



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:44 AM UTC

PDB ID : 9D1L / pdb_00009d1l
Title : Lucilia cuprina alpha esterase 7 directed evolution round 1
Authors : Frkic, R.L.; Fraser, N.; Mabbitt, P.D.; Jackson, C.J.
Deposited on : 2024-08-07
Resolution : 1.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

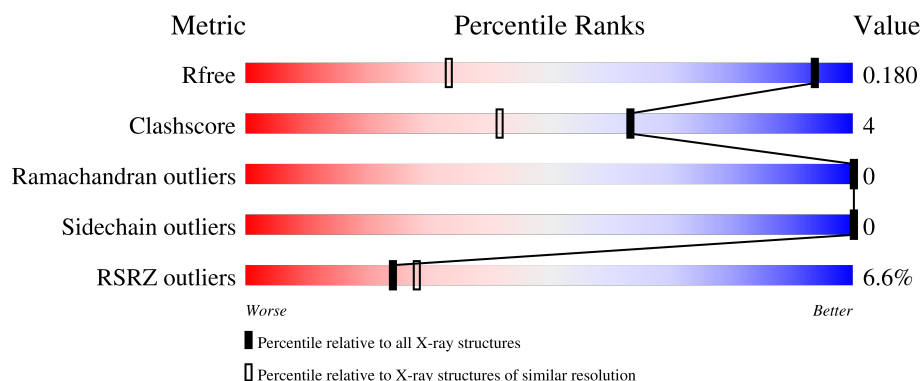
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.10 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}	180053	1625 (1.12-1.08)
Clashscore	190562	1656 (1.12-1.08)
Ramachandran outliers	187476	1616 (1.12-1.08)
Sidechain outliers	187428	1612 (1.12-1.08)
RSRZ outliers	180081	1625 (1.12-1.08)

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	570	<div> <div>6%</div> <div>93%</div> <div>6%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PEG	A	617	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5539 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
1	A	566	Total	C	N	O	S	0	15	0
			4682	3012	774	858	38			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	137	ASP	GLY	conflict	UNP Q25252
A	434	TYR	ASN	conflict	UNP Q25252

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

Continued on next page...

Continued from previous page...

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

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



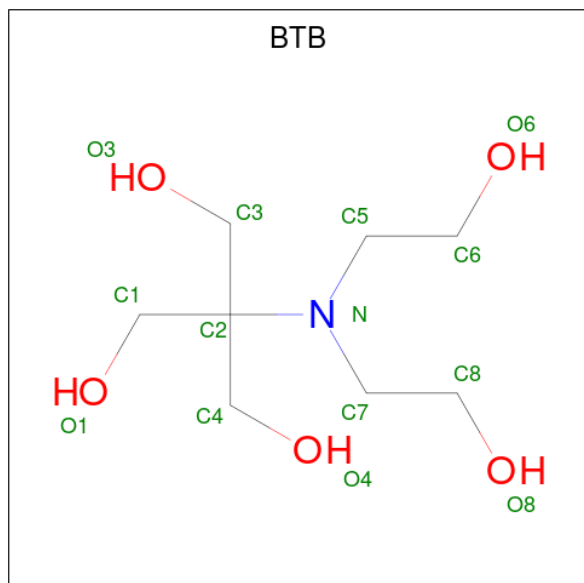
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: $C_8H_{19}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	1
			28	16	2	10		

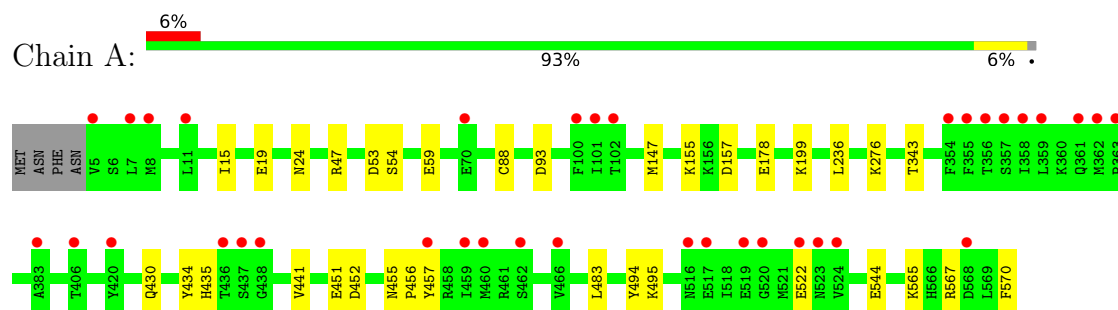
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	740	Total	O	0	0
			740	740		

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, α , β , γ	57.96Å 92.14Å 104.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.45 – 1.10 44.45 – 1.10	Depositor EDS
% Data completeness (in resolution range)	97.4 (44.45-1.10) 97.4 (44.45-1.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 1.10Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.161 , 0.173 (Not available) , 0.180	Depositor DCC
R_{free} test set	10976 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	12.6	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	5539	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% 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: M3L, ACT, MLZ, PEG, MLY, MPD, BTB, EDO

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	0.23	0/4587	0.51	0/6219

There are no bond length outliers.

There are no bond angle outliers.

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	4682	0	4651	34	0
2	A	40	0	60	8	0
3	A	4	0	3	0	0
4	A	24	0	42	2	0
5	A	21	0	30	11	0
6	A	28	0	38	3	0
7	A	740	0	0	5	0
All	All	5539	0	4824	38	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 4.

All (38) 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:434:TYR:HE1	5:A:617:PEG:H41	1.39	0.86
1:A:54:SER:H	2:A:610:EDO:H11	1.39	0.86
1:A:157:ASP:HB2	2:A:605:EDO:H21	1.65	0.79
1:A:343:THR:HB	1:A:441[B]:VAL:HG22	1.69	0.74
1:A:53:ASP:HB3	2:A:610:EDO:H22	1.72	0.71
1:A:430:GLN:HB3	5:A:617:PEG:H42	1.72	0.70
1:A:276:LYS:HE2	5:A:609:PEG:H12	1.76	0.68
1:A:544:GLU:HG2	2:A:618:EDO:H11	1.80	0.63
1:A:567:ARG:HH22	5:A:617:PEG:H22	1.66	0.60
1:A:451:GLU:H	2:A:616:EDO:H22	1.68	0.59
1:A:434:TYR:CE1	5:A:617:PEG:H41	2.30	0.55
4:A:607:MPD:H11	7:A:1313:HOH:O	2.06	0.55
1:A:59:GLU:O	1:A:88:CYS:HB3	2.05	0.55
1:A:15:ILE:O	1:A:19:GLU:HG3	2.07	0.55
1:A:567:ARG:HH22	5:A:617:PEG:C2	2.22	0.53
1:A:147[B]:MET:HE1	1:A:456:PRO:HB2	1.90	0.52
1:A:24[A]:ASN:OD1	7:A:701:HOH:O	2.19	0.51
1:A:430:GLN:OE1	5:A:617:PEG:H12	2.11	0.50
1:A:483:LEU:HD22	2:A:615:EDO:H12	1.94	0.50
1:A:155:M3L:HM11	1:A:494:TYR:CZ	2.48	0.49
1:A:435:HIS:HA	6:A:613[A]:BTB:H61	1.94	0.49
1:A:570:PHE:CD2	5:A:617:PEG:H31	2.49	0.48
1:A:178:GLU:OE2	7:A:702:HOH:O	2.20	0.47
1:A:434:TYR:O	6:A:613[A]:BTB:H41	2.14	0.47
1:A:522:GLU:H	1:A:522:GLU:CD	2.24	0.46
1:A:452:ASP:OD1	2:A:616:EDO:O1	2.28	0.46
1:A:199[B]:MLZ:HA	1:A:199[B]:MLZ:HD2	1.82	0.45
4:A:607:MPD:O4	4:A:607:MPD:H13	2.17	0.45
1:A:155:M3L:HM11	1:A:494:TYR:CE2	2.53	0.44
1:A:455:ASN:OD1	1:A:457:TYR:HB2	2.18	0.44
1:A:93[B]:ASP:OD2	7:A:703:HOH:O	2.21	0.43
1:A:570:PHE:HD2	5:A:617:PEG:H31	1.83	0.43
1:A:451:GLU:H	2:A:616:EDO:H11	1.84	0.43
1:A:199[B]:MLZ:HE2	1:A:236:LEU:O	2.19	0.43
1:A:47:ARG:HH12	5:A:612:PEG:H31	1.83	0.43
1:A:495:MLY:HH22	1:A:495:MLY:HD3	1.75	0.42
5:A:612:PEG:H32	7:A:1025:HOH:O	2.20	0.42
6:A:613[A]:BTB:H11	6:A:613[A]:BTB:H72	1.67	0.42

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	557/570 (98%)	546 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	492/485 (101%)	492 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	162	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

22 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	495	1	9,10,11	0.55	0	6,11,13	0.88	0
1	MLY	A	398	1	9,10,11	0.54	0	6,11,13	0.77	0
1	MLZ	A	199[A]	-	8,9,10	0.75	0	4,9,11	0.45	0
1	MLY	A	360	1	9,10,11	0.57	0	6,11,13	0.70	0
1	M3L	A	155	1	10,11,12	0.55	0	9,14,16	0.54	0
1	MLY	A	41	1	9,10,11	0.60	0	6,11,13	0.70	0
1	MLY	A	565	1	9,10,11	0.55	0	6,11,13	1.08	1 (16%)
1	M3L	A	156	1	10,11,12	0.56	0	9,14,16	0.47	0
1	MLY	A	467	1	9,10,11	0.57	0	6,11,13	0.81	0
1	MLZ	A	199[B]	-	8,9,10	0.84	0	4,9,11	0.65	0
1	MLY	A	126	1	9,10,11	0.64	0	6,11,13	0.70	0
1	MLZ	A	306	1	8,9,10	0.80	0	4,9,11	0.57	0
1	M3L	A	537	1	10,11,12	0.56	0	9,14,16	0.44	0
1	MLY	A	557	1	9,10,11	0.55	0	6,11,13	0.84	0
1	MLZ	A	334	1	8,9,10	0.78	0	4,9,11	0.72	0
1	MLY	A	46	1	9,10,11	0.63	0	6,11,13	0.75	0
1	MLY	A	74	1	9,10,11	0.55	0	6,11,13	0.79	0
1	MLY	A	16	1	9,10,11	0.54	0	6,11,13	0.80	0
1	MLY	A	396	1	9,10,11	0.53	0	6,11,13	0.78	0
1	MLZ	A	92	1	8,9,10	0.80	0	4,9,11	0.69	0
1	MLZ	A	10	1	8,9,10	0.76	0	4,9,11	0.66	0
1	MLY	A	555	1	9,10,11	0.56	0	6,11,13	0.80	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	495	1	-	0/8/9/11	-
1	MLY	A	398	1	-	0/8/9/11	-
1	MLZ	A	199[A]	-	-	2/7/8/10	-
1	MLY	A	360	1	-	0/8/9/11	-
1	M3L	A	155	1	-	0/9/10/12	-
1	MLY	A	41	1	-	0/8/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	565	1	-	1/8/9/11	-
1	M3L	A	156	1	-	0/9/10/12	-
1	MLY	A	467	1	-	0/8/9/11	-
1	MLZ	A	199[B]	-	-	3/7/8/10	-
1	MLY	A	126	1	-	1/8/9/11	-
1	MLZ	A	306	1	-	2/7/8/10	-
1	M3L	A	537	1	-	5/9/10/12	-
1	MLY	A	557	1	-	0/8/9/11	-
1	MLZ	A	334	1	-	1/7/8/10	-
1	MLY	A	46	1	-	0/8/9/11	-
1	MLY	A	74	1	-	0/8/9/11	-
1	MLY	A	16	1	-	1/8/9/11	-
1	MLY	A	396	1	-	0/8/9/11	-
1	MLZ	A	92	1	-	1/7/8/10	-
1	MLZ	A	10	1	-	0/7/8/10	-
1	MLY	A	555	1	-	0/8/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	565	MLY	CD-CE-NZ	-2.32	107.71	113.71

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	126	MLY	O-C-CA-CB
1	A	199[A]	MLZ	C-CA-CB-CG
1	A	199[A]	MLZ	CD-CE-NZ-CM
1	A	199[B]	MLZ	CD-CE-NZ-CM
1	A	306	MLZ	CD-CE-NZ-CM
1	A	565	MLY	O-C-CA-CB
1	A	537	M3L	CG-CD-CE-NZ
1	A	199[B]	MLZ	CE-CD-CG-CB
1	A	92	MLZ	CE-CD-CG-CB
1	A	537	M3L	CE-CD-CG-CB
1	A	537	M3L	CD-CE-NZ-CM3
1	A	537	M3L	CD-CE-NZ-CM2
1	A	16	MLY	C-CA-CB-CG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	A	537	M3L	CD-CE-NZ-CM1
1	A	334	MLZ	CE-CD-CG-CB
1	A	199[B]	MLZ	CA-CB-CG-CD
1	A	306	MLZ	N-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	495	MLY	1	0
1	A	155	M3L	2	0
1	A	199[B]	MLZ	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

19 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	EDO	A	616	-	3,3,3	0.42	0	2,2,2	0.29	0
2	EDO	A	605	-	3,3,3	0.41	0	2,2,2	0.37	0
2	EDO	A	614	-	3,3,3	0.44	0	2,2,2	0.28	0
4	MPD	A	611	-	7,7,7	0.31	0	9,10,10	0.35	0
2	EDO	A	604	-	3,3,3	0.40	0	2,2,2	0.36	0
6	BTB	A	613[A]	-	13,13,13	0.90	0	7,16,16	0.76	0
5	PEG	A	617	-	6,6,6	0.14	0	5,5,5	0.16	0
2	EDO	A	610	-	3,3,3	0.42	0	2,2,2	0.37	0
2	EDO	A	601	-	3,3,3	0.42	0	2,2,2	0.36	0
5	PEG	A	609	-	6,6,6	0.10	0	5,5,5	0.11	0
6	BTB	A	613[B]	-	13,13,13	0.88	0	7,16,16	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ACT	A	602	-	3,3,3	1.36	0	3,3,3	1.35	0
5	PEG	A	612	-	6,6,6	0.14	0	5,5,5	0.17	0
4	MPD	A	606	-	7,7,7	0.34	0	9,10,10	0.59	0
2	EDO	A	603	-	3,3,3	0.38	0	2,2,2	0.38	0
2	EDO	A	615	-	3,3,3	0.37	0	2,2,2	0.40	0
2	EDO	A	618	-	3,3,3	0.42	0	2,2,2	0.34	0
4	MPD	A	607	-	7,7,7	0.30	0	9,10,10	0.60	0
2	EDO	A	608	-	3,3,3	0.36	0	2,2,2	0.35	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	EDO	A	616	-	-	1/1/1/1	-
5	PEG	A	609	-	-	2/4/4/4	-
2	EDO	A	610	-	-	1/1/1/1	-
6	BTB	A	613[A]	-	-	9/21/21/21	-
2	EDO	A	605	-	-	1/1/1/1	-
6	BTB	A	613[B]	-	-	3/21/21/21	-
2	EDO	A	615	-	-	1/1/1/1	-
2	EDO	A	618	-	-	1/1/1/1	-
2	EDO	A	614	-	-	0/1/1/1	-
4	MPD	A	611	-	-	1/5/5/5	-
5	PEG	A	617	-	-	2/4/4/4	-
4	MPD	A	607	-	-	0/5/5/5	-
2	EDO	A	608	-	-	0/1/1/1	-
5	PEG	A	612	-	-	4/4/4/4	-
2	EDO	A	604	-	-	0/1/1/1	-
2	EDO	A	601	-	-	0/1/1/1	-
4	MPD	A	606	-	-	0/5/5/5	-
2	EDO	A	603	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	613[A]	BTB	O1-C1-C2-C4
6	A	613[A]	BTB	C1-C2-N-C5
6	A	613[A]	BTB	C1-C2-N-C7
6	A	613[A]	BTB	C3-C2-N-C5
6	A	613[A]	BTB	C3-C2-N-C7
6	A	613[A]	BTB	C4-C2-N-C5
6	A	613[A]	BTB	C4-C2-N-C7
6	A	613[B]	BTB	O1-C1-C2-N
5	A	612	PEG	C4-C3-O2-C2
5	A	617	PEG	O1-C1-C2-O2
5	A	612	PEG	O2-C3-C4-O4
2	A	616	EDO	O1-C1-C2-O2
5	A	609	PEG	O1-C1-C2-O2
5	A	617	PEG	O2-C3-C4-O4
2	A	610	EDO	O1-C1-C2-O2
2	A	618	EDO	O1-C1-C2-O2
6	A	613[B]	BTB	O1-C1-C2-C3
6	A	613[B]	BTB	O1-C1-C2-C4
5	A	612	PEG	C1-C2-O2-C3
6	A	613[A]	BTB	N-C5-C6-O6
5	A	612	PEG	O1-C1-C2-O2
4	A	611	MPD	O2-C2-C3-C4
2	A	605	EDO	O1-C1-C2-O2
2	A	615	EDO	O1-C1-C2-O2
5	A	609	PEG	C4-C3-O2-C2
6	A	613[A]	BTB	O1-C1-C2-N

There are no ring outliers.

10 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	616	EDO	3	0
2	A	605	EDO	1	0
6	A	613[A]	BTB	3	0
5	A	617	PEG	8	0
2	A	610	EDO	2	0
5	A	609	PEG	1	0
5	A	612	PEG	2	0
2	A	615	EDO	1	0
2	A	618	EDO	1	0
4	A	607	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 ⓘ

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	545/570 (95%)	0.48	36 (6%) 24 28	7, 14, 29, 48	14 (2%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	354	PHE	5.5
1	A	457	TYR	5.0
1	A	100	PHE	4.6
1	A	5	VAL	4.0
1	A	459	ILE	3.6
1	A	460	MET	3.6
1	A	358	ILE	3.4
1	A	523	ASN	3.2
1	A	101	ILE	3.2
1	A	357	SER	3.1
1	A	361	GLN	2.8
1	A	355	PHE	2.8
1	A	7	LEU	2.8
1	A	359	LEU	2.7
1	A	406	THR	2.7
1	A	362	MET	2.6
1	A	437	SER	2.6
1	A	520	GLY	2.5
1	A	102	THR	2.5
1	A	462	SER	2.5
1	A	519	GLU	2.4
1	A	466	VAL	2.4
1	A	8	MET	2.4
1	A	383	ALA	2.3
1	A	420	TYR	2.3
1	A	436	THR	2.3
1	A	524	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	522	GLU	2.3
1	A	356	THR	2.2
1	A	438	GLY	2.2
1	A	568[A]	ASP	2.1
1	A	363	PRO	2.1
1	A	516	ASN	2.1
1	A	70	GLU	2.0
1	A	517	GLU	2.0
1	A	11	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	MLY	A	360	11/12	0.83	0.14	30,35,40,43	0
1	MLZ	A	10	10/11	0.91	0.12	23,28,35,38	0
1	MLZ	A	306	10/11	0.93	0.10	18,21,27,27	0
1	MLY	A	16	11/12	0.93	0.11	15,19,26,30	0
1	M3L	A	537	12/13	0.93	0.14	12,31,39,40	0
1	MLZ	A	92	10/11	0.94	0.10	13,15,23,30	0
1	MLY	A	467	11/12	0.94	0.10	17,21,33,34	0
1	MLZ	A	334	10/11	0.94	0.11	13,18,36,38	0
1	MLY	A	565	11/12	0.94	0.09	15,17,20,21	0
1	MLY	A	495	11/12	0.95	0.10	13,15,34,37	0
1	MLY	A	398	11/12	0.95	0.09	15,17,28,33	0
1	MLY	A	557	11/12	0.95	0.11	12,16,28,29	0
1	MLY	A	396	11/12	0.95	0.09	17,19,25,27	0
1	MLY	A	46	11/12	0.96	0.08	11,13,22,23	0
1	MLY	A	126	11/12	0.96	0.08	13,15,20,23	0
1	M3L	A	156	12/13	0.96	0.11	12,17,36,38	0
1	MLY	A	555	11/12	0.96	0.09	13,14,30,30	0
1	MLZ	A	199[A]	10/11	0.96	0.10	11,14,19,20	7
1	MLZ	A	199[B]	10/11	0.96	0.10	11,13,22,26	7
1	M3L	A	155	12/13	0.97	0.08	11,14,21,32	0
1	MLY	A	41	11/12	0.97	0.08	14,16,28,30	0
1	MLY	A	74	11/12	0.97	0.07	11,13,22,22	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ACT	A	602	4/4	0.57	0.28	28,28,29,32	4
5	PEG	A	609	7/7	0.61	0.24	25,30,34,34	7
6	BTB	A	613[A]	14/14	0.66	0.18	26,29,31,31	14
6	BTB	A	613[B]	14/14	0.66	0.18	25,28,31,31	14
4	MPD	A	606	8/8	0.72	0.22	17,29,34,41	8
2	EDO	A	616	4/4	0.76	0.20	19,26,27,33	4
2	EDO	A	601	4/4	0.76	0.17	20,25,25,30	0
2	EDO	A	608	4/4	0.77	0.37	17,20,22,28	4
2	EDO	A	605	4/4	0.78	0.22	24,26,27,29	4
5	PEG	A	617	7/7	0.79	0.29	17,24,29,29	7
5	PEG	A	612	7/7	0.80	0.24	18,20,26,27	7
2	EDO	A	614	4/4	0.82	0.16	20,20,25,26	4
2	EDO	A	615	4/4	0.82	0.20	18,29,30,33	4
2	EDO	A	603	4/4	0.83	0.18	20,23,26,35	4
2	EDO	A	610	4/4	0.84	0.16	14,18,18,29	4
2	EDO	A	618	4/4	0.85	0.18	26,28,30,30	4
2	EDO	A	604	4/4	0.85	0.18	23,26,29,32	4
4	MPD	A	611	8/8	0.89	0.12	20,25,29,30	0
4	MPD	A	607	8/8	0.90	0.12	12,16,21,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.