



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:36 PM UTC

PDB ID : 6OK3 / pdb_00006ok3
Title : Crystal structure of Sell repeat protein from *Oxalobacter formigenes*
Authors : Chang, C.; Tesar, C.; Endres, M.; Babnigg, G.; Hassan, H.; Joachimiak, A.;
Midwest Center for Structural Genomics (MCSG)
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 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

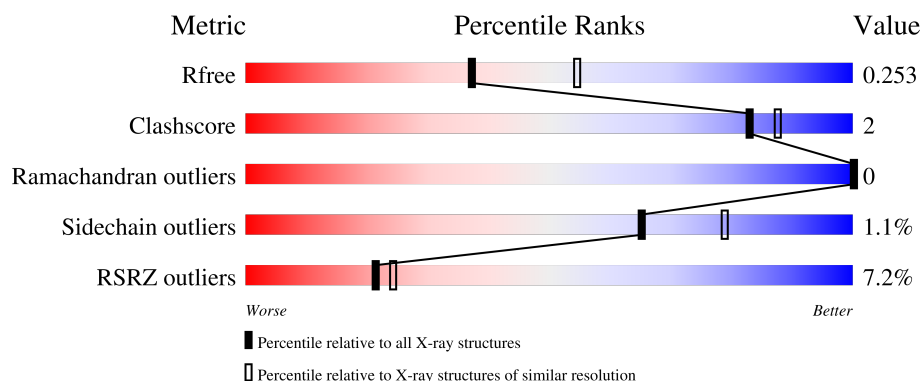
1 Overall quality at a glance

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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (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 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	523	% 92% 5% •
2	B	523	13% 90% 7% •

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.

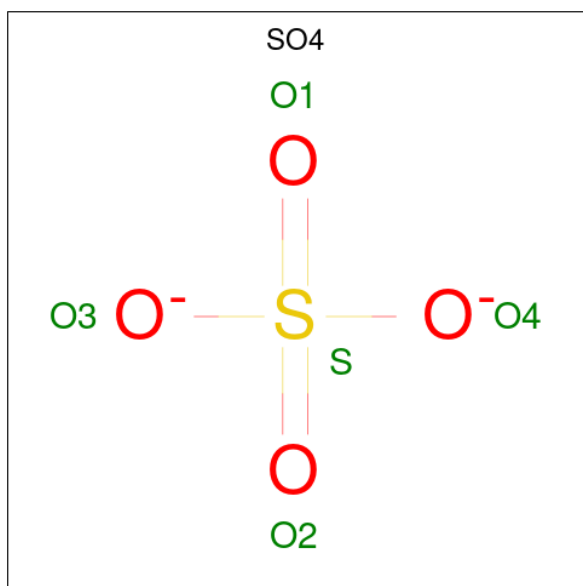
- Molecule 1 is a protein called Sel1 repeat protein.

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 Sel1 repeat protein.

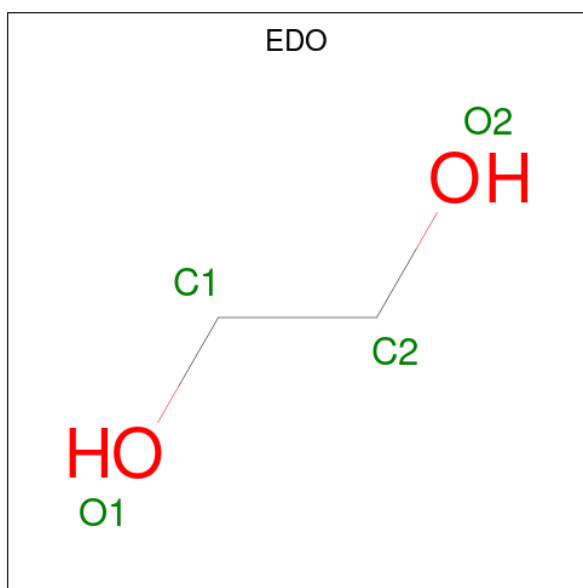
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
2	B	506	3992	2568	684	730	5	5	0	2	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



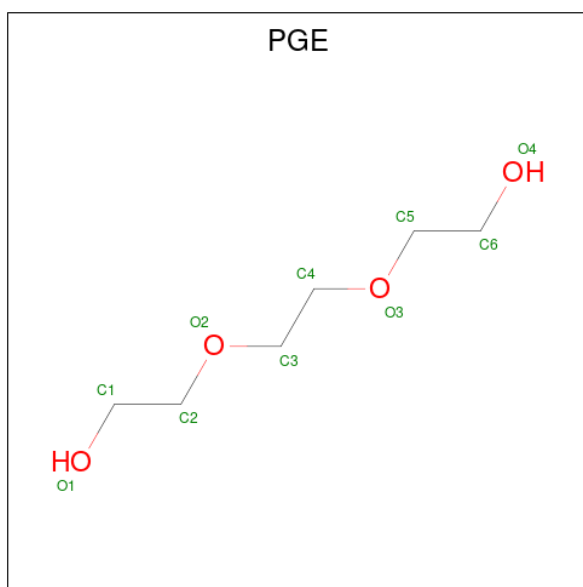
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	A	1	5	4	1	0	0
3	B	1	5	4	1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



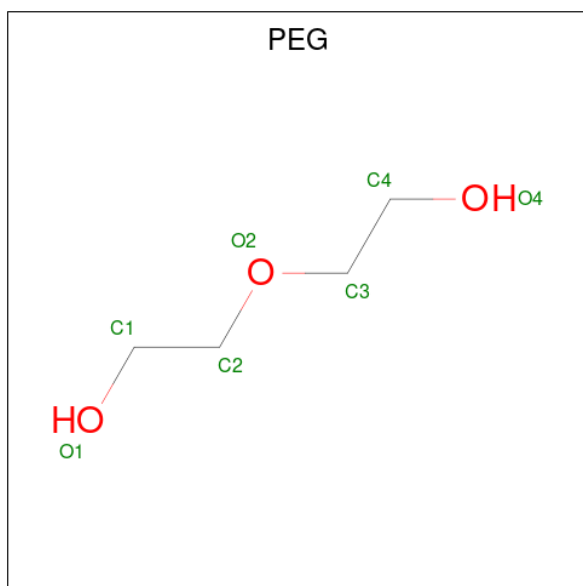
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total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

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: 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 (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

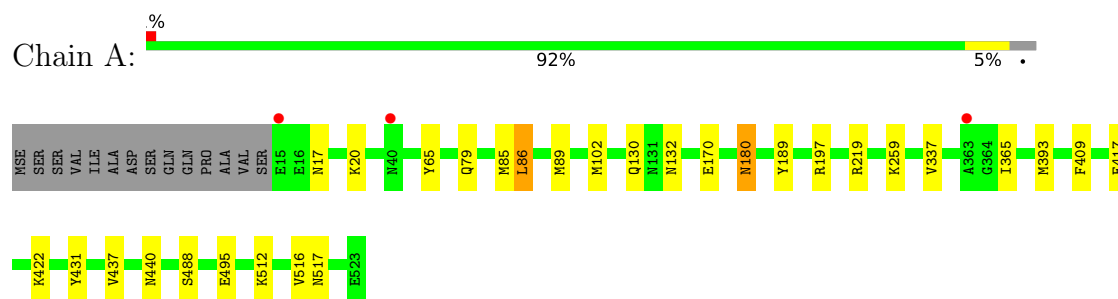
- Molecule 7 is water.

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

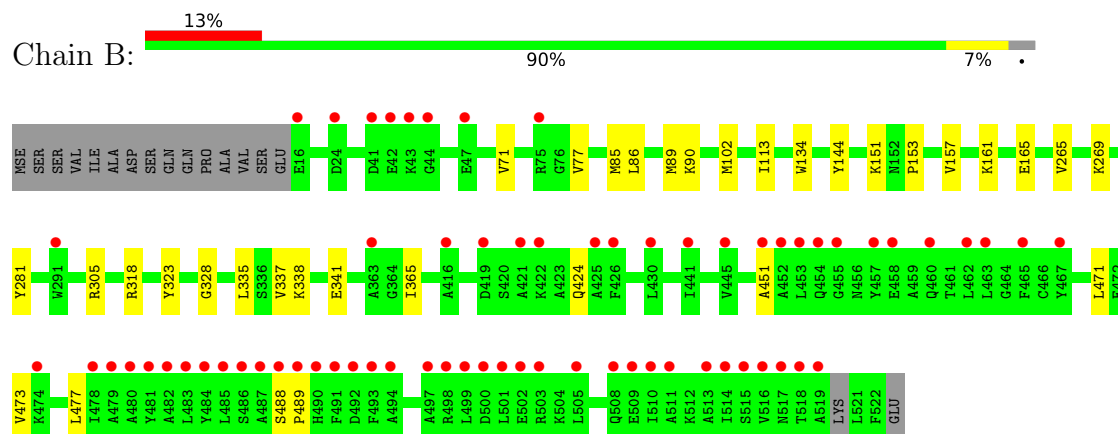
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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: 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)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.190 , 0.247 0.200 , 0.253	Depositor DCC
R_{free} test set	2463 reflections (4.30%)	wwPDB-VP
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
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

Xtriage'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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, PGE, SO4, MLZ, MLY, 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	0.10	0/4060	0.24	0/5479
2	B	0.09	0/3988	0.23	0/5399
All	All	0.09	0/8048	0.23	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

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	19	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	38	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 (38) 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:86:LEU:HA	2:B:89:MSE:HE3	1.97	0.45
2:B:144:TYR:O	2:B:151:MLY:HE3	2.16	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	372 (98%)	6 (2%)	55	70
2	B	359/389 (92%)	357 (99%)	2 (1%)	78	87
All	All	737/774 (95%)	729 (99%)	8 (1%)	65	79

All (8) 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
1	A	259	LYS
1	A	417	GLU
2	B	113	ILE
2	B	477	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	130	GLN
1	A	172	GLN
1	A	208	GLN
1	A	238	GLN
1	A	274	GLN
1	A	316	GLN
1	A	346	GLN
1	A	424	GLN
1	A	490	HIS
2	B	40	ASN
2	B	64	GLN
2	B	94	GLN
2	B	172	GLN
2	B	274	GLN
2	B	317	ASN
2	B	354	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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
2	MLY	B	234	2	9,10,11	0.47	0	6,11,13	0.93	0
2	MLY	B	161	2	9,10,11	0.48	0	6,11,13	0.83	0
2	MLY	B	306	2	9,10,11	0.49	0	6,11,13	0.82	0
1	MLZ	A	198	1	8,9,10	0.78	0	4,9,11	0.69	0
1	MLY	A	403	1	9,10,11	0.55	0	6,11,13	0.79	0
1	MLY	A	151	1	9,10,11	0.50	0	6,11,13	0.87	0
2	MLY	B	263	2	9,10,11	0.56	0	6,11,13	0.79	0
2	MLY	B	378	2	9,10,11	0.52	0	6,11,13	0.91	0
2	MLY	B	151	2	9,10,11	0.47	0	6,11,13	0.91	0
2	MLY	B	90	2	9,10,11	0.50	0	6,11,13	0.89	0
1	MLZ	A	162	1	8,9,10	0.78	0	4,9,11	0.75	0
1	MLY	A	397	1	9,10,11	0.53	0	6,11,13	0.80	0
1	MLY	A	57	1	9,10,11	0.51	0	6,11,13	0.93	0
1	MLZ	A	306	1	8,9,10	0.79	0	4,9,11	0.64	0
1	MLY	A	98	1	9,10,11	0.48	0	6,11,13	0.91	0
1	MLZ	A	27	1	8,9,10	0.78	0	4,9,11	0.64	0
1	MLY	A	422	1	9,10,11	0.54	0	6,11,13	0.85	0
1	MLZ	A	269	1	8,9,10	0.80	0	4,9,11	0.66	0
1	MLY	A	161	1	9,10,11	0.49	0	6,11,13	0.87	0
2	MLY	B	331	2	9,10,11	0.56	0	6,11,13	0.82	0
2	MLY	B	403	2	9,10,11	0.51	0	6,11,13	0.84	0
1	MLY	A	270	1	9,10,11	0.65	0	6,11,13	0.60	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
2	MLY	B	234	2	-	1/8/9/11	-
2	MLY	B	161	2	-	1/8/9/11	-
2	MLY	B	306	2	-	3/8/9/11	-
1	MLZ	A	198	1	-	2/7/8/10	-
1	MLY	A	403	1	-	3/8/9/11	-
1	MLY	A	151	1	-	0/8/9/11	-
2	MLY	B	263	2	-	1/8/9/11	-
2	MLY	B	378	2	-	3/8/9/11	-
2	MLY	B	151	2	-	4/8/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLY	B	90	2	-	1/8/9/11	-
1	MLZ	A	162	1	-	6/7/8/10	-
1	MLY	A	397	1	-	1/8/9/11	-
1	MLY	A	57	1	-	0/8/9/11	-
1	MLZ	A	306	1	-	1/7/8/10	-
1	MLY	A	98	1	-	2/8/9/11	-
1	MLZ	A	27	1	-	0/7/8/10	-
1	MLY	A	422	1	-	1/8/9/11	-
1	MLZ	A	269	1	-	1/7/8/10	-
1	MLY	A	161	1	-	1/8/9/11	-
2	MLY	B	331	2	-	0/8/9/11	-
2	MLY	B	403	2	-	0/8/9/11	-
1	MLY	A	270	1	-	6/8/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (38) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	A	162	MLZ	CE-CD-CG-CB
1	A	270	MLY	CG-CD-CE-NZ
1	A	270	MLY	CE-CD-CG-CB
1	A	162	MLZ	CG-CD-CE-NZ
1	A	270	MLY	CD-CE-NZ-CH1
1	A	270	MLY	CA-CB-CG-CD
1	A	403	MLY	CD-CE-NZ-CH1
1	A	162	MLZ	CA-CB-CG-CD
1	A	161	MLY	C-CA-CB-CG
1	A	269	MLZ	C-CA-CB-CG
1	A	403	MLY	C-CA-CB-CG
2	B	161	MLY	C-CA-CB-CG
1	A	397	MLY	CG-CD-CE-NZ
2	B	378	MLY	CG-CD-CE-NZ
1	A	198	MLZ	CA-CB-CG-CD
2	B	90	MLY	CA-CB-CG-CD
1	A	270	MLY	C-CA-CB-CG
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	151	MLY	1	0
2	B	90	MLY	1	0
1	A	422	MLY	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	B	605	-	3,3,3	0.44	0	2,2,2	0.30	0
5	PGE	A	608	-	9,9,9	0.47	0	8,8,8	0.32	0
4	EDO	B	604	-	3,3,3	0.42	0	2,2,2	0.39	0
4	EDO	B	606	-	3,3,3	0.43	0	2,2,2	0.37	0
4	EDO	A	606	-	3,3,3	0.43	0	2,2,2	0.37	0
4	EDO	A	603	-	3,3,3	0.41	0	2,2,2	0.39	0
3	SO4	B	601	-	4,4,4	0.23	0	6,6,6	0.10	0
6	PEG	B	607	-	6,6,6	0.44	0	5,5,5	0.26	0
4	EDO	A	605	-	3,3,3	0.44	0	2,2,2	0.29	0
4	EDO	A	602	-	3,3,3	0.43	0	2,2,2	0.36	0
4	EDO	A	607	-	3,3,3	0.43	0	2,2,2	0.41	0
3	SO4	A	601	-	4,4,4	0.24	0	6,6,6	0.08	0
4	EDO	B	602	-	3,3,3	0.43	0	2,2,2	0.35	0
4	EDO	B	603	-	3,3,3	0.45	0	2,2,2	0.37	0
4	EDO	A	604	-	3,3,3	0.43	0	2,2,2	0.36	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	B	605	-	-	0/1/1/1	-
5	PGE	A	608	-	-	2/7/7/7	-
4	EDO	B	604	-	-	0/1/1/1	-
4	EDO	B	606	-	-	0/1/1/1	-
4	EDO	A	606	-	-	0/1/1/1	-
4	EDO	A	603	-	-	0/1/1/1	-
6	PEG	B	607	-	-	1/4/4/4	-
4	EDO	A	605	-	-	0/1/1/1	-
4	EDO	A	602	-	-	0/1/1/1	-
4	EDO	A	607	-	-	0/1/1/1	-
4	EDO	B	602	-	-	0/1/1/1	-
4	EDO	B	603	-	-	0/1/1/1	-
4	EDO	A	604	-	-	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	B	605	EDO	1	0
5	A	608	PGE	2	0
4	A	606	EDO	2	0
6	B	607	PEG	1	0
4	A	604	EDO	2	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

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%)	-0.20	3 (0%) 85 89	11, 31, 58, 100	4 (0%)
2	B	492/523 (94%)	0.57	68 (13%) 6 7	12, 41, 90, 146	2 (0%)
All	All	983/1046 (93%)	0.19	71 (7%) 21 24	11, 34, 83, 146	6 (0%)

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	291[A]	TRP	5.3
2	B	453	LEU	5.0
2	B	500	ASP	4.8
2	B	486	SER	4.8
2	B	498	ARG	4.8
2	B	416	ALA	4.7
2	B	441	ILE	4.6
2	B	462	LEU	4.5
2	B	482	ALA	4.3
2	B	480	ALA	4.3
2	B	499	LEU	4.1
2	B	485	LEU	4.0
2	B	421	ALA	3.9
2	B	478	ILE	3.8
2	B	43	LYS	3.6
2	B	497	ALA	3.6
2	B	467	TYR	3.5
2	B	505	LEU	3.5
2	B	479	ALA	3.5
2	B	465	PHE	3.4
2	B	363	ALA	3.4
2	B	41	ASP	3.4
2	B	489	PRO	3.3
2	B	455	GLY	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	492	ASP	3.3
2	B	460	GLN	3.2
2	B	513	ALA	3.2
2	B	494	ALA	3.1
2	B	516	VAL	3.1
2	B	474	LYS	3.1
2	B	425	ALA	3.1
2	B	457	TYR	3.0
2	B	515	SER	3.0
2	B	509	GLU	3.0
2	B	491	PHE	2.9
2	B	493	PHE	2.9
2	B	75	ARG	2.9
2	B	42	GLU	2.9
2	B	483	LEU	2.8
1	A	363	ALA	2.8
2	B	487	ALA	2.8
2	B	502	GLU	2.8
2	B	463	LEU	2.7
2	B	484	TYR	2.7
2	B	452	ALA	2.6
2	B	510	ILE	2.6
2	B	44	GLY	2.6
2	B	426	PHE	2.6
2	B	47	GLU	2.5
2	B	511	ALA	2.4
1	A	15	GLU	2.4
2	B	481	TYR	2.3
2	B	488	SER	2.3
2	B	490	HIS	2.3
2	B	454	GLN	2.3
2	B	517	ASN	2.3
2	B	430	LEU	2.2
2	B	419	ASP	2.2
2	B	16	GLU	2.2
2	B	519	ALA	2.2
2	B	518	THR	2.2
2	B	501	LEU	2.2
2	B	451	ALA	2.2
2	B	503	ARG	2.1
2	B	422	LYS	2.1
2	B	508	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	458	GLU	2.1
2	B	24	ASP	2.1
2	B	445	VAL	2.1
1	A	40	ASN	2.1
2	B	514	ILE	2.1

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	0.77	0.17	40,56,66,71	0
2	MLY	B	151	11/12	0.83	0.14	34,42,58,65	0
1	MLY	A	397	11/12	0.87	0.19	24,42,77,78	0
1	MLZ	A	306	10/11	0.88	0.12	29,37,43,44	0
2	MLY	B	161	11/12	0.89	0.14	32,40,64,64	0
2	MLY	B	378	11/12	0.89	0.17	42,48,70,71	0
2	MLY	B	403	11/12	0.90	0.13	34,45,68,73	0
2	MLY	B	306	11/12	0.91	0.13	18,31,60,62	0
2	MLY	B	263	11/12	0.91	0.15	16,28,56,63	0
1	MLY	A	403	11/12	0.92	0.10	30,33,48,56	0
2	MLY	B	234	11/12	0.94	0.09	18,27,37,47	0
1	MLY	A	151	11/12	0.94	0.10	11,20,33,41	0
1	MLY	A	422	11/12	0.95	0.09	20,30,32,35	0
2	MLY	B	90	11/12	0.95	0.09	21,29,39,45	0
1	MLY	A	57	11/12	0.95	0.09	21,33,49,50	0
1	MLZ	A	269	10/11	0.95	0.09	21,28,40,44	0
1	MLY	A	270	11/12	0.95	0.09	20,33,46,48	0
1	MLY	A	98	11/12	0.96	0.10	16,25,46,48	0
1	MLZ	A	27	10/11	0.96	0.07	14,25,35,36	0
1	MLY	A	161	11/12	0.96	0.09	9,21,46,46	0
1	MLZ	A	198	10/11	0.97	0.07	10,20,30,32	0
1	MLZ	A	162	10/11	0.97	0.07	14,20,31,40	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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
4	EDO	B	606	4/4	0.48	0.33	105,109,114,115	0
4	EDO	A	607	4/4	0.60	0.26	60,63,64,64	0
4	EDO	B	605	4/4	0.74	0.19	59,62,64,66	0
4	EDO	A	605	4/4	0.75	0.26	59,67,77,87	0
6	PEG	B	607	7/7	0.75	0.28	65,73,89,95	0
4	EDO	B	603	4/4	0.77	0.20	44,46,47,49	0
5	PGE	A	608	10/10	0.78	0.25	34,69,86,89	0
4	EDO	A	602	4/4	0.82	0.19	40,46,47,60	0
3	SO4	B	601	5/5	0.83	0.14	84,87,97,97	0
4	EDO	A	606	4/4	0.85	0.14	42,44,50,54	0
4	EDO	B	604	4/4	0.85	0.16	47,48,54,57	0
4	EDO	A	604	4/4	0.86	0.15	50,55,55,57	0
4	EDO	B	602	4/4	0.86	0.12	29,36,47,48	0
3	SO4	A	601	5/5	0.88	0.10	74,81,85,89	0
4	EDO	A	603	4/4	0.91	0.16	45,52,58,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.