



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2025 – 02:50 PM EDT

PDB ID : 9D1S / pdb\_00009d1s  
Title : Lucilia cuprina alpha esterase 7 directed evolution round 8  
Authors : Frkic, R.L.; Fraser, N.; Mabbitt, P.D.; Jackson, C.J.  
Deposited on : 2024-08-07  
Resolution : 1.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

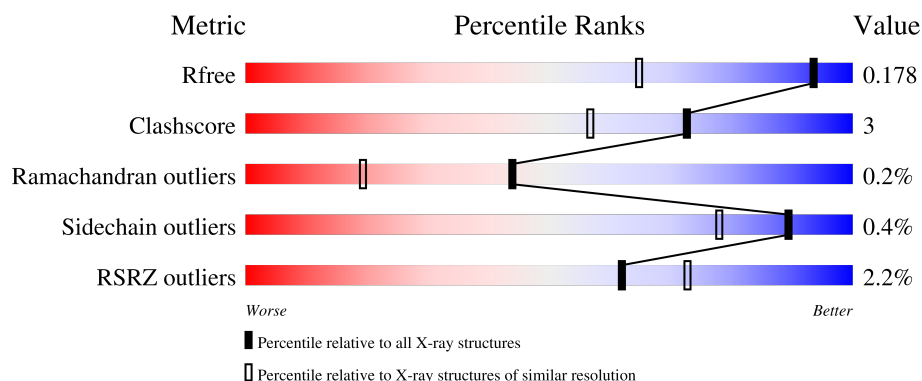
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

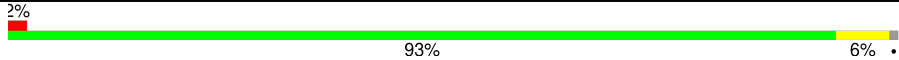
The reported resolution of this entry is 1.35 Å.

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	1089 (1.36-1.36)
Clashscore	180529	1157 (1.36-1.36)
Ramachandran outliers	177936	1146 (1.36-1.36)
Sidechain outliers	177891	1146 (1.36-1.36)
RSRZ outliers	164620	1088 (1.36-1.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	570	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5375 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.

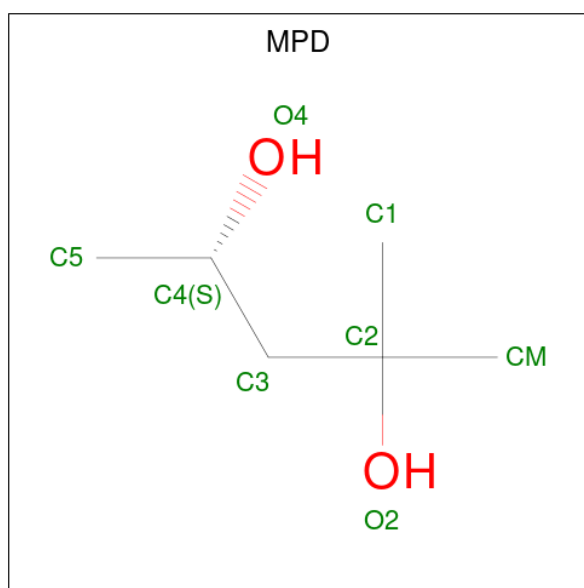
- Molecule 1 is a protein called Carboxylic ester hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	565	4746	3037	790	884	35	0	25	0

There are 7 discrepancies between the modelled and reference sequences:

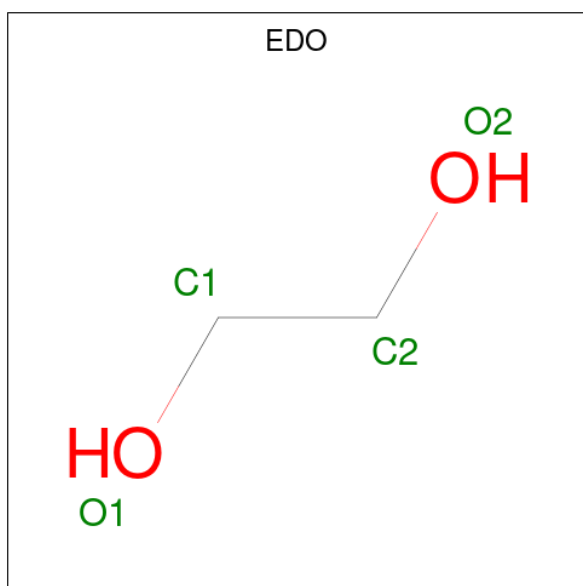
Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	THR	conflict	UNP Q25252
A	137	ASP	GLY	conflict	UNP Q25252
A	306	MET	LYS	conflict	UNP Q25252
A	308	VAL	MET	conflict	UNP Q25252
A	362	THR	MET	conflict	UNP Q25252
A	373	ALA	VAL	conflict	UNP Q25252
A	476	SER	THR	conflict	UNP Q25252

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



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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



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

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

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula:  $C_2H_3O_2$ ).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



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

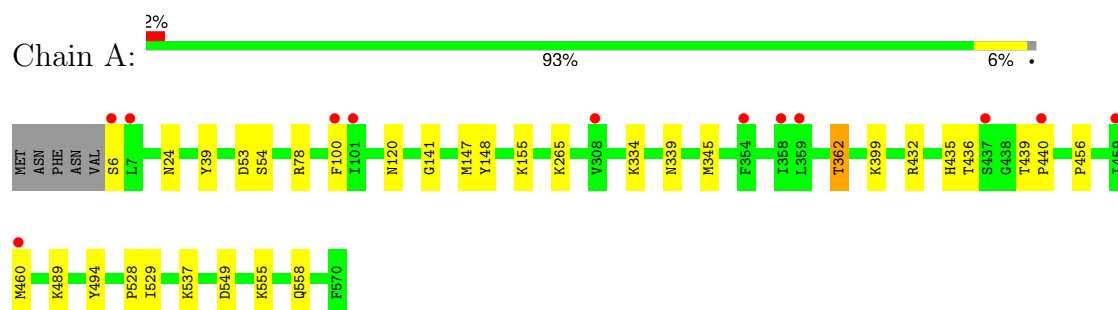
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	547	Total	O	0	0
			547	547		

### 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: Carboxylic ester hydrolase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.24Å 92.13Å 104.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.56 – 1.35 44.56 – 1.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.56-1.35) 99.9 (44.56-1.35)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.45 (at 1.35Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.143 , 0.178 0.143 , 0.178	Depositor DCC
$R_{free}$ test set	6232 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.1	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 47.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	5375	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, MLZ, M3L, MLY, MPD, EDO, GOL

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	0.26	0/4681	0.50	1/6353 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	345	MET	N-CA-CB	-5.88	100.59	111.53

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	4746	0	4652	27	0
2	A	40	0	70	5	0
3	A	32	0	48	5	0
4	A	4	0	3	1	0
5	A	6	0	8	0	0
6	A	547	0	0	4	0
All	All	5375	0	4781	30	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 3.

All (30) 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:54:SER:H	3:A:603:EDO:H11	1.44	0.82
1:A:53:ASP:HB3	3:A:603:EDO:H22	1.71	0.71
1:A:432:ARG:NH2	1:A:439[B]:THR:O	2.26	0.68
1:A:141:GLY:HA2	3:A:614:EDO:H12	1.75	0.68
1:A:24[A]:ASN:ND2	6:A:705:HOH:O	2.29	0.62
2:A:602:MPD:H11	6:A:1201:HOH:O	2.02	0.60
1:A:339:ASN:HD22	1:A:436[B]:THR:HG21	1.69	0.58
1:A:334:LYS:O	3:A:604:EDO:H12	2.06	0.55
1:A:432:ARG:NH1	1:A:439[B]:THR:O	2.41	0.53
1:A:120:ASN:HD22	4:A:609:ACT:H1	1.76	0.51
1:A:555:MLY:HH21	2:A:611:MPD:H13	1.93	0.51
1:A:537:MLY:HE3	2:A:606:MPD:H12	1.93	0.49
3:A:607:EDO:O2	6:A:701:HOH:O	2.20	0.49
1:A:362:THR:O	1:A:362:THR:OG1	2.29	0.47
1:A:440[B]:PRO:HB2	1:A:528:PRO:HB2	1.97	0.47
1:A:440[B]:PRO:HB3	1:A:529:ILE:O	2.15	0.47
1:A:100:PHE:HD2	1:A:460:MET:HG3	1.80	0.46
2:A:602:MPD:O4	2:A:602:MPD:H13	2.16	0.46
1:A:549:ASP:OD1	2:A:606:MPD:H13	2.15	0.45
1:A:489:LYS:HE3	1:A:489:LYS:HB3	1.65	0.43
1:A:155:M3L:HM11	1:A:494:TYR:CE2	2.53	0.43
1:A:399:LYS:HD2	1:A:558:GLN:OE1	2.17	0.43
1:A:147:MET:SD	1:A:456:PRO:HD2	2.59	0.42
1:A:432:ARG:NH2	1:A:439[B]:THR:OG1	2.53	0.41
1:A:265:MLY:HH12	6:A:907:HOH:O	2.20	0.41
1:A:432:ARG:HH22	1:A:439[B]:THR:C	2.24	0.41
1:A:39:TYR:OH	1:A:78:ARG:HG3	2.21	0.41
1:A:147:MET:HG3	1:A:148:TYR:CE2	2.56	0.41
1:A:432:ARG:HH22	1:A:439[B]:THR:N	2.18	0.41
1:A:432:ARG:CZ	1:A:439[B]:THR:O	2.69	0.40

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	570/570 (100%)	554 (97%)	14 (2%)	2 (0%)	30	12

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	435[A]	HIS
1	A	435[B]	HIS

### 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	502/486 (103%)	500 (100%)	2 (0%)	89	78

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	362	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	162	ASN
1	A	339	ASN
1	A	430	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

18 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	M3L	A	155	1	10,11,12	0.53	0	9,14,16	0.60	0
1	MLY	A	360	1	9,10,11	0.60	0	6,11,13	0.79	0
1	MLY	A	398	1	9,10,11	0.56	0	6,11,13	0.80	0
1	MLY	A	467	1	9,10,11	0.67	0	6,11,13	0.74	0
1	MLY	A	74	1	9,10,11	0.54	0	6,11,13	0.74	0
1	MLY	A	537	1	9,10,11	0.55	0	6,11,13	0.71	0
1	MLY	A	555	1	9,10,11	0.59	0	6,11,13	0.68	0
1	MLY	A	126	1	9,10,11	0.57	0	6,11,13	0.75	0
1	MLY	A	199	1	9,10,11	0.49	0	6,11,13	0.96	0
1	MLY	A	557	1	9,10,11	0.52	0	6,11,13	0.77	0
1	MLY	A	396	1	9,10,11	0.51	0	6,11,13	0.79	0
1	MLY	A	46	1	9,10,11	0.60	0	6,11,13	0.95	0
1	MLY	A	41	1	9,10,11	0.55	0	6,11,13	0.70	0
1	MLY	A	565	1	9,10,11	0.55	0	6,11,13	0.70	0
1	MLY	A	16	1	9,10,11	0.52	0	6,11,13	0.91	0
1	MLZ	A	92	1	8,9,10	0.77	0	4,9,11	0.72	0
1	MLY	A	495	1	9,10,11	0.54	0	6,11,13	0.96	0
1	MLY	A	265	1	9,10,11	0.56	0	6,11,13	0.59	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	M3L	A	155	1	-	0/9/10/12	-
1	MLY	A	360	1	-	2/8/9/11	-
1	MLY	A	398	1	-	0/8/9/11	-
1	MLY	A	467	1	-	0/8/9/11	-
1	MLY	A	74	1	-	0/8/9/11	-
1	MLY	A	537	1	-	2/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	555	1	-	0/8/9/11	-
1	MLY	A	126	1	-	1/8/9/11	-
1	MLY	A	199	1	-	0/8/9/11	-
1	MLY	A	557	1	-	0/8/9/11	-
1	MLY	A	396	1	-	0/8/9/11	-
1	MLY	A	46	1	-	0/8/9/11	-
1	MLY	A	41	1	-	0/8/9/11	-
1	MLY	A	565	1	-	0/8/9/11	-
1	MLY	A	16	1	-	3/8/9/11	-
1	MLZ	A	92	1	-	1/7/8/10	-
1	MLY	A	495	1	-	0/8/9/11	-
1	MLY	A	265	1	-	2/8/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	16	MLY	C-CA-CB-CG
1	A	126	MLY	O-C-CA-CB
1	A	16	MLY	CD-CE-NZ-CH1
1	A	537	MLY	CG-CD-CE-NZ
1	A	16	MLY	CD-CE-NZ-CH2
1	A	360	MLY	CD-CE-NZ-CH2
1	A	265	MLY	CD-CE-NZ-CH1
1	A	537	MLY	CD-CE-NZ-CH1
1	A	92	MLZ	CE-CD-CG-CB
1	A	265	MLY	CE-CD-CG-CB
1	A	360	MLY	CD-CE-NZ-CH1

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	155	M3L	1	0
1	A	537	MLY	1	0
1	A	555	MLY	1	0
1	A	265	MLY	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

15 ligands 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	MPD	A	611	-	7,7,7	0.31	0	9,10,10	0.26	0
2	MPD	A	602	-	7,7,7	0.31	0	9,10,10	0.57	0
3	EDO	A	614	-	3,3,3	0.44	0	2,2,2	0.30	0
4	ACT	A	609	-	3,3,3	1.45	1 (33%)	3,3,3	1.35	0
5	GOL	A	613	-	5,5,5	0.91	0	5,5,5	1.03	0
2	MPD	A	601	-	7,7,7	0.30	0	9,10,10	0.64	0
3	EDO	A	603	-	3,3,3	0.45	0	2,2,2	0.34	0
3	EDO	A	604	-	3,3,3	0.42	0	2,2,2	0.43	0
2	MPD	A	605	-	7,7,7	0.32	0	9,10,10	0.48	0
3	EDO	A	607	-	3,3,3	0.38	0	2,2,2	0.46	0
3	EDO	A	610	-	3,3,3	0.43	0	2,2,2	0.43	0
3	EDO	A	615	-	3,3,3	0.43	0	2,2,2	0.40	0
3	EDO	A	608	-	3,3,3	0.43	0	2,2,2	0.28	0
2	MPD	A	606	-	7,7,7	0.28	0	9,10,10	0.35	0
3	EDO	A	612	-	3,3,3	0.47	0	2,2,2	0.26	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MPD	A	611	-	-	1/5/5/5	-
2	MPD	A	602	-	-	0/5/5/5	-
3	EDO	A	614	-	-	0/1/1/1	-
5	GOL	A	613	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MPD	A	601	-	-	0/5/5/5	-
3	EDO	A	603	-	-	1/1/1/1	-
3	EDO	A	604	-	-	1/1/1/1	-
2	MPD	A	605	-	-	1/5/5/5	-
3	EDO	A	607	-	-	0/1/1/1	-
3	EDO	A	610	-	-	0/1/1/1	-
3	EDO	A	615	-	-	0/1/1/1	-
3	EDO	A	608	-	-	0/1/1/1	-
2	MPD	A	606	-	-	5/5/5/5	-
3	EDO	A	612	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	609	ACT	CH3-C	2.12	1.57	1.49

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	606	MPD	CM-C2-C3-C4
2	A	606	MPD	C2-C3-C4-O4
2	A	606	MPD	C2-C3-C4-C5
5	A	613	GOL	O1-C1-C2-O2
5	A	613	GOL	O1-C1-C2-C3
2	A	606	MPD	O2-C2-C3-C4
2	A	606	MPD	C1-C2-C3-C4
2	A	605	MPD	C2-C3-C4-C5
2	A	611	MPD	C2-C3-C4-C5
3	A	603	EDO	O1-C1-C2-O2
3	A	604	EDO	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	611	MPD	1	0
2	A	602	MPD	2	0
3	A	614	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	609	ACT	1	0
3	A	603	EDO	2	0
3	A	604	EDO	1	0
3	A	607	EDO	1	0
2	A	606	MPD	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	547/570 (95%)	-0.14	12 (2%) 62 73	6, 16, 37, 54	25 (4%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	100	PHE	7.7
1	A	437[A]	SER	3.2
1	A	7	LEU	3.0
1	A	354	PHE	2.9
1	A	440[A]	PRO	2.5
1	A	308	VAL	2.5
1	A	460	MET	2.5
1	A	358	ILE	2.3
1	A	459	ILE	2.2
1	A	359	LEU	2.2
1	A	101	ILE	2.0
1	A	6	SER	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	MLY	A	360	11/12	0.87	0.13	42,44,51,52	0
1	MLY	A	265	11/12	0.93	0.09	19,24,34,36	0
1	MLY	A	16	11/12	0.93	0.09	25,27,31,32	0
1	MLY	A	467	11/12	0.93	0.11	21,27,44,45	0
1	MLY	A	537	11/12	0.95	0.08	14,17,28,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MLY	A	495	11/12	0.96	0.10	14,18,37,38	0
1	MLY	A	396	11/12	0.96	0.07	20,23,30,31	0
1	M3L	A	155	12/13	0.97	0.06	13,17,23,28	0
1	MLY	A	398	11/12	0.97	0.07	18,21,35,35	0
1	MLY	A	199	11/12	0.97	0.07	11,14,27,28	0
1	MLZ	A	92	10/11	0.97	0.07	14,19,29,30	0
1	MLY	A	126	11/12	0.97	0.06	16,20,29,31	0
1	MLY	A	557	11/12	0.97	0.07	14,17,31,33	0
1	MLY	A	565	11/12	0.97	0.06	17,19,22,23	0
1	MLY	A	46	11/12	0.98	0.07	12,14,29,29	0
1	MLY	A	555	11/12	0.98	0.06	14,15,26,27	0
1	MLY	A	74	11/12	0.98	0.06	13,15,24,26	0
1	MLY	A	41	11/12	0.98	0.06	14,17,32,32	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	A	615	4/4	0.66	0.15	55,58,62,71	0
3	EDO	A	604	4/4	0.69	0.25	30,77,78,161	0
2	MPD	A	611	8/8	0.71	0.26	58,80,102,134	0
4	ACT	A	609	4/4	0.72	0.16	44,64,65,91	0
3	EDO	A	610	4/4	0.74	0.18	50,51,67,70	0
3	EDO	A	607	4/4	0.75	0.21	39,53,57,76	0
3	EDO	A	614	4/4	0.77	0.26	33,50,65,89	0
3	EDO	A	612	4/4	0.78	0.20	31,40,66,67	0
2	MPD	A	605	8/8	0.79	0.28	49,52,88,170	0
5	GOL	A	613	6/6	0.80	0.25	35,58,78,92	0
3	EDO	A	603	4/4	0.83	0.19	27,33,35,98	4
2	MPD	A	606	8/8	0.87	0.17	33,51,68,74	0
2	MPD	A	601	8/8	0.88	0.15	29,41,49,84	0
3	EDO	A	608	4/4	0.91	0.25	24,115,119,144	0
2	MPD	A	602	8/8	0.93	0.09	14,19,23,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.