



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:55 PM UTC

PDB ID : 2IU7 / pdb_00002iu7
Title : Site directed mutagenesis of key residues involved in the catalytic mechanism of Cyanase
Authors : Guilloton, M.; Walsh, M.A.; Joachimiak, A.; Anderson, P.M.
Deposited on : 2006-05-30
Resolution : 1.91 Å(reported)

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

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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)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

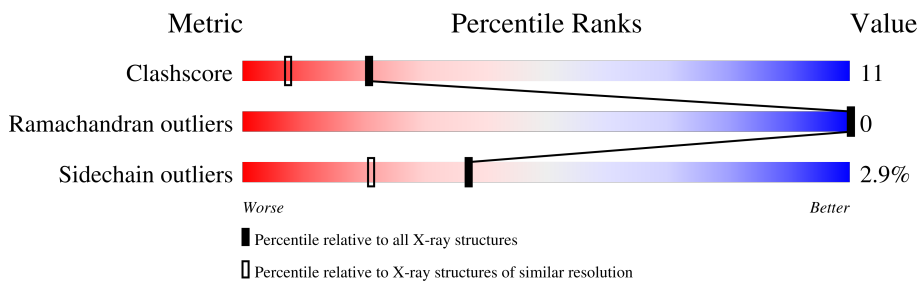
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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))
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)



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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	156	88% 12% .
1	B	156	85% 14% .
1	C	156	83% 15% ..
1	D	156	87% 12% .
1	E	156	85% 15% .
1	F	156	82% 17% .
1	G	156	81% 17% ..
1	H	156	84% 14% .

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Mol	Chain	Length	Quality of chain
1	I	156	 89% 10% .
1	J	156	 83% 15% ..

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
2	OXL	A	1157	-	X	-	-
2	OXL	C	1157	-	X	-	-
2	OXL	D	1157	-	X	-	-
2	OXL	F	1157	-	X	-	-
2	OXL	G	1157	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 15456 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 CYANATE HYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	156	1219	783	201	230	5	0	3	0
1	B	156	1219	783	201	230	5	0	3	0
1	C	156	1221	787	200	229	5	0	4	0
1	D	156	1208	776	199	228	5	0	2	0
1	E	156	1228	794	200	229	5	0	6	0
1	F	156	1213	781	199	228	5	0	3	0
1	G	156	1208	776	199	228	5	0	2	0
1	H	156	1217	784	199	229	5	0	4	0
1	I	156	1213	781	199	228	5	0	3	0
1	J	156	1218	786	199	228	5	0	4	0

There are 10 discrepancies between the modelled and reference sequences:

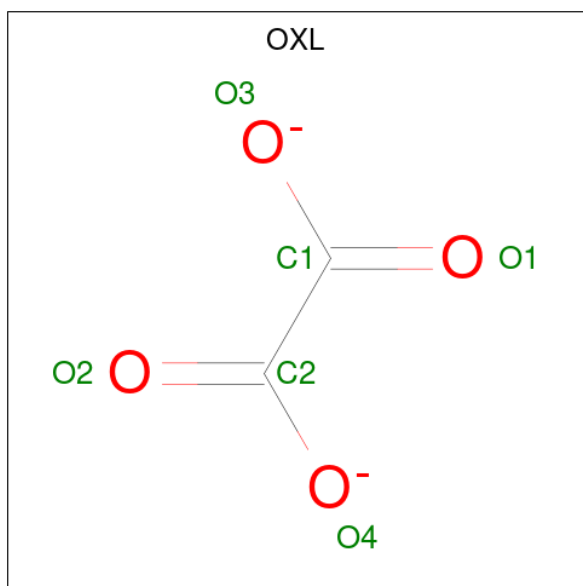
Chain	Residue	Modelled	Actual	Comment	Reference
A	95	PHE	TYR	engineered mutation	UNP P00816
B	95	PHE	TYR	engineered mutation	UNP P00816
C	95	PHE	TYR	engineered mutation	UNP P00816
D	95	PHE	TYR	engineered mutation	UNP P00816
E	95	PHE	TYR	engineered mutation	UNP P00816
F	95	PHE	TYR	engineered mutation	UNP P00816
G	95	PHE	TYR	engineered mutation	UNP P00816
H	95	PHE	TYR	engineered mutation	UNP P00816
I	95	PHE	TYR	engineered mutation	UNP P00816

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Chain	Residue	Modelled	Actual	Comment	Reference
J	95	PHE	TYR	engineered mutation	UNP P00816

- Molecule 2 is OXALATE ION (CCD ID: OXL) (formula: C_2O_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	6	2	4	0	0
2	C	1	6	2	4	0	0
2	D	1	6	2	4	0	0
2	F	1	6	2	4	0	0
2	G	1	6	2	4	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0

- Molecule 4 is water.


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	282	Total O 282 282	0	0
4	B	315	Total O 315 315	0	0
4	C	311	Total O 311 311	0	0
4	D	304	Total O 304 304	0	0
4	E	295	Total O 295 295	0	0
4	F	326	Total O 326 326	0	0
4	G	291	Total O 291 291	0	0
4	H	327	Total O 327 327	0	0
4	I	332	Total O 332 332	0	0
4	J	374	Total O 374 374	0	0

3 Residue-property plots

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. 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. 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.


Note EDS was not executed.

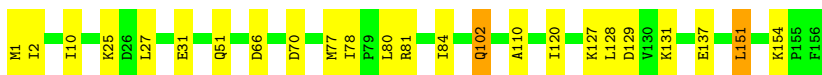
- Molecule 1: CYANATE HYDRATASE

Chain A:  88% 12%




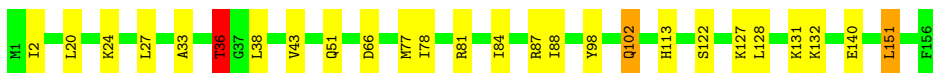
- Molecule 1: CYANATE HYDRATASE

Chain B:  85% 14%




- Molecule 1: CYANATE HYDRATASE

Chain C:  83% 15%




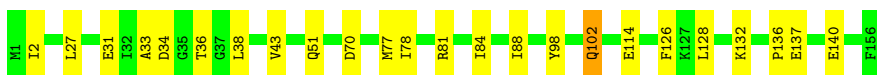
- Molecule 1: CYANATE HYDRATASE

Chain D:  87% 12%




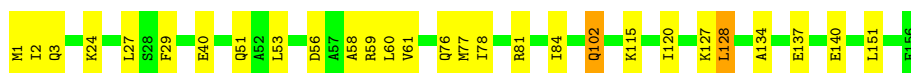
- Molecule 1: CYANATE HYDRATASE

Chain E:  85% 15%



- Molecule 1: CYANATE HYDRATASE

Chain F:  82% 17%



- Molecule 1: CYANATE HYDRATASE

Chain G: 81% 17% ..



- Molecule 1: CYANATE HYDRATASE

Chain H: 84% 14% .



- Molecule 1: CYANATE HYDRATASE

Chain I: 89% 10% .



- Molecule 1: CYANATE HYDRATASE

Chain J: 83% 15% ..



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	82.51Å 82.44Å 84.50Å 61.90° 72.56° 69.59°	Depositor
Resolution (Å)	76.25 – 1.91	Depositor
% Data completeness (in resolution range)	96.9 (76.25-1.91)	Depositor
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.131 , 0.186	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	15456	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

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: OXL, SO4

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	1.03	1/1239 (0.1%)	0.96	3/1674 (0.2%)
1	B	1.03	0/1239	0.88	0/1674
1	C	1.05	0/1247	0.95	1/1686 (0.1%)
1	D	1.07	0/1231	0.92	0/1663
1	E	1.04	0/1263	0.91	0/1707
1	F	1.01	0/1239	0.93	0/1674
1	G	1.04	0/1231	0.96	1/1663 (0.1%)
1	H	1.03	0/1246	0.94	1/1684 (0.1%)
1	I	1.07	1/1239 (0.1%)	0.98	0/1674
1	J	1.08	0/1247	0.98	2/1686 (0.1%)
All	All	1.05	2/12421 (0.0%)	0.94	8/16785 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	43	VAL	CA-CB	5.44	1.61	1.54
1	A	61	VAL	CA-CB	5.42	1.61	1.54

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	ILE	CA-C-N	-6.56	114.02	120.52
1	A	78	ILE	C-N-CA	-6.56	114.02	120.52
1	C	36	THR	N-CA-C	-6.18	105.56	113.23
1	J	36	THR	N-CA-C	-5.96	105.84	113.23
1	A	88	ILE	CB-CA-C	-5.59	104.39	110.37

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	1219	0	1269	23	0
1	B	1219	0	1270	33	0
1	C	1221	0	1281	32	0
1	D	1208	0	1260	25	0
1	E	1228	0	1302	33	0
1	F	1213	0	1271	38	0
1	G	1208	0	1260	28	0
1	H	1217	0	1278	37	0
1	I	1213	0	1271	25	0
1	J	1218	0	1282	38	0
2	A	6	0	0	0	0
2	C	6	0	0	0	0
2	D	6	0	0	0	0
2	F	6	0	0	0	0
2	G	6	0	0	0	0
3	A	15	0	0	0	0
3	B	10	0	0	0	0
3	C	5	0	0	0	0
3	D	10	0	0	0	0
3	E	15	0	0	0	0
3	F	10	0	0	0	0
3	G	5	0	0	0	0
3	H	10	0	0	0	0
3	I	15	0	0	0	0
3	J	10	0	0	0	0
4	A	282	0	0	7	0
4	B	315	0	0	11	0
4	C	311	0	0	9	0
4	D	304	0	0	7	1
4	E	295	0	0	13	1
4	F	326	0	0	19	0
4	G	291	0	0	7	0
4	H	327	0	0	10	0
4	I	332	0	0	9	0
4	J	374	0	0	15	0
All	All	15456	0	12744	277	1

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 11.

The worst 5 of 277 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:I:1:MET:CE	1:I:2:ILE:HG22	1.61	1.30
1:E:140[A]:GLU:HG2	4:E:2269:HOH:O	1.34	1.25
1:J:1:MET:CE	1:J:2:ILE:HG22	1.66	1.25
1:C:20:LEU:HD11	4:G:2187:HOH:O	1.36	1.25
1:D:1:MET:CE	1:D:2:ILE:HG22	1.69	1.22

All (1) 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)
4:D:2166:HOH:O	4:E:2114:HOH:O[1_546]	2.08	0.12

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	157/156 (101%)	154 (98%)	3 (2%)	0	100	100
1	B	157/156 (101%)	154 (98%)	3 (2%)	0	100	100
1	C	158/156 (101%)	155 (98%)	3 (2%)	0	100	100
1	D	156/156 (100%)	153 (98%)	3 (2%)	0	100	100
1	E	160/156 (103%)	157 (98%)	3 (2%)	0	100	100
1	F	157/156 (101%)	154 (98%)	3 (2%)	0	100	100
1	G	156/156 (100%)	152 (97%)	4 (3%)	0	100	100
1	H	158/156 (101%)	155 (98%)	3 (2%)	0	100	100
1	I	157/156 (101%)	154 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	158/156 (101%)	155 (98%)	3 (2%)	0	100	100
All	All	1574/1560 (101%)	1543 (98%)	31 (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	130/127 (102%)	129 (99%)	1 (1%)	73	71
1	B	130/127 (102%)	126 (97%)	4 (3%)	35	19
1	C	131/127 (103%)	124 (95%)	7 (5%)	20	7
1	D	129/127 (102%)	125 (97%)	4 (3%)	35	19
1	E	133/127 (105%)	130 (98%)	3 (2%)	44	30
1	F	130/127 (102%)	125 (96%)	5 (4%)	29	14
1	G	129/127 (102%)	124 (96%)	5 (4%)	28	13
1	H	131/127 (103%)	126 (96%)	5 (4%)	29	14
1	I	130/127 (102%)	126 (97%)	4 (3%)	35	19
1	J	131/127 (103%)	125 (95%)	6 (5%)	24	9
All	All	1304/1270 (103%)	1260 (97%)	44 (3%)	37	16

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	151	LEU
1	I	128[A]	LEU
1	H	27	LEU
1	H	128[B]	LEU
1	I	151	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	102	GLN
1	I	9	ASN
1	H	102	GLN
1	I	51	GLN
1	C	102	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

26 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
3	SO4	B	1157	-	4,4,4	0.25	0	6,6,6	0.25	0
2	OXL	D	1157	-	5,5,5	2.09	3 (60%)	6,6,6	4.06	4 (66%)
3	SO4	E	1157	-	4,4,4	0.36	0	6,6,6	0.37	0
3	SO4	C	1158	-	4,4,4	0.27	0	6,6,6	0.30	0
3	SO4	F	1158	-	4,4,4	0.30	0	6,6,6	0.48	0
3	SO4	H	1157	-	4,4,4	0.29	0	6,6,6	0.23	0
3	SO4	F	1159	-	4,4,4	0.23	0	6,6,6	0.14	0
2	OXL	C	1157	-	5,5,5	2.19	1 (20%)	6,6,6	3.42	3 (50%)
2	OXL	F	1157	-	5,5,5	2.04	1 (20%)	6,6,6	2.50	4 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	I	1159	-	4,4,4	0.24	0	6,6,6	0.21	0
3	SO4	E	1158	-	4,4,4	0.42	0	6,6,6	0.57	0
3	SO4	A	1160	-	4,4,4	0.46	0	6,6,6	0.69	0
3	SO4	I	1158	-	4,4,4	0.28	0	6,6,6	0.60	0
2	OXL	G	1157	-	5,5,5	2.34	1 (20%)	6,6,6	2.46	3 (50%)
3	SO4	A	1159	-	4,4,4	0.25	0	6,6,6	0.76	0
3	SO4	H	1158	-	4,4,4	0.28	0	6,6,6	0.20	0
3	SO4	E	1159	-	4,4,4	0.22	0	6,6,6	0.15	0
3	SO4	I	1157	-	4,4,4	0.28	0	6,6,6	0.56	0
2	OXL	A	1157	-	5,5,5	2.17	1 (20%)	6,6,6	3.15	4 (66%)
3	SO4	B	1158	-	4,4,4	0.31	0	6,6,6	0.51	0
3	SO4	G	1158	-	4,4,4	0.28	0	6,6,6	0.37	0
3	SO4	J	1157	-	4,4,4	0.30	0	6,6,6	0.38	0
3	SO4	A	1158	-	4,4,4	0.21	0	6,6,6	0.29	0
3	SO4	J	1158	-	4,4,4	0.23	0	6,6,6	0.32	0
3	SO4	D	1158	-	4,4,4	0.25	0	6,6,6	0.15	0
3	SO4	D	1159	-	4,4,4	0.26	0	6,6,6	0.18	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	OXL	A	1157	-	-	4/4/4/4	-
2	OXL	D	1157	-	-	4/4/4/4	-
2	OXL	G	1157	-	-	4/4/4/4	-
2	OXL	C	1157	-	-	4/4/4/4	-
2	OXL	F	1157	-	-	4/4/4/4	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1157	OXL	C2-C1	-4.30	1.47	1.54
2	C	1157	OXL	C2-C1	-3.86	1.48	1.54
2	F	1157	OXL	C2-C1	-3.60	1.48	1.54
2	A	1157	OXL	C2-C1	-3.54	1.48	1.54
2	D	1157	OXL	C2-C1	-2.85	1.49	1.54

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1157	OXL	O4-C2-C1	6.90	126.21	112.83
2	C	1157	OXL	O3-C1-C2	5.58	123.66	112.83
2	D	1157	OXL	O3-C1-C2	5.55	123.60	112.83
2	A	1157	OXL	O3-C1-C2	5.15	122.83	112.83
2	C	1157	OXL	O4-C2-C1	5.13	122.79	112.83

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	1157	OXL	O1-C1-C2-O2
2	G	1157	OXL	O1-C1-C2-O2
2	D	1157	OXL	O3-C1-C2-O4
2	A	1157	OXL	O3-C1-C2-O4
2	F	1157	OXL	O3-C1-C2-O4

There are no ring outliers.

No monomer is involved in short contacts.

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.