



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 11:31 am BST

PDB ID : 2ETV
Title : Crystal structure of a putative fe(iii) abc transporter (tm0189) from thermotoga maritima msb8 at 1.70 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2005-10-27
Resolution : 1.70 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

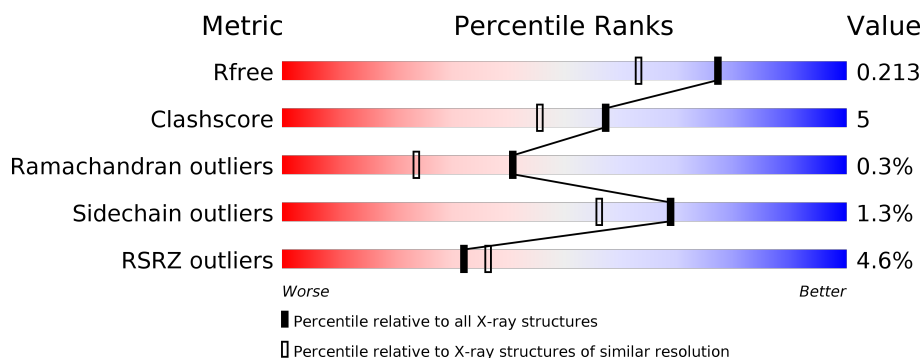
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	346	<div> <div>4%</div> <div>88%</div> <div>11%</div> </div>
1	B	346	<div> <div>4%</div> <div>90%</div> <div>7%</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
5	EDO	A	12	-	-	X	-
5	EDO	B	10	-	-	X	-
5	EDO	B	22	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6360 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 iron(III) ABC transporter, periplasmic iron-binding protein, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	Se	0	10	0
			2789	1815	454	518	2			
1	B	336	Total	C	N	O	Se	0	9	0
			2707	1764	432	509	2			

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MSE	-	MODIFIED RESIDUE	GB 4980685
A	-10	GLY	-	LEADER SEQUENCE	GB 4980685
A	-9	SER	-	LEADER SEQUENCE	GB 4980685
A	-8	ASP	-	LEADER SEQUENCE	GB 4980685
A	-7	MLY	-	MODIFIED RESIDUE	GB 4980685
A	-6	ILE	-	LEADER SEQUENCE	GB 4980685
A	-5	HIS	-	LEADER SEQUENCE	GB 4980685
A	-4	HIS	-	LEADER SEQUENCE	GB 4980685
A	-3	HIS	-	LEADER SEQUENCE	GB 4980685
A	-2	HIS	-	LEADER SEQUENCE	GB 4980685
A	-1	HIS	-	LEADER SEQUENCE	GB 4980685
A	0	HIS	-	LEADER SEQUENCE	GB 4980685
A	25	MLY	LYS	MODIFIED RESIDUE	GB 4980685
A	56	MLY	LYS	MODIFIED RESIDUE	GB 4980685
A	60	MSE	MET	MODIFIED RESIDUE	GB 4980685
A	69	MLY	LYS	MODIFIED RESIDUE	GB 4980685
A	85	MLY	LYS	MODIFIED RESIDUE	GB 4980685
A	86	MLY	LYS	MODIFIED RESIDUE	GB 4980685
A	97	MLY	LYS	MODIFIED RESIDUE	GB 4980685
A	120	MLY	LYS	MODIFIED RESIDUE	GB 4980685
A	123	MLY	LYS	MODIFIED RESIDUE	GB 4980685
A	128	MLY	LYS	MODIFIED RESIDUE	GB 4980685
A	158	MLY	LYS	MODIFIED RESIDUE	GB 4980685
A	175	MLY	LYS	MODIFIED RESIDUE	GB 4980685

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	200	MLY	LYS	MODIFIED RESIDUE	GB 4980685
A	211	MLY	LYS	MODIFIED RESIDUE	GB 4980685
A	232	MLY	LYS	MODIFIED RESIDUE	GB 4980685
A	238	MLY	LYS	MODIFIED RESIDUE	GB 4980685
A	263	MLY	LYS	MODIFIED RESIDUE	GB 4980685
A	275	MLY	LYS	MODIFIED RESIDUE	GB 4980685
A	278	MLY	LYS	MODIFIED RESIDUE	GB 4980685
A	319	MLY	LYS	MODIFIED RESIDUE	GB 4980685
A	330	MLY	LYS	MODIFIED RESIDUE	GB 4980685
A	336	MSE	MET	MODIFIED RESIDUE	GB 4980685
A	345	MLY	LYS	MODIFIED RESIDUE	GB 4980685
B	-11	MSE	-	MODIFIED RESIDUE	GB 4980685
B	-10	GLY	-	LEADER SEQUENCE	GB 4980685
B	-9	SER	-	LEADER SEQUENCE	GB 4980685
B	-8	ASP	-	LEADER SEQUENCE	GB 4980685
B	-7	MLY	-	MODIFIED RESIDUE	GB 4980685
B	-6	ILE	-	LEADER SEQUENCE	GB 4980685
B	-5	HIS	-	LEADER SEQUENCE	GB 4980685
B	-4	HIS	-	LEADER SEQUENCE	GB 4980685
B	-3	HIS	-	LEADER SEQUENCE	GB 4980685
B	-2	HIS	-	LEADER SEQUENCE	GB 4980685
B	-1	HIS	-	LEADER SEQUENCE	GB 4980685
B	0	HIS	-	LEADER SEQUENCE	GB 4980685
B	25	MLY	LYS	MODIFIED RESIDUE	GB 4980685
B	56	MLY	LYS	MODIFIED RESIDUE	GB 4980685
B	60	MSE	MET	MODIFIED RESIDUE	GB 4980685
B	69	MLY	LYS	MODIFIED RESIDUE	GB 4980685
B	85	MLY	LYS	MODIFIED RESIDUE	GB 4980685
B	86	MLY	LYS	MODIFIED RESIDUE	GB 4980685
B	97	MLY	LYS	MODIFIED RESIDUE	GB 4980685
B	120	MLY	LYS	MODIFIED RESIDUE	GB 4980685
B	123	MLY	LYS	MODIFIED RESIDUE	GB 4980685
B	128	MLY	LYS	MODIFIED RESIDUE	GB 4980685
B	158	MLY	LYS	MODIFIED RESIDUE	GB 4980685
B	175	MLY	LYS	MODIFIED RESIDUE	GB 4980685
B	200	MLY	LYS	MODIFIED RESIDUE	GB 4980685
B	211	MLY	LYS	MODIFIED RESIDUE	GB 4980685
B	232	MLY	LYS	MODIFIED RESIDUE	GB 4980685
B	238	MLY	LYS	MODIFIED RESIDUE	GB 4980685
B	263	MLY	LYS	MODIFIED RESIDUE	GB 4980685
B	275	MLY	LYS	MODIFIED RESIDUE	GB 4980685
B	278	MLY	LYS	MODIFIED RESIDUE	GB 4980685

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	319	MLY	LYS	MODIFIED RESIDUE	GB 4980685
B	330	MLY	LYS	MODIFIED RESIDUE	GB 4980685
B	336	MSE	MET	MODIFIED RESIDUE	GB 4980685
B	345	MLY	LYS	MODIFIED RESIDUE	GB 4980685

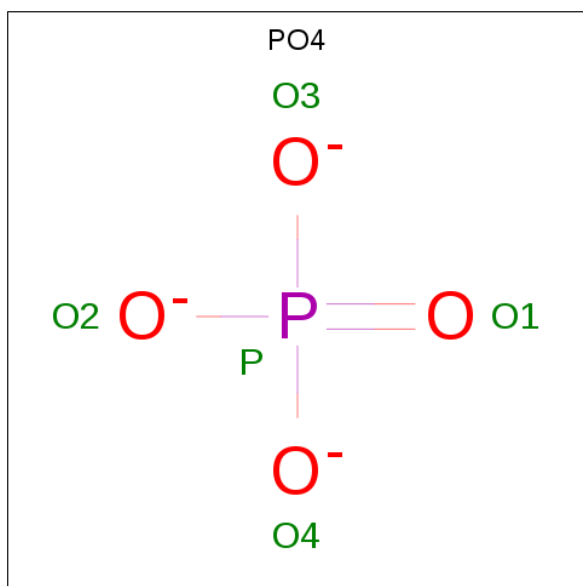
- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ni 1 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Cl 1 1	0	0
3	A	1	Total Cl 1 1	0	0

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



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

Continued on next page...

Continued from previous page...

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

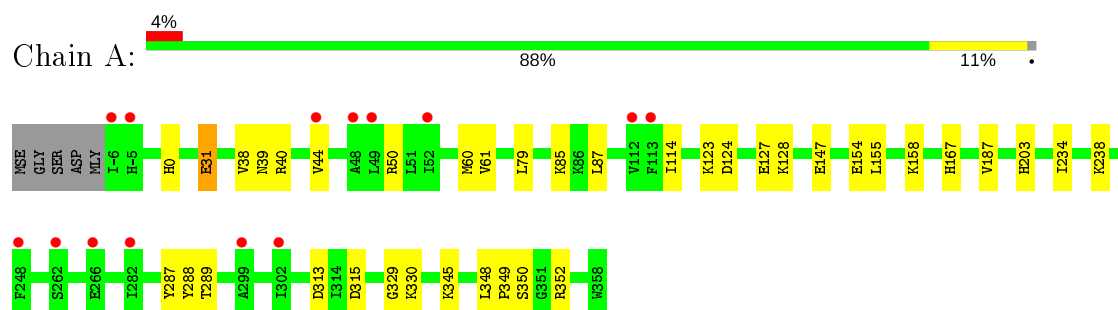
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	414	Total O 414 414	0	0
6	B	364	Total O 366 366	0	2

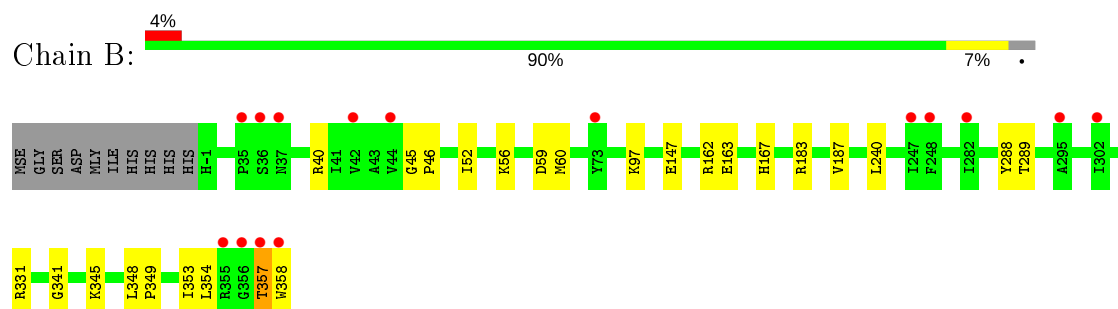
3 Residue-property plots [i](#)

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: iron(III) ABC transporter, periplasmic iron-binding protein, putative



- Molecule 1: iron(III) ABC transporter, periplasmic iron-binding protein, putative



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	109.82Å 109.82Å 122.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.70 29.19 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-1.70) 99.9 (29.19-1.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.163 , 0.207 0.176 , 0.213	Depositor DCC
R_{free} test set	4608 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	20.3	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.045 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6360	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.63% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NI, PO4, MLY, EDO, CL

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	0.83	1/2665 (0.0%)	0.82	3/3634 (0.1%)
1	B	0.82	1/2587 (0.0%)	0.78	4/3530 (0.1%)
All	All	0.82	2/5252 (0.0%)	0.80	7/7164 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	147	GLU	CG-CD	5.25	1.59	1.51
1	A	147	GLU	CG-CD	5.06	1.59	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	ARG	NE-CZ-NH1	-6.13	117.23	120.30
1	B	331	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	B	183	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	315	ASP	CB-CG-OD1	5.45	123.20	118.30
1	B	331	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	A	50	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	B	40	ARG	NE-CZ-NH1	-5.02	117.79	120.30

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	2789	0	2755	35	0
1	B	2707	0	2663	17	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	0	0
5	A	36	0	54	9	0
5	B	40	0	60	11	0
6	A	414	0	0	8	0
6	B	366	0	0	3	0
All	All	6360	0	5532	55	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 (55) 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:124:ASP:OD2	1:A:128:MLY:HH23	1.88	0.73
1:A:330[A]:MLY:NZ	5:A:12:EDO:H11	2.12	0.64
1:A:345:MLY:HH23	5:A:14:EDO:H12	1.82	0.61
1:A:350:SER:HB2	1:A:352[B]:ARG:CZ	2.30	0.61
1:B:162:ARG:HH21	5:B:22:EDO:H12	1.64	0.61
1:B:163:GLU:O	1:B:167[B]:HIS:HD2	1.85	0.60
1:B:97:MLY:O	5:B:10:EDO:C1	2.49	0.60
5:B:10:EDO:C1	6:B:498:HOH:O	2.49	0.59
1:A:154[B]:GLU:HG3	6:A:764:HOH:O	2.05	0.55
1:A:85:MLY:HH13	6:A:653:HOH:O	2.06	0.55
1:A:313:ASP:OD1	5:A:5:EDO:H12	2.05	0.55
1:B:60:MSE:HE2	1:B:162:ARG:NH2	2.22	0.55
1:A:154[B]:GLU:CG	6:A:764:HOH:O	2.54	0.55
1:A:350:SER:HB2	1:A:352[B]:ARG:NH1	2.23	0.54
1:A:287:TYR:CD1	5:A:19:EDO:H22	2.43	0.54
1:A:38:VAL:O	1:A:60:MSE:HE1	2.10	0.52
1:A:330[A]:MLY:NZ	5:A:12:EDO:C1	2.72	0.51
1:A:123:MLY:CH1	1:A:127:GLU:OE2	2.59	0.51
1:A:38:VAL:O	1:A:60:MSE:CE	2.59	0.50
1:B:345:MLY:H	1:B:357[A]:THR:HG22	1.76	0.50
1:A:238:MLY:HH23	6:A:405:HOH:O	2.12	0.49
1:B:341:GLY:HA3	1:B:353:ILE:CD1	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31[A]:GLU:OE1	6:A:469:HOH:O	2.20	0.49
1:A:330[A]:MLY:HG3	5:A:12:EDO:H22	1.95	0.49
1:A:123:MLY:HH13	1:A:123:MLY:HG2	1.94	0.49
1:A:85:MLY:HD2	6:A:653:HOH:O	2.12	0.48
1:A:123:MLY:CG	1:A:123:MLY:HH13	2.43	0.48
1:B:162:ARG:NH2	5:B:22:EDO:H12	2.28	0.47
1:A:167:HIS:HE1	6:A:688:HOH:O	1.98	0.47
1:A:345:MLY:HH23	5:A:14:EDO:C1	2.46	0.46
1:B:46:PRO:HD3	5:B:10:EDO:H21	1.98	0.46
1:B:348:LEU:N	1:B:349:PRO:CD	2.79	0.46
1:A:203:HIS:ND1	5:A:16:EDO:H12	2.31	0.45
1:B:59:ASP:HB2	5:B:22:EDO:C1	2.46	0.45
1:A:350:SER:CB	1:A:352[B]:ARG:CZ	2.94	0.45
1:B:45:GLY:HA2	5:B:10:EDO:H11	1.99	0.44
5:B:10:EDO:H12	6:B:498:HOH:O	2.15	0.44
1:B:97:MLY:O	5:B:10:EDO:O1	2.35	0.44
1:A:234:ILE:C	1:A:234:ILE:HD12	2.38	0.44
1:A:44:VAL:O	1:A:114:ILE:HA	2.18	0.44
1:B:345:MLY:H	1:B:357[A]:THR:CG2	2.31	0.43
1:A:158:MLY:HH22	6:A:503:HOH:O	2.19	0.43
1:A:330[A]:MLY:CG	5:A:12:EDO:H22	2.49	0.43
5:B:10:EDO:H11	6:B:498:HOH:O	2.18	0.42
1:A:79:LEU:O	1:A:330[B]:MLY:HH23	2.19	0.42
1:B:56:MLY:O	5:B:22:EDO:C2	2.68	0.42
1:B:354:LEU:O	1:B:357[A]:THR:HG22	2.19	0.42
1:A:0:HIS:HB3	1:A:155:LEU:HD11	2.02	0.42
1:A:329:GLY:O	1:A:330[A]:MLY:HH22	2.20	0.41
1:A:348:LEU:N	1:A:349:PRO:CD	2.83	0.41
1:A:39:ASN:HA	1:A:60:MSE:CE	2.51	0.41
1:A:61:VAL:HG12	1:A:87:LEU:HD13	2.02	0.41
1:B:345:MLY:HB2	1:B:357[A]:THR:HG21	2.02	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	327/346 (94%)	321 (98%)	5 (2%)	1 (0%)	41	24
1	B	321/346 (93%)	315 (98%)	5 (2%)	1 (0%)	41	24
All	All	648/692 (94%)	636 (98%)	10 (2%)	2 (0%)	41	24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	289	THR
1	B	289	THR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	274/268 (102%)	271 (99%)	3 (1%)	73	63
1	B	268/268 (100%)	262 (98%)	6 (2%)	52	34
All	All	542/536 (101%)	533 (98%)	9 (2%)	69	46

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

Mol	Chain	Res	Type
1	A	31[A]	GLU
1	A	31[B]	GLU
1	A	288	TYR
1	B	52	ILE
1	B	240	LEU
1	B	288	TYR
1	B	357[A]	THR
1	B	357[B]	THR
1	B	358	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

44 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	MLY	B	238[A]	-	7,8,11	0.52	0	3,8,13	0.49	0
1	MLY	A	120	1	9,10,11	1.23	1 (11%)	6,11,13	0.34	0
1	MLY	A	211	1	9,10,11	1.04	1 (11%)	6,11,13	0.80	0
1	MLY	A	86	1	7,8,11	0.59	0	3,8,13	0.25	0
1	MLY	B	275	1	9,10,11	0.73	0	6,11,13	0.54	0
1	MLY	A	275	1	9,10,11	0.88	0	6,11,13	0.45	0
1	MLY	A	69	1	4,5,11	0.75	0	1,5,13	1.06	0
1	MLY	B	330	1	7,8,11	0.62	0	3,8,13	0.44	0
1	MLY	B	200	1	7,8,11	0.72	0	3,8,13	0.72	0
1	MLY	B	175	1	5,6,11	0.85	0	2,6,13	0.13	0
1	MLY	B	123	1	9,10,11	0.62	0	6,11,13	1.09	0
1	MLY	A	97	1	9,10,11	0.98	1 (11%)	6,11,13	0.36	0
1	MLY	A	319	1	9,10,11	1.06	0	6,11,13	0.45	0
1	MLY	B	56	1	9,10,11	0.94	0	6,11,13	0.71	0
1	MLY	A	330[A]	-	9,10,11	0.61	0	6,11,13	0.50	0
1	MLY	A	128	1	9,10,11	0.87	0	6,11,13	0.78	0
1	MLY	B	128	1	9,10,11	0.65	0	6,11,13	0.51	0
1	MLY	A	330[B]	-	9,10,11	0.80	0	6,11,13	1.13	1 (16%)
1	MLY	B	85	1	9,10,11	0.91	0	6,11,13	0.37	0
1	MLY	A	56	1	9,10,11	0.97	1 (11%)	6,11,13	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	B	25	1	9,10,11	1.04	1 (11%)	6,11,13	0.45	0
1	MLY	B	232	1	9,10,11	1.08	1 (11%)	6,11,13	0.46	0
1	MLY	A	123	1	9,10,11	0.46	0	6,11,13	0.78	0
1	MLY	A	263	1	9,10,11	0.63	0	6,11,13	0.48	0
1	MLY	B	86	1	7,8,11	0.75	0	3,8,13	0.46	0
1	MLY	A	238	1	9,10,11	0.82	0	6,11,13	0.71	0
1	MLY	A	345	1	9,10,11	0.86	0	6,11,13	1.36	1 (16%)
1	MLY	B	120	1	5,6,11	0.54	0	2,6,13	0.54	0
1	MLY	A	175	1	7,8,11	1.35	0	3,8,13	0.39	0
1	MLY	A	200	1	9,10,11	0.89	1 (11%)	6,11,13	0.47	0
1	MLY	A	232	1	9,10,11	1.19	1 (11%)	6,11,13	0.62	0
1	MLY	B	319	1	9,10,11	0.94	0	6,11,13	0.93	0
1	MLY	A	158	1	9,10,11	1.21	1 (11%)	6,11,13	1.37	0
1	MLY	B	345	1	9,10,11	0.97	0	6,11,13	0.55	0
1	MLY	B	69	1	6,7,11	0.48	0	2,7,13	0.21	0
1	MLY	A	278	1	9,10,11	0.80	0	6,11,13	0.58	0
1	MLY	B	211	1	9,10,11	0.85	0	6,11,13	0.48	0
1	MLY	B	278	1	9,10,11	0.85	0	6,11,13	0.38	0
1	MLY	B	158	1	7,8,11	0.70	0	3,8,13	0.23	0
1	MLY	A	25	1	7,8,11	0.80	0	3,8,13	1.01	0
1	MLY	A	85	1	9,10,11	0.79	0	6,11,13	0.59	0
1	MLY	B	97	1	9,10,11	0.82	0	6,11,13	0.46	0
1	MLY	B	238[B]	-	7,8,11	0.43	0	3,8,13	0.12	0
1	MLY	B	263	1	7,8,11	0.64	0	3,8,13	0.22	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	B	238[A]	-	-	2/6/7/11	-
1	MLY	A	120	1	-	1/8/9/11	-
1	MLY	A	211	1	-	0/8/9/11	-
1	MLY	A	86	1	-	0/6/7/11	-
1	MLY	B	275	1	-	0/8/9/11	-
1	MLY	A	275	1	-	0/8/9/11	-
1	MLY	A	69	1	-	0/3/4/11	-
1	MLY	B	330	1	-	0/6/7/11	-
1	MLY	B	200	1	-	0/6/7/11	-
1	MLY	B	175	1	-	0/4/5/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	B	123	1	-	0/8/9/11	-
1	MLY	A	97	1	-	1/8/9/11	-
1	MLY	A	319	1	-	0/8/9/11	-
1	MLY	B	56	1	-	0/8/9/11	-
1	MLY	A	330[A]	-	-	1/8/9/11	-
1	MLY	A	128	1	-	2/8/9/11	-
1	MLY	B	128	1	-	0/8/9/11	-
1	MLY	A	330[B]	-	-	0/8/9/11	-
1	MLY	B	85	1	-	1/8/9/11	-
1	MLY	A	56	1	-	0/8/9/11	-
1	MLY	B	25	1	-	1/8/9/11	-
1	MLY	B	232	1	-	1/8/9/11	-
1	MLY	A	123	1	-	2/8/9/11	-
1	MLY	A	263	1	-	0/8/9/11	-
1	MLY	B	86	1	-	0/6/7/11	-
1	MLY	A	238	1	-	1/8/9/11	-
1	MLY	A	345	1	-	3/8/9/11	-
1	MLY	B	120	1	-	0/4/5/11	-
1	MLY	A	175	1	-	1/6/7/11	-
1	MLY	A	200	1	-	0/8/9/11	-
1	MLY	A	232	1	-	0/8/9/11	-
1	MLY	B	319	1	-	0/8/9/11	-
1	MLY	A	158	1	-	3/8/9/11	-
1	MLY	B	345	1	-	0/8/9/11	-
1	MLY	B	69	1	-	0/5/6/11	-
1	MLY	A	278	1	-	0/8/9/11	-
1	MLY	B	211	1	-	1/8/9/11	-
1	MLY	B	278	1	-	0/8/9/11	-
1	MLY	B	158	1	-	0/6/7/11	-
1	MLY	A	25	1	-	1/6/7/11	-
1	MLY	A	85	1	-	0/8/9/11	-
1	MLY	B	97	1	-	0/8/9/11	-
1	MLY	B	238[B]	-	-	0/6/7/11	-
1	MLY	B	263	1	-	0/6/7/11	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	232	MLY	CE-NZ	2.44	1.55	1.46
1	A	97	MLY	CE-NZ	2.41	1.55	1.46
1	A	158	MLY	CE-NZ	2.35	1.54	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	120	MLY	CE-NZ	2.24	1.54	1.46
1	B	232	MLY	CE-NZ	2.22	1.54	1.46
1	A	211	MLY	CB-CA	2.18	1.56	1.53
1	B	25	MLY	CE-NZ	2.16	1.54	1.46
1	A	200	MLY	CE-NZ	2.03	1.53	1.46
1	A	56	MLY	CE-NZ	2.01	1.53	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330[B]	MLY	CD-CE-NZ	-2.06	108.21	113.79
1	A	345	MLY	CH2-NZ-CH1	2.02	114.95	109.73

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	238[A]	MLY	O-C-CA-CB
1	B	232	MLY	O-C-CA-CB
1	A	345	MLY	O-C-CA-CB
1	A	128	MLY	CD-CE-NZ-CH1
1	A	345	MLY	CD-CE-NZ-CH2
1	A	128	MLY	CD-CE-NZ-CH2
1	A	123	MLY	CD-CE-NZ-CH1
1	A	345	MLY	CD-CE-NZ-CH1
1	A	158	MLY	CD-CE-NZ-CH2
1	A	158	MLY	CG-CD-CE-NZ
1	B	25	MLY	CD-CE-NZ-CH2
1	B	238[A]	MLY	CA-CB-CG-CD
1	A	330[A]	MLY	CG-CD-CE-NZ
1	A	175	MLY	CA-CB-CG-CD
1	A	158	MLY	CD-CE-NZ-CH1
1	A	97	MLY	CD-CE-NZ-CH1
1	A	120	MLY	CE-CD-CG-CB
1	A	123	MLY	CE-CD-CG-CB
1	A	25	MLY	CE-CD-CG-CB
1	A	238	MLY	CD-CE-NZ-CH2
1	B	85	MLY	CD-CE-NZ-CH1
1	B	211	MLY	CD-CE-NZ-CH2

There are no ring outliers.

11 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	56	MLY	1	0
1	A	330[A]	MLY	5	0
1	A	128	MLY	1	0
1	A	330[B]	MLY	1	0
1	A	123	MLY	3	0
1	A	238	MLY	1	0
1	A	345	MLY	2	0
1	A	158	MLY	1	0
1	B	345	MLY	3	0
1	A	85	MLY	2	0
1	B	97	MLY	2	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 23 ligands modelled in this entry, 3 are monoatomic - leaving 20 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	$\# Z > 2$
5	EDO	A	17	-	3,3,3	0.63	0	2,2,2	0.35	0
5	EDO	B	7	-	3,3,3	0.74	0	2,2,2	0.43	0
5	EDO	A	16	-	3,3,3	0.49	0	2,2,2	0.22	0
5	EDO	A	13	-	3,3,3	0.43	0	2,2,2	0.55	0
5	EDO	B	23	-	3,3,3	0.34	0	2,2,2	0.58	0
5	EDO	A	12	-	3,3,3	0.61	0	2,2,2	0.51	0
5	EDO	A	14	-	3,3,3	0.40	0	2,2,2	0.39	0
5	EDO	B	9	-	3,3,3	0.63	0	2,2,2	0.08	0
5	EDO	B	20	-	3,3,3	0.45	0	2,2,2	0.42	0
4	PO4	A	4	-	4,4,4	0.68	0	6,6,6	0.57	0
5	EDO	B	22	-	3,3,3	0.34	0	2,2,2	0.25	0
5	EDO	A	11	-	3,3,3	0.64	0	2,2,2	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	B	18	-	3,3,3	0.61	0	2,2,2	0.02	0
5	EDO	B	6	-	3,3,3	0.45	0	2,2,2	0.19	0
5	EDO	A	21	-	3,3,3	0.40	0	2,2,2	0.33	0
5	EDO	B	8	-	3,3,3	0.38	0	2,2,2	0.21	0
5	EDO	A	19	-	3,3,3	0.46	0	2,2,2	0.29	0
5	EDO	B	15	-	3,3,3	0.54	0	2,2,2	0.21	0
5	EDO	B	10	-	3,3,3	0.66	0	2,2,2	0.50	0
5	EDO	A	5	-	3,3,3	1.48	0	2,2,2	1.27	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
5	EDO	A	17	-	-	1/1/1/1	-
5	EDO	B	7	-	-	1/1/1/1	-
5	EDO	A	16	-	-	1/1/1/1	-
5	EDO	A	13	-	-	1/1/1/1	-
5	EDO	B	23	-	-	1/1/1/1	-
5	EDO	A	12	-	-	1/1/1/1	-
5	EDO	A	14	-	-	1/1/1/1	-
5	EDO	B	9	-	-	1/1/1/1	-
5	EDO	B	20	-	-	1/1/1/1	-
5	EDO	B	22	-	-	0/1/1/1	-
5	EDO	A	11	-	-	0/1/1/1	-
5	EDO	B	18	-	-	1/1/1/1	-
5	EDO	B	6	-	-	1/1/1/1	-
5	EDO	A	21	-	-	1/1/1/1	-
5	EDO	B	8	-	-	0/1/1/1	-
5	EDO	A	19	-	-	1/1/1/1	-
5	EDO	B	15	-	-	1/1/1/1	-
5	EDO	B	10	-	-	1/1/1/1	-
5	EDO	A	5	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	14	EDO	O1-C1-C2-O2
5	A	16	EDO	O1-C1-C2-O2
5	A	17	EDO	O1-C1-C2-O2
5	B	18	EDO	O1-C1-C2-O2
5	A	12	EDO	O1-C1-C2-O2
5	B	7	EDO	O1-C1-C2-O2
5	A	13	EDO	O1-C1-C2-O2
5	B	20	EDO	O1-C1-C2-O2
5	B	23	EDO	O1-C1-C2-O2
5	B	9	EDO	O1-C1-C2-O2
5	B	6	EDO	O1-C1-C2-O2
5	B	15	EDO	O1-C1-C2-O2
5	A	5	EDO	O1-C1-C2-O2
5	A	19	EDO	O1-C1-C2-O2
5	A	21	EDO	O1-C1-C2-O2
5	B	10	EDO	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	16	EDO	1	0
5	A	12	EDO	4	0
5	A	14	EDO	2	0
5	B	22	EDO	4	0
5	A	19	EDO	1	0
5	B	10	EDO	7	0
5	A	5	EDO	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

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, 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	318/346 (91%)	0.22	14 (4%) 34 38	20, 24, 35, 47	0
1	B	313/346 (90%)	0.35	15 (4%) 30 34	19, 24, 35, 47	0
All	All	631/692 (91%)	0.28	29 (4%) 32 36	19, 24, 35, 47	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	36	SER	6.4
1	A	-6	ILE	5.9
1	B	37	ASN	5.0
1	B	358	TRP	4.8
1	B	356	GLY	4.7
1	B	35	PRO	4.5
1	B	357[A]	THR	4.2
1	A	282	ILE	3.4
1	B	355	ARG	3.2
1	B	282	ILE	2.8
1	A	112	VAL	2.7
1	A	302	ILE	2.6
1	A	262	SER	2.6
1	B	302	ILE	2.5
1	A	44	VAL	2.5
1	A	48	ALA	2.4
1	A	-5	HIS	2.4
1	A	52	ILE	2.3
1	A	49	LEU	2.3
1	A	248	PHE	2.3
1	A	113	PHE	2.3
1	B	44	VAL	2.2
1	B	42	VAL	2.2
1	B	295	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	247	ILE	2.1
1	B	73	TYR	2.1
1	B	248	PHE	2.1
1	A	299	ALA	2.0
1	A	266	GLU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	MLY	B	263	9/12	0.80	0.18	29,31,38,43	0
1	MLY	B	275	11/12	0.83	0.21	25,27,40,42	0
1	MLY	A	200	11/12	0.86	0.15	32,36,50,58	0
1	MLY	A	263	11/12	0.87	0.21	29,31,46,50	0
1	MLY	B	85	11/12	0.88	0.13	27,33,37,38	0
1	MLY	B	86	9/12	0.89	0.12	28,30,41,45	0
1	MLY	B	345	11/12	0.90	0.11	22,26,35,38	0
1	MLY	B	238[B]	9/12	0.90	0.18	22,26,29,35	5
1	MLY	B	238[A]	9/12	0.90	0.18	22,26,36,38	5
1	MLY	A	97	11/12	0.91	0.09	24,28,43,45	0
1	MLY	A	85	11/12	0.91	0.10	27,31,39,39	0
1	MLY	B	123	11/12	0.91	0.09	22,24,34,36	0
1	MLY	A	56	11/12	0.91	0.12	21,26,41,43	0
1	MLY	A	25	9/12	0.92	0.12	20,25,39,47	0
1	MLY	A	211	11/12	0.92	0.16	30,33,51,55	0
1	MLY	A	158	11/12	0.92	0.13	20,23,41,45	0
1	MLY	B	120	7/12	0.92	0.11	22,25,34,36	0
1	MLY	B	211	11/12	0.93	0.14	30,32,51,54	0
1	MLY	A	123	11/12	0.93	0.13	23,28,39,40	0
1	MLY	A	120	11/12	0.93	0.14	23,29,46,49	0
1	MLY	B	128	11/12	0.93	0.12	24,27,40,41	0
1	MLY	A	345	11/12	0.93	0.11	21,24,34,34	0
1	MLY	B	25	11/12	0.94	0.09	20,24,41,41	0
1	MLY	A	232	11/12	0.94	0.10	25,28,35,40	0
1	MLY	B	319	11/12	0.94	0.11	20,22,28,32	0
1	MLY	B	232	11/12	0.94	0.09	24,27,35,36	0
1	MLY	B	56	11/12	0.94	0.10	21,24,41,41	0
1	MLY	A	128	11/12	0.94	0.09	25,27,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	MLY	B	158	9/12	0.94	0.09	20,22,38,40	0
1	MLY	B	200	9/12	0.94	0.09	31,33,47,52	0
1	MLY	A	86	9/12	0.94	0.10	28,30,43,45	0
1	MLY	B	97	11/12	0.94	0.11	26,30,42,45	0
1	MLY	A	275	11/12	0.94	0.10	25,27,38,38	0
1	MLY	A	175	9/12	0.94	0.12	22,23,49,51	0
1	MLY	A	278	11/12	0.95	0.07	20,23,30,31	0
1	MLY	A	319	11/12	0.95	0.09	20,23,28,31	0
1	MLY	A	238	11/12	0.95	0.11	21,28,50,52	0
1	MLY	B	69	8/12	0.95	0.18	26,28,38,42	0
1	MLY	A	330[B]	11/12	0.96	0.11	18,23,38,40	7
1	MLY	B	330	9/12	0.96	0.09	22,24,38,48	0
1	MLY	A	330[A]	11/12	0.96	0.11	21,23,30,32	7
1	MLY	A	69	6/12	0.96	0.08	24,28,28,34	0
1	MLY	B	175	7/12	0.96	0.06	22,22,29,38	0
1	MLY	B	278	11/12	0.96	0.07	21,23,31,32	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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
5	EDO	A	11	4/4	0.59	0.18	35,43,44,46	0
5	EDO	B	7	4/4	0.62	0.18	48,52,57,58	0
5	EDO	A	5	4/4	0.69	0.18	28,31,34,36	0
5	EDO	B	18	4/4	0.70	0.18	58,62,62,64	0
5	EDO	B	15	4/4	0.74	0.21	52,55,56,57	0
5	EDO	A	17	4/4	0.81	0.11	39,44,46,49	0
5	EDO	B	10	4/4	0.81	0.30	36,38,41,46	0
5	EDO	B	20	4/4	0.83	0.15	55,62,64,69	0
5	EDO	A	12	4/4	0.86	0.34	28,30,37,50	0
5	EDO	A	19	4/4	0.87	0.30	39,46,47,55	0
5	EDO	B	22	4/4	0.87	0.33	46,46,50,55	0
4	PO4	A	4	5/5	0.87	0.20	24,30,40,40	5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EDO	A	21	4/4	0.87	0.11	42,44,48,55	0
5	EDO	A	16	4/4	0.88	0.15	28,42,43,55	0
5	EDO	A	13	4/4	0.89	0.11	35,36,37,45	0
5	EDO	B	23	4/4	0.91	0.23	35,40,47,51	0
5	EDO	B	6	4/4	0.92	0.14	28,37,42,45	0
5	EDO	B	9	4/4	0.92	0.16	34,38,49,57	0
5	EDO	A	14	4/4	0.93	0.11	46,47,52,53	0
5	EDO	B	8	4/4	0.95	0.11	35,37,38,41	0
2	NI	A	1	1/1	0.99	0.07	17,17,17,17	0
3	CL	B	3	1/1	0.99	0.04	17,17,17,17	0
3	CL	A	2	1/1	1.00	0.03	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.