



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 23, 2023 – 03:00 AM EDT

PDB ID : 3BJK
Title : Crystal structure of HI0827, a hexameric broad specificity acyl-coenzyme A thioesterase: The Asp44Ala mutant enzyme
Authors : Willis, M.A.; Herzberg, O.; Structure 2 Function Project (S2F)
Deposited on : 2007-12-04
Resolution : 1.90 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

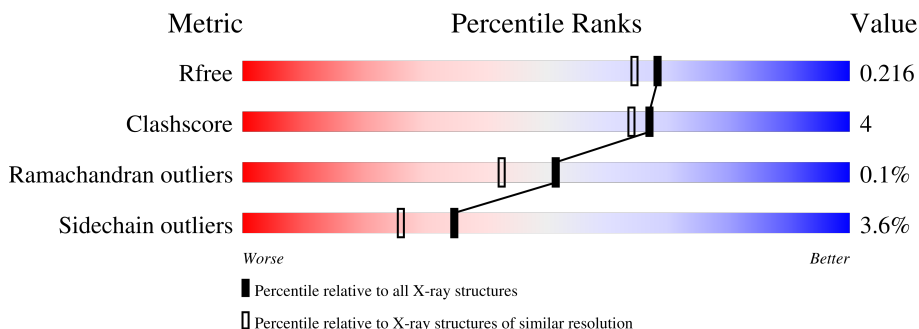
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	153	
1	B	153	
1	C	153	
1	D	153	
1	E	153	
1	F	153	

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	CIT	A	155	-	X	-	-
2	CIT	D	155	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6970 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 Acyl-CoA thioester hydrolase HI0827.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	140	1058	667	185	197	9	0	0	0
1	B	142	1072	675	189	199	9	0	0	0
1	C	143	1080	679	191	201	9	0	0	1
1	D	139	1054	665	184	196	9	0	1	0
1	E	140	1058	667	185	197	9	0	0	0
1	F	139	1046	661	183	193	9	0	0	1

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	ALA	ASP	engineered mutation	UNP P44886
B	44	ALA	ASP	engineered mutation	UNP P44886
C	44	ALA	ASP	engineered mutation	UNP P44886
D	44	ALA	ASP	engineered mutation	UNP P44886
E	44	ALA	ASP	engineered mutation	UNP P44886
F	44	ALA	ASP	engineered mutation	UNP P44886

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	A	1	Total	C	O	0	0
			13	6	7		
2	D	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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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	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0

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


- Molecule 4 is water.

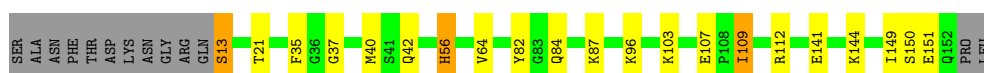
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	89	Total	O	0	0
			89	89		
4	B	77	Total	O	0	0
			77	77		
4	C	77	Total	O	0	0
			77	77		
4	D	98	Total	O	0	0
			98	98		
4	E	77	Total	O	0	0
			77	77		
4	F	45	Total	O	0	0
			45	45		

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. 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.

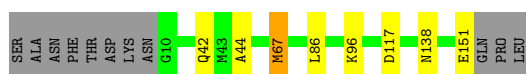
- Molecule 1: Acyl-CoA thioester hydrolase HI0827

Chain A: 




- Molecule 1: Acyl-CoA thioester hydrolase HI0827

Chain B: 




- Molecule 1: Acyl-CoA thioester hydrolase HI0827

Chain C: 




- Molecule 1: Acyl-CoA thioester hydrolase HI0827

Chain D: 




- Molecule 1: Acyl-CoA thioester hydrolase HI0827

Chain E: 



- Molecule 1: Acyl-CoA thioester hydrolase HI0827

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.49Å 63.11Å 104.72Å 90.00° 100.14° 90.00°	Depositor
Resolution (Å)	29.88 – 1.90 29.87 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.88-1.90) 98.0 (29.87-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 1.91Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.169 , 0.210 0.177 , 0.216	Depositor DCC
R_{free} test set	6357 reflections (8.14%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtrriage
Anisotropy	0.174	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6970	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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: EDO, CIT

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	0.90	0/1072	0.84	0/1447
1	B	0.88	0/1086	0.86	1/1465 (0.1%)
1	C	0.93	1/1094 (0.1%)	0.87	2/1475 (0.1%)
1	D	0.98	1/1072 (0.1%)	0.90	3/1447 (0.2%)
1	E	0.89	1/1072 (0.1%)	0.92	5/1447 (0.3%)
1	F	0.74	0/1058	0.77	0/1424
All	All	0.89	3/6454 (0.0%)	0.86	11/8705 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	152	GLN	C-O	11.04	1.44	1.23
1	C	137	GLU	CD-OE1	6.83	1.33	1.25
1	D	80	CYS	CB-SG	-6.41	1.71	1.82

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	132	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	B	67	MET	CA-CB-CG	7.32	125.74	113.30
1	D	77	ASP	CB-CG-OD2	-6.54	112.41	118.30
1	E	90	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	E	90	ARG	NE-CZ-NH1	6.19	123.39	120.30

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	1058	0	1090	18	0
1	B	1072	0	1104	5	0
1	C	1080	0	1112	6	0
1	D	1054	0	1086	16	0
1	E	1058	0	1090	7	0
1	F	1046	0	1080	4	0
2	A	26	0	10	2	0
2	D	13	0	5	0	0
3	A	24	0	36	1	0
3	B	16	0	24	1	0
3	C	12	0	18	0	0
3	D	28	0	42	7	0
3	E	16	0	24	2	0
3	F	4	0	6	0	0
4	A	89	0	0	7	0
4	B	77	0	0	1	0
4	C	77	0	0	1	0
4	D	98	0	0	4	0
4	E	77	0	0	3	1
4	F	45	0	0	1	0
All	All	6970	0	6727	52	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 4.

The worst 5 of 52 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:D:114:CYS:O	3:D:160:EDO:H11	1.86	0.74
1:A:144:LYS:NZ	4:A:187:HOH:O	2.26	0.69
1:A:87:LYS:HD3	4:A:202:HOH:O	1.93	0.69
1:D:42:GLN:OE1	4:D:296:HOH:O	2.13	0.66
1:E:19:LEU:CD2	4:E:212:HOH:O	2.43	0.66

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:207:HOH:O	4:E:234:HOH:O[2_545]	1.81	0.39

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	138/153 (90%)	136 (99%)	1 (1%)	1 (1%)	22	12
1	B	140/153 (92%)	139 (99%)	1 (1%)	0	100	100
1	C	141/153 (92%)	139 (99%)	2 (1%)	0	100	100
1	D	138/153 (90%)	138 (100%)	0	0	100	100
1	E	138/153 (90%)	138 (100%)	0	0	100	100
1	F	133/153 (87%)	131 (98%)	2 (2%)	0	100	100
All	All	828/918 (90%)	821 (99%)	6 (1%)	1 (0%)	51	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	150	SER

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	116/127 (91%)	112 (97%)	4 (3%)	37	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	117/127 (92%)	115 (98%)	2 (2%)	60	57
1	C	118/127 (93%)	112 (95%)	6 (5%)	24	14
1	D	116/127 (91%)	112 (97%)	4 (3%)	37	28
1	E	116/127 (91%)	111 (96%)	5 (4%)	29	19
1	F	114/127 (90%)	110 (96%)	4 (4%)	36	27
All	All	697/762 (92%)	672 (96%)	25 (4%)	35	26

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	148	LEU
1	E	90	ARG
1	F	116	THR
1	E	65	GLU
1	E	138	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	84	GLN
1	E	128	ASN
1	E	138	ASN
1	C	42	GLN
1	C	152	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 monosaccharides in this entry.

5.6 Ligand geometry

28 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	EDO	B	158	-	3,3,3	0.61	0	2,2,2	0.31	0
3	EDO	D	159	-	3,3,3	0.53	0	2,2,2	0.31	0
3	EDO	D	162	-	3,3,3	0.57	0	2,2,2	0.30	0
3	EDO	A	157	-	3,3,3	0.75	0	2,2,2	0.31	0
3	EDO	D	158	-	3,3,3	0.94	0	2,2,2	0.55	0
3	EDO	A	160	-	3,3,3	0.53	0	2,2,2	0.46	0
3	EDO	C	155	-	3,3,3	0.59	0	2,2,2	0.26	0
3	EDO	E	157	-	3,3,3	0.57	0	2,2,2	0.26	0
3	EDO	A	159	-	3,3,3	0.98	0	2,2,2	0.63	0
3	EDO	B	155	-	3,3,3	0.50	0	2,2,2	0.09	0
3	EDO	A	161	-	3,3,3	0.59	0	2,2,2	0.22	0
3	EDO	C	156	-	3,3,3	0.65	0	2,2,2	0.40	0
3	EDO	A	156	-	3,3,3	0.67	0	2,2,2	0.51	0
3	EDO	E	155	-	3,3,3	0.49	0	2,2,2	0.52	0
3	EDO	D	160	-	3,3,3	0.88	0	2,2,2	1.01	0
3	EDO	D	156	-	3,3,3	0.50	0	2,2,2	0.09	0
3	EDO	B	156	-	3,3,3	0.71	0	2,2,2	0.23	0
3	EDO	E	158	-	3,3,3	0.66	0	2,2,2	0.49	0
3	EDO	E	156	-	3,3,3	0.33	0	2,2,2	0.42	0
3	EDO	F	155	-	3,3,3	0.69	0	2,2,2	0.20	0
2	CIT	A	1	-	12,12,12	1.66	5 (41%)	17,17,17	1.43	2 (11%)
2	CIT	D	155	-	12,12,12	1.31	2 (16%)	17,17,17	2.64	9 (52%)
3	EDO	C	157	-	3,3,3	0.54	0	2,2,2	0.12	0
3	EDO	D	161	-	3,3,3	0.61	0	2,2,2	0.82	0
3	EDO	A	158	-	3,3,3	0.54	0	2,2,2	0.60	0
2	CIT	A	155	-	12,12,12	1.27	3 (25%)	17,17,17	2.59	5 (29%)
3	EDO	D	157	-	3,3,3	0.42	0	2,2,2	0.42	0
3	EDO	B	157	-	3,3,3	0.47	0	2,2,2	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
3	EDO	B	158	-	-	0/1/1/1	-
3	EDO	D	159	-	-	0/1/1/1	-
3	EDO	D	162	-	-	0/1/1/1	-
3	EDO	A	157	-	-	1/1/1/1	-
3	EDO	D	158	-	-	0/1/1/1	-
3	EDO	A	160	-	-	0/1/1/1	-
3	EDO	C	155	-	-	0/1/1/1	-
3	EDO	E	157	-	-	1/1/1/1	-
3	EDO	A	159	-	-	1/1/1/1	-
3	EDO	B	155	-	-	0/1/1/1	-
3	EDO	A	161	-	-	0/1/1/1	-
3	EDO	C	156	-	-	1/1/1/1	-
3	EDO	A	156	-	-	0/1/1/1	-
3	EDO	E	155	-	-	0/1/1/1	-
3	EDO	D	160	-	-	1/1/1/1	-
3	EDO	D	156	-	-	0/1/1/1	-
3	EDO	B	156	-	-	1/1/1/1	-
3	EDO	E	158	-	-	1/1/1/1	-
3	EDO	E	156	-	-	0/1/1/1	-
3	EDO	F	155	-	-	0/1/1/1	-
2	CIT	A	1	-	-	8/16/16/16	-
2	CIT	D	155	-	-	9/16/16/16	-
3	EDO	C	157	-	-	1/1/1/1	-
3	EDO	D	161	-	-	1/1/1/1	-
3	EDO	A	158	-	-	1/1/1/1	-
2	CIT	A	155	-	-	11/16/16/16	-
3	EDO	D	157	-	-	1/1/1/1	-
3	EDO	B	157	-	-	0/1/1/1	-

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	155	CIT	O4-C5	-2.85	1.21	1.30
2	A	1	CIT	O7-C3	2.66	1.48	1.43
2	A	1	CIT	O5-C6	2.38	1.29	1.22
2	A	155	CIT	O2-C1	-2.31	1.23	1.30
2	A	1	CIT	O1-C1	2.24	1.29	1.22

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	155	CIT	C3-C2-C1	-5.56	100.34	113.81
2	D	155	CIT	O6-C6-C3	5.44	122.50	113.05
2	A	155	CIT	O7-C3-C6	-5.29	101.44	108.86
2	D	155	CIT	O4-C5-O3	-4.61	111.80	123.30
2	A	155	CIT	O6-C6-C3	4.34	120.58	113.05

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	CIT	O7-C3-C6-O6
2	A	155	CIT	C1-C2-C3-O7
2	A	155	CIT	C1-C2-C3-C4
2	A	155	CIT	C2-C3-C6-O5
2	A	155	CIT	C2-C3-C6-O6

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	158	EDO	1	0
3	A	160	EDO	1	0
3	D	160	EDO	3	0
3	E	158	EDO	1	0
3	E	156	EDO	1	0
3	D	161	EDO	3	0
2	A	155	CIT	2	0
3	D	157	EDO	1	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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.