



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 1, 2025 – 11:09 pm BST

PDB ID : 6FND / pdb_00006fnd
Title : Crystal structure of Toxoplasma gondii AKMT
Authors : Pivovarova, Y.; Dong, G.
Deposited on : 2018-02-02
Resolution : 2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

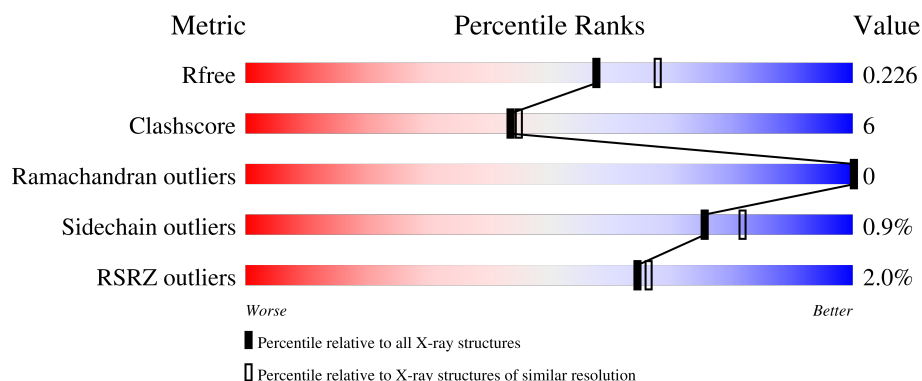
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

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 ≥ 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	423	<div> <div>6%</div> <div> <div></div> <div>83%</div> <div>16%</div> <div>.</div> </div> </div>
2	B	418	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>13%</div> </div> </div>
3	C	424	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div>..</div> </div> </div>
4	D	425	<div> <div></div> <div> <div></div> <div>91%</div> <div>8%</div> <div>.</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
6	SO4	D	803	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14140 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 Apical complex lysine methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	423	Total	C	N	O	S	0	0	0
			3390	2155	572	638	25			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	285	GLY	-	expression tag	UNP A0A151H4R7
A	286	SER	-	expression tag	UNP A0A151H4R7
A	287	HIS	-	expression tag	UNP A0A151H4R7
A	288	MET	-	expression tag	UNP A0A151H4R7

- Molecule 2 is a protein called Apical complex lysine methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	418	Total	C	N	O	S	0	2	0
			3377	2150	568	635	24			

- Molecule 3 is a protein called Apical complex lysine methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	420	Total	C	N	O	S	0	1	0
			3378	2149	569	636	24			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	285	GLY	-	expression tag	UNP A0A151H4R7
C	286	SER	-	expression tag	UNP A0A151H4R7
C	287	HIS	-	expression tag	UNP A0A151H4R7
C	288	MET	-	expression tag	UNP A0A151H4R7

- Molecule 4 is a protein called Apical complex lysine methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	422	Total	C	N	O	S	0	0	0
			3389	2157	569	638	25			

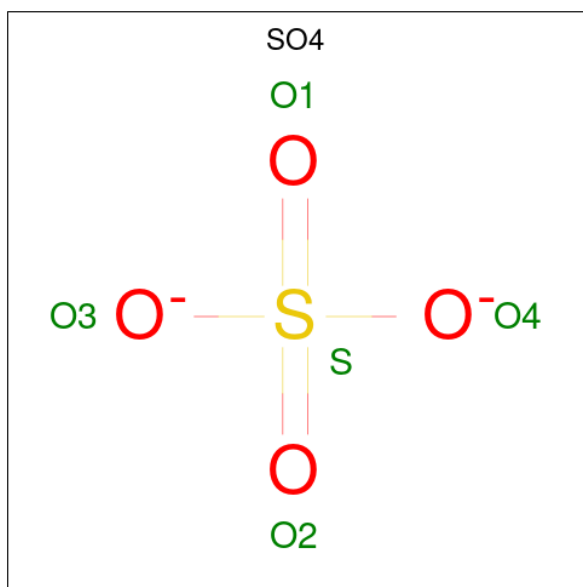
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	285	GLY	-	expression tag	UNP A0A151H4R7
D	286	SER	-	expression tag	UNP A0A151H4R7
D	287	HIS	-	expression tag	UNP A0A151H4R7
D	288	MET	-	expression tag	UNP A0A151H4R7

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

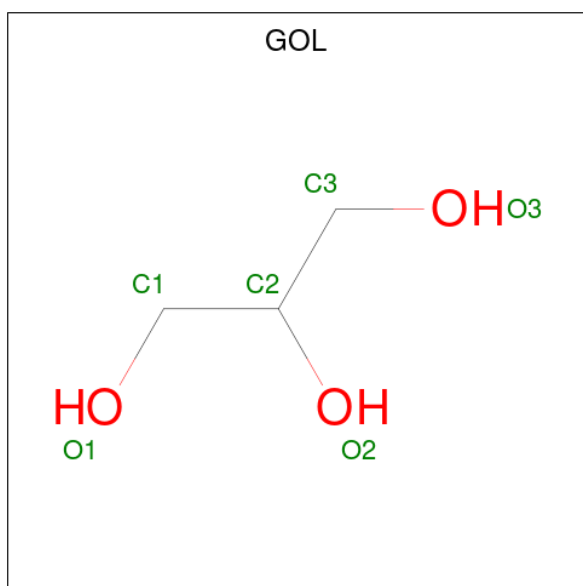
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Zn	0	2
			2	2		
5	B	2	Total	Zn	0	2
			2	2		
5	C	2	Total	Zn	0	2
			2	2		
5	D	2	Total	Zn	0	0
			2	2		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



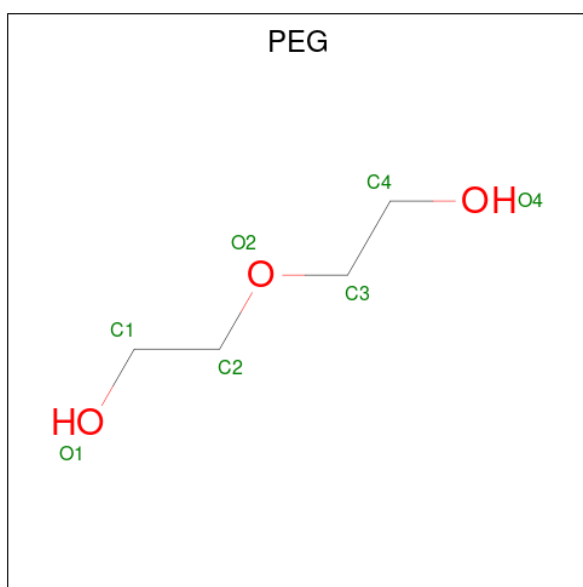
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total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

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

- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			7	4	3		

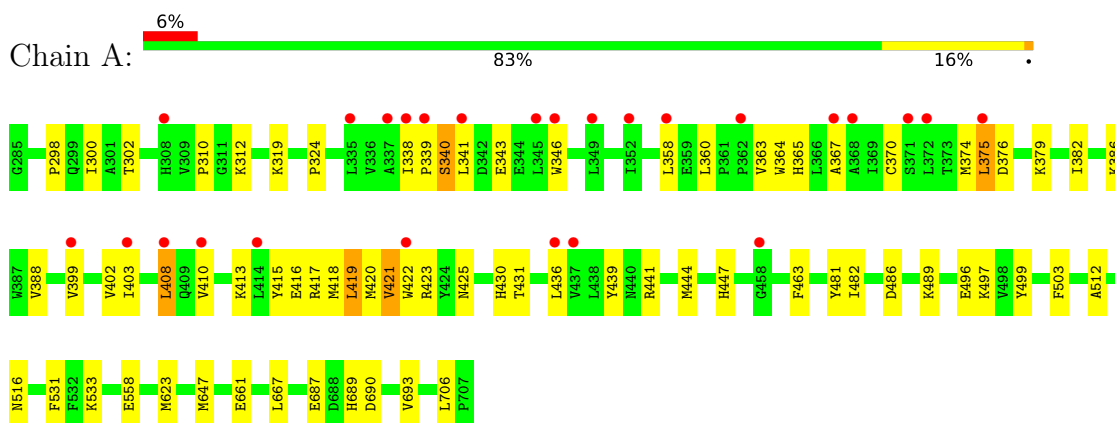
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	69	Total	O	0	0
			69	69		
10	B	117	Total	O	0	0
			117	117		
10	C	134	Total	O	0	0
			134	134		
10	D	114	Total	O	0	0
			114	114		

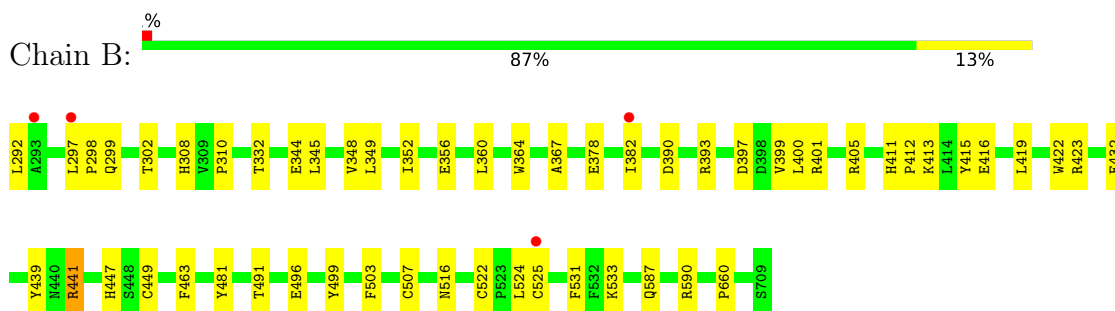
3 Residue-property plots [i](#)

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.

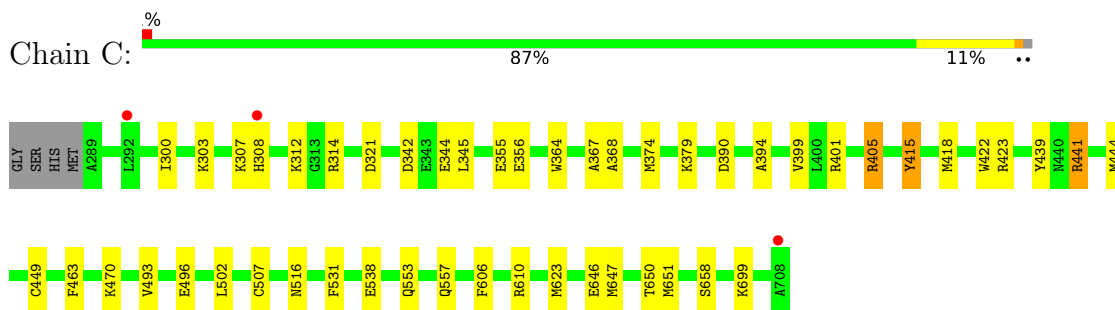
- Molecule 1: Apical complex lysine methyltransferase



- Molecule 2: Apical complex lysine methyltransferase



- Molecule 3: Apical complex lysine methyltransferase

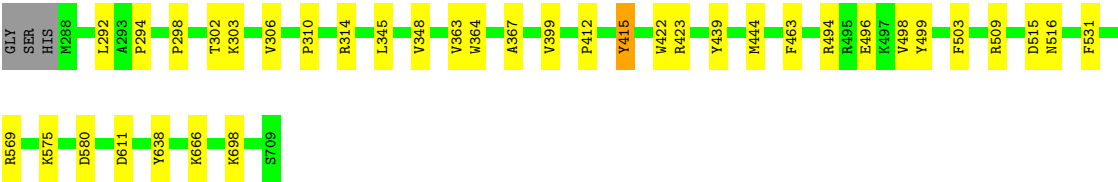


- Molecule 4: Apical complex lysine methyltransferase

Chain D:

91%

8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.94Å 89.37Å 91.72Å 108.69° 101.31° 103.41°	Depositor
Resolution (Å)	20.07 – 2.10 20.07 – 2.10	Depositor EDS
% Data completeness (in resolution range)	83.1 (20.07-2.10) 82.6 (20.07-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.09Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.191 , 0.226 0.191 , 0.226	Depositor DCC
R_{free} test set	98993 reflections (2.33%)	wwPDB-VP
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14140	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% 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: MLY, SO4, ZN, EDO, GOL, MLZ, PEG

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	0.30	0/3376	0.52	2/4599 (0.0%)
2	B	0.27	0/3286	0.46	0/4470
3	C	0.27	0/3352	0.46	1/4569 (0.0%)
4	D	0.26	0/3319	0.45	0/4522
All	All	0.28	0/13333	0.47	3/18160 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	419	LEU	CA-CB-CG	7.34	132.19	115.30
3	C	441	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	421	VAL	CG1-CB-CG2	5.04	118.97	110.90

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	3390	0	3278	59	0
2	B	3377	0	3272	46	0
3	C	3378	0	3271	36	0
4	D	3389	0	3281	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	A	5	0	0	0	0
6	B	10	0	0	0	0
6	C	5	0	0	0	0
6	D	5	0	0	3	0
7	A	24	0	32	0	0
7	C	12	0	16	0	0
7	D	12	0	16	1	0
8	A	16	0	24	0	0
8	B	28	0	42	0	0
8	C	28	0	42	1	0
8	D	12	0	18	0	0
9	B	7	0	10	1	0
10	A	69	0	0	5	0
10	B	117	0	0	5	0
10	C	134	0	0	7	0
10	D	114	0	0	7	0
All	All	14140	0	13302	162	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 6.

The worst 5 of 162 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:496:GLU:OE1	10:A:901:HOH:O	1.86	0.93
1:A:512:ALA:O	1:A:533:LYS:NZ	2.07	0.88
2:B:348:VAL:HG12	2:B:352:ILE:HD11	1.59	0.84
4:D:292:LEU:O	10:D:901:HOH:O	1.99	0.78
2:B:352:ILE:HG22	2:B:401:ARG:HH21	1.50	0.77

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	412/423 (97%)	403 (98%)	9 (2%)	0	100	100
2	B	402/418 (96%)	386 (96%)	16 (4%)	0	100	100
3	C	409/424 (96%)	397 (97%)	12 (3%)	0	100	100
4	D	406/425 (96%)	393 (97%)	13 (3%)	0	100	100
All	All	1629/1690 (96%)	1579 (97%)	50 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	357/357 (100%)	353 (99%)	4 (1%)	70	77
2	B	348/348 (100%)	346 (99%)	2 (1%)	84	89
3	C	354/356 (99%)	350 (99%)	4 (1%)	70	77
4	D	351/353 (99%)	349 (99%)	2 (1%)	84	89
All	All	1410/1414 (100%)	1398 (99%)	12 (1%)	75	82

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	405	ARG
3	C	415	TYR
4	D	444	MET

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Mol	Chain	Res	Type
3	C	658	SER
1	A	444	MET

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	308	HIS
4	D	553	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

49 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	$\# Z > 2$
4	MLY	D	319	4	9,10,11	0.52	0	6,11,13	0.85	0
3	MLY	C	319	3	9,10,11	0.55	0	6,11,13	0.76	0
3	MLY	C	575	3	9,10,11	0.48	0	6,11,13	0.83	0
4	MLY	D	307	4	9,10,11	0.54	0	6,11,13	0.87	0
2	MLZ	B	379[A]	2	8,9,10	0.79	0	4,9,11	0.62	0
2	MLZ	B	497	2	8,9,10	0.75	0	4,9,11	0.67	0
2	MLZ	B	533	2	8,9,10	0.76	0	4,9,11	0.65	0
2	MLY	B	489	2	9,10,11	0.56	0	6,11,13	0.62	0
2	MLZ	B	699[A]	2	8,9,10	0.81	0	4,9,11	0.58	0
2	MLZ	B	575	2	8,9,10	0.75	0	4,9,11	0.70	0
3	MLY	C	489	3	9,10,11	0.53	0	6,11,13	0.66	0
4	MLY	D	497	4	9,10,11	0.56	0	6,11,13	0.65	0
1	MLZ	A	470	1	8,9,10	0.77	0	4,9,11	0.68	0
2	MLZ	B	319	2	8,9,10	0.76	0	4,9,11	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MLZ	D	666	4	8,9,10	0.81	0	4,9,11	0.56	0
4	MLY	D	627	4	9,10,11	0.73	0	6,11,13	0.66	0
3	MLZ	C	699	3	8,9,10	0.84	1 (12%)	4,9,11	0.64	0
3	MLY	C	627	3	9,10,11	0.68	0	6,11,13	0.68	0
1	MLY	A	303	1	9,10,11	0.55	0	6,11,13	0.58	0
2	MLY	B	413	2	9,10,11	0.49	0	6,11,13	1.06	0
4	MLY	D	470	4	9,10,11	0.56	0	6,11,13	0.79	0
2	MLZ	B	666	2	8,9,10	0.75	0	4,9,11	0.54	0
1	MLY	A	627	1	9,10,11	0.66	0	6,11,13	0.75	0
2	MLY	B	627	2	9,10,11	0.77	0	6,11,13	0.99	0
1	MLY	A	307	1	9,10,11	0.62	0	6,11,13	0.89	0
3	MLY	C	470	3	9,10,11	0.59	0	6,11,13	0.89	0
1	MLY	A	489	1	9,10,11	0.59	0	6,11,13	0.82	0
4	MLY	D	413	4	9,10,11	0.59	0	6,11,13	0.78	0
2	MLZ	B	654	2	8,9,10	0.77	0	4,9,11	0.63	0
3	MLY	C	497	3	9,10,11	0.51	0	6,11,13	0.82	0
1	MLZ	A	380	1	8,9,10	0.76	0	4,9,11	0.61	0
4	MLZ	D	698	4	8,9,10	0.83	1 (12%)	4,9,11	0.69	0
4	MLY	D	312	4	9,10,11	0.48	0	6,11,13	0.85	0
2	MLY	B	307	2	9,10,11	0.59	0	6,11,13	0.74	0
2	MLZ	B	379[B]	2	8,9,10	0.77	0	4,9,11	0.57	0
2	MLZ	B	699[B]	2	8,9,10	0.80	0	4,9,11	0.60	0
3	MLZ	C	380	3	8,9,10	0.75	0	4,9,11	0.53	0
4	MLZ	D	380	4	8,9,10	0.77	0	4,9,11	0.60	0
1	MLY	A	497	1	9,10,11	0.49	0	6,11,13	0.86	0
2	MLY	B	312	2	9,10,11	0.53	0	6,11,13	0.84	0
4	MLY	D	379	4	9,10,11	0.51	0	6,11,13	0.85	0
4	MLZ	D	533	4	8,9,10	0.77	0	4,9,11	0.73	0
4	MLY	D	489	4	9,10,11	0.52	0	6,11,13	0.66	0
3	MLY	C	666	3	9,10,11	0.56	0	6,11,13	0.87	0
3	MLY	C	312	3	9,10,11	0.62	0	6,11,13	0.77	0
1	MLY	A	312	1	9,10,11	0.51	0	6,11,13	0.88	0
1	MLY	A	666	1	9,10,11	0.54	0	6,11,13	0.85	0
2	MLZ	B	303	2	8,9,10	0.76	0	4,9,11	0.68	0
4	MLZ	D	303	4	8,9,10	0.78	0	4,9,11	0.55	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
4	MLY	D	319	4	-	0/8/9/11	-
3	MLY	C	319	3	-	0/8/9/11	-
3	MLY	C	575	3	-	0/8/9/11	-
4	MLY	D	307	4	-	0/8/9/11	-
2	MLZ	B	379[A]	2	-	4/7/8/10	-
2	MLZ	B	497	2	-	0/7/8/10	-
2	MLZ	B	533	2	-	4/7/8/10	-
2	MLY	B	489	2	-	0/8/9/11	-
2	MLZ	B	699[A]	2	-	4/7/8/10	-
2	MLZ	B	575	2	-	0/7/8/10	-
3	MLY	C	489	3	-	0/8/9/11	-
4	MLY	D	497	4	-	0/8/9/11	-
1	MLZ	A	470	1	-	3/7/8/10	-
2	MLZ	B	319	2	-	0/7/8/10	-
4	MLZ	D	666	4	-	4/7/8/10	-
4	MLY	D	627	4	-	1/8/9/11	-
3	MLZ	C	699	3	-	3/7/8/10	-
3	MLY	C	627	3	-	1/8/9/11	-
1	MLY	A	303	1	-	0/8/9/11	-
2	MLY	B	413	2	-	6/8/9/11	-
4	MLY	D	470	4	-	0/8/9/11	-
2	MLZ	B	666	2	-	1/7/8/10	-
1	MLY	A	627	1	-	0/8/9/11	-
2	MLY	B	627	2	-	0/8/9/11	-
1	MLY	A	307	1	-	2/8/9/11	-
3	MLY	C	470	3	-	3/8/9/11	-
1	MLY	A	489	1	-	1/8/9/11	-
4	MLY	D	413	4	-	2/8/9/11	-
2	MLZ	B	654	2	-	3/7/8/10	-
3	MLY	C	497	3	-	4/8/9/11	-
1	MLZ	A	380	1	-	1/7/8/10	-
4	MLZ	D	698	4	-	0/7/8/10	-
4	MLY	D	312	4	-	1/8/9/11	-
2	MLY	B	307	2	-	1/8/9/11	-
2	MLZ	B	379[B]	2	-	3/7/8/10	-
2	MLZ	B	699[B]	2	-	3/7/8/10	-
3	MLZ	C	380	3	-	1/7/8/10	-
4	MLZ	D	380	4	-	1/7/8/10	-
1	MLY	A	497	1	-	0/8/9/11	-
2	MLY	B	312	2	-	0/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MLY	D	379	4	-	2/8/9/11	-
4	MLZ	D	533	4	-	2/7/8/10	-
4	MLY	D	489	4	-	0/8/9/11	-
3	MLY	C	666	3	-	2/8/9/11	-
3	MLY	C	312	3	-	3/8/9/11	-
1	MLY	A	312	1	-	1/8/9/11	-
1	MLY	A	666	1	-	3/8/9/11	-
2	MLZ	B	303	2	-	0/7/8/10	-
4	MLZ	D	303	4	-	3/7/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	699	MLZ	O-C	2.05	1.28	1.19
4	D	698	MLZ	O-C	2.05	1.28	1.19

There are no bond angle outliers.

There are no chirality outliers.

5 of 73 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	312	MLY	O-C-CA-CB
1	A	380	MLZ	CD-CE-NZ-CM
2	B	379[A]	MLZ	C-CA-CB-CG
2	B	379[B]	MLZ	N-CA-CB-CG
2	B	379[B]	MLZ	C-CA-CB-CG

There are no ring outliers.

9 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	533	MLZ	1	0
4	D	666	MLZ	1	0
2	B	413	MLY	1	0
3	C	470	MLY	2	0
1	A	489	MLY	1	0
1	A	497	MLY	1	0
3	C	312	MLY	1	0
1	A	312	MLY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	303	MLZ	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 43 ligands modelled in this entry, 8 are monoatomic - leaving 35 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	$\# Z > 2$
8	EDO	B	808	-	3,3,3	0.45	0	2,2,2	0.36	0
6	SO4	D	803	-	4,4,4	0.14	0	6,6,6	0.05	0
8	EDO	B	807	-	3,3,3	0.46	0	2,2,2	0.36	0
8	EDO	A	810	-	3,3,3	0.46	0	2,2,2	0.29	0
8	EDO	C	809	-	3,3,3	0.45	0	2,2,2	0.37	0
8	EDO	C	812	-	3,3,3	0.46	0	2,2,2	0.30	0
6	SO4	C	803	-	4,4,4	0.14	0	6,6,6	0.05	0
6	SO4	B	803	-	4,4,4	0.14	0	6,6,6	0.04	0
7	GOL	D	805	-	5,5,5	0.37	0	5,5,5	0.32	0
8	EDO	B	806	-	3,3,3	0.45	0	2,2,2	0.35	0
8	EDO	A	809	-	3,3,3	0.46	0	2,2,2	0.26	0
8	EDO	C	808	-	3,3,3	0.45	0	2,2,2	0.40	0
8	EDO	B	809	-	3,3,3	0.46	0	2,2,2	0.28	0
8	EDO	A	808	-	3,3,3	0.46	0	2,2,2	0.29	0
7	GOL	C	804	-	5,5,5	0.37	0	5,5,5	0.27	0
8	EDO	C	806	-	3,3,3	0.46	0	2,2,2	0.31	0
7	GOL	A	806	-	5,5,5	0.34	0	5,5,5	0.42	0
7	GOL	A	804	-	5,5,5	0.38	0	5,5,5	0.29	0
8	EDO	B	805	-	3,3,3	0.44	0	2,2,2	0.34	0
8	EDO	A	811	-	3,3,3	0.41	0	2,2,2	0.43	0
9	PEG	B	812	-	6,6,6	0.49	0	5,5,5	0.35	0
6	SO4	B	804	-	4,4,4	0.15	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	EDO	B	811	-	3,3,3	0.46	0	2,2,2	0.36	0
7	GOL	C	805	-	5,5,5	0.37	0	5,5,5	0.21	0
7	GOL	A	805	-	5,5,5	0.38	0	5,5,5	0.26	0
8	EDO	C	810	-	3,3,3	0.43	0	2,2,2	0.40	0
8	EDO	D	808	-	3,3,3	0.46	0	2,2,2	0.32	0
8	EDO	C	811	-	3,3,3	0.45	0	2,2,2	0.30	0
7	GOL	A	807	-	5,5,5	0.38	0	5,5,5	0.26	0
6	SO4	A	803	-	4,4,4	0.14	0	6,6,6	0.07	0
8	EDO	B	810	-	3,3,3	0.45	0	2,2,2	0.37	0
7	GOL	D	804	-	5,5,5	0.38	0	5,5,5	0.10	0
8	EDO	D	807	-	3,3,3	0.45	0	2,2,2	0.29	0
8	EDO	D	806	-	3,3,3	0.45	0	2,2,2	0.35	0
8	EDO	C	807	-	3,3,3	0.46	0	2,2,2	0.34	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
8	EDO	B	808	-	-	1/1/1/1	-
8	EDO	B	807	-	-	1/1/1/1	-
8	EDO	A	810	-	-	1/1/1/1	-
8	EDO	C	809	-	-	1/1/1/1	-
8	EDO	C	812	-	-	0/1/1/1	-
7	GOL	D	805	-	-	2/4/4/4	-
8	EDO	B	806	-	-	0/1/1/1	-
8	EDO	A	809	-	-	1/1/1/1	-
8	EDO	C	808	-	-	0/1/1/1	-
8	EDO	B	809	-	-	1/1/1/1	-
8	EDO	A	808	-	-	0/1/1/1	-
7	GOL	C	804	-	-	0/4/4/4	-
8	EDO	C	806	-	-	0/1/1/1	-
7	GOL	A	806	-	-	3/4/4/4	-
7	GOL	A	804	-	-	0/4/4/4	-
8	EDO	B	805	-	-	0/1/1/1	-
8	EDO	A	811	-	-	1/1/1/1	-
9	PEG	B	812	-	-	1/4/4/4	-
8	EDO	B	811	-	-	1/1/1/1	-
7	GOL	C	805	-	-	2/4/4/4	-
7	GOL	A	805	-	-	2/4/4/4	-
8	EDO	C	810	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	D	808	-	-	0/1/1/1	-
8	EDO	C	811	-	-	0/1/1/1	-
7	GOL	A	807	-	-	2/4/4/4	-
8	EDO	B	810	-	-	0/1/1/1	-
7	GOL	D	804	-	-	3/4/4/4	-
8	EDO	D	807	-	-	0/1/1/1	-
8	EDO	D	806	-	-	0/1/1/1	-
8	EDO	C	807	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	807	GOL	C1-C2-C3-O3
7	C	805	GOL	O1-C1-C2-C3
7	D	804	GOL	C1-C2-C3-O3
7	C	805	GOL	O1-C1-C2-O2
7	D	804	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	803	SO4	3	0
9	B	812	PEG	1	0
8	C	811	EDO	1	0
7	D	804	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	414/423 (97%)	0.22	26 (6%) 27 29	31, 61, 140, 170	0
2	B	404/418 (96%)	-0.22	4 (0%) 79 80	32, 50, 100, 120	0
3	C	410/424 (96%)	-0.30	3 (0%) 84 85	17, 46, 91, 123	1 (0%)
4	D	408/425 (96%)	-0.34	0 100 100	29, 48, 84, 111	0
All	All	1636/1690 (96%)	-0.16	33 (2%) 64 66	17, 51, 107, 170	1 (0%)

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	349	LEU	4.1
1	A	345	LEU	3.9
1	A	372	LEU	3.4
1	A	337	ALA	3.4
1	A	371	SER	3.3

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
2	MLZ	B	379[A]	10/11	0.71	0.18	74,79,80,83	10
2	MLZ	B	379[B]	10/11	0.71	0.18	74,79,80,83	10
2	MLY	B	413	11/12	0.71	0.13	79,84,91,92	0
1	MLZ	A	380	10/11	0.78	0.19	108,116,121,122	0
2	MLZ	B	699[A]	10/11	0.81	0.17	38,42,44,45	10
2	MLZ	B	699[B]	10/11	0.81	0.17	38,42,44,45	10
1	MLY	A	307	11/12	0.83	0.11	51,58,63,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MLY	D	413	11/12	0.83	0.12	62,68,82,83	0
2	MLZ	B	654	10/11	0.85	0.11	50,60,69,70	0
4	MLY	D	379	11/12	0.85	0.13	57,71,73,73	0
2	MLY	B	307	11/12	0.85	0.12	53,59,64,66	0
4	MLY	D	627	11/12	0.85	0.11	35,42,58,59	0
2	MLZ	B	666	10/11	0.86	0.11	46,50,64,65	0
1	MLZ	A	470	10/11	0.86	0.11	54,60,71,71	0
3	MLZ	C	699	10/11	0.87	0.11	50,55,63,65	0
1	MLY	A	666	11/12	0.87	0.11	52,56,62,62	0
2	MLZ	B	575	10/11	0.87	0.11	56,62,64,72	0
1	MLY	A	312	11/12	0.87	0.11	63,65,68,69	0
4	MLY	D	307	11/12	0.88	0.10	50,60,65,66	0
3	MLY	C	497	11/12	0.88	0.09	34,45,59,59	0
3	MLY	C	627	11/12	0.88	0.11	35,40,64,64	0
3	MLZ	C	380	10/11	0.88	0.09	61,63,73,73	0
4	MLZ	D	666	10/11	0.88	0.09	41,48,64,65	0
4	MLZ	D	380	10/11	0.89	0.08	60,63,65,71	0
1	MLY	A	627	11/12	0.89	0.10	32,38,60,61	0
4	MLZ	D	698	10/11	0.89	0.09	44,53,57,58	0
4	MLZ	D	533	10/11	0.90	0.11	39,49,63,64	0
1	MLY	A	497	11/12	0.90	0.08	48,54,66,67	0
3	MLY	C	319	11/12	0.91	0.09	36,40,46,48	0
3	MLY	C	666	11/12	0.91	0.12	54,57,67,70	0
2	MLZ	B	533	10/11	0.91	0.12	50,60,68,70	0
4	MLZ	D	303	10/11	0.91	0.09	49,52,62,64	0
2	MLZ	B	303	10/11	0.91	0.13	51,59,75,77	0
3	MLY	C	575	11/12	0.91	0.10	42,47,54,59	0
1	MLY	A	489	11/12	0.92	0.08	34,40,49,49	0
2	MLY	B	312	11/12	0.92	0.08	45,48,54,58	0
2	MLZ	B	319	10/11	0.92	0.07	43,49,52,54	0
4	MLY	D	497	11/12	0.92	0.08	35,44,60,62	0
2	MLZ	B	497	10/11	0.93	0.08	47,49,63,63	0
4	MLY	D	319	11/12	0.93	0.07	35,37,47,50	0
4	MLY	D	312	11/12	0.94	0.08	33,39,44,46	0
3	MLY	C	470	11/12	0.94	0.09	31,35,56,58	0
4	MLY	D	470	11/12	0.94	0.08	35,43,48,49	0
1	MLY	A	303	11/12	0.94	0.09	32,39,51,54	0
3	MLY	C	312	11/12	0.95	0.07	41,43,50,56	0
2	MLY	B	489	11/12	0.95	0.07	33,38,40,41	0
4	MLY	D	489	11/12	0.95	0.08	31,36,44,46	0
2	MLY	B	627	11/12	0.95	0.07	29,33,58,60	0
3	MLY	C	489	11/12	0.97	0.05	32,35,41,45	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	SO4	D	803	5/5	0.67	0.14	102,102,103,104	0
8	EDO	C	807	4/4	0.67	0.21	71,71,73,73	0
6	SO4	C	803	5/5	0.73	0.15	103,104,105,106	0
8	EDO	B	810	4/4	0.74	0.15	79,80,80,83	0
8	EDO	B	807	4/4	0.75	0.19	73,76,78,78	0
6	SO4	A	803	5/5	0.79	0.10	94,94,97,99	0
8	EDO	C	808	4/4	0.79	0.16	62,63,66,68	0
8	EDO	A	811	4/4	0.80	0.13	73,75,75,77	0
9	PEG	B	812	7/7	0.80	0.14	78,79,84,85	0
8	EDO	C	811	4/4	0.81	0.15	77,78,78,80	0
5	ZN	A	801[L]	1/1	0.82	0.15	42,42,42,42	1
8	EDO	D	807	4/4	0.83	0.15	61,62,65,67	0
7	GOL	D	804	6/6	0.83	0.14	38,46,52,56	0
8	EDO	A	810	4/4	0.84	0.18	72,73,73,73	0
8	EDO	B	809	4/4	0.84	0.12	74,78,80,80	0
8	EDO	B	811	4/4	0.85	0.14	73,74,75,76	0
8	EDO	B	806	4/4	0.85	0.16	53,54,57,58	0
8	EDO	A	809	4/4	0.85	0.11	61,65,66,67	0
8	EDO	D	808	4/4	0.86	0.14	67,68,69,69	0
8	EDO	C	809	4/4	0.86	0.15	63,66,67,68	0
7	GOL	A	807	6/6	0.87	0.11	93,93,94,94	0
8	EDO	B	808	4/4	0.87	0.12	80,81,82,82	0
8	EDO	A	808	4/4	0.87	0.11	73,74,74,77	0
7	GOL	A	805	6/6	0.88	0.14	77,79,79,80	0
7	GOL	D	805	6/6	0.88	0.09	84,88,89,90	0
8	EDO	C	812	4/4	0.88	0.14	78,79,81,81	0
7	GOL	A	806	6/6	0.89	0.12	64,69,70,72	0
6	SO4	B	804	5/5	0.89	0.10	117,117,117,117	0
8	EDO	C	810	4/4	0.90	0.14	75,76,76,77	0
5	ZN	B	802[L]	1/1	0.90	0.12	45,45,45,45	1
6	SO4	B	803	5/5	0.91	0.09	123,124,125,126	0
8	EDO	B	805	4/4	0.91	0.11	66,68,70,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	EDO	D	806	4/4	0.91	0.12	77,77,77,77	0
5	ZN	D	801	1/1	0.92	0.08	40,40,40,40	0
5	ZN	C	801[L]	1/1	0.92	0.13	36,36,36,36	1
7	GOL	A	804	6/6	0.93	0.09	44,49,55,59	0
8	EDO	C	806	4/4	0.93	0.10	56,63,68,70	0
5	ZN	D	802	1/1	0.93	0.09	46,46,46,46	0
5	ZN	C	802[L]	1/1	0.94	0.11	37,37,37,37	1
5	ZN	B	801[L]	1/1	0.94	0.12	39,39,39,39	1
7	GOL	C	804	6/6	0.94	0.07	40,44,53,58	0
7	GOL	C	805	6/6	0.94	0.11	58,63,64,67	0
5	ZN	A	802[L]	1/1	0.96	0.13	38,38,38,38	1

6.5 Other polymers [i](#)

There are no such residues in this entry.