



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2025 – 06:36 AM 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 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 : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.21
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

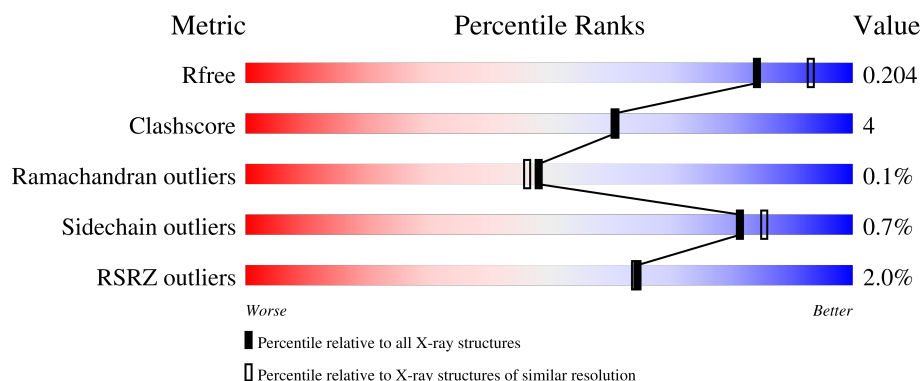
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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}	164625	12358 (2.04-2.00)
Clashscore	180529	13897 (2.04-2.00)
Ramachandran outliers	177936	13770 (2.04-2.00)
Sidechain outliers	177891	13769 (2.04-2.00)
RSRZ outliers	164620	12358 (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 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	1014	
2	B	1014	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	CAS	A	313	-	-	X	-
1	CAS	A	556	-	-	X	-
2	CAS	B	112	-	-	X	-
2	CAS	B	313	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17046 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 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 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	MET	-	expression tag	UNP Q5JRX3
A	25	HIS	-	expression tag	UNP Q5JRX3
A	26	HIS	-	expression tag	UNP Q5JRX3
A	27	HIS	-	expression tag	UNP Q5JRX3
A	28	HIS	-	expression tag	UNP Q5JRX3
A	29	HIS	-	expression tag	UNP Q5JRX3
A	30	HIS	-	expression tag	UNP Q5JRX3
A	31	ALA	-	expression tag	UNP Q5JRX3
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 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	24	MET	-	expression tag	UNP Q5JRX3
B	25	HIS	-	expression tag	UNP Q5JRX3
B	26	HIS	-	expression tag	UNP Q5JRX3

Continued on next page...

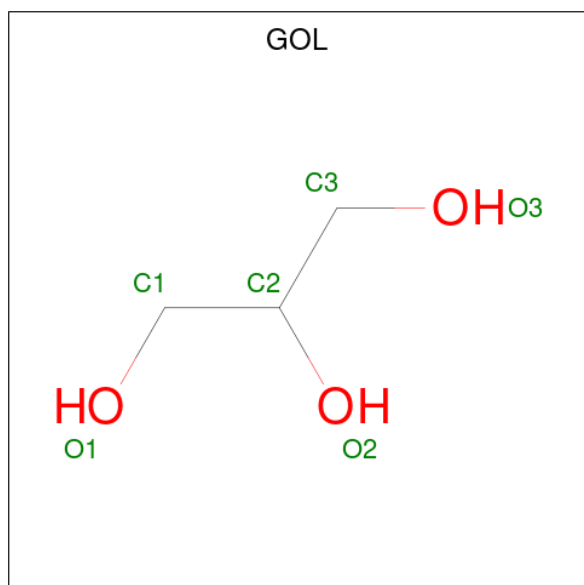
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	27	HIS	-	expression tag	UNP Q5JRX3
B	28	HIS	-	expression tag	UNP Q5JRX3
B	29	HIS	-	expression tag	UNP Q5JRX3
B	30	HIS	-	expression tag	UNP Q5JRX3
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	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



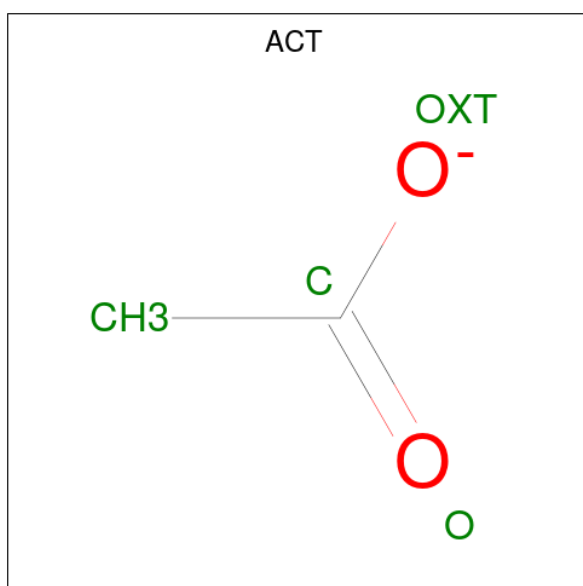
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		

Continued on next page...

Continued from previous page...

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

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) 84.9 (42.55-2.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 2.03Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.171 , 0.210 0.169 , 0.204	Depositor DCC
R_{free} test set	7469 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 60.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -h-2*k,l	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 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MLY, ACT, CAS, GOL, ZN, MLZ

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 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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
5	A	16	0	12	0	0
5	B	36	0	27	1	0

Continued on next page...

Continued from previous page...

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

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 4.

The worst 5 of 131 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: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	Interatomic distance (Å)	Clash overlap (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%)	48 46

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	926/1014 (91%)	909 (98%)	16 (2%)	1 (0%)	48	46
All	All	1863/2028 (92%)	1828 (98%)	33 (2%)	2 (0%)	48	46

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%)	84	88
2	B	827/855 (97%)	819 (99%)	8 (1%)	73	77
All	All	1665/1713 (97%)	1652 (99%)	13 (1%)	81	83

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

Mol	Chain	Res	Type
2	B	403	THR
2	B	604	LEU
2	B	1011	THR
2	B	814	ARG
2	B	843	VAL

Sometimes 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 molecules 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	$\# Z > 2$
2	CAS	B	477	2	5,8,9	1.17	0	1,9,11	0.45	0
1	MLY	A	290	1	9,10,11	0.54	0	6,11,13	0.74	0
1	CAS	A	477	1	5,8,9	1.15	0	1,9,11	0.36	0
2	MLZ	B	324	2	8,9,10	0.88	0	4,9,11	0.86	0
1	MLZ	A	550	1	8,9,10	0.83	0	4,9,11	0.81	0
2	CAS	B	692	2	5,8,9	1.14	0	1,9,11	0.49	0
1	MLY	A	513	1	9,10,11	0.53	0	6,11,13	0.66	0
1	MLY	A	911	1	9,10,11	0.63	0	6,11,13	0.80	0
2	MLY	B	116	2	9,10,11	0.60	0	6,11,13	0.79	0
1	MLY	A	704	1	9,10,11	0.56	0	6,11,13	0.73	0
1	MLY	A	854	1	9,10,11	0.67	0	6,11,13	0.75	0
1	CAS	A	692	1	5,8,9	1.13	0	1,9,11	1.43	0
1	MLY	A	937	1	9,10,11	0.66	0	6,11,13	0.71	0
2	MLY	B	1013	2	9,10,11	0.58	0	6,11,13	0.76	0
1	MLY	A	884	1	9,10,11	0.55	0	6,11,13	0.78	0
1	MLY	A	431	1	9,10,11	0.59	0	6,11,13	0.81	0
1	MLY	A	466	1	9,10,11	0.54	0	6,11,13	0.86	0
1	MLY	A	794	1	9,10,11	0.63	0	6,11,13	0.67	0
1	MLY	A	278	1	9,10,11	0.51	0	6,11,13	0.72	0
1	MLY	A	1013	1	9,10,11	0.56	0	6,11,13	0.67	0
1	MLY	A	972	1	9,10,11	0.56	0	6,11,13	0.84	0
2	MLZ	B	764	2	8,9,10	0.88	0	4,9,11	0.91	0
2	MLY	B	488	2	9,10,11	0.57	0	6,11,13	0.77	0
1	MLY	A	956	1	9,10,11	0.51	0	6,11,13	1.52	2 (33%)
2	MLY	B	986	2	9,10,11	0.59	0	6,11,13	0.62	0
2	MLY	B	278	2	9,10,11	0.54	0	6,11,13	0.86	0
2	MLY	B	431	2	9,10,11	0.56	0	6,11,13	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MLY	B	473	2	9,10,11	0.52	0	6,11,13	0.83	0
2	MLY	B	525	2	9,10,11	0.57	0	6,11,13	0.73	0
2	CAS	B	171	2	5,8,9	1.14	0	1,9,11	0.31	0
2	MLZ	B	769	2	8,9,10	0.84	0	4,9,11	0.87	0
2	MLZ	B	494	2	8,9,10	0.78	0	4,9,11	0.82	0
2	MLY	B	66	2	9,10,11	0.57	0	6,11,13	0.82	0
2	MLY	B	642	2	9,10,11	0.60	0	6,11,13	0.80	0
2	MLZ	B	937	2	8,9,10	0.84	0	4,9,11	0.94	0
1	MLY	A	943	1	9,10,11	0.69	0	6,11,13	0.65	0
2	MLY	B	199	2	9,10,11	0.48	0	6,11,13	0.95	0
2	MLY	B	943	2	9,10,11	0.62	0	6,11,13	0.71	0
1	MLY	A	700	1	9,10,11	0.55	0	6,11,13	0.77	0
2	CAS	B	556	2	5,8,9	1.16	0	1,9,11	0.68	0
1	CAS	A	313	1	5,8,9	1.15	0	1,9,11	8.25	1 (100%)
2	MLY	B	550	2	9,10,11	0.63	0	6,11,13	0.82	0
2	MLY	B	290	2	9,10,11	0.52	0	6,11,13	0.89	0
1	MLZ	A	769	1	8,9,10	0.76	0	4,9,11	0.60	0
1	MLY	A	363	1	9,10,11	0.58	0	6,11,13	0.70	0
1	MLY	A	642	1	9,10,11	0.53	0	6,11,13	0.87	0
1	MLY	A	764	1	9,10,11	0.54	0	6,11,13	0.89	0
1	MLZ	A	525	1	8,9,10	0.87	0	4,9,11	0.95	0
2	MLY	B	972	2	9,10,11	0.51	0	6,11,13	0.82	0
1	CAS	A	556	1	5,8,9	1.16	0	1,9,11	1.86	0
1	MLY	A	946	1	9,10,11	0.53	0	6,11,13	0.96	0
2	MLY	B	624	2	9,10,11	0.47	0	6,11,13	0.93	0
1	MLY	A	540	1	9,10,11	0.54	0	6,11,13	0.67	0
2	MLY	B	251	2	9,10,11	0.52	0	6,11,13	0.80	0
1	MLY	A	116	1	9,10,11	0.46	0	6,11,13	1.18	0
2	CAS	B	112	2	5,8,9	1.13	0	1,9,11	0.45	0
2	CAS	B	313	2	5,8,9	1.16	0	1,9,11	0.63	0
1	MLY	A	1000	1	9,10,11	0.56	0	6,11,13	0.72	0
2	MLY	B	287	2	9,10,11	0.53	0	6,11,13	0.88	0
2	MLZ	B	490	2	8,9,10	0.92	0	4,9,11	1.08	0
2	MLZ	B	759	2	8,9,10	0.77	0	4,9,11	0.87	0
1	MLY	A	154	1	9,10,11	0.56	0	6,11,13	0.95	0
1	CAS	A	171	1	5,8,9	1.14	0	1,9,11	0.30	0
1	MLY	A	287	1	9,10,11	0.49	0	6,11,13	0.86	0
2	MLY	B	363	2	9,10,11	0.69	0	6,11,13	0.62	0
1	MLY	A	759	1	9,10,11	0.54	0	6,11,13	0.77	0
2	MLY	B	902	2	9,10,11	0.58	0	6,11,13	0.71	0
1	MLY	A	750	1	9,10,11	0.55	0	6,11,13	0.66	0
2	MLY	B	499	2	9,10,11	0.55	0	6,11,13	0.90	0
2	MLY	B	956	2	9,10,11	0.64	0	6,11,13	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	A	251	1	9,10,11	0.60	0	6,11,13	0.85	0
2	MLY	B	750	2	9,10,11	0.57	0	6,11,13	0.76	0
2	MLY	B	540	2	9,10,11	0.56	0	6,11,13	0.60	0
2	MLY	B	704	2	9,10,11	0.51	0	6,11,13	0.84	0
2	MLZ	B	1000	2	8,9,10	0.92	0	4,9,11	0.98	0
2	MLY	B	911	2	9,10,11	0.52	0	6,11,13	0.96	0
2	MLY	B	41	2	9,10,11	0.57	0	6,11,13	0.89	0
1	MLY	A	521	1	9,10,11	0.55	0	6,11,13	0.73	0
1	MLZ	A	437	1	8,9,10	0.80	0	4,9,11	0.93	0
1	MLY	A	902	1	9,10,11	0.59	0	6,11,13	0.68	0
2	MLZ	B	884	2	8,9,10	0.83	0	4,9,11	0.86	0
1	MLY	A	66	1	9,10,11	0.56	0	6,11,13	0.75	0
2	MLY	B	466	2	9,10,11	0.58	0	6,11,13	0.88	0
1	CAS	A	241	1	5,8,9	1.17	0	1,9,11	0.51	0
1	MLY	A	488	1	9,10,11	0.56	0	6,11,13	0.57	0
2	MLY	B	946	2	9,10,11	0.58	0	6,11,13	0.92	0
1	MLZ	A	207	1	8,9,10	0.87	0	4,9,11	1.11	0
2	MLZ	B	854	2	8,9,10	0.87	0	4,9,11	0.91	0
2	MLY	B	513	2	9,10,11	0.57	0	6,11,13	0.71	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
2	CAS	B	477	2	-	0/0/7/9	-
1	MLY	A	290	1	-	2/8/9/11	-
1	CAS	A	477	1	-	0/0/7/9	-
2	MLZ	B	324	2	-	2/7/8/10	-
1	MLZ	A	550	1	-	1/7/8/10	-
2	CAS	B	692	2	-	0/0/7/9	-
1	MLY	A	513	1	-	0/8/9/11	-
1	MLY	A	911	1	-	0/8/9/11	-
2	MLY	B	116	2	-	2/8/9/11	-
1	MLY	A	704	1	-	0/8/9/11	-
1	MLY	A	854	1	-	2/8/9/11	-
1	CAS	A	692	1	-	0/0/7/9	-
1	MLY	A	937	1	-	3/8/9/11	-
2	MLY	B	1013	2	-	1/8/9/11	-
1	MLY	A	884	1	-	3/8/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	431	1	-	0/8/9/11	-
1	MLY	A	466	1	-	0/8/9/11	-
1	MLY	A	794	1	-	3/8/9/11	-
1	MLY	A	278	1	-	0/8/9/11	-
1	MLY	A	1013	1	-	1/8/9/11	-
1	MLY	A	972	1	-	1/8/9/11	-
2	MLZ	B	764	2	-	2/7/8/10	-
2	MLY	B	488	2	-	0/8/9/11	-
1	MLY	A	956	1	-	0/8/9/11	-
2	MLY	B	986	2	-	2/8/9/11	-
2	MLY	B	278	2	-	2/8/9/11	-
2	MLY	B	431	2	-	0/8/9/11	-
2	MLY	B	473	2	-	0/8/9/11	-
2	MLY	B	525	2	-	0/8/9/11	-
2	CAS	B	171	2	-	0/0/7/9	-
2	MLZ	B	769	2	-	1/7/8/10	-
2	MLZ	B	494	2	-	3/7/8/10	-
2	MLY	B	66	2	-	1/8/9/11	-
2	MLY	B	642	2	-	0/8/9/11	-
2	MLZ	B	937	2	-	2/7/8/10	-
1	MLY	A	943	1	-	2/8/9/11	-
2	MLY	B	199	2	-	0/8/9/11	-
2	MLY	B	943	2	-	2/8/9/11	-
1	MLY	A	700	1	-	1/8/9/11	-
2	CAS	B	556	2	-	0/0/7/9	-
1	CAS	A	313	1	-	0/0/7/9	-
2	MLY	B	550	2	-	1/8/9/11	-
2	MLY	B	290	2	-	1/8/9/11	-
1	MLZ	A	769	1	-	1/7/8/10	-
1	MLY	A	363	1	-	0/8/9/11	-
1	MLY	A	642	1	-	0/8/9/11	-
1	MLY	A	764	1	-	0/8/9/11	-
1	MLZ	A	525	1	-	1/7/8/10	-
2	MLY	B	972	2	-	3/8/9/11	-
1	CAS	A	556	1	-	0/0/7/9	-
1	MLY	A	946	1	-	2/8/9/11	-
2	MLY	B	624	2	-	2/8/9/11	-
1	MLY	A	540	1	-	1/8/9/11	-
2	MLY	B	251	2	-	0/8/9/11	-
1	MLY	A	116	1	-	1/8/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CAS	B	112	2	-	0/0/7/9	-
2	CAS	B	313	2	-	0/0/7/9	-
1	MLY	A	1000	1	-	4/8/9/11	-
2	MLY	B	287	2	-	0/8/9/11	-
2	MLZ	B	490	2	-	2/7/8/10	-
2	MLZ	B	759	2	-	0/7/8/10	-
1	MLY	A	154	1	-	2/8/9/11	-
1	CAS	A	171	1	-	0/0/7/9	-
1	MLY	A	287	1	-	1/8/9/11	-
2	MLY	B	363	2	-	1/8/9/11	-
1	MLY	A	759	1	-	2/8/9/11	-
2	MLY	B	902	2	-	0/8/9/11	-
1	MLY	A	750	1	-	1/8/9/11	-
2	MLY	B	499	2	-	1/8/9/11	-
2	MLY	B	956	2	-	2/8/9/11	-
1	MLY	A	251	1	-	0/8/9/11	-
2	MLY	B	750	2	-	0/8/9/11	-
2	MLY	B	540	2	-	3/8/9/11	-
2	MLY	B	704	2	-	1/8/9/11	-
2	MLZ	B	1000	2	-	1/7/8/10	-
2	MLY	B	911	2	-	0/8/9/11	-
2	MLY	B	41	2	-	0/8/9/11	-
1	MLY	A	521	1	-	1/8/9/11	-
1	MLZ	A	437	1	-	1/7/8/10	-
1	MLY	A	902	1	-	2/8/9/11	-
2	MLZ	B	884	2	-	1/7/8/10	-
1	MLY	A	66	1	-	1/8/9/11	-
2	MLY	B	466	2	-	0/8/9/11	-
1	CAS	A	241	1	-	0/0/7/9	-
1	MLY	A	488	1	-	1/8/9/11	-
2	MLY	B	946	2	-	0/8/9/11	-
1	MLZ	A	207	1	-	0/7/8/10	-
2	MLZ	B	854	2	-	1/7/8/10	-
2	MLY	B	513	2	-	0/8/9/11	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	313	CAS	CB-CA-C	-8.25	88.39	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	956	MLY	CD-CE-NZ	-2.46	107.36	113.71
1	A	956	MLY	CH2-NZ-CH1	-2.39	103.60	109.72

There are no chirality outliers.

5 of 81 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	437	MLZ	O-C-CA-CB
1	A	769	MLZ	C-CA-CB-CG
1	A	794	MLY	C-CA-CB-CG
1	A	937	MLY	O-C-CA-CB
1	A	943	MLY	O-C-CA-CB

There are no ring outliers.

21 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	324	MLZ	1	0
1	A	692	CAS	1	0
2	B	278	MLY	1	0
2	B	171	CAS	1	0
2	B	769	MLZ	1	0
1	A	700	MLY	1	0
1	A	313	CAS	6	0
1	A	769	MLZ	1	0
1	A	363	MLY	2	0
1	A	556	CAS	6	0
1	A	540	MLY	1	0
2	B	112	CAS	7	0
2	B	313	CAS	7	0
1	A	171	CAS	1	0
2	B	902	MLY	1	0
1	A	750	MLY	1	0
2	B	540	MLY	1	0
2	B	1000	MLZ	1	0
2	B	911	MLY	1	0
1	A	66	MLY	1	0
2	B	466	MLY	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	1112	-	5,5,5	0.36	0	5,5,5	0.36	0
5	ACT	B	1109	-	3,3,3	0.81	0	3,3,3	1.33	0
5	ACT	B	1114	-	3,3,3	0.80	0	3,3,3	1.30	0
4	GOL	B	1102	-	5,5,5	0.37	0	5,5,5	0.56	0
5	ACT	B	1108	-	3,3,3	0.81	0	3,3,3	1.35	0
5	ACT	A	1106	-	3,3,3	0.81	0	3,3,3	1.38	0
5	ACT	B	1111	-	3,3,3	0.82	0	3,3,3	1.32	0
4	GOL	B	1103	-	5,5,5	0.34	0	5,5,5	0.43	0
4	GOL	B	1104	-	5,5,5	0.38	0	5,5,5	0.16	0
5	ACT	B	1113	-	3,3,3	0.79	0	3,3,3	1.42	0
5	ACT	B	1110	-	3,3,3	0.87	0	3,3,3	1.42	0
5	ACT	A	1105	-	3,3,3	0.78	0	3,3,3	1.51	0
5	ACT	B	1106	-	3,3,3	0.81	0	3,3,3	0.73	0
5	ACT	A	1104	-	3,3,3	0.82	0	3,3,3	1.32	0
4	GOL	A	1102	-	5,5,5	0.35	0	5,5,5	0.39	0
4	GOL	A	1103	-	5,5,5	0.31	0	5,5,5	0.40	0
5	ACT	A	1108	3	3,3,3	1.09	0	3,3,3	1.13	0
5	ACT	B	1105	-	3,3,3	0.81	0	3,3,3	1.37	0
5	ACT	B	1107	-	3,3,3	0.82	0	3,3,3	1.30	0
4	GOL	A	1107	-	5,5,5	0.34	0	5,5,5	0.48	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	GOL	B	1112	-	-	0/4/4/4	-
4	GOL	B	1103	-	-	0/4/4/4	-
4	GOL	B	1104	-	-	2/4/4/4	-
4	GOL	A	1102	-	-	0/4/4/4	-
4	GOL	A	1103	-	-	1/4/4/4	-
4	GOL	B	1102	-	-	2/4/4/4	-
4	GOL	A	1107	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1107	GOL	O1-C1-C2-C3
4	B	1102	GOL	O1-C1-C2-C3
4	B	1104	GOL	C1-C2-C3-O3
4	A	1107	GOL	O1-C1-C2-O2
4	B	1102	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1102	GOL	1	1
5	B	1110	ACT	1	0
4	A	1107	GOL	2	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	938/1014 (92%)	-0.21	17 (1%) 67 67	12, 30, 58, 93	7 (0%)
2	B	932/1014 (91%)	-0.18	21 (2%) 61 60	13, 32, 58, 98	3 (0%)
All	All	1870/2028 (92%)	-0.20	38 (2%) 64 64	12, 31, 58, 98	10 (0%)

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	316	ASP	7.2
2	B	838	VAL	5.6
2	B	31	ALA	5.4
2	B	817	THR	4.5
2	B	851	TRP	4.3

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
1	CAS	A	556	9/10	0.73	0.27	24,32,90,102	0
1	CAS	A	692	9/10	0.74	0.25	39,44,108,242	0
1	CAS	A	313	9/10	0.76	0.32	54,56,93,287	0
2	CAS	B	313	9/10	0.78	0.26	48,54,100,262	0
2	CAS	B	692	9/10	0.82	0.19	28,41,70,165	0
2	MLZ	B	324	10/11	0.83	0.17	47,62,75,75	0
1	CAS	A	477	9/10	0.83	0.16	40,44,77,147	0
2	CAS	B	556	9/10	0.84	0.20	34,42,114,157	0
2	MLY	B	1013	11/12	0.86	0.15	31,39,54,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MLY	B	499	11/12	0.87	0.15	28,33,64,67	0
2	MLY	B	513	11/12	0.87	0.15	46,49,53,56	0
2	CAS	B	171	9/10	0.87	0.19	24,32,90,102	0
1	MLY	A	700	11/12	0.87	0.18	28,40,73,74	0
1	MLY	A	1013	11/12	0.87	0.12	35,38,56,58	0
1	MLY	A	521	11/12	0.88	0.17	44,59,87,89	0
1	CAS	A	241	9/10	0.89	0.16	22,39,71,190	0
2	MLY	B	290	11/12	0.89	0.15	36,39,65,65	0
1	MLY	A	794	11/12	0.89	0.16	38,52,69,69	0
1	CAS	A	171	9/10	0.89	0.18	19,34,86,100	0
2	MLY	B	750	11/12	0.89	0.15	24,36,65,65	0
2	CAS	B	477	9/10	0.89	0.17	35,47,118,187	0
2	CAS	B	112	9/10	0.90	0.21	25,33,104,226	0
2	MLY	B	986	11/12	0.90	0.16	35,43,70,70	0
2	MLZ	B	494	10/11	0.90	0.15	29,42,61,62	0
2	MLZ	B	769	10/11	0.91	0.12	30,41,50,52	0
2	MLY	B	943	11/12	0.91	0.12	24,31,56,58	0
2	MLY	B	972	11/12	0.91	0.17	27,36,71,71	0
2	MLY	B	550	11/12	0.91	0.13	29,37,51,58	0
1	MLY	A	750	11/12	0.91	0.15	27,41,61,66	0
1	MLY	A	513	11/12	0.92	0.10	43,48,53,60	0
2	MLY	B	287	11/12	0.92	0.11	31,35,50,52	0
2	MLZ	B	854	10/11	0.92	0.10	29,33,46,48	0
1	MLY	A	937	11/12	0.92	0.15	24,31,62,65	0
2	MLY	B	956	11/12	0.92	0.13	25,34,64,67	0
1	MLY	A	972	11/12	0.92	0.14	22,35,63,64	0
1	MLY	A	704	11/12	0.92	0.13	25,29,50,52	0
1	MLY	A	363	11/12	0.92	0.14	24,31,59,60	0
2	MLY	B	473	11/12	0.93	0.13	31,37,68,69	0
2	MLY	B	624	11/12	0.93	0.10	27,31,57,58	0
1	MLZ	A	525	10/11	0.93	0.10	41,45,51,53	0
2	MLY	B	525	11/12	0.93	0.11	25,39,47,51	0
2	MLZ	B	759	10/11	0.93	0.11	41,47,64,65	0
1	MLY	A	290	11/12	0.93	0.12	34,39,59,60	0
1	MLZ	A	550	10/11	0.94	0.09	28,35,45,46	0
1	MLY	A	902	11/12	0.94	0.09	25,27,42,43	0
2	MLY	B	642	11/12	0.94	0.08	27,28,39,43	0
1	MLY	A	488	11/12	0.94	0.08	28,35,39,40	0
2	MLY	B	363	11/12	0.94	0.11	28,34,59,60	0
2	MLY	B	466	11/12	0.94	0.09	26,36,47,49	0
2	MLZ	B	764	10/11	0.94	0.09	35,44,48,50	0
1	MLY	A	946	11/12	0.94	0.12	22,33,57,60	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	A	431	11/12	0.94	0.12	24,33,63,63	0
2	MLZ	B	884	10/11	0.94	0.09	22,27,53,54	0
2	MLY	B	911	11/12	0.94	0.11	20,28,54,55	0
1	MLY	A	466	11/12	0.94	0.09	28,32,50,51	0
2	MLY	B	946	11/12	0.94	0.09	26,34,46,48	0
1	MLY	A	66	11/12	0.94	0.11	25,36,54,55	0
1	MLY	A	540	11/12	0.94	0.10	28,30,45,47	0
2	MLY	B	199	11/12	0.94	0.13	22,31,62,62	0
1	MLY	A	759	11/12	0.94	0.12	32,42,63,64	0
2	MLY	B	66	11/12	0.95	0.11	20,24,58,59	0
1	MLY	A	854	11/12	0.95	0.09	20,29,46,46	0
2	MLY	B	116	11/12	0.95	0.11	21,35,57,58	0
2	MLZ	B	490	10/11	0.95	0.11	31,37,66,68	0
1	MLY	A	278	11/12	0.95	0.09	22,35,41,41	0
1	MLY	A	911	11/12	0.95	0.10	20,22,42,44	0
2	MLY	B	251	11/12	0.95	0.10	23,26,55,56	0
2	MLZ	B	937	10/11	0.95	0.11	23,28,64,67	0
2	MLY	B	278	11/12	0.95	0.11	24,29,60,62	0
1	MLZ	A	207	10/11	0.95	0.10	19,28,53,56	0
1	MLY	A	116	11/12	0.95	0.09	25,30,42,46	0
1	MLY	A	764	11/12	0.95	0.07	35,38,49,50	0
1	MLY	A	251	11/12	0.95	0.10	24,27,53,54	0
2	MLZ	B	1000	10/11	0.95	0.12	25,31,64,65	0
2	MLY	B	41	11/12	0.95	0.08	27,29,44,49	0
1	MLY	A	1000	11/12	0.96	0.10	20,27,60,64	0
2	MLY	B	704	11/12	0.96	0.11	24,31,59,60	0
1	MLZ	A	769	10/11	0.96	0.09	27,31,43,43	0
2	MLY	B	540	11/12	0.96	0.07	20,26,41,45	0
2	MLY	B	488	11/12	0.96	0.07	27,30,42,43	0
1	MLY	A	956	11/12	0.96	0.12	18,22,62,69	0
2	MLY	B	431	11/12	0.96	0.10	25,32,60,62	0
1	MLY	A	943	11/12	0.96	0.08	20,29,43,47	0
2	MLY	B	902	11/12	0.96	0.08	27,31,40,41	0
1	MLY	A	884	11/12	0.97	0.08	20,25,46,51	0
1	MLY	A	154	11/12	0.97	0.09	23,28,61,63	0
1	MLY	A	287	11/12	0.97	0.07	22,26,34,34	0
1	MLZ	A	437	10/11	0.97	0.08	28,32,56,56	0
1	MLY	A	642	11/12	0.98	0.06	22,24,42,43	0

6.3 Carbohydrates ⓘ

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
5	ACT	A	1106	4/4	0.49	0.34	58,65,67,67	0
5	ACT	A	1105	4/4	0.60	0.38	58,64,65,72	0
5	ACT	B	1105	4/4	0.66	0.20	49,59,60,66	0
5	ACT	B	1111	4/4	0.69	0.24	72,76,77,81	0
5	ACT	B	1113	4/4	0.73	0.19	49,56,60,62	0
4	GOL	B	1112	6/6	0.75	0.22	84,89,91,92	0
5	ACT	B	1109	4/4	0.76	0.33	91,91,92,93	0
5	ACT	B	1114	4/4	0.77	0.23	61,70,71,74	0
5	ACT	A	1104	4/4	0.84	0.23	49,57,57,58	0
5	ACT	B	1107	4/4	0.85	0.24	69,71,73,77	0
4	GOL	A	1107	6/6	0.87	0.16	40,53,63,68	0
5	ACT	B	1106	4/4	0.88	0.22	69,71,71,74	0
5	ACT	A	1108	4/4	0.88	0.16	34,35,35,36	0
4	GOL	A	1103	6/6	0.91	0.10	40,41,50,56	0
4	GOL	B	1104	6/6	0.93	0.09	35,47,50,52	0
5	ACT	B	1108	4/4	0.93	0.12	38,40,43,47	0
4	GOL	B	1102	6/6	0.93	0.17	11,48,54,64	0
5	ACT	B	1110	4/4	0.94	0.15	8,31,41,45	0
4	GOL	A	1102	6/6	0.96	0.08	23,33,34,35	0
4	GOL	B	1103	6/6	0.97	0.09	23,32,36,39	0
3	ZN	A	1101	1/1	0.97	0.04	28,28,28,28	0
3	ZN	B	1101	1/1	0.99	0.02	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.