



wwPDB X-ray Structure Validation Summary Report i

Jul 14, 2014 – 05:32 PM EDT

PDB ID : 4L3T
Title : Crystal Structure of Substrate-free Human Presequence Protease
Authors : King, J.V.; Liang, W.G.; Tang, W.J.
Deposited on : 2013-06-06
Resolution : 2.03 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

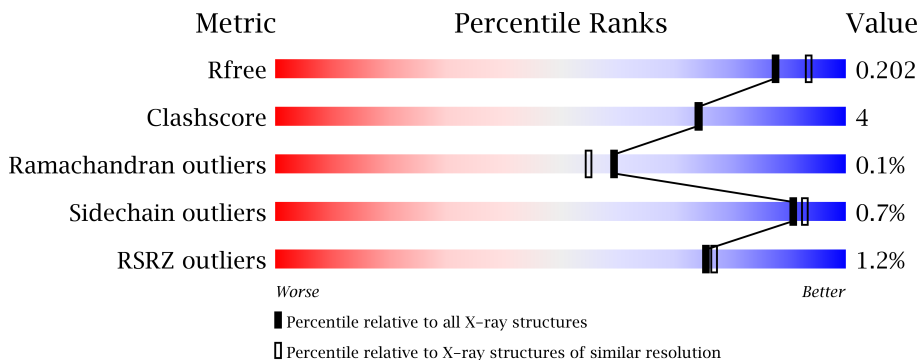
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23161
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23161

1 Overall quality at a glance

The reported resolution of this entry is 2.03 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}	66092	6003 (2.04-2.00)
Clashscore	79885	7467 (2.04-2.00)
Ramachandran outliers	78287	7370 (2.04-2.00)
Sidechain outliers	78261	7368 (2.04-2.00)
RSRZ outliers	66119	6006 (2.04-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1014	
2	B	1014	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	GOL	A	1107	-	X
4	GOL	B	1102	-	X
4	GOL	B	1112	-	X
5	ACT	A	1104	-	X
5	ACT	A	1105	-	X
5	ACT	A	1106	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
5	ACT	A	1108	-	X
5	ACT	B	1105	-	X
5	ACT	B	1106	-	X
5	ACT	B	1107	-	X
5	ACT	B	1109	-	X
5	ACT	B	1110	-	X
5	ACT	B	1111	-	X
5	ACT	B	1113	-	X
5	ACT	B	1114	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17046 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Presequence protease, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	As	C	N	O	S			
1	A	981	7977	6	5098	1349	1484	40	0	7	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	ALA	-	EXPRESSION TAG	UNP Q5JRX3
A	107	GLN	GLU	ENGINEERED MUTATION	UNP Q5JRX3
A	328	VAL	ILE	SEE REMARK 999	UNP Q5JRX3
A	397	VAL	ALA	SEE REMARK 999	UNP Q5JRX3
A	1037	ARG	GLN	SEE REMARK 999	UNP Q5JRX3

- Molecule 2 is a protein called Presequence protease, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	As	C	N	O	S			
2	B	978	7915	6	5064	1331	1474	40	0	3	0

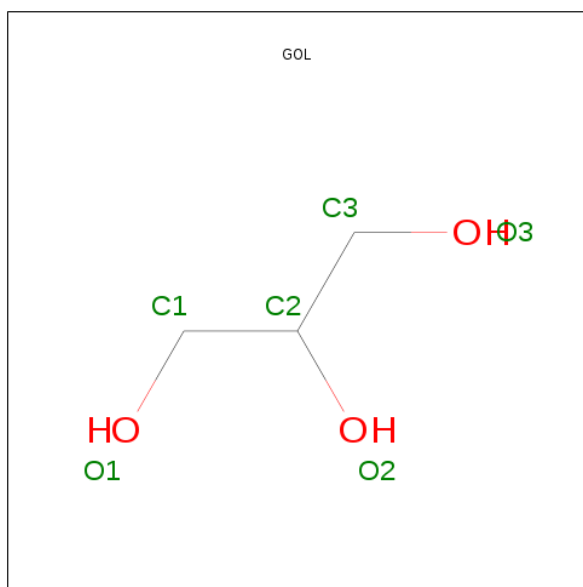
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	31	ALA	-	EXPRESSION TAG	UNP Q5JRX3
B	32	ALA	-	EXPRESSION TAG	UNP Q5JRX3
B	107	GLN	GLU	ENGINEERED MUTATION	UNP Q5JRX3
B	328	VAL	ILE	SEE REMARK 999	UNP Q5JRX3
B	397	VAL	ALA	SEE REMARK 999	UNP Q5JRX3
B	1037	ARG	GLN	SEE REMARK 999	UNP Q5JRX3

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

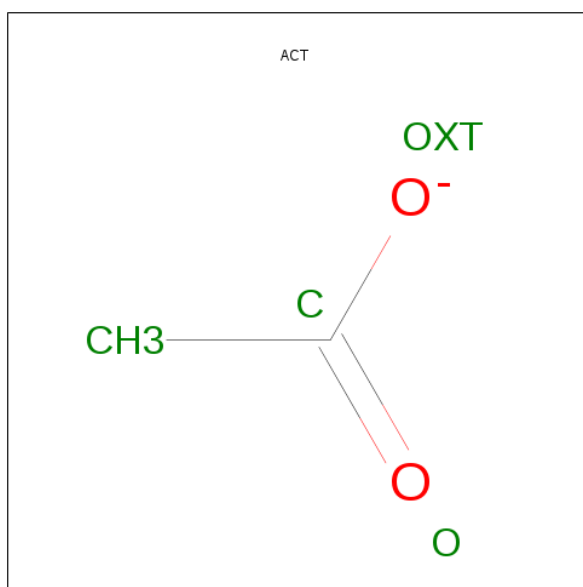
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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	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		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	553	Total 553	O 553	0	0
6	B	505	Total 505	O 505	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	245.78Å 85.09Å 158.46Å 90.00° 127.54° 90.00°	Depositor
Resolution (Å)	42.55 – 2.03 42.55 – 2.03	Depositor EDS
% Data completeness (in resolution range)	89.3 (42.55-2.03) 84.8 (42.55-2.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.67 (at 2.03Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.171 , 0.210 0.167 , 0.202	Depositor DCC
R_{free} test set	7099 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	27.2	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.0	EDS
Estimated twinning fraction	0.013 for -h-2*k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 149408 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17046	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, CAS, ACT, MLZ, 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	0.28	0/7704	0.47	1/10467 (0.0%)
2	B	0.28	0/7607	0.45	0/10329
All	All	0.28	0/15311	0.46	1/20796 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	316	ASP	CB-CG-OD2	5.17	122.95	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7977	0	7860	57	1
2	B	7915	0	7797	74	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	18	0	24	2	0
4	B	24	0	32	1	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	16	0	12	0	0
5	B	36	0	27	1	0
6	A	553	0	0	8	4
6	B	505	0	0	7	4
All	All	17046	0	15752	131	5

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

The worst 5 of 131 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:118:PRO:HG2	1:A:556:CAS:CE2	1.51	1.40
2:B:609:GLU:CD	2:B:814:ARG:NH1	1.78	1.35
2:B:609:GLU:OE2	2:B:814:ARG:NH1	1.58	1.31
1:A:313:CAS:CE1	1:A:506:PRO:HB3	1.65	1.26
2:B:609:GLU:OE1	2:B:814:ARG:NH1	1.66	1.24

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:A:1593:HOH:O	6:B:1534:HOH:O[3_556]	1.96	0.24
6:A:1557:HOH:O	6:B:1550:HOH:O[4_554]	2.10	0.10
1:A:682:GLN:NE2	4:B:1102:GOL:O3[3_556]	2.13	0.07
6:A:1601:HOH:O	6:B:1564:HOH:O[3_556]	2.16	0.04
6:A:1557:HOH:O	6:B:1548:HOH:O[4_554]	2.19	0.01

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	937/1014 (92%)	919 (98%)	17 (2%)	1 (0%)	59 55
2	B	926/1014 (91%)	909 (98%)	16 (2%)	1 (0%)	59 55
All	All	1863/2028 (92%)	1828 (98%)	33 (2%)	2 (0%)	59 55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	PRO
2	B	147	PRO

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	838/858 (98%)	833 (99%)	5 (1%)	92	94
2	B	827/855 (97%)	819 (99%)	8 (1%)	85	88
All	All	1665/1713 (97%)	1652 (99%)	13 (1%)	91	91

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	75	ARG
2	B	294	SER
2	B	814	ARG
1	A	981	LEU
2	B	728	ARG

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

Mol	Chain	Res	Type
1	A	498	HIS
1	A	989	HIS
2	B	498	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

89 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	1000	1	10,10,11	5.59	1 (10%)	9,11,13	0.91	1 (11%)
1	MLY	A	1013	1	10,10,11	5.72	1 (10%)	9,11,13	0.60	0
1	MLY	A	116	1	10,10,11	5.64	1 (10%)	9,11,13	1.37	1 (11%)
1	MLY	A	154	1	10,10,11	5.82	1 (10%)	9,11,13	1.56	1 (11%)
1	CAS	A	171	1	8,8,9	7.42	3 (37%)	7,9,11	3.68	3 (42%)
1	MLZ	A	207	1	9,9,10	7.05	2 (22%)	7,9,11	2.38	1 (14%)
1	CAS	A	241	1	8,8,9	7.46	3 (37%)	7,9,11	3.86	4 (57%)
1	MLY	A	251	1	10,10,11	5.78	2 (20%)	9,11,13	0.80	0
1	MLY	A	278	1	10,10,11	5.71	1 (10%)	9,11,13	1.05	1 (11%)
1	MLY	A	287	1	10,10,11	5.67	2 (20%)	9,11,13	0.84	0
1	MLY	A	290	1	10,10,11	5.53	1 (10%)	9,11,13	0.62	0
1	CAS	A	313	1	8,8,9	7.41	3 (37%)	7,9,11	5.23	4 (57%)
1	MLY	A	363	1	10,10,11	5.44	1 (10%)	9,11,13	1.02	1 (11%)
1	MLY	A	431	1	10,10,11	5.81	1 (10%)	9,11,13	1.01	1 (11%)
1	MLZ	A	437	1	9,9,10	7.20	1 (11%)	7,9,11	0.87	0
1	MLY	A	466	1	10,10,11	5.60	1 (10%)	9,11,13	1.25	1 (11%)
1	CAS	A	477	1	8,8,9	7.44	2 (25%)	7,9,11	3.90	4 (57%)
1	MLY	A	488	1	10,10,11	5.65	1 (10%)	9,11,13	1.05	1 (11%)
1	MLY	A	513	1	10,10,11	5.55	1 (10%)	9,11,13	1.13	1 (11%)
1	MLY	A	521	1	10,10,11	5.83	1 (10%)	9,11,13	1.10	1 (11%)
1	MLZ	A	525	1	9,9,10	7.26	1 (11%)	7,9,11	1.89	1 (14%)
1	MLY	A	540	1	10,10,11	5.58	1 (10%)	9,11,13	1.02	1 (11%)
1	MLZ	A	550	1	9,9,10	7.19	1 (11%)	7,9,11	1.22	1 (14%)
1	CAS	A	556	1	8,8,9	7.42	3 (37%)	7,9,11	4.75	4 (57%)
1	MLY	A	642	1	10,10,11	5.60	1 (10%)	9,11,13	0.74	0
1	MLY	A	66	1	10,10,11	5.74	1 (10%)	9,11,13	1.32	1 (11%)
1	CAS	A	692	1	8,8,9	7.42	3 (37%)	7,9,11	3.75	3 (42%)
1	MLY	A	700	1	10,10,11	5.60	1 (10%)	9,11,13	0.82	0
1	MLY	A	704	1	10,10,11	5.66	1 (10%)	9,11,13	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	A	750	1	10,10,11	5.84	2 (20%)	9,11,13	0.98	1 (11%)
1	MLY	A	759	1	10,10,11	5.72	2 (20%)	9,11,13	1.25	1 (11%)
1	MLY	A	764	1	10,10,11	5.75	1 (10%)	9,11,13	1.34	1 (11%)
1	MLZ	A	769	1	9,9,10	7.14	1 (11%)	7,9,11	1.82	1 (14%)
1	MLY	A	794	1	10,10,11	5.71	1 (10%)	9,11,13	0.86	0
1	MLY	A	854	1	10,10,11	5.71	1 (10%)	9,11,13	2.49	1 (11%)
1	MLY	A	884	1	10,10,11	5.63	1 (10%)	9,11,13	1.39	1 (11%)
1	MLY	A	902	1	10,10,11	5.52	1 (10%)	9,11,13	0.87	1 (11%)
1	MLY	A	911	1	10,10,11	5.69	1 (10%)	9,11,13	1.47	1 (11%)
1	MLY	A	937	1	10,10,11	5.80	1 (10%)	9,11,13	0.92	1 (11%)
1	MLY	A	943	1	10,10,11	5.71	2 (20%)	9,11,13	0.67	0
1	MLY	A	946	1	10,10,11	5.65	2 (20%)	9,11,13	0.78	0
1	MLY	A	956	1	10,10,11	5.60	1 (10%)	9,11,13	1.41	3 (33%)
1	MLY	A	972	1	10,10,11	5.60	1 (10%)	9,11,13	1.32	1 (11%)
2	MLZ	B	1000	2	9,9,10	7.24	2 (22%)	7,9,11	1.70	1 (14%)
2	MLY	B	1013	2	10,10,11	5.77	1 (10%)	9,11,13	0.90	1 (11%)
2	CAS	B	112	2	8,8,9	7.41	3 (37%)	7,9,11	3.66	3 (42%)
2	MLY	B	116	2	10,10,11	5.75	1 (10%)	9,11,13	1.02	1 (11%)
2	CAS	B	171	2	8,8,9	7.40	3 (37%)	7,9,11	3.75	4 (57%)
2	MLY	B	199	2	10,10,11	5.58	1 (10%)	9,11,13	1.40	1 (11%)
2	MLY	B	251	2	10,10,11	5.63	1 (10%)	9,11,13	0.86	0
2	MLY	B	278	2	10,10,11	5.81	1 (10%)	9,11,13	0.90	0
2	MLY	B	287	2	10,10,11	5.63	1 (10%)	9,11,13	0.92	0
2	MLY	B	290	2	10,10,11	5.50	1 (10%)	9,11,13	0.89	0
2	CAS	B	313	2	8,8,9	7.45	3 (37%)	7,9,11	4.05	4 (57%)
2	MLZ	B	324	2	9,9,10	7.26	1 (11%)	7,9,11	2.15	1 (14%)
2	MLY	B	363	2	10,10,11	5.69	2 (20%)	9,11,13	0.68	0
2	MLY	B	41	2	10,10,11	5.62	1 (10%)	9,11,13	1.67	1 (11%)
2	MLY	B	431	2	10,10,11	5.77	1 (10%)	9,11,13	1.21	1 (11%)
2	MLY	B	466	2	10,10,11	5.78	1 (10%)	9,11,13	1.05	1 (11%)
2	MLY	B	473	2	10,10,11	5.79	1 (10%)	9,11,13	0.96	1 (11%)
2	CAS	B	477	2	8,8,9	7.44	3 (37%)	7,9,11	3.85	4 (57%)
2	MLY	B	488	2	10,10,11	5.79	1 (10%)	9,11,13	1.07	1 (11%)
2	MLZ	B	490	2	9,9,10	7.28	1 (11%)	7,9,11	1.82	1 (14%)
2	MLZ	B	494	2	9,9,10	7.15	1 (11%)	7,9,11	1.11	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MLY	B	499	2	10,10,11	5.67	1 (10%)	9,11,13	1.38	1 (11%)
2	MLY	B	513	2	10,10,11	5.69	1 (10%)	9,11,13	1.18	1 (11%)
2	MLY	B	525	2	10,10,11	5.67	1 (10%)	9,11,13	0.97	1 (11%)
2	MLY	B	540	2	10,10,11	5.70	1 (10%)	9,11,13	0.67	0
2	MLY	B	550	2	10,10,11	5.78	1 (10%)	9,11,13	0.84	0
2	CAS	B	556	2	8,8,9	7.42	3 (37%)	7,9,11	3.86	4 (57%)
2	MLY	B	624	2	10,10,11	5.50	1 (10%)	9,11,13	0.82	0
2	MLY	B	642	2	10,10,11	5.72	1 (10%)	9,11,13	0.85	0
2	MLY	B	66	2	10,10,11	5.48	1 (10%)	9,11,13	1.79	1 (11%)
2	CAS	B	692	2	8,8,9	7.40	3 (37%)	7,9,11	3.80	4 (57%)
2	MLY	B	704	2	10,10,11	5.73	1 (10%)	9,11,13	0.79	0
2	MLY	B	750	2	10,10,11	5.56	1 (10%)	9,11,13	1.05	1 (11%)
2	MLZ	B	759	2	9,9,10	7.25	1 (11%)	7,9,11	0.95	0
2	MLZ	B	764	2	9,9,10	7.31	1 (11%)	7,9,11	1.66	1 (14%)
2	MLZ	B	769	2	9,9,10	7.39	1 (11%)	7,9,11	1.51	1 (14%)
2	MLZ	B	854	2	9,9,10	7.22	1 (11%)	7,9,11	2.76	1 (14%)
2	MLZ	B	884	2	9,9,10	7.23	1 (11%)	7,9,11	1.96	1 (14%)
2	MLY	B	902	2	10,10,11	5.55	1 (10%)	9,11,13	0.99	1 (11%)
2	MLY	B	911	2	10,10,11	5.64	1 (10%)	9,11,13	1.29	1 (11%)
2	MLZ	B	937	2	9,9,10	7.15	1 (11%)	7,9,11	1.49	1 (14%)
2	MLY	B	943	2	10,10,11	5.73	2 (20%)	9,11,13	0.61	0
2	MLY	B	946	2	10,10,11	5.77	2 (20%)	9,11,13	0.94	0
2	MLY	B	956	2	10,10,11	5.72	1 (10%)	9,11,13	0.93	0
2	MLY	B	972	2	10,10,11	5.56	1 (10%)	9,11,13	1.14	1 (11%)
2	MLY	B	986	2	10,10,11	5.63	1 (10%)	9,11,13	0.84	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	1000	1	-	0/7/9/11	0/0/0/0
1	MLY	A	1013	1	-	0/7/9/11	0/0/0/0
1	MLY	A	116	1	-	0/7/9/11	0/0/0/0
1	MLY	A	154	1	-	0/7/9/11	0/0/0/0
1	CAS	A	171	1	-	0/2/7/9	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLZ	A	207	1	-	0/6/8/10	0/0/0/0
1	CAS	A	241	1	-	0/2/7/9	0/0/0/0
1	MLY	A	251	1	-	0/7/9/11	0/0/0/0
1	MLY	A	278	1	-	0/7/9/11	0/0/0/0
1	MLY	A	287	1	-	0/7/9/11	0/0/0/0
1	MLY	A	290	1	-	0/7/9/11	0/0/0/0
1	CAS	A	313	1	-	0/2/7/9	0/0/0/0
1	MLY	A	363	1	-	0/7/9/11	0/0/0/0
1	MLY	A	431	1	-	0/7/9/11	0/0/0/0
1	MLZ	A	437	1	-	0/6/8/10	0/0/0/0
1	MLY	A	466	1	-	0/7/9/11	0/0/0/0
1	CAS	A	477	1	-	0/2/7/9	0/0/0/0
1	MLY	A	488	1	-	0/7/9/11	0/0/0/0
1	MLY	A	513	1	-	0/7/9/11	0/0/0/0
1	MLY	A	521	1	-	0/7/9/11	0/0/0/0
1	MLZ	A	525	1	-	0/6/8/10	0/0/0/0
1	MLY	A	540	1	-	0/7/9/11	0/0/0/0
1	MLZ	A	550	1	-	0/6/8/10	0/0/0/0
1	CAS	A	556	1	-	0/2/7/9	0/0/0/0
1	MLY	A	642	1	-	0/7/9/11	0/0/0/0
1	MLY	A	66	1	-	0/7/9/11	0/0/0/0
1	CAS	A	692	1	-	0/2/7/9	0/0/0/0
1	MLY	A	700	1	-	0/7/9/11	0/0/0/0
1	MLY	A	704	1	-	0/7/9/11	0/0/0/0
1	MLY	A	750	1	-	0/7/9/11	0/0/0/0
1	MLY	A	759	1	-	0/7/9/11	0/0/0/0
1	MLY	A	764	1	-	0/7/9/11	0/0/0/0
1	MLZ	A	769	1	-	0/6/8/10	0/0/0/0
1	MLY	A	794	1	-	0/7/9/11	0/0/0/0
1	MLY	A	854	1	-	0/7/9/11	0/0/0/0
1	MLY	A	884	1	-	0/7/9/11	0/0/0/0
1	MLY	A	902	1	-	0/7/9/11	0/0/0/0
1	MLY	A	911	1	-	0/7/9/11	0/0/0/0
1	MLY	A	937	1	-	0/7/9/11	0/0/0/0
1	MLY	A	943	1	-	0/7/9/11	0/0/0/0
1	MLY	A	946	1	-	0/7/9/11	0/0/0/0
1	MLY	A	956	1	-	0/7/9/11	0/0/0/0
1	MLY	A	972	1	-	0/7/9/11	0/0/0/0
2	MLZ	B	1000	2	-	0/6/8/10	0/0/0/0
2	MLY	B	1013	2	-	0/7/9/11	0/0/0/0
2	CAS	B	112	2	-	0/2/7/9	0/0/0/0
2	MLY	B	116	2	-	0/7/9/11	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CAS	B	171	2	-	0/2/7/9	0/0/0/0
2	MLY	B	199	2	-	0/7/9/11	0/0/0/0
2	MLY	B	251	2	-	0/7/9/11	0/0/0/0
2	MLY	B	278	2	-	0/7/9/11	0/0/0/0
2	MLY	B	287	2	-	0/7/9/11	0/0/0/0
2	MLY	B	290	2	-	0/7/9/11	0/0/0/0
2	CAS	B	313	2	-	0/2/7/9	0/0/0/0
2	MLZ	B	324	2	-	0/6/8/10	0/0/0/0
2	MLY	B	363	2	-	0/7/9/11	0/0/0/0
2	MLY	B	41	2	-	0/7/9/11	0/0/0/0
2	MLY	B	431	2	-	0/7/9/11	0/0/0/0
2	MLY	B	466	2	-	0/7/9/11	0/0/0/0
2	MLY	B	473	2	-	0/7/9/11	0/0/0/0
2	CAS	B	477	2	-	0/2/7/9	0/0/0/0
2	MLY	B	488	2	-	0/7/9/11	0/0/0/0
2	MLZ	B	490	2	-	0/6/8/10	0/0/0/0
2	MLZ	B	494	2	-	0/6/8/10	0/0/0/0
2	MLY	B	499	2	-	0/7/9/11	0/0/0/0
2	MLY	B	513	2	-	0/7/9/11	0/0/0/0
2	MLY	B	525	2	-	0/7/9/11	0/0/0/0
2	MLY	B	540	2	-	0/7/9/11	0/0/0/0
2	MLY	B	550	2	-	0/7/9/11	0/0/0/0
2	CAS	B	556	2	-	0/2/7/9	0/0/0/0
2	MLY	B	624	2	-	0/7/9/11	0/0/0/0
2	MLY	B	642	2	-	0/7/9/11	0/0/0/0
2	MLY	B	66	2	-	0/7/9/11	0/0/0/0
2	CAS	B	692	2	-	0/2/7/9	0/0/0/0
2	MLY	B	704	2	-	0/7/9/11	0/0/0/0
2	MLY	B	750	2	-	0/7/9/11	0/0/0/0
2	MLZ	B	759	2	-	0/6/8/10	0/0/0/0
2	MLZ	B	764	2	-	0/6/8/10	0/0/0/0
2	MLZ	B	769	2	-	0/6/8/10	0/0/0/0
2	MLZ	B	854	2	-	0/6/8/10	0/0/0/0
2	MLZ	B	884	2	-	0/6/8/10	0/0/0/0
2	MLY	B	902	2	-	0/7/9/11	0/0/0/0
2	MLY	B	911	2	-	0/7/9/11	0/0/0/0
2	MLZ	B	937	2	-	0/6/8/10	0/0/0/0
2	MLY	B	943	2	-	0/7/9/11	0/0/0/0
2	MLY	B	946	2	-	0/7/9/11	0/0/0/0
2	MLY	B	956	2	-	0/7/9/11	0/0/0/0
2	MLY	B	972	2	-	0/7/9/11	0/0/0/0
2	MLY	B	986	2	-	0/7/9/11	0/0/0/0

The worst 5 of 123 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	769	MLZ	O-C	22.09	1.26	1.11
2	B	764	MLZ	O-C	21.81	1.26	1.11
2	B	490	MLZ	O-C	21.71	1.26	1.11
1	A	525	MLZ	O-C	21.68	1.26	1.11
2	B	324	MLZ	O-C	21.66	1.26	1.11

The worst 5 of 98 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	313	CAS	C-CA-N	-9.86	103.98	113.83
1	A	692	CAS	CE2-AS-CE1	8.20	109.56	96.77
2	B	477	CAS	CE2-AS-CE1	8.19	109.53	96.77
1	A	556	CAS	CE2-AS-CE1	8.18	109.52	96.77
1	A	241	CAS	CE2-AS-CE1	8.17	109.51	96.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 2 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	$\# Z > 2$
4	GOL	A	1102	-	5,5,5	0.30	0	5,5,5	0.32	0
4	GOL	A	1103	-	5,5,5	0.27	0	5,5,5	0.34	0
5	ACT	A	1104	-	1,3,3	1.02	0	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ACT	A	1105	-	1,3,3	1.13	0	0,3,3	0.00	-
5	ACT	A	1106	-	1,3,3	1.33	0	0,3,3	0.00	-
4	GOL	A	1107	-	5,5,5	0.32	0	5,5,5	0.42	0
5	ACT	A	1108	3	1,3,3	1.36	0	0,3,3	0.00	-
4	GOL	B	1102	-	5,5,5	0.36	0	5,5,5	0.51	0
4	GOL	B	1103	-	5,5,5	0.28	0	5,5,5	0.33	0
4	GOL	B	1104	-	5,5,5	0.33	0	5,5,5	0.12	0
5	ACT	B	1105	-	1,3,3	1.36	0	0,3,3	0.00	-
5	ACT	B	1106	-	1,3,3	1.14	0	0,3,3	0.00	-
5	ACT	B	1107	-	1,3,3	0.97	0	0,3,3	0.00	-
5	ACT	B	1108	-	1,3,3	1.21	0	0,3,3	0.00	-
5	ACT	B	1109	-	1,3,3	1.10	0	0,3,3	0.00	-
5	ACT	B	1110	-	1,3,3	1.18	0	0,3,3	0.00	-
5	ACT	B	1111	-	1,3,3	1.19	0	0,3,3	0.00	-
4	GOL	B	1112	-	5,5,5	0.32	0	5,5,5	0.30	0
5	ACT	B	1113	-	1,3,3	1.32	0	0,3,3	0.00	-
5	ACT	B	1114	-	1,3,3	0.90	0	0,3,3	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	1102	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1103	-	-	0/4/4/4	0/0/0/0
5	ACT	A	1104	-	-	0/0/0/0	0/0/0/0
5	ACT	A	1105	-	-	0/0/0/0	0/0/0/0
5	ACT	A	1106	-	-	0/0/0/0	0/0/0/0
4	GOL	A	1107	-	-	0/4/4/4	0/0/0/0
5	ACT	A	1108	3	-	0/0/0/0	0/0/0/0
4	GOL	B	1102	-	-	0/4/4/4	0/0/0/0
4	GOL	B	1103	-	-	0/4/4/4	0/0/0/0
4	GOL	B	1104	-	-	0/4/4/4	0/0/0/0
5	ACT	B	1105	-	-	0/0/0/0	0/0/0/0
5	ACT	B	1106	-	-	0/0/0/0	0/0/0/0
5	ACT	B	1107	-	-	0/0/0/0	0/0/0/0
5	ACT	B	1108	-	-	0/0/0/0	0/0/0/0
5	ACT	B	1109	-	-	0/0/0/0	0/0/0/0
5	ACT	B	1110	-	-	0/0/0/0	0/0/0/0
5	ACT	B	1111	-	-	0/0/0/0	0/0/0/0
4	GOL	B	1112	-	-	0/4/4/4	0/0/0/0
5	ACT	B	1113	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ACT	B	1114	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	981/1014 (96%)	-0.37	11 (1%) 77 78	18, 30, 58, 93	0
2	B	978/1014 (96%)	-0.43	13 (1%) 74 75	20, 32, 59, 98	0
All	All	1959/2028 (96%)	-0.40	24 (1%) 75 77	18, 31, 59, 98	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	838	VAL	6.0
1	A	313	CAS	5.0
1	A	838	VAL	4.9
1	A	316	ASP	4.7
2	B	313	CAS	4.5

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	CAS	A	556	9/10	0.23	7.27	24,32,90,102	0
2	MLZ	B	937	10/11	0.13	6.37	23,28,64,67	0
2	MLY	B	66	11/12	0.13	5.20	20,24,58,59	0
2	CAS	B	171	9/10	0.17	4.49	24,32,90,102	0
2	MLZ	B	494	10/11	0.20	4.03	29,42,61,62	0
2	CAS	B	556	9/10	0.17	3.75	34,42,114,157	0
1	MLY	A	937	11/12	0.13	3.48	24,31,62,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MLZ	B	324	10/11	0.20	3.35	47,62,75,75	0
2	MLY	B	525	11/12	0.12	2.98	25,39,47,51	0
1	CAS	A	692	9/10	0.18	2.79	39,44,108,242	0
2	MLY	B	499	11/12	0.13	2.56	28,33,64,67	0
2	CAS	B	112	9/10	0.18	2.42	25,33,104,226	0
2	MLZ	B	1000	10/11	0.12	2.35	25,31,64,65	0
1	MLY	A	946	11/12	0.12	2.35	22,33,57,60	0
2	MLY	B	956	11/12	0.12	2.23	25,34,64,67	0
1	MLY	A	1000	11/12	0.11	2.20	20,27,60,64	0
2	CAS	B	313	9/10	0.26	2.16	48,54,100,262	0
1	MLY	A	956	11/12	0.12	2.12	18,22,62,69	0
2	MLY	B	624	11/12	0.14	2.11	27,31,57,58	0
2	MLY	B	550	11/12	0.14	1.88	29,37,51,58	0
1	MLY	A	1013	11/12	0.14	1.81	35,38,56,58	0
2	MLY	B	473	11/12	0.13	1.78	31,37,68,69	0
2	CAS	B	692	9/10	0.13	1.74	28,41,70,165	0
2	MLY	B	199	11/12	0.14	1.68	22,31,62,62	0
1	CAS	A	171	9/10	0.14	1.57	19,34,86,100	0
1	MLY	A	972	11/12	0.13	1.56	22,35,63,64	0
1	MLY	A	700	11/12	0.18	1.56	28,40,73,74	0
2	MLY	B	363	11/12	0.10	1.50	28,34,59,60	0
1	MLY	A	66	11/12	0.11	1.50	25,36,54,55	0
1	CAS	A	313	9/10	0.27	1.48	54,56,93,287	0
2	MLY	B	41	11/12	0.10	1.36	27,29,44,49	0
1	MLY	A	794	11/12	0.15	1.22	38,52,69,69	0
1	MLY	A	116	11/12	0.09	1.21	25,30,42,46	0
1	MLY	A	521	11/12	0.21	1.18	44,59,87,89	0
2	MLY	B	431	11/12	0.13	1.17	25,32,60,62	0
2	MLZ	B	490	10/11	0.14	1.13	31,37,66,68	0
1	CAS	A	241	9/10	0.13	1.12	22,39,71,190	0
1	MLY	A	911	11/12	0.13	1.00	20,22,42,44	0
1	MLY	A	466	11/12	0.11	0.93	28,32,50,51	0
2	MLY	B	750	11/12	0.16	0.92	24,36,65,65	0
2	MLY	B	278	11/12	0.10	0.89	24,29,60,62	0
2	MLY	B	116	11/12	0.12	0.88	21,35,57,58	0
1	MLY	A	902	11/12	0.12	0.83	25,27,42,43	0
1	MLY	A	154	11/12	0.08	0.79	23,28,61,63	0
1	MLY	A	290	11/12	0.12	0.72	34,39,59,60	0
2	MLY	B	287	11/12	0.13	0.70	31,35,50,52	0
1	MLZ	A	207	10/11	0.12	0.70	19,28,53,56	0
1	MLY	A	759	11/12	0.16	0.69	32,42,63,64	0
1	MLY	A	704	11/12	0.12	0.61	25,29,50,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	MLY	A	943	11/12	0.10	0.58	20,29,43,47	0
2	MLY	B	972	11/12	0.12	0.49	27,36,71,71	0
2	MLY	B	466	11/12	0.10	0.49	26,36,47,49	0
2	MLY	B	986	11/12	0.16	0.44	35,43,70,70	0
2	MLY	B	946	11/12	0.10	0.42	26,34,46,48	0
1	MLY	A	513	11/12	0.17	0.37	43,48,53,60	0
2	MLY	B	290	11/12	0.12	0.30	36,39,65,65	0
2	MLY	B	704	11/12	0.10	0.30	24,31,59,60	0
2	MLY	B	911	11/12	0.10	0.27	20,28,54,55	0
1	MLY	A	251	11/12	0.10	0.26	24,27,53,54	0
2	MLY	B	513	11/12	0.16	0.24	46,49,53,56	0
1	MLY	A	278	11/12	0.08	0.22	22,35,41,41	0
1	MLY	A	363	11/12	0.10	0.19	24,31,59,60	0
1	MLY	A	884	11/12	0.09	0.19	20,25,46,51	0
2	MLZ	B	769	10/11	0.10	0.17	30,41,50,52	0
1	MLY	A	287	11/12	0.10	0.15	22,26,34,34	0
2	MLZ	B	759	10/11	0.14	0.15	41,47,64,65	0
2	MLY	B	642	11/12	0.10	0.15	27,28,39,43	0
1	MLZ	A	550	10/11	0.11	0.14	28,35,45,46	0
1	MLY	A	431	11/12	0.10	0.12	24,33,63,63	0
2	MLY	B	540	11/12	0.10	0.10	20,26,41,45	0
1	MLY	A	764	11/12	0.11	0.07	35,38,49,50	0
2	MLY	B	943	11/12	0.10	0.05	24,31,56,58	0
2	MLY	B	488	11/12	0.10	-0.06	27,30,42,43	0
1	MLY	A	750	11/12	0.12	-0.08	27,41,61,66	0
1	MLZ	A	437	10/11	0.08	-0.13	28,32,56,56	0
2	MLY	B	251	11/12	0.10	-0.17	23,26,55,56	0
1	MLY	A	854	11/12	0.09	-0.19	20,29,46,46	0
2	MLY	B	1013	11/12	0.09	-0.29	31,39,54,55	0
1	MLY	A	488	11/12	0.09	-0.38	28,35,39,40	0
1	MLZ	A	525	10/11	0.14	-0.38	41,45,51,53	0
1	CAS	A	477	9/10	0.11	-0.41	40,44,77,147	0
1	MLY	A	642	11/12	0.09	-0.44	22,24,42,43	0
1	MLZ	A	769	10/11	0.08	-0.45	27,31,43,43	0
2	CAS	B	477	9/10	0.10	-0.46	35,47,118,187	0
2	MLZ	B	764	10/11	0.08	-0.59	35,44,48,50	0
1	MLY	A	540	11/12	0.09	-0.59	28,30,45,47	0
2	MLZ	B	884	10/11	0.07	-0.73	22,27,53,54	0
2	MLY	B	902	11/12	0.08	-0.94	27,31,40,41	0
2	MLZ	B	854	10/11	0.08	-1.38	29,33,46,48	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	GOL	B	1112	6/6	0.31	16.17	84,89,91,92	0
5	ACT	B	1114	4/4	0.30	12.90	61,70,71,74	0
5	ACT	A	1104	4/4	0.26	8.03	49,57,57,58	0
5	ACT	B	1109	4/4	0.21	7.84	91,91,92,93	0
5	ACT	A	1105	4/4	0.34	5.89	58,64,65,72	0
5	ACT	B	1110	4/4	0.16	5.86	8,31,41,45	0
5	ACT	B	1113	4/4	0.18	5.67	49,56,60,62	0
5	ACT	A	1108	4/4	0.23	5.34	34,35,35,36	0
5	ACT	B	1107	4/4	0.16	4.47	69,71,73,77	0
4	GOL	B	1102	6/6	0.18	4.14	11,48,54,64	0
5	ACT	B	1106	4/4	0.13	3.26	69,71,71,74	0
5	ACT	B	1105	4/4	0.16	2.95	49,59,60,66	0
5	ACT	A	1106	4/4	0.23	2.78	58,65,67,67	0
4	GOL	A	1107	6/6	0.21	2.55	40,53,63,68	0
5	ACT	B	1111	4/4	0.15	2.01	72,76,77,81	0
5	ACT	B	1108	4/4	0.16	0.78	38,40,43,47	0
4	GOL	B	1104	6/6	0.09	0.30	35,47,50,52	0
4	GOL	A	1103	6/6	0.09	-0.13	40,41,50,56	0
3	ZN	A	1101	1/1	0.11	-0.40	28,28,28,28	0
4	GOL	A	1102	6/6	0.08	-1.06	23,33,34,35	0
4	GOL	B	1103	6/6	0.08	-1.19	23,32,36,39	0
3	ZN	B	1101	1/1	0.08	-1.90	25,25,25,25	0

6.5 Other polymers ⓘ

There are no such residues in this entry.