wwPDB X-ray Structure Validation Summary Report (i)

Jan 17, 2023 – 02:18 AM EST

PDB ID	:	2I6G
Title	:	Crystal structure of a putative methyltransferase (tehb, stm1608) from salmonella typhimurium lt2 at 1.90 A resolution
Authors	:	Joint Center for Structural Genomics (JCSG)
Deposited on	:	2006-08-28
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 (i) 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 (i)) were used in the production of this report:

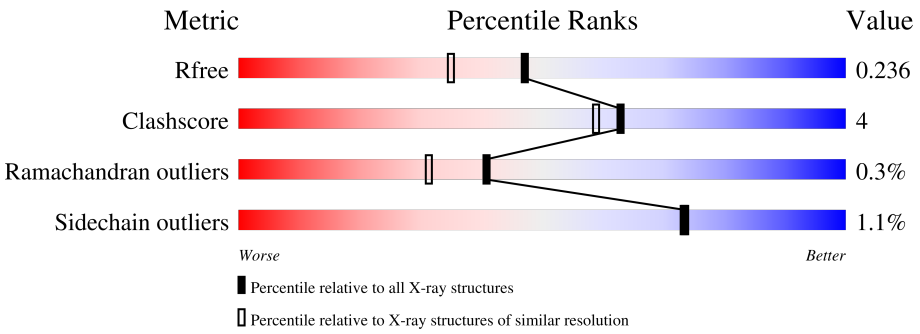
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	199	80% 9% • 11%
1	B	199	91% 9%

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	CL	B	199	-	-	X	-
3	EDO	A	200	-	-	X	-
4	ACY	B	204	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3423 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 Putative methyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	178	1414	905	236	263	2	8	0	6	0
1	B	199	1571	997	266	297	3	8	0	3	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q8ZPC3
A	1	MSE	MET	modified residue	UNP Q8ZPC3
A	12	MLY	LYS	SEE REMARK 999	UNP Q8ZPC3
A	27	MLY	LYS	SEE REMARK 999	UNP Q8ZPC3
A	60	MLY	LYS	SEE REMARK 999	UNP Q8ZPC3
A	65	MSE	MET	modified residue	UNP Q8ZPC3
A	72	MLY	LYS	SEE REMARK 999	UNP Q8ZPC3
A	105	MSE	MET	modified residue	UNP Q8ZPC3
A	106	MSE	MET	modified residue	UNP Q8ZPC3
A	120	MSE	MET	modified residue	UNP Q8ZPC3
A	125	MLY	LYS	SEE REMARK 999	UNP Q8ZPC3
A	136	MSE	MET	modified residue	UNP Q8ZPC3
A	152	MLY	LYS	SEE REMARK 999	UNP Q8ZPC3
A	165	MSE	MET	modified residue	UNP Q8ZPC3
A	167	MLY	LYS	SEE REMARK 999	UNP Q8ZPC3
A	186	MLY	LYS	SEE REMARK 999	UNP Q8ZPC3
A	192	MSE	MET	modified residue	UNP Q8ZPC3
A	196	MLY	LYS	SEE REMARK 999	UNP Q8ZPC3
B	0	GLY	-	expression tag	UNP Q8ZPC3
B	1	MSE	MET	modified residue	UNP Q8ZPC3
B	12	MLY	LYS	SEE REMARK 999	UNP Q8ZPC3
B	27	MLY	LYS	SEE REMARK 999	UNP Q8ZPC3
B	60	MLY	LYS	SEE REMARK 999	UNP Q8ZPC3
B	65	MSE	MET	modified residue	UNP Q8ZPC3
B	72	MLY	LYS	SEE REMARK 999	UNP Q8ZPC3

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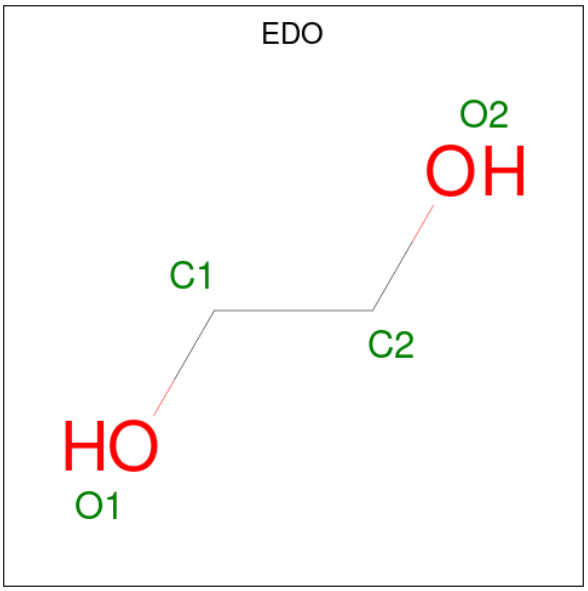
Chain	Residue	Modelled	Actual	Comment	Reference
B	105	MSE	MET	modified residue	UNP Q8ZPC3
B	106	MSE	MET	modified residue	UNP Q8ZPC3
B	120	MSE	MET	modified residue	UNP Q8ZPC3
B	125	MLY	LYS	SEE REMARK 999	UNP Q8ZPC3
B	136	MSE	MET	modified residue	UNP Q8ZPC3
B	152	MLY	LYS	SEE REMARK 999	UNP Q8ZPC3
B	165	MSE	MET	modified residue	UNP Q8ZPC3
B	167	MLY	LYS	SEE REMARK 999	UNP Q8ZPC3
B	186	MLY	LYS	SEE REMARK 999	UNP Q8ZPC3
B	192	MSE	MET	modified residue	UNP Q8ZPC3
B	196	MLY	LYS	SEE REMARK 999	UNP Q8ZPC3

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
2	A	1	1	1	0	0
			Total	Cl		
2	B	1	1	1	0	0

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



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

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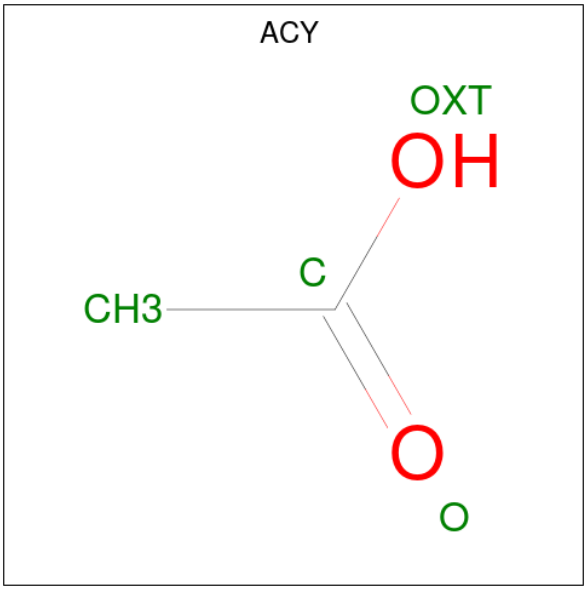
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	4	2	2	0	0
			Total	C	O		
3	A	1	4	2	2	0	0
			Total	C	O		
3	A	1	4	2	2	0	0
			Total	C	O		
3	A	1	4	2	2	0	0
			Total	C	O		
3	A	1	4	2	2	0	0
			Total	C	O		
3	B	1	4	2	2	0	0
			Total	C	O		
3	B	1	4	2	2	0	0

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



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

- Molecule 5 is water.

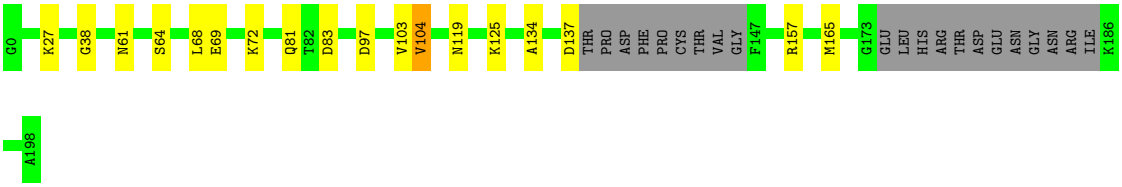
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	199	199	199	0	0
			Total	O		
5	B	189	189	189	0	0

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: Putative methyltransferase

Chain A:



- Molecule 1: Putative methyltransferase

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	100.89Å 60.16Å 72.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.60 – 1.90 29.61 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.60-1.90) 100.0 (29.61-1.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.190 , 0.233 0.198 , 0.236	Depositor DCC
R_{free} test set	1770 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	20.8	Xtriage
Anisotropy	0.606	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 35.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3423	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.25 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4263e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, MLY, CL, ACY

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	0.51	0/1359	0.70	0/1830
1	B	0.45	0/1514	0.67	0/2044
All	All	0.48	0/2873	0.69	0/3874

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 (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	1414	0	1403	14	0
1	B	1571	0	1528	11	0
2	A	1	0	0	1	0
2	B	1	0	0	2	0
3	A	24	0	36	6	0
3	B	8	0	12	0	0
4	A	4	0	3	0	0
4	B	12	0	9	2	0
5	A	199	0	0	3	0
5	B	189	0	0	0	0
All	All	3423	0	2991	26	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.

The worst 5 of 26 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)
3:A:200:EDO:H21	5:A:271:HOH:O	1.87	0.74
1:A:64:SER:O	3:A:200:EDO:H11	1.90	0.71
1:A:69:GLU:OE2	1:A:72:MLY:HH13	2.01	0.61
1:A:157:ARG:NH1	1:A:165:MSE:HG2	2.17	0.60
1:B:125:MLY:CH2	4:B:204:ACY:H1	2.36	0.55

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	169/199 (85%)	163 (96%)	5 (3%)	1 (1%)	25 15
1	B	191/199 (96%)	187 (98%)	4 (2%)	0	100 100
All	All	360/398 (90%)	350 (97%)	9 (2%)	1 (0%)	41 31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	ASN

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	136/146 (93%)	133 (98%)	3 (2%)	52	47
1	B	153/146 (105%)	152 (99%)	1 (1%)	84	84
All	All	289/292 (99%)	285 (99%)	4 (1%)	73	65

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104[A]	VAL
1	A	104[B]	VAL
1	A	119	ASN
1	B	119	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	MLY	A	196	1	7,8,11	0.54	0	3,8,13	0.66	0
1	MLY	B	125	1	9,10,11	0.61	0	6,11,13	0.94	0
1	MLY	A	12	1	9,10,11	0.45	0	6,11,13	0.76	0
1	MLY	B	167	1	5,6,11	0.71	0	2,6,13	0.53	0
1	MLY	A	72	1	9,10,11	0.77	0	6,11,13	0.71	0
1	MLY	A	186	1	3,4,11	0.81	0	2,4,13	0.75	0
1	MLY	A	27	1	9,10,11	0.65	0	6,11,13	1.03	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	MLY	B	186	1	5,6,11	0.75	0	2,6,13	0.65	0
1	MLY	B	12	1	9,10,11	0.49	0	6,11,13	0.99	0
1	MLY	B	27	1	7,8,11	0.53	0	3,8,13	0.31	0
1	MLY	A	60	1	9,10,11	0.66	0	6,11,13	0.60	0
1	MLY	A	167	1	9,10,11	0.64	0	6,11,13	0.78	0
1	MLY	B	60	1	9,10,11	0.66	0	6,11,13	1.01	0
1	MLY	B	196	1	9,10,11	0.69	0	6,11,13	0.97	0
1	MLY	B	152	1	7,8,11	0.66	0	3,8,13	0.32	0
1	MLY	A	125	1	9,10,11	0.60	0	6,11,13	0.77	0
1	MLY	B	72	1	9,10,11	0.55	0	6,11,13	0.51	0
1	MLY	A	152	1	5,6,11	0.55	0	2,6,13	0.45	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	196	1	-	0/6/7/11	-
1	MLY	B	125	1	-	2/8/9/11	-
1	MLY	A	12	1	-	1/8/9/11	-
1	MLY	B	167	1	-	0/4/5/11	-
1	MLY	A	72	1	-	2/8/9/11	-
1	MLY	A	186	1	-	0/0/2/11	-
1	MLY	A	27	1	-	2/8/9/11	-
1	MLY	B	186	1	-	1/4/5/11	-
1	MLY	B	12	1	-	4/8/9/11	-
1	MLY	B	27	1	-	0/6/7/11	-
1	MLY	A	60	1	-	0/8/9/11	-
1	MLY	A	167	1	-	2/8/9/11	-
1	MLY	B	60	1	-	2/8/9/11	-
1	MLY	B	196	1	-	1/8/9/11	-
1	MLY	B	152	1	-	1/6/7/11	-
1	MLY	A	125	1	-	2/8/9/11	-
1	MLY	B	72	1	-	0/8/9/11	-
1	MLY	A	152	1	-	1/4/5/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	27	MLY	CD-CE-NZ	-2.09	108.13	113.79

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	196	MLY	O-C-CA-CB
1	A	27	MLY	CD-CE-NZ-CH1
1	A	27	MLY	CD-CE-NZ-CH2
1	A	152	MLY	CA-CB-CG-CD
1	B	60	MLY	CD-CE-NZ-CH2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	125	MLY	2	0
1	A	72	MLY	1	0
1	A	125	MLY	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
3	EDO	A	204	-	3,3,3	0.46	0	2,2,2	0.21	0
3	EDO	A	201	-	3,3,3	0.52	0	2,2,2	0.16	0
3	EDO	A	202	-	3,3,3	0.59	0	2,2,2	0.07	0
3	EDO	B	200	-	3,3,3	0.47	0	2,2,2	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ACY	B	204	-	3,3,3	0.71	0	3,3,3	0.92	0
3	EDO	B	201	-	3,3,3	0.48	0	2,2,2	0.15	0
3	EDO	A	200	-	3,3,3	0.25	0	2,2,2	0.12	0
4	ACY	B	203	-	3,3,3	0.75	0	3,3,3	0.79	0
4	ACY	A	206	-	3,3,3	0.82	0	3,3,3	0.66	0
4	ACY	B	202	-	3,3,3	0.82	0	3,3,3	0.71	0
3	EDO	A	205	-	3,3,3	0.54	0	2,2,2	0.13	0
3	EDO	A	203	-	3,3,3	0.44	0	2,2,2	0.30	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	A	204	-	-	1/1/1/1	-
3	EDO	A	201	-	-	1/1/1/1	-
3	EDO	A	202	-	-	1/1/1/1	-
3	EDO	B	200	-	-	0/1/1/1	-
3	EDO	B	201	-	-	1/1/1/1	-
3	EDO	A	200	-	-	1/1/1/1	-
3	EDO	A	205	-	-	1/1/1/1	-
3	EDO	A	203	-	-	1/1/1/1	-

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
3	A	200	EDO	O1-C1-C2-O2
3	A	202	EDO	O1-C1-C2-O2
3	B	201	EDO	O1-C1-C2-O2
3	A	201	EDO	O1-C1-C2-O2
3	A	205	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	201	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	204	ACY	2	0
3	A	200	EDO	5	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)

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

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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