



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2022 – 04:39 PM EDT

PDB ID : 7SNJ
Title : Structure of Bacple_01701, a 6-O-galactose porphyran sulfatase
Authors : Ulaganathan, T.; Cygler, M.
Deposited on : 2021-10-28
Resolution : 1.74 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	:	4.02b-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

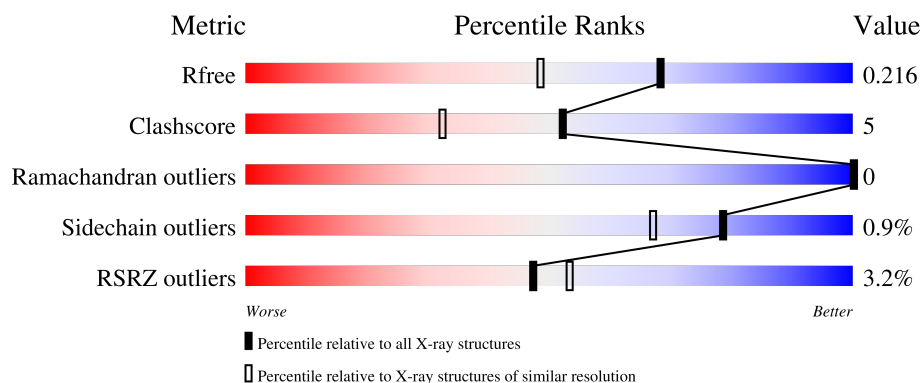
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 1.74 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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	536	

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	P4G	A	604	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 4473 atoms, of which 79 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 Arylsulfatase.

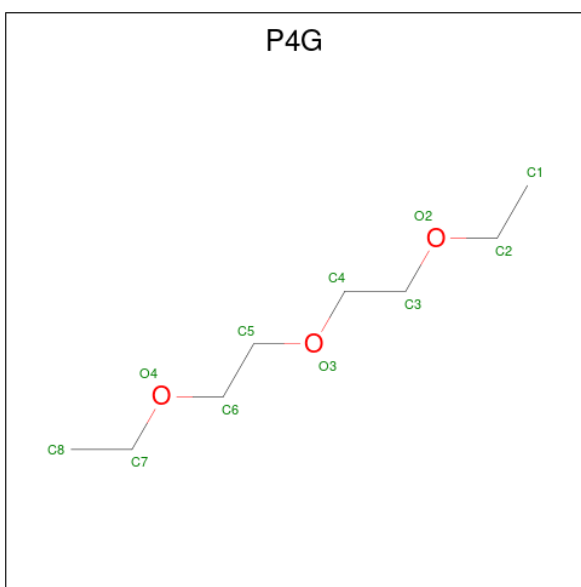
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	506	4134	2636	696	771	31	0	0	0

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



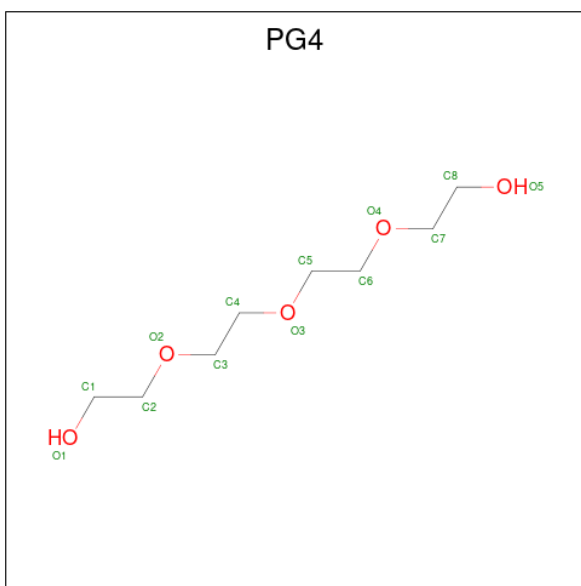
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	A	1	10	2	6	2	0	0
2	A	1	10	2	6	2	0	0
2	A	1	10	2	6	2	0	0

- Molecule 3 is 1-ETHOXY-2-(2-ETHOXYETHOXY)ETHANE (three-letter code: P4G) (formula: C₈H₁₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			29	8	18	3		

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



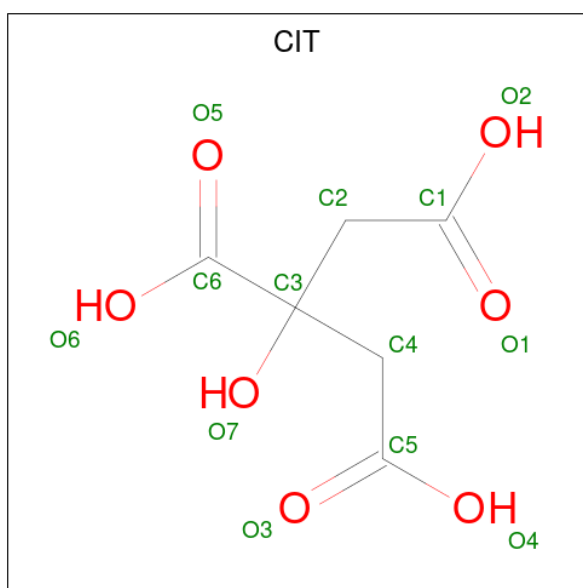
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			17	4	10	3		
5	A	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 6 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			18	6	5	7		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total 1	Na 1	0	0

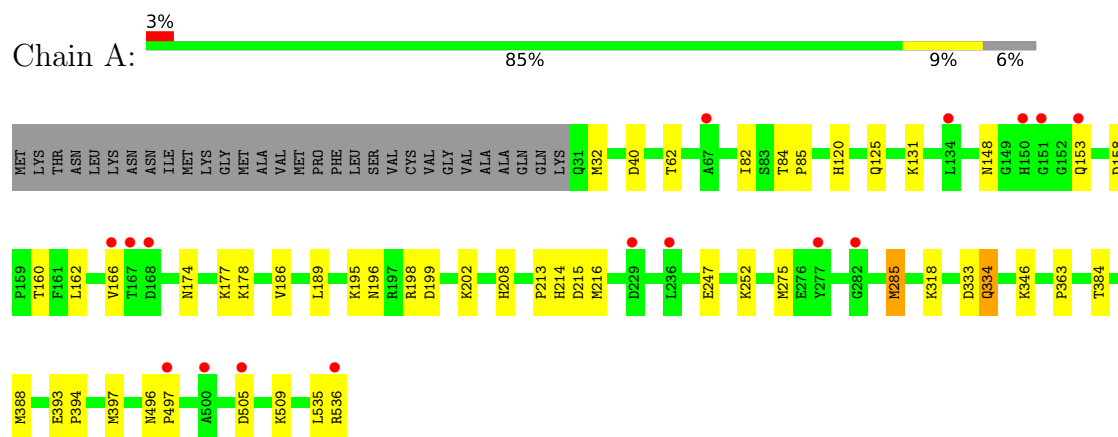
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	196	Total 196	O 196	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 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: Arylsulfatase



4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	154.86Å 154.86Å 46.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.70 – 1.74 44.70 – 1.74	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.70-1.74) 100.0 (44.70-1.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 1.74Å)	Xtriage
Refinement program	PHENIX 1.19rc4_4035	Depositor
R, R_{free}	0.188 , 0.218 0.186 , 0.216	Depositor DCC
R_{free} test set	3277 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	34.9	Xtriage
Anisotropy	0.567	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.028 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4473	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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: PEG, EDO, P4G, PG4, CIT, NA

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	0.38	0/4247	0.58	0/5742

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	4134	0	3945	43	0
2	A	12	18	18	1	0
3	A	11	18	18	7	0
4	A	13	18	18	1	0
5	A	14	20	20	2	0
6	A	13	5	5	0	0
7	A	1	0	0	0	0
8	A	196	0	0	6	0
All	All	4394	79	4024	45	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 5.

All (45) 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:318:LYS:HZ2	3:A:604:P4G:H13	1.47	0.79
1:A:131:LYS:HE3	1:A:153:GLN:HA	1.65	0.77
1:A:536:ARG:HG2	1:A:536:ARG:HH11	1.51	0.76
1:A:160:THR:HG22	1:A:177:LYS:HG3	1.69	0.73
1:A:148:ASN:OD1	1:A:160:THR:OG1	2.07	0.72
1:A:125:GLN:HE22	1:A:198:ARG:HG3	1.56	0.70
1:A:131:LYS:NZ	8:A:701:HOH:O	2.27	0.68
1:A:509:LYS:NZ	2:A:603:EDO:O2	2.28	0.66
1:A:536:ARG:HG2	1:A:536:ARG:NH1	2.09	0.66
1:A:148:ASN:HB3	1:A:162:LEU:HG	1.78	0.65
1:A:318:LYS:HZ2	3:A:604:P4G:C1	2.09	0.65
1:A:199:ASP:OD2	1:A:202:LYS:HD2	1.99	0.62
1:A:40:ASP:OD2	1:A:131:LYS:NZ	2.34	0.60
1:A:166:VAL:HB	1:A:174:ASN:HB2	1.84	0.60
1:A:384:THR:O	1:A:388:MET:HG3	2.07	0.54
1:A:247:GLU:CD	1:A:252:LYS:HG3	2.31	0.51
3:A:604:P4G:H13	3:A:604:P4G:H42	1.94	0.50
1:A:318:LYS:HZ1	3:A:604:P4G:H71	1.77	0.50
1:A:275:MET:HE2	8:A:877:HOH:O	2.13	0.49
1:A:40:ASP:O	1:A:213:PRO:HD2	2.13	0.48
1:A:393:GLU:HG3	8:A:727:HOH:O	2.13	0.48
1:A:174:ASN:OD1	1:A:174:ASN:N	2.42	0.48
1:A:84:THR:HB	1:A:85:PRO:HD3	1.96	0.48
1:A:198:ARG:HD2	8:A:711:HOH:O	2.13	0.48
1:A:333:ASP:C	1:A:334:GLN:HG3	2.34	0.47
1:A:195:LYS:HE3	1:A:196:ASN:ND2	2.30	0.47
1:A:125:GLN:NE2	1:A:198:ARG:HG3	2.28	0.47
1:A:189:LEU:HD23	4:A:605:PG4:H61	1.97	0.47
1:A:496:ASN:OD1	1:A:497:PRO:HD2	2.16	0.46
1:A:214:HIS:CE1	1:A:215:ASP:OD1	2.69	0.46
1:A:195:LYS:HE3	1:A:196:ASN:HD21	1.81	0.45
3:A:604:P4G:H13	3:A:604:P4G:C4	2.47	0.45
1:A:125:GLN:HB3	5:A:607:PEG:H22	1.99	0.44
1:A:32:MET:HE1	1:A:363:PRO:HG2	1.99	0.44
1:A:62:THR:HG23	3:A:604:P4G:C3	2.48	0.43
1:A:62:THR:HG23	3:A:604:P4G:H32	1.99	0.43
1:A:158:ASP:HA	1:A:178:LYS:O	2.18	0.43
1:A:505:ASP:O	1:A:509:LYS:HG3	2.18	0.43
1:A:535:LEU:O	1:A:536:ARG:HB2	2.19	0.42
1:A:215:ASP:HB2	1:A:216:MET:HA	2.01	0.42
1:A:186:VAL:HG12	1:A:208:HIS:CE1	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LYS:HZ3	5:A:607:PEG:H32	1.84	0.41
1:A:394:PRO:HB2	1:A:397:MET:HG3	2.01	0.41
1:A:285:MET:HG3	8:A:854:HOH:O	2.21	0.41
1:A:120:HIS:HD2	8:A:707:HOH:O	2.03	0.41

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	504/536 (94%)	488 (97%)	16 (3%)	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	444/481 (92%)	440 (99%)	4 (1%)	78	67

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

Mol	Chain	Res	Type
1	A	82	ILE
1	A	285	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	334	GLN
1	A	346	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	ASN

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 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	P4G	A	604	-	10,10,10	0.54	0	9,9,9	0.60	0
6	CIT	A	608	-	12,12,12	1.06	0	17,17,17	1.28	3 (17%)
2	EDO	A	603	-	3,3,3	0.47	0	2,2,2	0.49	0
2	EDO	A	602	-	3,3,3	0.41	0	2,2,2	0.53	0
5	PEG	A	606	-	6,6,6	0.49	0	5,5,5	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PEG	A	607	-	6,6,6	0.47	0	5,5,5	0.39	0
4	PG4	A	605	-	12,12,12	0.16	0	11,11,11	0.60	0
2	EDO	A	601	-	3,3,3	0.47	0	2,2,2	0.33	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	P4G	A	604	-	-	4/8/8/8	-
6	CIT	A	608	-	-	0/16/16/16	-
2	EDO	A	603	-	-	0/1/1/1	-
2	EDO	A	602	-	-	1/1/1/1	-
5	PEG	A	606	-	-	2/4/4/4	-
5	PEG	A	607	-	-	1/4/4/4	-
4	PG4	A	605	-	-	5/10/10/10	-
2	EDO	A	601	-	-	1/1/1/1	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	608	CIT	O6-C6-C3	2.78	117.87	113.05
6	A	608	CIT	O2-C1-O1	-2.50	117.08	123.30
6	A	608	CIT	O4-C5-O3	-2.12	118.01	123.30

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	604	P4G	O2-C3-C4-O3
5	A	606	PEG	O1-C1-C2-O2
4	A	605	PG4	O1-C1-C2-O2
4	A	605	PG4	O3-C5-C6-O4
5	A	607	PEG	O2-C3-C4-O4
2	A	601	EDO	O1-C1-C2-O2
4	A	605	PG4	O2-C3-C4-O3
4	A	605	PG4	C6-C5-O3-C4
5	A	606	PEG	O2-C3-C4-O4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	605	PG4	O4-C7-C8-O5
2	A	602	EDO	O1-C1-C2-O2
3	A	604	P4G	C1-C2-O2-C3
3	A	604	P4G	C8-C7-O4-C6
3	A	604	P4G	O3-C5-C6-O4

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	604	P4G	7	0
2	A	603	EDO	1	0
5	A	607	PEG	2	0
4	A	605	PG4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	506/536 (94%)	0.20	16 (3%)	47 53	37, 46, 66, 93	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	167	THR	5.3
1	A	153	GLN	3.6
1	A	150	HIS	3.5
1	A	229	ASP	3.1
1	A	134	LEU	3.0
1	A	497	PRO	2.8
1	A	282	GLY	2.7
1	A	536	ARG	2.7
1	A	505	ASP	2.6
1	A	151	GLY	2.4
1	A	166	VAL	2.3
1	A	277	TYR	2.2
1	A	67	ALA	2.2
1	A	500	ALA	2.2
1	A	168	ASP	2.1
1	A	236	LEU	2.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(Å ²)	Q<0.9
5	PEG	A	606	7/7	0.60	0.32	67,81,91,93	0
2	EDO	A	603	4/4	0.68	0.18	65,78,78,89	0
2	EDO	A	601	4/4	0.70	0.12	65,78,88,89	0
5	PEG	A	607	7/7	0.72	0.33	66,80,98,98	0
3	P4G	A	604	11/11	0.76	0.20	48,62,82,82	0
4	PG4	A	605	13/13	0.77	0.24	59,72,84,84	0
6	CIT	A	608	13/13	0.88	0.10	47,50,58,58	0
2	EDO	A	602	4/4	0.93	0.11	54,66,74,79	0
7	NA	A	609	1/1	0.95	0.11	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.