



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 07:39 pm BST

PDB ID : 6OK3
Title : Crystal structure of Sell repeat protein from *Oxalobacter formigenes*
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Deposited on : 2019-04-12
Resolution : 2.35 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 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 : 2.11
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) : 2.11

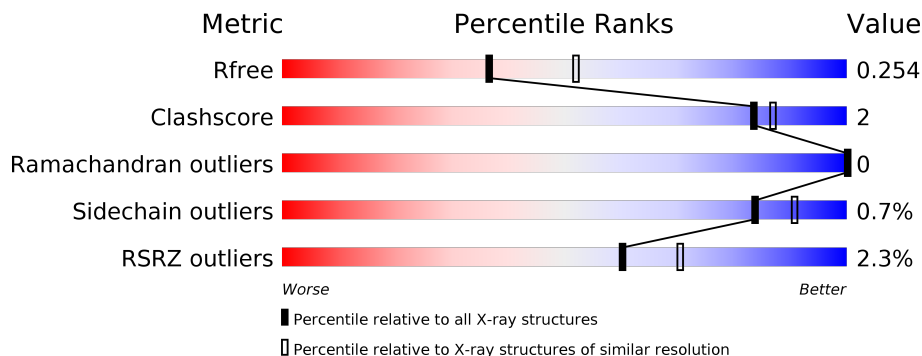
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 $\leq 5\%$. 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	523	<p>92% 5% .</p>
2	B	523	<p>4% 90% 7% .</p>

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
4	EDO	B	606	-	-	-	X
6	PEG	B	607	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8528 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.

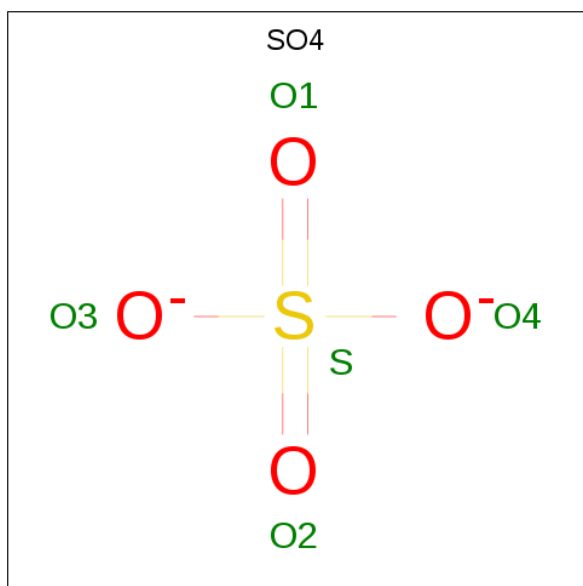
- Molecule 1 is a protein called Sell repeat protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	509	4109	2636	709	754	5	5	0	4	0

- Molecule 2 is a protein called Sell repeat protein.

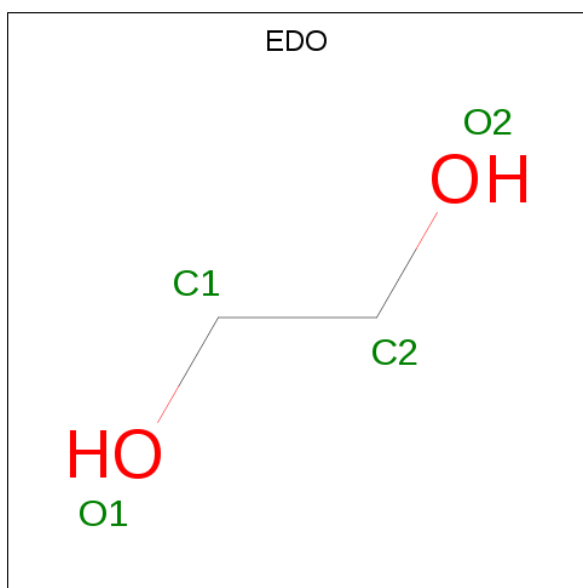
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
2	B	506	3992	2568	684	730	5	5	0	2	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



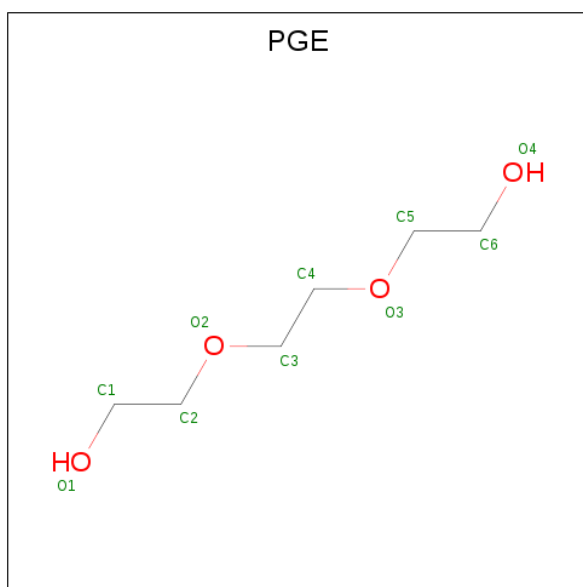
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	A	1	5	4	1	0	0
3	B	1	5	4	1	0	0

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



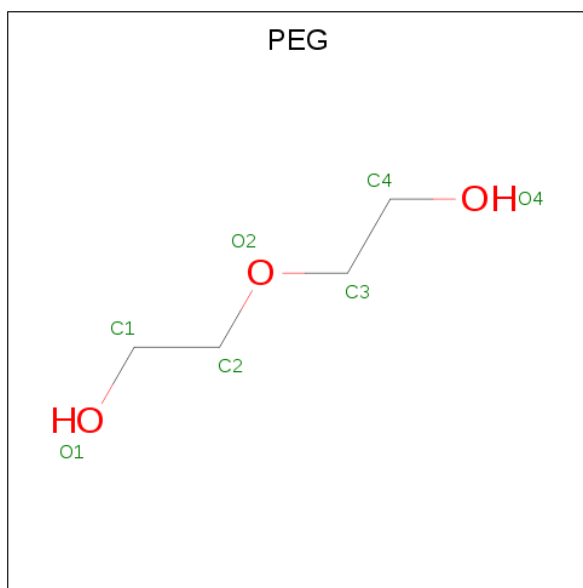
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0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

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

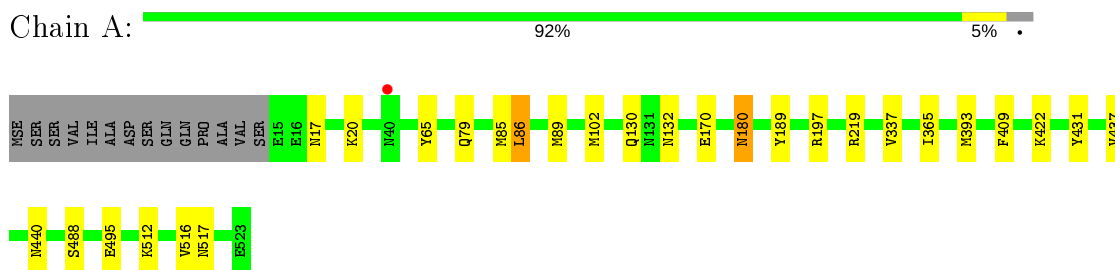
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	218	Total 218	O 218	0	0
7	B	138	Total 138	O 138	0	0

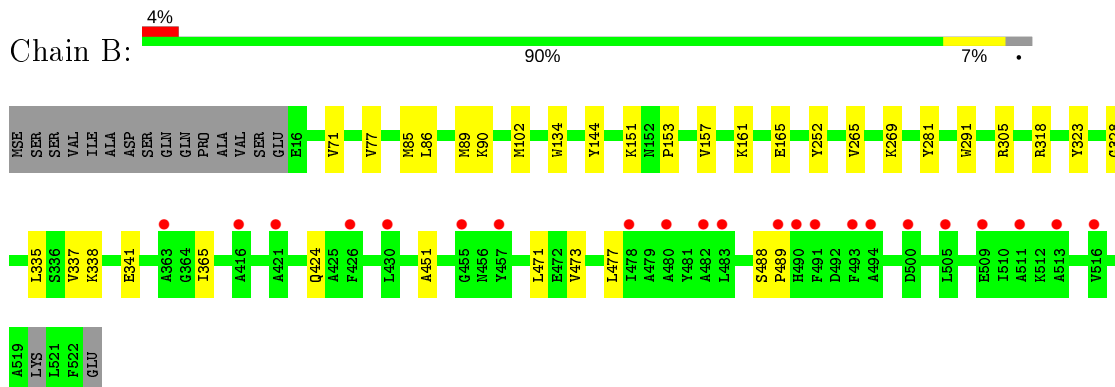
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Sell1 repeat protein



- Molecule 2: Sell1 repeat protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	213.06Å 44.98Å 142.73Å 90.00° 92.84° 90.00°	Depositor
Resolution (Å)	47.52 – 2.35 47.52 – 2.35	Depositor EDS
% Data completeness (in resolution range)	74.9 (47.52-2.35) 85.7 (47.52-2.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.27 (at 2.34Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.190 , 0.247 0.199 , 0.254	Depositor DCC
R_{free} test set	2463 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	29.6	Xtrriage
Anisotropy	0.229	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8528	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.13% 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, PGE, SO4, MLZ, MLY

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	0.24	0/4060	0.36	0/5479
2	B	0.24	0/3988	0.36	0/5399
All	All	0.24	0/8048	0.36	0/10878

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	4109	0	3979	19	0
2	B	3992	0	3795	20	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	24	0	36	4	0
4	B	20	0	30	1	0
5	A	10	0	14	2	0
6	B	7	0	10	1	0
7	A	218	0	0	2	0
7	B	138	0	0	0	0
All	All	8528	0	7864	39	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 2.

All (39) 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:85:MSE:HG2	1:A:89:MSE:HE2	1.68	0.74
2:B:85:MSE:HG2	2:B:89:MSE:HE2	1.70	0.73
1:A:197[B]:ARG:NH2	7:A:703:HOH:O	2.29	0.65
1:A:393:MSE:HE1	1:A:422:MLY:HG3	1.80	0.63
2:B:328:GLY:H	4:B:605:EDO:H22	1.64	0.63
1:A:409:PHE:HZ	1:A:437:VAL:HG11	1.67	0.59
1:A:17:ASN:HB3	1:A:20:LYS:HB3	1.85	0.59
1:A:132:ASN:HD22	4:A:604:EDO:H22	1.67	0.58
2:B:305:ARG:NH2	2:B:323:TYR:OH	2.39	0.56
2:B:337:VAL:HG21	2:B:365:ILE:HD13	1.88	0.55
2:B:71:VAL:HG22	2:B:77:VAL:HG11	1.90	0.53
2:B:424:GLN:HB2	2:B:451:ALA:HB2	1.90	0.53
2:B:161:MLY:O	2:B:165:GLU:HG2	2.10	0.52
1:A:170:GLU:HA	5:A:608:PGE:H52	1.93	0.51
2:B:281:TYR:HE1	2:B:318:ARG:HG3	1.75	0.51
1:A:488:SER:OG	1:A:495:GLU:OE1	2.29	0.50
2:B:90:MLY:HH22	6:B:607:PEG:H32	1.94	0.49
1:A:86:LEU:HA	1:A:89:MSE:HE3	1.95	0.48
2:B:471:LEU:O	2:B:473:VAL:N	2.47	0.48
1:A:337:VAL:HG21	1:A:365:ILE:HD13	1.95	0.48
1:A:517:ASN:HD22	4:A:606:EDO:H12	1.79	0.47
2:B:488:SER:HB3	2:B:489:PRO:HD3	1.96	0.46
2:B:335:LEU:HD23	2:B:338:LYS:HD2	1.97	0.46
2:B:144:TYR:O	2:B:151:MLY:HE3	2.16	0.45
2:B:86:LEU:HA	2:B:89:MSE:HE3	1.97	0.45
1:A:517:ASN:ND2	4:A:606:EDO:H12	2.32	0.45
1:A:65:TYR:HE1	1:A:102:MSE:HE3	1.81	0.45
2:B:102:MSE:HE1	2:B:134:TRP:CZ3	2.52	0.45
2:B:337:VAL:O	2:B:341:GLU:HB2	2.16	0.45
1:A:189:TYR:CZ	1:A:219:ARG:HD3	2.52	0.45
1:A:170:GLU:HG3	5:A:608:PGE:H52	1.98	0.44
2:B:265:VAL:HG12	2:B:269:LYS:HE3	1.99	0.44
2:B:281:TYR:CE1	2:B:318:ARG:HG3	2.53	0.44
1:A:512:LYS:O	1:A:516:VAL:HG23	2.19	0.43
1:A:180:ASN:ND2	7:A:707:HOH:O	2.40	0.43
1:A:431:TYR:HB3	1:A:440:ASN:O	2.21	0.41
2:B:153:PRO:O	2:B:157:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:252:TYR:HH	2:B:291[A]:TRP:HE3	1.69	0.41
1:A:132:ASN:ND2	4:A:604:EDO:H22	2.35	0.40

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	498/523 (95%)	487 (98%)	11 (2%)	0	100	100
2	B	495/523 (95%)	479 (97%)	16 (3%)	0	100	100
All	All	993/1046 (95%)	966 (97%)	27 (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	378/385 (98%)	374 (99%)	4 (1%)	73	84
2	B	359/389 (92%)	358 (100%)	1 (0%)	92	96
All	All	737/774 (95%)	732 (99%)	5 (1%)	84	91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	86	LEU
1	A	130	GLN
1	A	180	ASN
2	B	477	LEU

Some 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](#)

22 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	151	1	9,10,11	0.50	0	6,11,13	0.87	0
1	MLZ	A	269	1	8,9,10	0.78	0	4,9,11	0.66	0
2	MLY	B	331	2	9,10,11	0.55	0	6,11,13	0.83	0
1	MLY	A	403	1	9,10,11	0.54	0	6,11,13	0.79	0
2	MLY	B	161	2	9,10,11	0.48	0	6,11,13	0.83	0
1	MLY	A	98	1	9,10,11	0.48	0	6,11,13	0.92	0
2	MLY	B	90	2	9,10,11	0.50	0	6,11,13	0.89	0
2	MLY	B	378	2	9,10,11	0.51	0	6,11,13	0.90	0
1	MLY	A	397	1	9,10,11	0.53	0	6,11,13	0.80	0
1	MLY	A	422	1	9,10,11	0.53	0	6,11,13	0.85	0
2	MLY	B	403	2	9,10,11	0.50	0	6,11,13	0.85	0
1	MLZ	A	198	1	8,9,10	0.76	0	4,9,11	0.66	0
2	MLY	B	234	2	9,10,11	0.47	0	6,11,13	0.93	0
2	MLY	B	306	2	9,10,11	0.49	0	6,11,13	0.83	0
2	MLY	B	263	2	9,10,11	0.56	0	6,11,13	0.79	0
1	MLZ	A	27	1	8,9,10	0.76	0	4,9,11	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	A	161	1	9,10,11	0.49	0	6,11,13	0.87	0
1	MLY	A	270	1	9,10,11	0.65	0	6,11,13	0.58	0
1	MLZ	A	306	1	8,9,10	0.77	0	4,9,11	0.62	0
2	MLY	B	151	2	9,10,11	0.47	0	6,11,13	0.91	0
1	MLY	A	57	1	9,10,11	0.51	0	6,11,13	0.93	0
1	MLZ	A	162	1	8,9,10	0.76	0	4,9,11	0.73	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	151	1	-	0/8/9/11	-
1	MLZ	A	269	1	-	1/7/8/10	-
2	MLY	B	331	2	-	0/8/9/11	-
1	MLY	A	403	1	-	2/8/9/11	-
2	MLY	B	161	2	-	1/8/9/11	-
1	MLY	A	98	1	-	2/8/9/11	-
2	MLY	B	90	2	-	1/8/9/11	-
2	MLY	B	378	2	-	3/8/9/11	-
1	MLY	A	397	1	-	1/8/9/11	-
1	MLY	A	422	1	-	1/8/9/11	-
2	MLY	B	403	2	-	0/8/9/11	-
1	MLZ	A	198	1	-	2/7/8/10	-
2	MLY	B	234	2	-	1/8/9/11	-
2	MLY	B	306	2	-	3/8/9/11	-
2	MLY	B	263	2	-	1/8/9/11	-
1	MLZ	A	27	1	-	0/7/8/10	-
1	MLY	A	161	1	-	1/8/9/11	-
1	MLY	A	270	1	-	5/8/9/11	-
1	MLZ	A	306	1	-	1/7/8/10	-
2	MLY	B	151	2	-	4/8/9/11	-
1	MLY	A	57	1	-	0/8/9/11	-
1	MLZ	A	162	1	-	6/7/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	234	MLY	O-C-CA-CB
2	B	306	MLY	N-CA-CB-CG
2	B	306	MLY	C-CA-CB-CG
2	B	263	MLY	O-C-CA-CB
2	B	151	MLY	N-CA-CB-CG
2	B	151	MLY	C-CA-CB-CG
1	A	162	MLZ	C-CA-CB-CG
1	A	162	MLZ	CD-CE-NZ-CM
1	A	98	MLY	CD-CE-NZ-CH1
1	A	98	MLY	CD-CE-NZ-CH2
2	B	378	MLY	CD-CE-NZ-CH1
2	B	151	MLY	CD-CE-NZ-CH1
2	B	151	MLY	CD-CE-NZ-CH2
1	A	422	MLY	CG-CD-CE-NZ
2	B	306	MLY	CG-CD-CE-NZ
1	A	198	MLZ	CD-CE-NZ-CM
2	B	378	MLY	CD-CE-NZ-CH2
1	A	270	MLY	CD-CE-NZ-CH2
1	A	403	MLY	CA-CB-CG-CD
1	A	162	MLZ	CE-CD-CG-CB
1	A	162	MLZ	CG-CD-CE-NZ
1	A	270	MLY	CE-CD-CG-CB
1	A	270	MLY	CG-CD-CE-NZ
1	A	270	MLY	CA-CB-CG-CD
1	A	306	MLZ	CD-CE-NZ-CM
1	A	270	MLY	CD-CE-NZ-CH1
1	A	162	MLZ	CA-CB-CG-CD
1	A	403	MLY	CD-CE-NZ-CH1
2	B	161	MLY	C-CA-CB-CG
1	A	198	MLZ	CA-CB-CG-CD
2	B	90	MLY	CA-CB-CG-CD
1	A	269	MLZ	C-CA-CB-CG
1	A	161	MLY	C-CA-CB-CG
1	A	397	MLY	CG-CD-CE-NZ
2	B	378	MLY	CG-CD-CE-NZ
1	A	162	MLZ	N-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	161	MLY	1	0
2	B	90	MLY	1	0
1	A	422	MLY	1	0
2	B	151	MLY	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

15 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	$\# Z > 2$
4	EDO	A	605	-	3,3,3	0.47	0	2,2,2	0.25	0
4	EDO	A	604	-	3,3,3	0.46	0	2,2,2	0.32	0
4	EDO	B	604	-	3,3,3	0.46	0	2,2,2	0.35	0
4	EDO	B	602	-	3,3,3	0.46	0	2,2,2	0.30	0
4	EDO	A	607	-	3,3,3	0.46	0	2,2,2	0.36	0
3	SO4	B	601	-	4,4,4	0.13	0	6,6,6	0.07	0
4	EDO	B	605	-	3,3,3	0.47	0	2,2,2	0.26	0
4	EDO	A	603	-	3,3,3	0.44	0	2,2,2	0.35	0
6	PEG	B	607	-	6,6,6	0.43	0	5,5,5	0.26	0
4	EDO	B	606	-	3,3,3	0.47	0	2,2,2	0.33	0
4	EDO	A	606	-	3,3,3	0.46	0	2,2,2	0.33	0
4	EDO	B	603	-	3,3,3	0.48	0	2,2,2	0.32	0
3	SO4	A	601	-	4,4,4	0.14	0	6,6,6	0.05	0
4	EDO	A	602	-	3,3,3	0.46	0	2,2,2	0.31	0
5	PGE	A	608	-	9,9,9	0.46	0	8,8,8	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
4	EDO	A	605	-	-	0/1/1/1	-
4	EDO	A	604	-	-	0/1/1/1	-
4	EDO	B	604	-	-	0/1/1/1	-
4	EDO	A	607	-	-	0/1/1/1	-
5	PGE	A	608	-	-	2/7/7/7	-
4	EDO	B	605	-	-	0/1/1/1	-
4	EDO	A	603	-	-	0/1/1/1	-
6	PEG	B	607	-	-	1/4/4/4	-
4	EDO	B	606	-	-	0/1/1/1	-
4	EDO	A	606	-	-	0/1/1/1	-
4	EDO	B	602	-	-	0/1/1/1	-
4	EDO	A	602	-	-	0/1/1/1	-
4	EDO	B	603	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	608	PGE	O2-C3-C4-O3
6	B	607	PEG	O2-C3-C4-O4
5	A	608	PGE	C3-C4-O3-C5

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	604	EDO	2	0
4	B	605	EDO	1	0
6	B	607	PEG	1	0
4	A	606	EDO	2	0
5	A	608	PGE	2	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, 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	491/523 (93%)	-0.34	1 (0%) 95 97	14, 31, 58, 100	0
2	B	492/523 (94%)	0.06	22 (4%) 33 46	18, 41, 90, 146	0
All	All	983/1046 (93%)	-0.14	23 (2%) 60 70	14, 35, 83, 146	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	513	ALA	5.3
2	B	363	ALA	4.7
2	B	482	ALA	4.4
2	B	505	LEU	3.8
2	B	480	ALA	3.7
2	B	493	PHE	3.6
2	B	478	ILE	3.5
2	B	455	GLY	3.4
2	B	516	VAL	3.2
2	B	416	ALA	3.2
2	B	489	PRO	3.2
2	B	491	PHE	3.1
2	B	500	ASP	3.0
2	B	511	ALA	2.9
1	A	40	ASN	2.8
2	B	457	TYR	2.8
2	B	509	GLU	2.8
2	B	421	ALA	2.4
2	B	430	LEU	2.3
2	B	426	PHE	2.2
2	B	490	HIS	2.2
2	B	483	LEU	2.1
2	B	494	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	MLY	B	331	11/12	0.86	0.26	40,56,66,71	0
2	MLY	B	161	11/12	0.92	0.13	32,40,64,64	0
2	MLY	B	378	11/12	0.92	0.17	42,48,70,71	0
1	MLY	A	397	11/12	0.93	0.13	24,42,77,78	0
2	MLY	B	403	11/12	0.94	0.18	34,45,68,73	0
2	MLY	B	306	11/12	0.94	0.17	18,31,60,62	0
1	MLZ	A	306	10/11	0.94	0.13	29,37,43,44	0
1	MLY	A	403	11/12	0.95	0.17	30,33,48,56	0
2	MLY	B	151	11/12	0.95	0.15	34,42,58,65	0
2	MLY	B	263	11/12	0.96	0.14	16,28,56,63	0
1	MLY	A	161	11/12	0.96	0.14	9,21,46,46	0
1	MLY	A	270	11/12	0.96	0.12	20,33,46,48	0
1	MLZ	A	269	10/11	0.96	0.11	21,28,40,44	0
1	MLY	A	422	11/12	0.96	0.14	20,30,32,35	0
1	MLY	A	151	11/12	0.97	0.12	11,20,33,41	0
2	MLY	B	90	11/12	0.97	0.14	21,29,39,45	0
2	MLY	B	234	11/12	0.97	0.15	18,27,37,47	0
1	MLY	A	57	11/12	0.97	0.12	21,33,49,50	0
1	MLZ	A	27	10/11	0.98	0.10	14,25,35,36	0
1	MLZ	A	198	10/11	0.98	0.13	10,20,30,32	0
1	MLY	A	98	11/12	0.98	0.12	16,25,46,48	0
1	MLZ	A	162	10/11	0.98	0.13	14,20,31,40	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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(\AA^2)	Q<0.9
4	EDO	B	606	4/4	0.18	0.84	105,109,114,115	0
4	EDO	A	605	4/4	0.61	0.23	59,67,77,87	0
6	PEG	B	607	7/7	0.68	0.51	65,73,89,95	0
4	EDO	B	605	4/4	0.79	0.34	59,62,64,66	0
4	EDO	A	607	4/4	0.81	0.18	60,63,64,64	0
4	EDO	A	604	4/4	0.82	0.20	50,55,55,57	0
4	EDO	B	603	4/4	0.84	0.15	44,46,47,49	0
5	PGE	A	608	10/10	0.85	0.28	34,69,86,89	0
3	SO4	B	601	5/5	0.85	0.18	84,87,97,97	0
4	EDO	B	604	4/4	0.85	0.17	47,48,54,57	0
4	EDO	A	602	4/4	0.90	0.20	40,46,47,60	0
4	EDO	A	606	4/4	0.90	0.13	42,44,50,54	0
4	EDO	B	602	4/4	0.91	0.14	29,36,47,48	0
4	EDO	A	603	4/4	0.92	0.21	45,52,58,61	0
3	SO4	A	601	5/5	0.97	0.24	74,81,85,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.