-CB-CG
1	D	115	MLY	C-CA-CB-CG
1	A	142	MLY	C-CA-CB-CG
1	F	142	MLY	C-CA-CB-CG
1	C	161	MLY	N-CA-CB-CG
1	C	161	MLY	C-CA-CB-CG
1	F	69	MLY	CD-CE-NZ-CH1
1	B	133	MLY	CD-CE-NZ-CH2
1	A	187	MLY	CD-CE-NZ-CH1
1	A	187	MLY	CD-CE-NZ-CH2
1	E	69	MLY	CD-CE-NZ-CH1
1	E	69	MLY	CD-CE-NZ-CH2
1	C	43	MLY	CD-CE-NZ-CH1
1	C	43	MLY	CD-CE-NZ-CH2
1	E	133	MLY	CD-CE-NZ-CH1
1	F	144	MLY	CD-CE-NZ-CH2
1	C	133	MLY	CD-CE-NZ-CH1
1	C	133	MLY	CD-CE-NZ-CH2
1	D	115	MLY	CD-CE-NZ-CH1
1	D	115	MLY	CD-CE-NZ-CH2
1	D	69	MLY	CD-CE-NZ-CH1
1	D	69	MLY	CD-CE-NZ-CH2
1	E	115	MLY	CD-CE-NZ-CH1
1	B	133	MLY	CD-CE-NZ-CH1
1	E	187	MLY	CD-CE-NZ-CH1
1	D	195	MLY	CD-CE-NZ-CH1
1	D	195	MLY	CD-CE-NZ-CH2
1	F	187	MLY	CG-CD-CE-NZ
1	B	115	MLY	CG-CD-CE-NZ
1	E	195	MLY	CG-CD-CE-NZ
1	C	161	MLY	CG-CD-CE-NZ
1	A	43	MLY	CG-CD-CE-NZ
1	A	185	MLY	CD-CE-NZ-CH1
1	A	185	MLY	CD-CE-NZ-CH2
1	E	149	MLY	CD-CE-NZ-CH2
1	A	222	MLY	CD-CE-NZ-CH1

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Mol	Chain	Res	Type	Atoms
1	E	222	MLY	CD-CE-NZ-CH1
1	A	43	MLY	CD-CE-NZ-CH1
1	E	187	MLY	CD-CE-NZ-CH2
1	F	149	MLY	CG-CD-CE-NZ
1	F	28	MLY	CA-CB-CG-CD
1	D	28	MLY	CA-CB-CG-CD
1	B	195	MLY	CD-CE-NZ-CH1
1	E	149	MLY	CD-CE-NZ-CH1
1	B	185	MLY	CD-CE-NZ-CH1
1	B	149	MLY	CD-CE-NZ-CH1
1	E	133	MLY	CD-CE-NZ-CH2
1	C	185	MLY	CA-CB-CG-CD
1	B	195	MLY	CD-CE-NZ-CH2
1	F	69	MLY	CD-CE-NZ-CH2
1	B	161	MLY	CD-CE-NZ-CH2
1	F	144	MLY	CD-CE-NZ-CH1
1	F	222	MLY	CA-CB-CG-CD
1	E	195	MLY	CA-CB-CG-CD
1	E	115	MLY	CG-CD-CE-NZ
1	A	185	MLY	CA-CB-CG-CD
1	C	69	MLY	CA-CB-CG-CD
1	A	70	MLY	CG-CD-CE-NZ
1	D	101	MLY	CD-CE-NZ-CH1
1	F	202	MLY	CD-CE-NZ-CH1
1	F	70	MLY	CD-CE-NZ-CH2
1	F	195	MLY	CG-CD-CE-NZ
1	D	195	MLY	CA-CB-CG-CD
1	A	144	MLY	CG-CD-CE-NZ
1	E	195	MLY	CE-CD-CG-CB
1	E	70	MLY	CA-CB-CG-CD
1	D	195	MLY	CE-CD-CG-CB
1	A	28	MLY	CE-CD-CG-CB
1	D	133	MLY	CE-CD-CG-CB
1	B	222	MLY	CE-CD-CG-CB
1	F	187	MLY	CE-CD-CG-CB
1	F	195	MLY	CE-CD-CG-CB
1	A	70	MLY	CE-CD-CG-CB
1	A	115	MLY	CE-CD-CG-CB
1	A	144	MLY	CE-CD-CG-CB
1	C	161	MLY	CE-CD-CG-CB
1	C	28	MLY	CA-CB-CG-CD
1	F	101	MLY	CA-CB-CG-CD

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Mol	Chain	Res	Type	Atoms
1	D	70	MLY	CA-CB-CG-CD
1	F	161	MLY	CA-CB-CG-CD
1	A	202	MLY	CA-CB-CG-CD
1	F	142	MLY	CA-CB-CG-CD
1	C	70	MLY	CD-CE-NZ-CH1
1	A	43	MLY	CD-CE-NZ-CH2
1	F	69	MLY	CE-CD-CG-CB
1	F	161	MLY	CE-CD-CG-CB
1	E	202	MLY	CA-CB-CG-CD
1	F	222	MLY	C-CA-CB-CG
1	B	43	MLY	C-CA-CB-CG
1	B	185	MLY	CE-CD-CG-CB
1	B	222	MLY	CA-CB-CG-CD
1	D	191	MLY	CE-CD-CG-CB
1	A	43	MLY	CE-CD-CG-CB
1	A	144	MLY	CA-CB-CG-CD
1	D	69	MLY	CE-CD-CG-CB
1	F	28	MLY	CG-CD-CE-NZ
1	F	222	MLY	CE-CD-CG-CB
1	D	149	MLY	CE-CD-CG-CB
1	C	191	MLY	CD-CE-NZ-CH1
1	F	142	MLY	CD-CE-NZ-CH2
1	E	133	MLY	CA-CB-CG-CD
1	F	149	MLY	CD-CE-NZ-CH1
1	B	191	MLY	CD-CE-NZ-CH1
1	E	83	MLY	CD-CE-NZ-CH2
1	E	222	MLY	CD-CE-NZ-CH2
1	B	222	MLY	CG-CD-CE-NZ
1	F	115	MLY	CE-CD-CG-CB
1	D	43	MLY	N-CA-CB-CG
1	C	222	MLY	N-CA-CB-CG
1	C	69	MLY	N-CA-CB-CG
1	C	187	MLY	CD-CE-NZ-CH1
1	E	202	MLY	CE-CD-CG-CB
1	C	222	MLY	C-CA-CB-CG
1	D	161	MLY	CE-CD-CG-CB
1	C	144	MLY	CA-CB-CG-CD
1	E	133	MLY	CG-CD-CE-NZ
1	D	161	MLY	CD-CE-NZ-CH1
1	B	101	MLY	CD-CE-NZ-CH1
1	B	133	MLY	CA-CB-CG-CD
1	C	28	MLY	CE-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
1	C	187	MLY	CE-CD-CG-CB
1	F	202	MLY	CA-CB-CG-CD
1	A	115	MLY	CG-CD-CE-NZ
1	D	202	MLY	CE-CD-CG-CB
1	A	101	MLY	CA-CB-CG-CD
1	B	161	MLY	CD-CE-NZ-CH1
1	E	115	MLY	CD-CE-NZ-CH2
1	A	191	MLY	CD-CE-NZ-CH1
1	E	69	MLY	CG-CD-CE-NZ
1	B	191	MLY	C-CA-CB-CG
1	F	149	MLY	C-CA-CB-CG
1	C	195	MLY	C-CA-CB-CG
1	D	69	MLY	C-CA-CB-CG
1	B	70	MLY	C-CA-CB-CG
1	F	191	MLY	CD-CE-NZ-CH1
1	C	149	MLY	CE-CD-CG-CB
1	F	187	MLY	CA-CB-CG-CD
1	A	191	MLY	CE-CD-CG-CB
1	A	133	MLY	CG-CD-CE-NZ
1	C	202	MLY	CD-CE-NZ-CH1
1	E	43	MLY	CE-CD-CG-CB
1	E	185	MLY	CG-CD-CE-NZ
1	A	144	MLY	CD-CE-NZ-CH2
1	C	185	MLY	CE-CD-CG-CB
1	A	185	MLY	N-CA-CB-CG
1	D	142	MLY	N-CA-CB-CG
1	F	70	MLY	CE-CD-CG-CB

There are no ring outliers.

25 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	195	MLY	1	0
1	D	101	MLY	1	0
1	A	149	MLY	1	0
1	D	133	MLY	1	0
1	D	43	MLY	1	0
1	A	144	MLY	2	0
1	C	101	MLY	1	0
1	C	69	MLY	1	0
1	F	69	MLY	1	0
1	F	43	MLY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	28	MLY	1	0
1	A	69	MLY	1	0
1	A	161	MLY	1	0
1	B	202	MLY	1	0
1	E	70	MLY	1	0
1	C	70	MLY	1	0
1	A	43	MLY	1	0
1	E	133	MLY	2	0
1	D	222	MLY	1	0
1	B	69	MLY	2	0
1	C	133	MLY	1	0
1	E	191	MLY	1	0
1	D	69	MLY	1	0
1	C	161	MLY	1	0
1	D	161	MLY	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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	$\# Z > 2$
4	PO4	F	1226	-	4,4,4	0.92	0	6,6,6	0.43	0
3	GOL	F	1225	-	5,5,5	0.37	0	5,5,5	0.37	0
4	PO4	B	1232	-	4,4,4	0.92	0	6,6,6	0.45	0
3	GOL	E	1231	-	5,5,5	0.39	0	5,5,5	0.19	0
3	GOL	A	1234	-	5,5,5	0.38	0	5,5,5	0.20	0
2	PEG	A	1232	-	6,6,6	0.67	0	5,5,5	0.76	0
3	GOL	C	1227	-	5,5,5	0.42	0	5,5,5	0.22	0
3	GOL	B	1230	-	5,5,5	0.39	0	5,5,5	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	D	1228	-	5,5,5	0.39	0	5,5,5	0.17	0
3	GOL	A	1233	-	5,5,5	0.41	0	5,5,5	0.34	0
3	GOL	B	1231	-	5,5,5	0.38	0	5,5,5	0.24	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	GOL	F	1225	-	-	2/4/4/4	-
3	GOL	E	1231	-	-	2/4/4/4	-
3	GOL	A	1234	-	-	2/4/4/4	-
2	PEG	A	1232	-	-	3/4/4/4	-
3	GOL	C	1227	-	-	2/4/4/4	-
3	GOL	B	1230	-	-	2/4/4/4	-
3	GOL	D	1228	-	-	2/4/4/4	-
3	GOL	A	1233	-	-	4/4/4/4	-
3	GOL	B	1231	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	1225	GOL	C1-C2-C3-O3
3	E	1231	GOL	C1-C2-C3-O3
3	A	1234	GOL	C1-C2-C3-O3
3	D	1228	GOL	C1-C2-C3-O3
3	A	1233	GOL	C1-C2-C3-O3
3	B	1231	GOL	C1-C2-C3-O3
3	A	1233	GOL	O2-C2-C3-O3
2	A	1232	PEG	O1-C1-C2-O2
3	B	1230	GOL	C1-C2-C3-O3
3	F	1225	GOL	O2-C2-C3-O3
3	A	1234	GOL	O2-C2-C3-O3
3	B	1231	GOL	O2-C2-C3-O3
2	A	1232	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
3	C	1227	GOL	O2-C2-C3-O3
3	E	1231	GOL	O2-C2-C3-O3
3	D	1228	GOL	O2-C2-C3-O3
2	A	1232	PEG	C1-C2-O2-C3
3	C	1227	GOL	C1-C2-C3-O3
3	B	1230	GOL	O2-C2-C3-O3
3	A	1233	GOL	O1-C1-C2-C3
3	A	1233	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1225	GOL	1	0
3	E	1231	GOL	1	0
3	C	1227	GOL	1	0
3	A	1233	GOL	1	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	187/220 (85%)	-0.08	2 (1%) 80 80	31, 61, 150, 176	0
1	B	181/220 (82%)	-0.08	3 (1%) 70 67	26, 71, 161, 190	0
1	C	167/220 (75%)	0.05	1 (0%) 89 89	35, 86, 146, 193	0
1	D	176/220 (80%)	-0.10	2 (1%) 80 80	42, 88, 174, 204	0
1	E	175/220 (79%)	-0.07	3 (1%) 70 67	49, 90, 167, 189	0
1	F	149/220 (67%)	0.05	1 (0%) 87 88	42, 96, 154, 183	0
All	All	1035/1320 (78%)	-0.04	12 (1%) 79 77	26, 83, 163, 204	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	66	LEU	4.1
1	B	227	GLN	3.3
1	E	121	GLN	2.7
1	D	130	ILE	2.7
1	D	121	GLN	2.5
1	A	227	GLN	2.5
1	E	68	ILE	2.4
1	B	51	THR	2.3
1	B	228	GLU	2.3
1	A	228	GLU	2.2
1	C	225	TYR	2.0
1	F	116	ILE	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(\AA^2)	Q<0.9
1	MLY	E	70	11/12	0.80	0.45	123,150,159,163	0
1	MLY	F	101	11/12	0.82	0.33	101,132,153,154	0
1	MLY	D	115	11/12	0.82	0.50	113,136,145,147	0
1	MLY	E	43	11/12	0.86	0.45	124,140,155,163	0
1	MLY	F	115	11/12	0.89	0.62	124,136,153,158	0
1	MLY	C	133	11/12	0.89	0.41	127,154,169,170	0
1	MLY	D	133	11/12	0.89	0.42	148,153,169,186	0
1	MLY	E	133	11/12	0.90	0.20	115,121,129,133	0
1	MLY	E	69	11/12	0.91	0.22	152,158,168,178	0
1	MLY	F	144	11/12	0.91	0.33	112,121,123,123	0
1	MLY	C	101	11/12	0.91	0.29	84,102,126,128	0
1	MLY	F	69	11/12	0.91	0.22	107,120,132,132	0
1	MLY	C	142	11/12	0.91	0.39	83,101,124,124	0
1	MLY	E	115	11/12	0.91	0.28	77,92,119,123	0
1	MLY	B	133	11/12	0.91	0.34	112,127,139,141	0
1	MLY	B	222	11/12	0.92	0.20	102,118,144,151	0
1	MLY	C	222	11/12	0.92	0.30	110,118,127,128	0
1	MLY	F	222	11/12	0.92	0.35	122,137,155,156	0
1	MLY	F	149	11/12	0.92	0.39	114,126,135,137	0
1	MLY	E	28	11/12	0.92	0.22	113,117,126,136	0
1	MLY	C	69	11/12	0.92	0.27	85,104,137,141	0
1	MLY	B	115	11/12	0.92	0.27	97,109,116,117	0
1	MLY	C	43	11/12	0.93	0.43	130,145,163,163	0
1	MLY	D	101	11/12	0.93	0.38	100,105,125,126	0
1	MLY	C	115	11/12	0.93	0.37	87,114,121,122	0
1	MLY	C	28	11/12	0.93	0.32	81,100,127,128	0
1	MLY	F	70	11/12	0.93	0.34	107,114,120,121	0
1	MLY	B	28	11/12	0.94	0.28	63,79,116,116	0
1	MLY	D	70	11/12	0.94	0.23	78,93,136,137	0
1	MLY	E	185	11/12	0.94	0.23	54,69,81,81	0
1	MLY	E	101	11/12	0.94	0.29	77,96,138,139	0
1	MLY	D	222	11/12	0.94	0.32	146,156,170,171	0
1	MLY	D	191	11/12	0.94	0.24	43,56,92,102	0
1	MLY	D	144	11/12	0.94	0.30	94,102,113,115	0
1	MLY	A	115	11/12	0.94	0.32	75,80,110,113	0
1	MLY	E	222	11/12	0.94	0.24	76,98,134,134	0
1	MLY	F	187	11/12	0.94	0.26	53,69,92,100	0
1	MLY	F	43	11/12	0.94	0.26	93,114,126,129	0
1	MLY	D	69	11/12	0.94	0.20	83,100,119,119	0
1	MLY	D	28	11/12	0.94	0.30	68,84,107,113	0
1	MLY	F	142	11/12	0.94	0.29	114,133,147,148	0
1	MLY	D	43	11/12	0.94	0.28	87,118,125,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	MLY	B	43	11/12	0.94	0.19	63,89,127,131	0
1	MLY	E	195	11/12	0.95	0.21	57,75,112,117	0
1	MLY	A	43	11/12	0.95	0.23	50,67,125,127	0
1	MLY	D	185	11/12	0.95	0.20	44,61,71,75	0
1	MLY	A	133	11/12	0.95	0.20	96,108,112,113	0
1	MLY	E	161	11/12	0.95	0.32	70,94,112,113	0
1	MLY	D	142	11/12	0.95	0.25	105,114,133,139	0
1	MLY	E	191	11/12	0.95	0.19	54,74,123,124	0
1	MLY	C	191	11/12	0.95	0.21	52,58,97,103	0
1	MLY	F	191	11/12	0.95	0.26	37,65,126,132	0
1	MLY	C	144	11/12	0.95	0.34	51,79,84,85	0
1	MLY	B	191	11/12	0.95	0.27	42,58,91,92	0
1	MLY	B	185	11/12	0.95	0.23	42,55,78,80	0
1	MLY	F	28	11/12	0.95	0.25	115,139,155,159	0
1	MLY	F	161	11/12	0.95	0.25	47,82,106,107	0
1	MLY	E	144	11/12	0.95	0.22	68,74,83,87	0
1	MLY	C	83	11/12	0.95	0.22	54,72,88,91	0
1	MLY	E	202	11/12	0.96	0.19	45,65,123,125	0
1	MLY	B	101	11/12	0.96	0.19	41,60,100,109	0
1	MLY	E	83	11/12	0.96	0.30	65,85,109,116	0
1	MLY	F	83	11/12	0.96	0.21	57,72,98,106	0
1	MLY	C	195	11/12	0.96	0.25	39,67,96,101	0
1	MLY	A	101	11/12	0.96	0.23	48,60,93,101	0
1	MLY	C	202	11/12	0.96	0.16	43,61,95,101	0
1	MLY	A	222	11/12	0.96	0.26	82,90,99,100	0
1	MLY	D	202	11/12	0.96	0.24	45,68,128,130	0
1	MLY	A	28	11/12	0.96	0.23	54,65,99,101	0
1	MLY	A	202	11/12	0.96	0.23	39,58,120,121	0
1	MLY	F	195	11/12	0.96	0.23	60,69,118,119	0
1	MLY	B	144	11/12	0.96	0.23	62,71,87,89	0
1	MLY	A	142	11/12	0.96	0.45	65,87,99,101	0
1	MLY	A	191	11/12	0.96	0.21	26,39,108,112	0
1	MLY	F	202	11/12	0.96	0.23	63,75,98,98	0
1	MLY	B	195	11/12	0.96	0.24	47,60,107,110	0
1	MLY	B	142	11/12	0.96	0.23	77,89,138,143	0
1	MLY	A	161	11/12	0.96	0.22	32,43,81,81	0
1	MLY	A	195	11/12	0.96	0.23	25,52,102,105	0
1	MLY	D	161	11/12	0.96	0.16	39,55,86,90	0
1	MLY	B	187	11/12	0.96	0.20	41,51,65,71	0
1	MLY	B	161	11/12	0.96	0.27	40,52,91,93	0
1	MLY	B	202	11/12	0.96	0.21	54,65,106,110	0
1	MLY	D	187	11/12	0.97	0.19	35,64,119,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	MLY	A	185	11/12	0.97	0.20	39,42,64,66	0
1	MLY	E	149	11/12	0.97	0.31	67,70,75,76	0
1	MLY	A	69	11/12	0.97	0.27	30,41,115,120	0
1	MLY	C	187	11/12	0.97	0.21	55,72,104,104	0
1	MLY	E	142	11/12	0.97	0.31	48,96,107,108	0
1	MLY	A	83	11/12	0.97	0.31	30,47,79,81	0
1	MLY	B	69	11/12	0.97	0.25	48,57,97,99	0
1	MLY	C	161	11/12	0.97	0.21	54,61,92,94	0
1	MLY	C	185	11/12	0.97	0.18	59,71,98,103	0
1	MLY	F	185	11/12	0.97	0.27	42,52,70,74	0
1	MLY	C	70	11/12	0.97	0.20	79,91,111,111	0
1	MLY	D	149	11/12	0.97	0.20	57,77,94,95	0
1	MLY	E	187	11/12	0.97	0.22	49,74,94,100	0
1	MLY	A	187	11/12	0.97	0.20	41,54,69,87	0
1	MLY	D	195	11/12	0.97	0.18	38,48,95,98	0
1	MLY	B	149	11/12	0.97	0.21	63,79,86,92	0
1	MLY	C	149	11/12	0.97	0.26	54,64,78,79	0
1	MLY	B	70	11/12	0.98	0.20	33,45,57,63	0
1	MLY	A	144	11/12	0.98	0.32	48,58,83,85	0
1	MLY	D	83	11/12	0.98	0.21	32,53,68,69	0
1	MLY	A	149	11/12	0.98	0.28	57,62,77,80	0
1	MLY	B	83	11/12	0.98	0.25	27,35,93,98	0
1	MLY	A	70	11/12	0.99	0.20	23,32,50,54	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
3	GOL	E	1231	6/6	0.76	0.36	94,106,115,120	0
4	PO4	F	1226	5/5	0.83	0.20	160,162,167,173	0
3	GOL	B	1230	6/6	0.83	0.35	75,80,92,98	0
4	PO4	B	1232	5/5	0.84	0.25	150,153,156,156	0
3	GOL	D	1228	6/6	0.84	0.43	76,101,107,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	C	1227	6/6	0.88	0.55	95,103,111,122	0
5	K	D	1229	1/1	0.90	0.23	114,114,114,114	0
3	GOL	A	1234	6/6	0.91	0.26	104,111,115,119	0
3	GOL	F	1225	6/6	0.93	0.43	74,100,106,107	0
2	PEG	A	1232	7/7	0.94	0.19	95,100,106,110	0
3	GOL	B	1231	6/6	0.94	0.36	101,104,104,107	0
3	GOL	A	1233	6/6	0.95	0.26	73,96,108,110	0

6.5 Other polymers [i](#)

There are no such residues in this entry.