



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:29 AM UTC

PDB ID : 9DCZ / pdb\_00009dcz  
Title : Designed allosteric facilitated dissociation switch AS1 in complex state TH with methylated lysines, crystal #1  
Authors : Bera, A.K.; Broerman, A.; Baker, D.  
Deposited on : 2024-08-27  
Resolution : 2.90 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](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

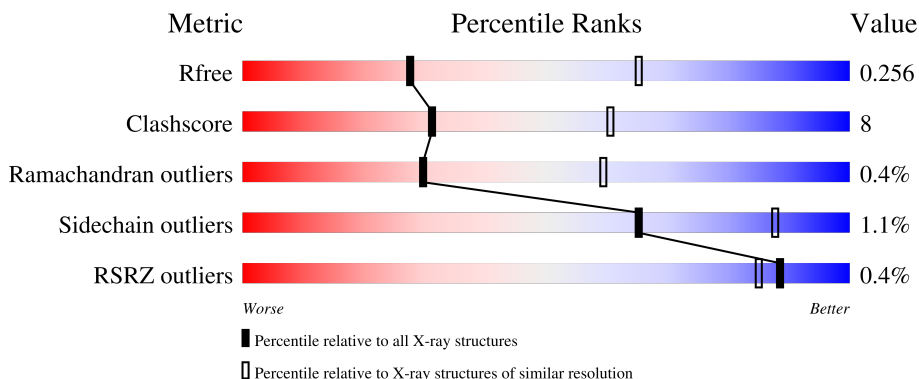
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 2.90 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))
$R_{free}$	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	263	 77% 20% .
1	C	263	 73% 24% . .
2	B	130	 77% 19% .
2	D	130	 78% 17% 5%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6025 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.

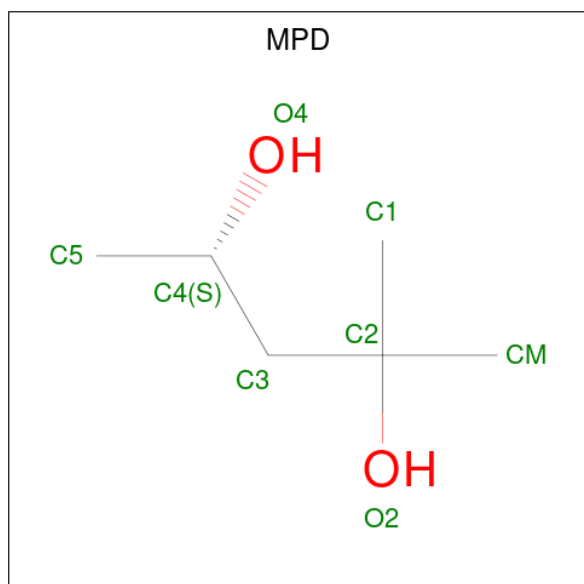
- Molecule 1 is a protein called Designed allosteric facilitated dissociation switch AS1 H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			2003	1282	340	376	5			
1	C	255	Total	C	N	O	S	0	0	0
			2003	1282	340	376	5			

- Molecule 2 is a protein called Designed allosteric facilitated dissociation switch AS1 T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	125	Total	C	N	O	S	0	0	0
			1004	621	188	191	4			
2	D	124	Total	C	N	O	S	0	0	0
			1000	619	187	190	4			

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			8	6	2		

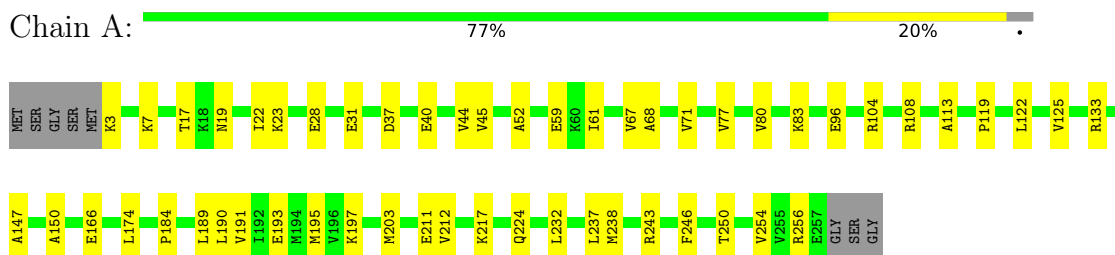
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	B	1	Total	O	0	0
			1	1		
4	D	5	Total	O	0	0
			5	5		

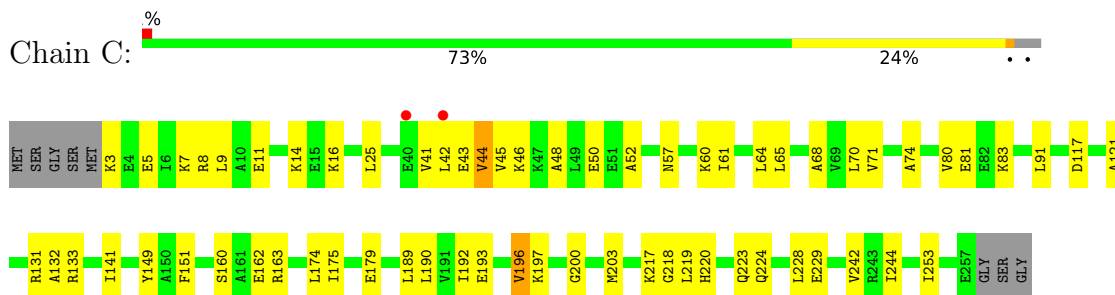
### 3 Residue-property plots [i](#)

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

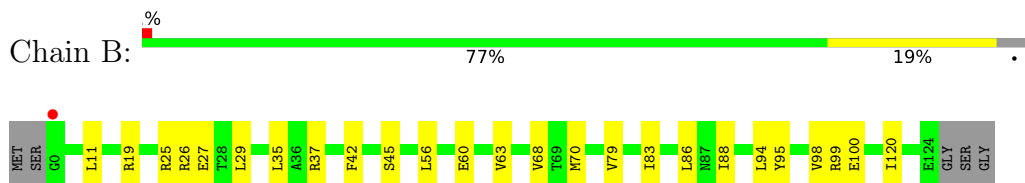
- Molecule 1: Designed allosteric facilitated dissociation switch AS1 H



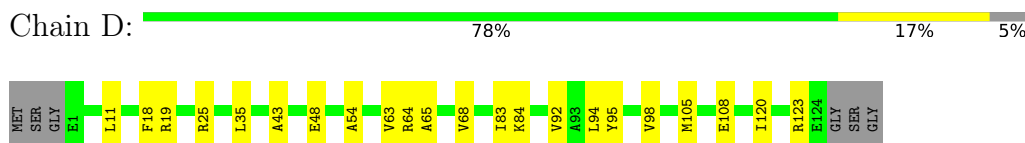
- Molecule 1: Designed allosteric facilitated dissociation switch AS1 H



- Molecule 2: Designed allosteric facilitated dissociation switch AS1 T



- Molecule 2: Designed allosteric facilitated dissociation switch AS1 T



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.71 Å 80.71 Å 546.86 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.75 – 2.90 34.75 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.75-2.90) 99.7 (34.75-2.90)	Depositor EDS
$R_{merge}$	0.37	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 2.90 Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, $R_{free}$	0.209 , 0.255 0.212 , 0.256	Depositor DCC
$R_{free}$ test set	2000 reflections (8.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.5	Xtriage
Anisotropy	0.485	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 78.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6025	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MPD, MLY

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.10	0/1749	0.25	0/2376
1	C	0.16	0/1749	0.32	0/2376
2	B	0.10	0/979	0.22	0/1317
2	D	0.11	0/975	0.24	0/1312
All	All	0.12	0/5452	0.27	0/7381

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	2003	0	2158	36	0
1	C	2003	0	2160	41	0
2	B	1004	0	1020	19	0
2	D	1000	0	1017	14	0
3	B	8	0	14	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	D	5	0	0	2	0
All	All	6025	0	6369	101	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 8.

All (101) 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:C:52:ALA:HB1	1:C:61:ILE:HG23	1.55	0.87
1:A:184:PRO:HB3	1:A:238:MET:HB3	1.67	0.76
2:B:56:LEU:HD21	2:B:79:VAL:HG11	1.67	0.75
1:A:147:ALA:HB2	1:A:174:LEU:HD22	1.70	0.71
2:D:98:VAL:HG21	2:D:120:ILE:HD13	1.78	0.65
1:A:211:GLU:HB3	1:A:256:ARG:HD3	1.81	0.63
2:B:68:VAL:HG11	2:B:86:LEU:HD23	1.82	0.62
1:C:80:VAL:HG13	1:C:83:MLY:HD3	1.82	0.61
1:C:57:ASN:HB3	1:C:60:MLY:HB3	1.82	0.60
1:C:3:MLY:HD3	1:C:5:GLU:HB2	1.84	0.60
1:A:17:THR:HG21	1:A:23:MLY:HB3	1.84	0.60
1:A:59:GLU:OE1	2:B:26:ARG:NH2	2.35	0.60
2:D:108:GLU:OE1	2:D:123:ARG:NH1	2.36	0.59
1:A:150:ALA:HB1	1:A:195:MET:HE3	1.85	0.58
1:C:132:ALA:HB1	1:C:141:ILE:HG13	1.85	0.58
1:C:131:ARG:NH1	1:C:179:GLU:OE1	2.36	0.58
1:A:37:ASP:OD2	1:A:37:ASP:N	2.36	0.58
1:A:246:PHE:HB3	2:B:99:ARG:HH22	1.68	0.58
2:B:83:ILE:HD13	2:B:94:LEU:HD21	1.86	0.58
1:C:70:LEU:HD11	1:C:83:MLY:HD2	1.85	0.57
1:C:174:LEU:HD23	1:C:190:LEU:HB2	1.86	0.57
1:A:189:LEU:HD11	1:A:212:VAL:HG21	1.84	0.57
1:C:25:LEU:HB3	1:C:65:LEU:HB3	1.86	0.57
1:A:193:GLU:HA	1:A:203:MET:HE1	1.88	0.56
2:B:37:ARG:NE	2:B:100:GLU:OE2	2.22	0.56
1:C:117:ASP:OD1	1:C:117:ASP:N	2.36	0.56
2:D:43:ALA:HB3	2:D:105:MET:HE1	1.88	0.55
1:C:217:MLY:O	1:C:219:LEU:N	2.40	0.54
2:B:19:ARG:HH22	3:B:401:MPD:HM3	1.73	0.53
2:D:63:VAL:HG13	2:D:68:VAL:HG23	1.89	0.53
2:B:98:VAL:HG21	2:B:120:ILE:HD13	1.90	0.53
1:C:193:GLU:HG2	1:C:203:MET:HE1	1.91	0.53
1:C:3:MLY:HD2	1:C:46:MLY:HH23	1.90	0.52
1:C:48:ALA:HA	1:C:64:LEU:HD22	1.92	0.52
1:C:149:TYR:OH	1:C:229:GLU:OE2	2.25	0.52
1:C:175:ILE:O	1:C:179:GLU:HG2	2.10	0.52
1:C:45:VAL:HG13	1:C:68:ALA:HB1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:64:ARG:NH2	4:D:401:HOH:O	2.41	0.52
2:D:83:ILE:HD13	2:D:94:LEU:HD21	1.92	0.51
1:A:166:GLU:HB3	1:A:197:MLY:HG3	1.93	0.51
1:A:224:GLN:OE1	2:B:99:ARG:NH1	2.44	0.51
2:B:42:PHE:O	2:B:45:SER:OG	2.29	0.51
1:C:224:GLN:OE1	2:D:95:TYR:OH	2.28	0.51
1:A:28:GLU:OE2	1:C:160:SER:OG	2.21	0.50
1:C:11:GLU:OE1	1:C:11:GLU:N	2.38	0.50
1:A:19:ASN:HB3	1:A:22:ILE:HB	1.94	0.50
1:C:81:GLU:N	1:C:81:GLU:OE1	2.45	0.50
2:B:95:TYR:OH	2:B:99:ARG:NH1	2.46	0.49
1:A:19:ASN:ND2	2:B:27:GLU:HB2	2.28	0.48
1:A:96:GLU:OE2	1:A:133:ARG:NH1	2.47	0.48
1:A:217:MLY:HG2	1:A:250:THR:HG22	1.96	0.48
1:C:80:VAL:N	1:C:81:GLU:OE1	2.47	0.48
2:D:54:ALA:HB1	2:D:105:MET:HE3	1.96	0.48
1:C:74:ALA:HB1	1:C:80:VAL:HG21	1.95	0.47
1:C:3:MLY:HH12	1:C:41:VAL:HG12	1.97	0.47
1:C:121:ALA:HA	1:C:151:PHE:HE2	1.78	0.47
2:B:25:ARG:O	2:B:29:LEU:HD23	2.13	0.47
1:A:232:LEU:HB3	2:B:88:ILE:HG13	1.95	0.47
1:C:163:ARG:HH21	1:C:197:MLY:HA	1.79	0.47
2:D:48:GLU:H	2:D:48:GLU:CD	2.22	0.46
1:A:80:VAL:HG12	1:A:83:MLY:HH13	1.97	0.46
1:C:163:ARG:CZ	1:C:200:GLY:HA2	2.46	0.46
1:A:189:LEU:HD21	1:A:212:VAL:HG11	1.97	0.46
1:A:174:LEU:HD12	1:A:190:LEU:HB3	1.97	0.46
1:A:40:GLU:HB3	1:A:77:VAL:HG21	1.97	0.45
1:A:7:MLY:HH23	1:A:7:MLY:HD2	1.78	0.45
1:A:237:LEU:HB3	1:A:238:MET:HE2	1.99	0.45
1:A:113:ALA:HB2	1:A:125:VAL:HG21	1.98	0.45
1:C:228:LEU:HD23	2:D:92:VAL:HG12	1.99	0.45
1:C:14:MLY:HH12	1:C:14:MLY:HD3	1.76	0.45
1:C:7:MLY:O	1:C:9:LEU:N	2.50	0.45
1:A:52:ALA:HB1	1:A:61:ILE:HG23	1.99	0.44
1:A:67:VAL:O	1:A:71:VAL:HG23	2.17	0.44
1:C:192:ILE:O	1:C:196:VAL:HG13	2.17	0.44
1:A:31:GLU:O	1:A:31:GLU:HG2	2.18	0.44
2:B:60:GLU:HG3	2:B:70:MET:HE1	1.99	0.44
1:A:174:LEU:HD11	1:A:191:VAL:HG23	2.00	0.44
1:C:9:LEU:HD13	1:C:50:GLU:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:ILE:HG23	1:C:253:ILE:HG12	2.00	0.43
2:B:25:ARG:HA	2:B:25:ARG:HD3	1.80	0.43
2:B:63:VAL:HG13	2:B:68:VAL:HG23	1.99	0.43
2:D:18:PHE:CE2	2:D:65:ALA:HB1	2.54	0.43
1:A:3:MLY:HE3	1:A:3:MLY:HB2	1.69	0.43
2:D:25:ARG:NH2	4:D:402:HOH:O	2.52	0.43
1:C:133:ARG:CZ	1:C:133:ARG:HB3	2.49	0.43
1:A:19:ASN:HD22	2:B:27:GLU:HB2	1.84	0.42
2:B:11:LEU:HD22	2:B:35:LEU:HD22	2.02	0.42
1:C:44:VAL:HG11	1:C:71:VAL:HG11	2.01	0.42
1:C:163:ARG:NE	1:C:197:MLY:O	2.48	0.42
1:C:43:GLU:O	1:C:45:VAL:N	2.53	0.42
1:A:243:ARG:HH21	1:A:254:VAL:HG21	1.84	0.42
1:C:16:MLY:HB3	1:C:16:MLY:HE3	1.73	0.42
1:A:44:VAL:HG11	1:A:71:VAL:HG21	2.02	0.41
1:A:119:PRO:HA	1:A:122:LEU:HD12	2.01	0.41
2:D:84:MLY:HH22	2:D:84:MLY:HD3	1.90	0.41
1:C:217:MLY:HH23	1:C:217:MLY:HD2	1.90	0.41
1:C:162:GLU:OE2	1:C:163:ARG:HD2	2.21	0.41
2:D:11:LEU:HD22	2:D:35:LEU:HD22	2.03	0.41
1:A:45:VAL:HG13	1:A:68:ALA:HB1	2.03	0.41
1:A:104:ARG:HD2	1:A:108:ARG:NH2	2.36	0.41
1:C:220:HIS:CE1	1:C:223:GLN:HG3	2.56	0.41

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	230/263 (88%)	226 (98%)	4 (2%)	0	100	100
1	C	230/263 (88%)	214 (93%)	13 (6%)	3 (1%)	9	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	120/130 (92%)	118 (98%)	2 (2%)	0	100	100
2	D	119/130 (92%)	114 (96%)	5 (4%)	0	100	100
All	All	699/786 (89%)	672 (96%)	24 (3%)	3 (0%)	30	59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	8	ARG
1	C	218	GLY
1	C	44	VAL

### 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	179/184 (97%)	179 (100%)	0	100	100
1	C	179/184 (97%)	174 (97%)	5 (3%)	38	72
2	B	101/104 (97%)	101 (100%)	0	100	100
2	D	101/104 (97%)	100 (99%)	1 (1%)	68	89
All	All	560/576 (97%)	554 (99%)	6 (1%)	65	88

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	42	LEU
1	C	91	LEU
1	C	189	LEU
1	C	196	VAL
1	C	242	VAL
2	D	19	ARG

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

Mol	Chain	Res	Type
2	B	118	GLN
2	D	118	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

54 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	54	1	9,10,11	0.44	0	6,11,13	0.25	0
2	MLY	B	80	2	9,10,11	0.44	0	6,11,13	0.25	0
1	MLY	A	47	1	9,10,11	0.45	0	6,11,13	0.26	0
1	MLY	C	123	1	9,10,11	0.43	0	6,11,13	0.29	0
2	MLY	D	80	2	9,10,11	0.46	0	6,11,13	0.23	0
1	MLY	C	18	1	9,10,11	0.44	0	6,11,13	0.34	0
1	MLY	C	3	1	9,10,11	0.45	0	6,11,13	0.22	0
1	MLY	C	136	1	9,10,11	0.45	0	6,11,13	0.35	0
1	MLY	C	83	1	9,10,11	0.43	0	6,11,13	0.25	0
1	MLY	C	180	1	9,10,11	0.44	0	6,11,13	0.41	0
2	MLY	D	84	2	9,10,11	0.42	0	6,11,13	0.25	0
1	MLY	A	180	1	9,10,11	0.43	0	6,11,13	0.21	0
2	MLY	B	103	2	9,10,11	0.44	0	6,11,13	0.30	0
1	MLY	A	3	1	9,10,11	0.43	0	6,11,13	0.51	0
1	MLY	A	83	1	9,10,11	0.43	0	6,11,13	0.28	0
2	MLY	D	103	2	9,10,11	0.44	0	6,11,13	0.37	0
1	MLY	A	217	1	9,10,11	0.39	0	6,11,13	0.27	0
1	MLY	A	23	1	9,10,11	0.45	0	6,11,13	0.25	0
1	MLY	A	98	1	9,10,11	0.45	0	6,11,13	0.54	0
1	MLY	C	16	1	9,10,11	0.45	0	6,11,13	0.25	0
1	MLY	A	247	1	9,10,11	0.44	0	6,11,13	0.38	0
1	MLY	A	46	1	9,10,11	0.42	0	6,11,13	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	A	123	1	9,10,11	0.44	0	6,11,13	0.26	0
1	MLY	A	16	1	9,10,11	0.42	0	6,11,13	0.32	0
1	MLY	C	197	1	9,10,11	0.44	0	6,11,13	0.27	0
1	MLY	A	60	1	9,10,11	0.43	0	6,11,13	0.29	0
1	MLY	C	126	1	9,10,11	0.41	0	6,11,13	0.29	0
1	MLY	A	213	1	9,10,11	0.43	0	6,11,13	0.22	0
1	MLY	C	23	1	9,10,11	0.44	0	6,11,13	0.28	0
1	MLY	C	98	1	9,10,11	0.45	0	6,11,13	0.37	0
1	MLY	A	56	1	9,10,11	0.43	0	6,11,13	0.26	0
1	MLY	A	126	1	9,10,11	0.43	0	6,11,13	0.40	0
1	MLY	A	197	1	9,10,11	0.44	0	6,11,13	0.29	0
2	MLY	B	84	2	9,10,11	0.43	0	6,11,13	0.34	0
1	MLY	C	92	1	9,10,11	0.43	0	6,11,13	0.32	0
1	MLY	C	172	1	9,10,11	0.45	0	6,11,13	0.28	0
1	MLY	A	165	1	9,10,11	0.44	0	6,11,13	0.21	0
1	MLY	A	18	1	9,10,11	0.46	0	6,11,13	0.29	0
1	MLY	C	217	1	9,10,11	0.43	0	6,11,13	0.25	0
1	MLY	A	7	1	9,10,11	0.43	0	6,11,13	0.29	0
1	MLY	C	14	1	9,10,11	0.42	0	6,11,13	0.29	0
1	MLY	A	92	1	9,10,11	0.44	0	6,11,13	0.29	0
1	MLY	C	60	1	9,10,11	0.44	0	6,11,13	0.30	0
1	MLY	A	172	1	9,10,11	0.46	0	6,11,13	0.29	0
1	MLY	C	213	1	9,10,11	0.45	0	6,11,13	0.25	0
1	MLY	C	54	1	9,10,11	0.47	0	6,11,13	0.30	0
1	MLY	C	56	1	9,10,11	0.44	0	6,11,13	0.37	0
1	MLY	C	247	1	9,10,11	0.43	0	6,11,13	0.31	0
1	MLY	A	136	1	9,10,11	0.45	0	6,11,13	0.27	0
1	MLY	C	7	1	9,10,11	0.45	0	6,11,13	0.31	0
1	MLY	C	165	1	9,10,11	0.44	0	6,11,13	0.33	0
1	MLY	C	46	1	9,10,11	0.45	0	6,11,13	0.28	0
1	MLY	A	14	1	9,10,11	0.42	0	6,11,13	0.27	0
1	MLY	C	47	1	9,10,11	0.43	0	6,11,13	0.26	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	54	1	-	2/8/9/11	-
2	MLY	B	80	2	-	1/8/9/11	-
1	MLY	A	47	1	-	5/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	C	123	1	-	3/8/9/11	-
2	MLY	D	80	2	-	3/8/9/11	-
1	MLY	C	18	1	-	3/8/9/11	-
1	MLY	C	3	1	-	6/8/9/11	-
1	MLY	C	136	1	-	3/8/9/11	-
1	MLY	C	83	1	-	4/8/9/11	-
1	MLY	C	180	1	-	3/8/9/11	-
2	MLY	D	84	2	-	1/8/9/11	-
1	MLY	A	180	1	-	1/8/9/11	-
2	MLY	B	103	2	-	3/8/9/11	-
1	MLY	A	3	1	-	5/8/9/11	-
1	MLY	A	83	1	-	2/8/9/11	-
2	MLY	D	103	2	-	1/8/9/11	-
1	MLY	A	217	1	-	2/8/9/11	-
1	MLY	A	23	1	-	2/8/9/11	-
1	MLY	A	98	1	-	5/8/9/11	-
1	MLY	C	16	1	-	5/8/9/11	-
1	MLY	A	247	1	-	3/8/9/11	-
1	MLY	A	46	1	-	3/8/9/11	-
1	MLY	A	123	1	-	2/8/9/11	-
1	MLY	A	16	1	-	2/8/9/11	-
1	MLY	C	197	1	-	4/8/9/11	-
1	MLY	A	60	1	-	1/8/9/11	-
1	MLY	C	126	1	-	2/8/9/11	-
1	MLY	A	213	1	-	4/8/9/11	-
1	MLY	C	23	1	-	1/8/9/11	-
1	MLY	C	98	1	-	2/8/9/11	-
1	MLY	A	56	1	-	4/8/9/11	-
1	MLY	A	126	1	-	1/8/9/11	-
1	MLY	A	197	1	-	4/8/9/11	-
2	MLY	B	84	2	-	0/8/9/11	-
1	MLY	C	92	1	-	2/8/9/11	-
1	MLY	C	172	1	-	4/8/9/11	-
1	MLY	A	165	1	-	5/8/9/11	-
1	MLY	A	18	1	-	2/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	C	217	1	-	3/8/9/11	-
1	MLY	A	7	1	-	5/8/9/11	-
1	MLY	C	14	1	-	4/8/9/11	-
1	MLY	A	92	1	-	1/8/9/11	-
1	MLY	C	60	1	-	4/8/9/11	-
1	MLY	A	172	1	-	2/8/9/11	-
1	MLY	C	213	1	-	0/8/9/11	-
1	MLY	C	54	1	-	3/8/9/11	-
1	MLY	C	56	1	-	1/8/9/11	-
1	MLY	C	247	1	-	6/8/9/11	-
1	MLY	A	136	1	-	2/8/9/11	-
1	MLY	C	7	1	-	0/8/9/11	-
1	MLY	C	165	1	-	1/8/9/11	-
1	MLY	C	46	1	-	2/8/9/11	-
1	MLY	A	14	1	-	3/8/9/11	-
1	MLY	C	47	1	-	3/8/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (146) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	3	MLY	N-CA-CB-CG
1	A	3	MLY	C-CA-CB-CG
1	C	3	MLY	N-CA-CB-CG
1	C	3	MLY	C-CA-CB-CG
1	A	14	MLY	O-C-CA-CB
1	C	14	MLY	N-CA-CB-CG
1	C	14	MLY	C-CA-CB-CG
1	C	16	MLY	O-C-CA-CB
1	A	23	MLY	C-CA-CB-CG
1	C	23	MLY	C-CA-CB-CG
1	C	46	MLY	N-CA-CB-CG
1	C	46	MLY	C-CA-CB-CG
1	A	47	MLY	N-CA-CB-CG
1	A	47	MLY	C-CA-CB-CG
1	A	54	MLY	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	A	54	MLY	C-CA-CB-CG
1	C	54	MLY	C-CA-CB-CG
1	C	54	MLY	O-C-CA-CB
1	A	56	MLY	N-CA-CB-CG
1	C	56	MLY	O-C-CA-CB
1	C	60	MLY	N-CA-CB-CG
1	C	60	MLY	C-CA-CB-CG
1	C	83	MLY	N-CA-CB-CG
1	C	83	MLY	C-CA-CB-CG
1	C	83	MLY	O-C-CA-CB
1	C	92	MLY	N-CA-CB-CG
1	C	92	MLY	C-CA-CB-CG
1	A	98	MLY	N-CA-CB-CG
1	A	98	MLY	C-CA-CB-CG
1	C	98	MLY	N-CA-CB-CG
1	C	98	MLY	C-CA-CB-CG
1	A	123	MLY	C-CA-CB-CG
1	C	123	MLY	N-CA-CB-CG
1	C	123	MLY	C-CA-CB-CG
1	A	136	MLY	O-C-CA-CB
1	C	136	MLY	N-CA-CB-CG
1	C	136	MLY	C-CA-CB-CG
1	C	136	MLY	O-C-CA-CB
1	A	165	MLY	N-CA-CB-CG
1	A	165	MLY	C-CA-CB-CG
1	A	172	MLY	C-CA-CB-CG
1	A	180	MLY	O-C-CA-CB
1	C	180	MLY	O-C-CA-CB
1	C	197	MLY	N-CA-CB-CG
1	C	197	MLY	C-CA-CB-CG
1	C	197	MLY	O-C-CA-CB
1	C	217	MLY	O-C-CA-CB
1	A	247	MLY	N-CA-CB-CG
1	A	247	MLY	C-CA-CB-CG
1	A	247	MLY	O-C-CA-CB
2	B	103	MLY	N-CA-CB-CG
2	B	103	MLY	C-CA-CB-CG
1	C	3	MLY	CD-CE-NZ-CH1
1	A	47	MLY	CD-CE-NZ-CH2
1	C	247	MLY	CD-CE-NZ-CH2
1	A	18	MLY	CG-CD-CE-NZ
1	C	47	MLY	CG-CD-CE-NZ

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Mol	Chain	Res	Type	Atoms
1	C	180	MLY	CG-CD-CE-NZ
1	A	197	MLY	CG-CD-CE-NZ
1	C	16	MLY	CE-CD-CG-CB
1	A	3	MLY	CD-CE-NZ-CH1
1	A	3	MLY	CD-CE-NZ-CH2
1	C	3	MLY	CD-CE-NZ-CH2
1	A	47	MLY	CD-CE-NZ-CH1
1	C	172	MLY	CD-CE-NZ-CH1
1	C	172	MLY	CD-CE-NZ-CH2
1	A	213	MLY	CD-CE-NZ-CH1
1	C	247	MLY	CD-CE-NZ-CH1
1	C	14	MLY	CG-CD-CE-NZ
1	C	16	MLY	CG-CD-CE-NZ
1	A	47	MLY	CA-CB-CG-CD
1	A	98	MLY	CD-CE-NZ-CH1
1	A	213	MLY	CD-CE-NZ-CH2
1	A	3	MLY	CE-CD-CG-CB
1	A	98	MLY	CG-CD-CE-NZ
1	A	16	MLY	CA-CB-CG-CD
1	A	7	MLY	CG-CD-CE-NZ
1	C	180	MLY	CD-CE-NZ-CH2
1	A	7	MLY	CA-CB-CG-CD
1	A	56	MLY	CA-CB-CG-CD
1	A	197	MLY	CA-CB-CG-CD
1	C	47	MLY	CE-CD-CG-CB
1	C	172	MLY	CG-CD-CE-NZ
1	A	16	MLY	CE-CD-CG-CB
1	A	165	MLY	CE-CD-CG-CB
1	C	3	MLY	CE-CD-CG-CB
1	C	83	MLY	CE-CD-CG-CB
2	B	103	MLY	CE-CD-CG-CB
1	A	92	MLY	CE-CD-CG-CB
2	D	103	MLY	CD-CE-NZ-CH2
1	A	14	MLY	CA-CB-CG-CD
1	C	247	MLY	CE-CD-CG-CB
1	A	56	MLY	CE-CD-CG-CB
1	A	23	MLY	CE-CD-CG-CB
1	A	217	MLY	CE-CD-CG-CB
1	C	126	MLY	CE-CD-CG-CB
1	C	247	MLY	CA-CB-CG-CD
1	C	18	MLY	CG-CD-CE-NZ
2	D	80	MLY	CG-CD-CE-NZ

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Mol	Chain	Res	Type	Atoms
1	C	16	MLY	CA-CB-CG-CD
1	A	136	MLY	CA-CB-CG-CD
1	A	213	MLY	CA-CB-CG-CD
1	C	123	MLY	CA-CB-CG-CD
1	C	18	MLY	CD-CE-NZ-CH2
1	A	126	MLY	CD-CE-NZ-CH1
1	A	7	MLY	C-CA-CB-CG
1	A	46	MLY	C-CA-CB-CG
1	A	56	MLY	C-CA-CB-CG
2	B	80	MLY	C-CA-CB-CG
1	C	60	MLY	CD-CE-NZ-CH2
1	C	247	MLY	CG-CD-CE-NZ
1	A	83	MLY	CG-CD-CE-NZ
1	A	7	MLY	N-CA-CB-CG
1	A	14	MLY	N-CA-CB-CG
1	A	46	MLY	N-CA-CB-CG
1	A	123	MLY	N-CA-CB-CG
1	A	197	MLY	N-CA-CB-CG
1	A	217	MLY	N-CA-CB-CG
1	C	247	MLY	N-CA-CB-CG
1	C	60	MLY	CE-CD-CG-CB
2	D	80	MLY	CD-CE-NZ-CH1
1	A	98	MLY	CA-CB-CG-CD
1	C	16	MLY	CD-CE-NZ-CH1
1	C	217	MLY	CG-CD-CE-NZ
1	A	197	MLY	CE-CD-CG-CB
1	A	213	MLY	CG-CD-CE-NZ
1	A	7	MLY	CD-CE-NZ-CH2
1	C	3	MLY	CA-CB-CG-CD
1	A	172	MLY	CD-CE-NZ-CH2
2	D	84	MLY	CG-CD-CE-NZ
1	C	217	MLY	CA-CB-CG-CD
1	A	46	MLY	CD-CE-NZ-CH2
1	A	60	MLY	CE-CD-CG-CB
1	C	14	MLY	CD-CE-NZ-CH1
1	A	165	MLY	CD-CE-NZ-CH1
2	D	80	MLY	CD-CE-NZ-CH2
1	C	126	MLY	CD-CE-NZ-CH1
1	C	165	MLY	CE-CD-CG-CB
1	A	18	MLY	C-CA-CB-CG
1	C	47	MLY	C-CA-CB-CG
1	C	172	MLY	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	A	165	MLY	CG-CD-CE-NZ
1	C	197	MLY	CE-CD-CG-CB
1	C	18	MLY	N-CA-CB-CG
1	C	54	MLY	N-CA-CB-CG
1	A	83	MLY	N-CA-CB-CG

There are no ring outliers.

16 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	3	MLY	3	0
1	C	83	MLY	2	0
2	D	84	MLY	1	0
1	A	3	MLY	1	0
1	A	83	MLY	1	0
1	A	217	MLY	1	0
1	A	23	MLY	1	0
1	C	16	MLY	1	0
1	C	197	MLY	2	0
1	A	197	MLY	1	0
1	C	217	MLY	2	0
1	A	7	MLY	1	0
1	C	14	MLY	1	0
1	C	60	MLY	1	0
1	C	7	MLY	1	0
1	C	46	MLY	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	MPD	B	401	-	7,7,7	0.39	0	9,10,10	0.46	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	MPD	B	401	-	-	4/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	MPD	CM-C2-C3-C4
3	B	401	MPD	C2-C3-C4-C5
3	B	401	MPD	O2-C2-C3-C4
3	B	401	MPD	C1-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	MPD	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	231/263 (87%)	-0.34	0 <b>100</b> <b>100</b>	48, 76, 122, 168	0
1	C	231/263 (87%)	-0.13	2 (0%) 81 75	50, 84, 165, 196	0
2	B	122/130 (93%)	-0.37	1 (0%) 82 77	43, 61, 121, 179	0
2	D	121/130 (93%)	-0.47	0 <b>100</b> <b>100</b>	41, 58, 117, 139	0
All	All	705/786 (89%)	-0.30	3 (0%) 88 85	41, 73, 140, 196	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	0	GLY	2.5
1	C	42	LEU	2.4
1	C	40	GLU	2.2

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	MLY	A	3	11/12	0.48	0.18	96,112,125,141	0
1	MLY	C	3	11/12	0.49	0.23	145,157,167,168	0
1	MLY	C	16	11/12	0.60	0.17	138,150,158,163	0
1	MLY	C	56	11/12	0.61	0.14	97,109,119,121	0
1	MLY	A	98	11/12	0.69	0.18	90,104,142,147	0
1	MLY	C	92	11/12	0.73	0.13	64,83,140,144	0
1	MLY	C	98	11/12	0.74	0.15	65,81,132,136	0
1	MLY	C	7	11/12	0.75	0.16	116,135,166,166	0
1	MLY	C	18	11/12	0.76	0.15	111,135,146,150	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MLY	C	54	11/12	0.76	0.14	99,113,133,134	0
1	MLY	C	136	11/12	0.76	0.15	73,113,131,136	0
1	MLY	A	18	11/12	0.77	0.18	125,141,165,168	0
1	MLY	C	83	11/12	0.79	0.20	130,138,162,170	0
1	MLY	C	165	11/12	0.79	0.16	87,101,126,132	0
1	MLY	C	47	11/12	0.80	0.11	116,124,133,136	0
1	MLY	A	16	11/12	0.80	0.12	77,112,120,122	0
1	MLY	C	46	11/12	0.80	0.14	114,129,149,150	0
1	MLY	A	217	11/12	0.83	0.15	69,78,134,144	0
1	MLY	C	247	11/12	0.83	0.14	66,94,124,136	0
1	MLY	A	136	11/12	0.84	0.12	83,100,127,128	0
2	MLY	B	103	11/12	0.84	0.16	59,72,108,115	0
1	MLY	A	47	11/12	0.85	0.13	84,101,143,151	0
1	MLY	A	54	11/12	0.85	0.14	92,105,130,131	0
1	MLY	A	46	11/12	0.86	0.13	80,95,118,120	0
1	MLY	C	60	11/12	0.86	0.14	75,83,108,115	0
1	MLY	A	197	11/12	0.87	0.15	82,90,122,123	0
1	MLY	C	126	11/12	0.87	0.12	80,88,120,139	0
1	MLY	A	23	11/12	0.87	0.12	89,103,123,128	0
1	MLY	A	180	11/12	0.87	0.12	74,93,102,112	0
1	MLY	C	197	11/12	0.88	0.17	63,85,130,134	0
1	MLY	C	14	11/12	0.88	0.13	122,133,140,143	0
1	MLY	A	7	11/12	0.88	0.11	108,116,135,135	0
1	MLY	A	14	11/12	0.88	0.13	117,128,144,147	0
1	MLY	A	165	11/12	0.89	0.11	70,83,111,112	0
1	MLY	C	23	11/12	0.89	0.11	98,103,116,119	0
1	MLY	C	217	11/12	0.89	0.13	67,83,99,101	0
1	MLY	A	56	11/12	0.89	0.11	75,90,125,131	0
1	MLY	C	123	11/12	0.89	0.10	85,89,109,111	0
2	MLY	B	84	11/12	0.90	0.13	45,59,139,140	0
2	MLY	D	103	11/12	0.90	0.10	44,53,69,75	0
1	MLY	C	172	11/12	0.91	0.14	66,82,132,133	0
1	MLY	A	123	11/12	0.91	0.11	59,73,114,116	0
1	MLY	A	60	11/12	0.92	0.16	58,68,116,125	0
1	MLY	C	180	11/12	0.92	0.11	64,70,108,110	0
1	MLY	A	126	11/12	0.93	0.08	66,70,82,102	0
1	MLY	A	247	11/12	0.93	0.09	57,87,110,120	0
1	MLY	A	92	11/12	0.93	0.10	77,85,126,128	0
1	MLY	A	213	11/12	0.93	0.10	62,74,81,83	0
1	MLY	C	213	11/12	0.93	0.10	62,75,101,105	0
1	MLY	A	172	11/12	0.93	0.11	70,80,126,128	0
2	MLY	B	80	11/12	0.94	0.08	58,65,69,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MLY	D	80	11/12	0.95	0.10	46,61,73,74	0
1	MLY	A	83	11/12	0.96	0.08	59,75,89,99	0
2	MLY	D	84	11/12	0.96	0.11	46,58,82,84	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	MPD	B	401	8/8	0.66	0.18	57,73,92,106	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.