wwPDB X-ray Structure Validation Summary Report (i)

Aug 30, 2020 – 10:50 AM BST

PDB ID	:	4U6D
Title	:	Zg3615, a family 117 glycoside hydrolase in complex with beta-3,6-anhydro-L-galactose
Authors	:	Ficko-Blean, E.
Deposited on	:	2014-07-28
Resolution	:	1.70 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 following versions of software and data (see references (1)) were used in the production of this report:

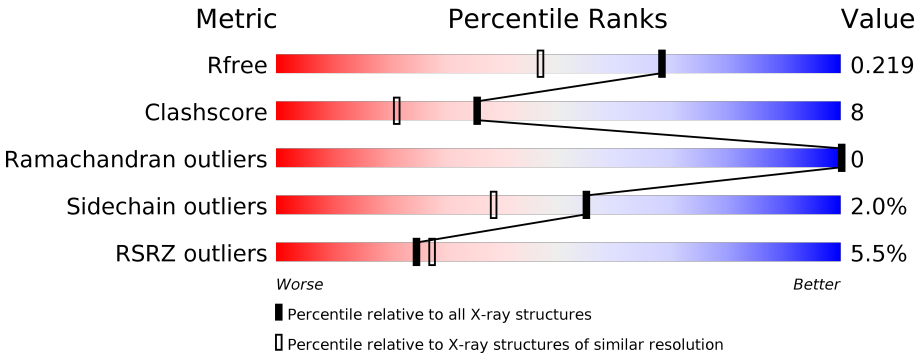
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

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 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 on 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% 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	414	% 82% 10% • 8%
1	B	414	9% 79% 14% • 7%

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
3	PEG	A	503	-	-	X	-
4	EDO	A	514	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7043 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.

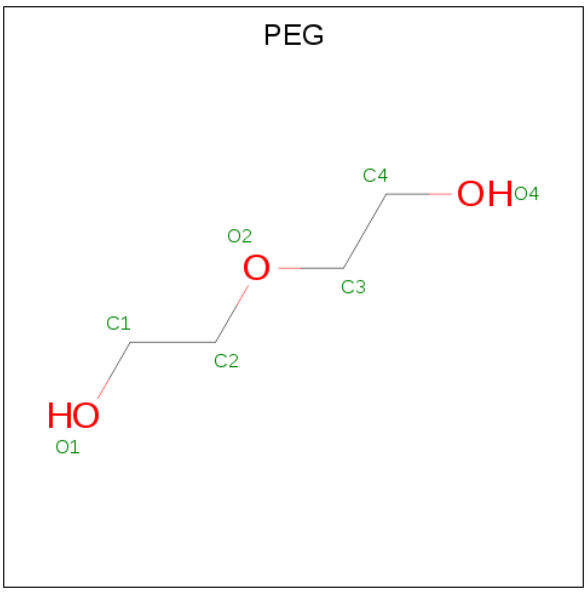
- Molecule 1 is a protein called Conserved hypothetical periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	4	0
			3108	1989	519	589	11			
1	B	385	Total	C	N	O	S	0	1	0
			3095	1985	512	588	10			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

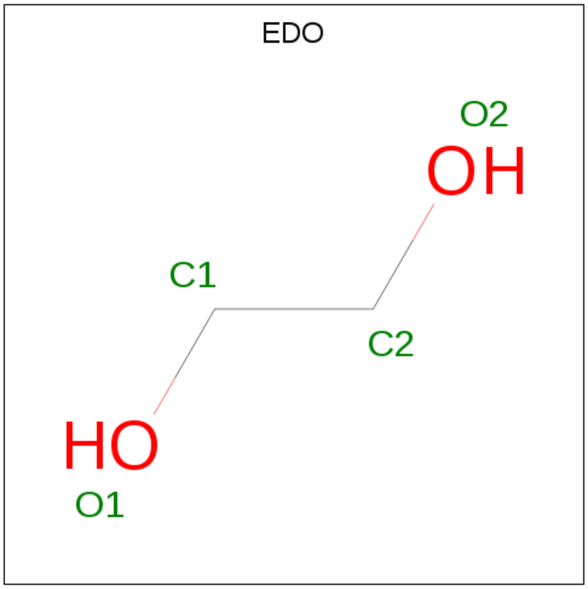
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Ca	0	0
			2	2		
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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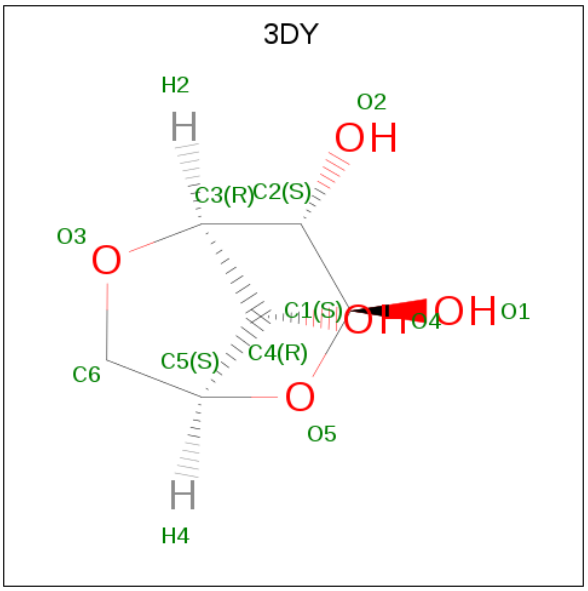
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0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

- Molecule 5 is 3,6-anhydro-beta-L-galactopyranose (three-letter code: 3DY) (formula: $C_6H_{10}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 11 6 5	0	0

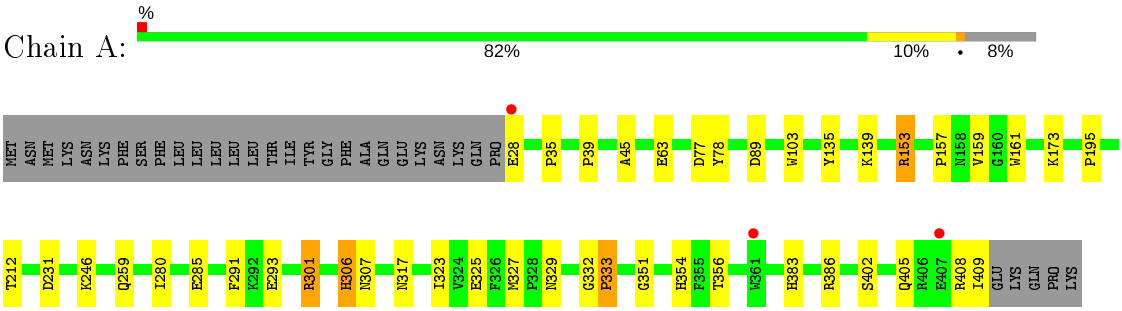
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	433	Total O 448 448	0	14
6	B	275	Total O 282 282	0	7

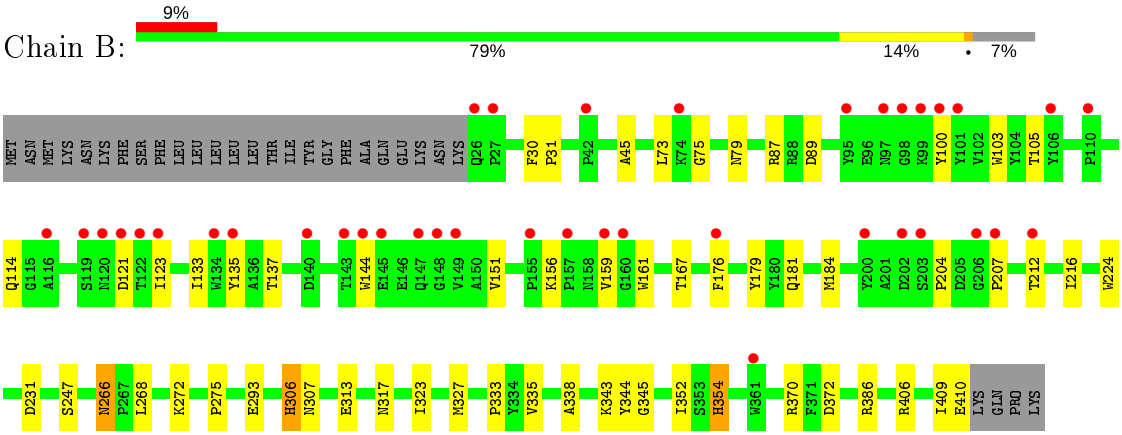
3 Residue-property plots (i)

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: Conserved hypothetical periplasmic protein



- Molecule 1: Conserved hypothetical periplasmic protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.11Å 226.13Å 67.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.70 45.52 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-1.70) 100.0 (45.52-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.35 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.185 , 0.219 0.184 , 0.219	Depositor DCC
R_{free} test set	4838 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	18.0	Xtriage
Anisotropy	0.615	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7043	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, PEG, 3DY, 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	0.84	4/3212 (0.1%)	0.85	6/4381 (0.1%)
1	B	0.70	1/3203 (0.0%)	0.74	0/4373
All	All	0.77	5/6415 (0.1%)	0.80	6/8754 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	293	GLU	CD-OE1	-5.66	1.19	1.25
1	A	333	PRO	N-CD	5.22	1.55	1.47
1	A	291	PHE	C-O	-5.21	1.13	1.23
1	A	332	GLY	C-O	-5.05	1.15	1.23
1	B	333	PRO	N-CD	5.02	1.54	1.47

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	153	ARG	NE-CZ-NH1	9.41	125.01	120.30
1	A	301[A]	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	A	301[B]	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	A	153	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	301[A]	ARG	NE-CZ-NH1	5.65	123.12	120.30

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	3108	0	2903	55	0
1	B	3095	0	2892	46	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	7	0	10	11	0
4	A	68	0	101	15	0
4	B	20	0	30	1	0
5	A	11	0	10	1	0
6	A	448	0	0	12	1
6	B	282	0	0	12	0
All	All	7043	0	5946	99	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 8.

The worst 5 of 99 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:B:144:TRP:O	6:B:832:HOH:O	1.67	1.12
1:B:75:GLY:HA3	6:B:832:HOH:O	1.48	1.11
1:B:89:ASP:H	1:B:354:HIS:HD2	1.06	0.97
1:A:301[B]:ARG:NH2	3:A:503:PEG:O1	1.98	0.97
1:A:405:GLN:N	6:A:991:HOH:O	1.99	0.95

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)
6:A:662:HOH:O	6:A:665:HOH:O[4_554]	2.06	0.14

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	384/414 (93%)	362 (94%)	22 (6%)	0	100	100
1	B	384/414 (93%)	364 (95%)	20 (5%)	0	100	100
All	All	768/828 (93%)	726 (94%)	42 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	328/359 (91%)	324 (99%)	4 (1%)	71	59
1	B	327/359 (91%)	318 (97%)	9 (3%)	43	25
All	All	655/718 (91%)	642 (98%)	13 (2%)	55	38

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	121	ASP
1	B	216	ILE
1	B	354	HIS
1	B	79	ASN
1	B	343	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	354	HIS
1	A	383	HIS
1	B	317	ASN
1	A	329	ASN
1	B	306	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 28 ligands modelled in this entry, 4 are monoatomic - leaving 24 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	$\#\|Z\| > 2$
4	EDO	A	509	2	3,3,3	0.60	0	2,2,2	0.45	0
4	EDO	A	520	-	3,3,3	0.39	0	2,2,2	0.88	0
4	EDO	A	511	-	3,3,3	0.34	0	2,2,2	0.65	0
4	EDO	A	510	-	3,3,3	0.41	0	2,2,2	0.51	0
4	EDO	A	504	-	3,3,3	0.50	0	2,2,2	0.61	0
4	EDO	A	516	-	3,3,3	0.44	0	2,2,2	0.25	0
4	EDO	A	512	-	3,3,3	0.54	0	2,2,2	0.75	0
3	PEG	A	503	-	6,6,6	0.57	0	5,5,5	0.57	0
4	EDO	A	514	-	3,3,3	0.30	0	2,2,2	0.44	0
4	EDO	B	506	-	3,3,3	0.47	0	2,2,2	0.29	0
4	EDO	A	519	-	3,3,3	1.15	0	2,2,2	0.83	0
4	EDO	A	517	-	3,3,3	0.38	0	2,2,2	0.38	0
4	EDO	A	518	-	3,3,3	0.37	0	2,2,2	0.58	0
4	EDO	B	503	-	3,3,3	0.45	0	2,2,2	0.49	0
4	EDO	B	507	-	3,3,3	0.49	0	2,2,2	0.36	0
4	EDO	A	515	-	3,3,3	0.44	0	2,2,2	0.52	0
4	EDO	A	506	-	3,3,3	0.71	0	2,2,2	0.75	0
4	EDO	A	507	-	3,3,3	0.45	0	2,2,2	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	3DY	A	521	-	12,12,12	2.31	5 (41%)	18,18,18	1.23	2 (11%)
4	EDO	B	505	-	3,3,3	0.56	0	2,2,2	0.64	0
4	EDO	B	504	-	3,3,3	0.49	0	2,2,2	0.02	0
4	EDO	A	513	-	3,3,3	0.36	0	2,2,2	0.67	0
4	EDO	A	508	-	3,3,3	0.44	0	2,2,2	0.51	0
4	EDO	A	505	-	3,3,3	0.35	0	2,2,2	0.66	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
4	EDO	A	509	2	-	0/1/1/1	-
4	EDO	A	520	-	-	1/1/1/1	-
4	EDO	A	511	-	-	1/1/1/1	-
4	EDO	A	510	-	-	1/1/1/1	-
4	EDO	A	504	-	-	0/1/1/1	-
4	EDO	A	516	-	-	0/1/1/1	-
4	EDO	A	512	-	-	1/1/1/1	-
3	PEG	A	503	-	-	3/4/4/4	-
4	EDO	A	514	-	-	0/1/1/1	-
4	EDO	B	506	-	-	1/1/1/1	-
4	EDO	A	519	-	-	0/1/1/1	-
4	EDO	A	517	-	-	0/1/1/1	-
4	EDO	A	518	-	-	1/1/1/1	-
4	EDO	B	503	-	-	1/1/1/1	-
4	EDO	B	507	-	-	0/1/1/1	-
4	EDO	A	515	-	-	0/1/1/1	-
4	EDO	A	506	-	-	0/1/1/1	-
4	EDO	A	507	-	-	1/1/1/1	-
5	3DY	A	521	-	-	-	0/3/2/2
4	EDO	B	505	-	-	0/1/1/1	-
4	EDO	B	504	-	-	0/1/1/1	-
4	EDO	A	513	-	-	1/1/1/1	-
4	EDO	A	508	-	-	1/1/1/1	-
4	EDO	A	505	-	-	0/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	521	3DY	O1-C1	3.74	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	521	3DY	O5-C1	3.31	1.51	1.42
5	A	521	3DY	O2-C2	3.19	1.50	1.43
5	A	521	3DY	O5-C5	2.97	1.51	1.44
5	A	521	3DY	C1-C2	2.68	1.58	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	521	3DY	O1-C1-O5	2.67	118.38	110.38
5	A	521	3DY	O5-C5-C6	-2.09	110.21	113.35

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	511	EDO	O1-C1-C2-O2
3	A	503	PEG	O1-C1-C2-O2
3	A	503	PEG	O2-C3-C4-O4
4	A	518	EDO	O1-C1-C2-O2
4	A	512	EDO	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	509	EDO	1	0
3	A	503	PEG	11	0
4	A	514	EDO	6	0
4	B	506	EDO	1	0
4	A	519	EDO	2	0
4	A	517	EDO	3	0
5	A	521	3DY	1	0
4	A	513	EDO	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	382/414 (92%)	-0.25	3 (0%) 86 88	10, 14, 29, 53	0
1	B	385/414 (92%)	0.56	39 (10%) 7 8	12, 25, 41, 55	0
All	All	767/828 (92%)	0.15	42 (5%) 25 27	10, 19, 39, 55	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	361	TRP	5.1
1	B	106	TYR	4.8
1	B	101	TYR	4.3
1	B	97	ASN	4.3
1	B	123	ILE	4.2

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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^{th} 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
4	EDO	A	510	4/4	0.59	0.16	55,55,56,56	0
4	EDO	A	519	4/4	0.63	0.27	31,32,34,36	0
4	EDO	B	506	4/4	0.78	0.13	43,46,46,46	0
4	EDO	A	518	4/4	0.81	0.20	51,52,53,53	0
3	PEG	A	503	7/7	0.82	0.19	36,38,47,49	0
4	EDO	A	515	4/4	0.82	0.24	30,37,38,45	0
4	EDO	A	508	4/4	0.83	0.16	49,52,53,53	0
5	3DY	A	521	11/11	0.88	0.15	17,18,20,20	0
4	EDO	B	507	4/4	0.88	0.10	40,40,43,43	0
4	EDO	B	505	4/4	0.89	0.09	24,25,28,29	0
4	EDO	A	513	4/4	0.90	0.19	23,33,38,41	0
4	EDO	A	516	4/4	0.90	0.19	36,38,39,46	0
4	EDO	A	505	4/4	0.90	0.11	31,32,35,40	0
4	EDO	A	507	4/4	0.91	0.09	27,29,33,35	0
4	EDO	A	514	4/4	0.91	0.18	29,30,30,31	0
4	EDO	A	517	4/4	0.92	0.16	26,29,32,36	0
4	EDO	B	503	4/4	0.92	0.10	34,35,38,39	0
4	EDO	A	509	4/4	0.94	0.13	16,19,20,20	0
4	EDO	A	520	4/4	0.94	0.15	23,30,31,32	0
4	EDO	B	504	4/4	0.94	0.16	27,28,28,29	0
4	EDO	A	511	4/4	0.95	0.22	25,33,37,43	0
2	CA	B	501	1/1	0.96	0.06	20,20,20,20	0
2	CA	B	502	1/1	0.97	0.07	24,24,24,24	0
4	EDO	A	506	4/4	0.97	0.09	17,19,19,19	0
4	EDO	A	512	4/4	0.97	0.11	19,20,21,22	0
4	EDO	A	504	4/4	0.98	0.12	13,16,19,20	0
2	CA	A	502	1/1	1.00	0.07	10,10,10,10	0
2	CA	A	501	1/1	1.00	0.05	13,13,13,13	0

6.5 Other polymers (i)

There are no such residues in this entry.