



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 14, 2024 – 07:40 am GMT

PDB ID : 6YQ6
Title : Promiscuous Reductase LugOII Catalyzes Keto-reduction at C1 during Lugdunomycin Biosynthesis
Authors : Xiao, X.; Elsayed, S.S.; Wu, C.; van der Heul, H.; Protá, A.; Huang, J.; Guo, R.; Abrahams, J.P.; van Wezel, G.P.
Deposited on : 2020-04-16
Resolution : 2.08 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 ⓘ 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

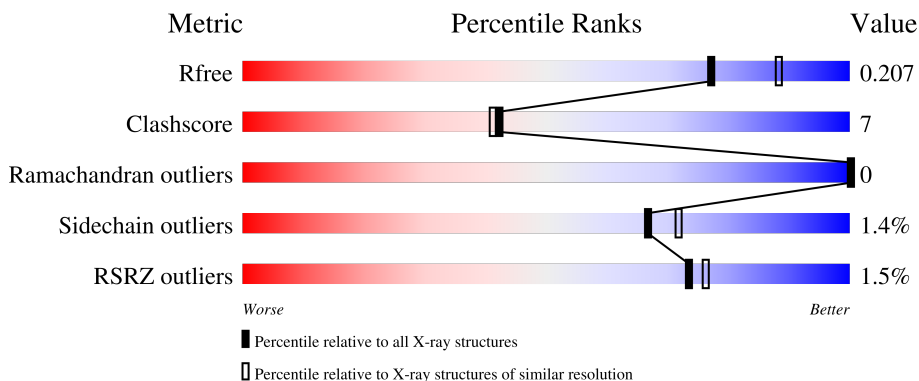
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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	AAA	255	
1	BBB	255	

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	AAA	404	-	-	X	-
3	PEG	AAA	405	-	-	X	-
3	PEG	BBB	501	-	-	X	-

2 Entry composition [i](#)

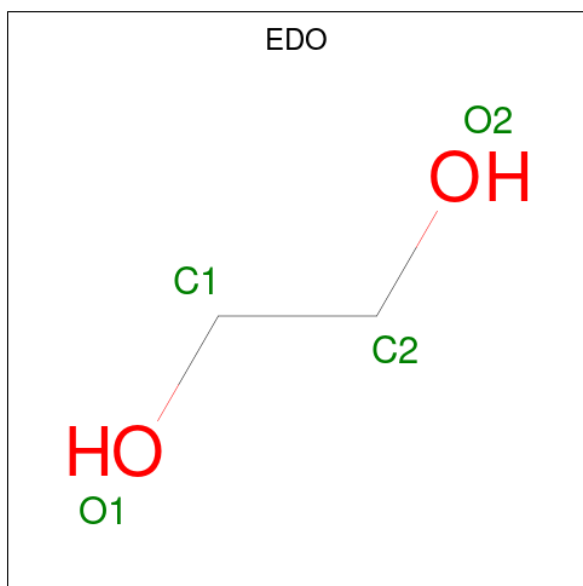
There are 5 unique types of molecules in this entry. The entry contains 4027 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	231	Total 1731	C 1077	N 316	O 332	S 6	0	4	0
1	BBB	244	Total 1825	C 1138	N 327	O 353	S 7	0	4	0

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



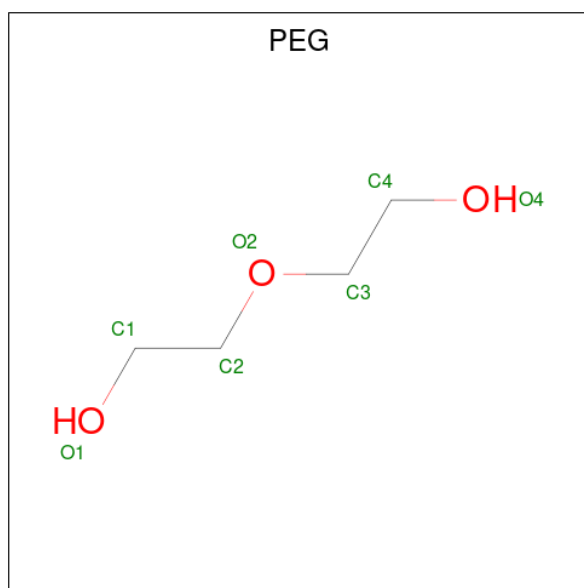
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	AAA	1	Total 4	C 2	O 2	0	0
2	AAA	1	Total 4	C 2	O 2	0	0
2	AAA	1	Total 4	C 2	O 2	0	0
2	AAA	1	Total 4	C 2	O 2	0	0

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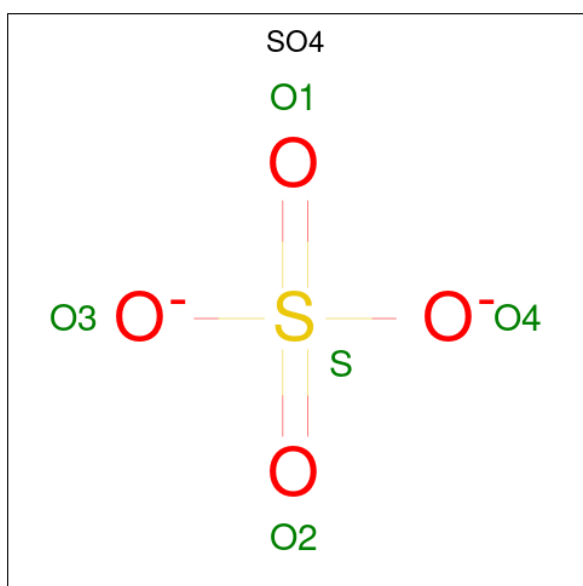
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	BBB	1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

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total O S 5 4 1	0	0
4	BBB	1	Total O S 5 4 1	0	0
4	BBB	1	Total O S 5 4 1	0	0


- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	194	Total O 194 194	0	0
5	BBB	170	Total O 170 170	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.

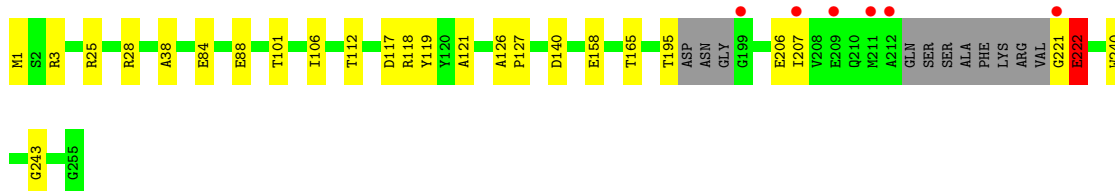
- Molecule 1: Monooxygenase

Chain AAA: 



- Molecule 1: Monooxygenase

Chain BBB: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	185.99Å 185.99Å 75.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.47 – 2.08 47.43 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.47-2.08) 99.9 (47.43-2.08)	Depositor EDS
R_{merge}	0.40	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.08Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.168 , 0.203 0.177 , 0.207	Depositor DCC
R_{free} test set	2313 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtrriage
Anisotropy	0.058	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4027	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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, SO4, 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	AAA	0.97	6/1764 (0.3%)	0.98	4/2389 (0.2%)
1	BBB	0.91	3/1859 (0.2%)	0.95	3/2518 (0.1%)
All	All	0.94	9/3623 (0.2%)	0.96	7/4907 (0.1%)

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	158	GLU	CD-OE1	11.09	1.37	1.25
1	BBB	88	GLU	CD-OE2	7.95	1.34	1.25
1	BBB	84	GLU	CD-OE2	6.90	1.33	1.25
1	BBB	88	GLU	CD-OE1	6.48	1.32	1.25
1	AAA	222	GLU	CD-OE1	5.98	1.32	1.25

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	118[A]	ARG	NE-CZ-NH1	-7.50	116.55	120.30
1	BBB	118[B]	ARG	NE-CZ-NH1	-7.50	116.55	120.30
1	AAA	53	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	AAA	118[A]	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	AAA	118[B]	ARG	NE-CZ-NH2	-5.53	117.53	120.30

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	AAA	1731	0	1760	32	0
1	BBB	1825	0	1846	23	0
2	AAA	40	0	60	5	0
2	BBB	24	0	36	7	0
3	AAA	14	0	20	16	0
3	BBB	14	0	20	4	0
4	AAA	5	0	0	1	0
4	BBB	10	0	0	0	0
5	AAA	194	0	0	0	0
5	BBB	170	0	0	2	0
All	All	4027	0	3742	51	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 7.

The worst 5 of 51 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:BBB:112:THR:HA	2:BBB:507:EDO:H12	1.46	0.96
1:AAA:65:LEU:HB2	3:AAA:405:PEG:H42	1.59	0.84
1:BBB:117:ASP:HB3	2:BBB:505:EDO:H12	1.58	0.82
1:AAA:20:ARG:HG2	3:AAA:404:PEG:H32	1.64	0.77
1:BBB:25:ARG:HH12	3:BBB:501:PEG:C2	2.02	0.72

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	AAA	231/255 (91%)	225 (97%)	6 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BBB	242/255 (95%)	237 (98%)	5 (2%)	0	100	100
All	All	473/510 (93%)	462 (98%)	11 (2%)	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	AAA	177/192 (92%)	174 (98%)	3 (2%)	60	65
1	BBB	187/192 (97%)	184 (98%)	3 (2%)	62	67
All	All	364/384 (95%)	358 (98%)	6 (2%)	67	67

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	106	ILE
1	BBB	222	GLU
1	BBB	240	TRP
1	AAA	120[B]	TYR
1	AAA	120[A]	TYR

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](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

23 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	$\# Z > 2$
2	EDO	AAA	407	-	3,3,3	0.09	0	2,2,2	0.15	0
2	EDO	BBB	507	-	3,3,3	0.43	0	2,2,2	0.64	0
2	EDO	BBB	502	-	3,3,3	0.38	0	2,2,2	0.23	0
3	PEG	AAA	404	-	6,6,6	0.93	0	5,5,5	0.76	0
2	EDO	AAA	403	-	3,3,3	0.38	0	2,2,2	0.37	0
4	SO4	BBB	510	-	4,4,4	0.36	0	6,6,6	0.10	0
3	PEG	BBB	506	-	6,6,6	0.66	0	5,5,5	0.67	0
4	SO4	BBB	509	-	4,4,4	0.37	0	6,6,6	0.29	0
2	EDO	AAA	411	-	3,3,3	0.41	0	2,2,2	0.62	0
2	EDO	BBB	503	-	3,3,3	0.47	0	2,2,2	0.70	0
2	EDO	AAA	412	-	3,3,3	0.63	0	2,2,2	0.93	0
2	EDO	BBB	508	-	3,3,3	0.73	0	2,2,2	0.83	0
3	PEG	AAA	405	-	6,6,6	0.43	0	5,5,5	0.30	0
4	SO4	AAA	413	-	4,4,4	0.41	0	6,6,6	0.51	0
2	EDO	BBB	505	-	3,3,3	0.30	0	2,2,2	1.01	0
2	EDO	AAA	410	-	3,3,3	0.26	0	2,2,2	0.14	0
2	EDO	BBB	504	-	3,3,3	0.30	0	2,2,2	0.11	0
2	EDO	AAA	401	-	3,3,3	0.56	0	2,2,2	0.24	0
2	EDO	AAA	409	-	3,3,3	0.37	0	2,2,2	0.51	0
2	EDO	AAA	402	-	3,3,3	0.36	0	2,2,2	0.37	0
2	EDO	AAA	408	-	3,3,3	0.48	0	2,2,2	0.53	0
2	EDO	AAA	406	-	3,3,3	0.16	0	2,2,2	0.14	0
3	PEG	BBB	501	-	6,6,6	0.66	0	5,5,5	0.47	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	EDO	AAA	407	-	-	1/1/1/1	-
2	EDO	BBB	507	-	-	0/1/1/1	-
2	EDO	BBB	502	-	-	1/1/1/1	-
3	PEG	AAA	404	-	-	1/4/4/4	-
2	EDO	AAA	403	-	-	1/1/1/1	-
3	PEG	BBB	506	-	-	3/4/4/4	-
2	EDO	AAA	411	-	-	0/1/1/1	-
2	EDO	BBB	503	-	-	1/1/1/1	-
2	EDO	AAA	412	-	-	0/1/1/1	-
2	EDO	BBB	508	-	-	1/1/1/1	-
3	PEG	AAA	405	-	-	1/4/4/4	-
2	EDO	BBB	505	-	-	1/1/1/1	-
2	EDO	AAA	410	-	-	1/1/1/1	-
2	EDO	BBB	504	-	-	1/1/1/1	-
2	EDO	AAA	401	-	-	1/1/1/1	-
2	EDO	AAA	409	-	-	0/1/1/1	-
2	EDO	AAA	402	-	-	0/1/1/1	-
2	EDO	AAA	408	-	-	1/1/1/1	-
2	EDO	AAA	406	-	-	1/1/1/1	-
3	PEG	BBB	501	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	BBB	506	PEG	C1-C2-O2-C3
2	AAA	403	EDO	O1-C1-C2-O2
3	BBB	506	PEG	O1-C1-C2-O2
2	BBB	503	EDO	O1-C1-C2-O2
2	BBB	508	EDO	O1-C1-C2-O2

There are no ring outliers.

10 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BBB	507	EDO	1	0
2	BBB	502	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	404	PEG	10	0
2	BBB	503	EDO	2	0
2	AAA	412	EDO	2	0
3	AAA	405	PEG	6	0
4	AAA	413	SO4	1	0
2	BBB	505	EDO	3	0
2	AAA	410	EDO	3	0
3	BBB	501	PEG	4	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	AAA	231/255 (90%)	-0.65	1 (0%) 92 93	18, 24, 43, 78	0
1	BBB	244/255 (95%)	-0.49	6 (2%) 57 62	18, 26, 57, 81	0
All	All	475/510 (93%)	-0.57	7 (1%) 73 76	18, 25, 53, 81	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	211	MET	4.3
1	AAA	103	VAL	3.6
1	BBB	221	GLY	2.9
1	BBB	212	ALA	2.7
1	BBB	209	GLU	2.7

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(\AA^2)	Q<0.9
2	EDO	BBB	508	4/4	0.64	0.20	60,60,62,64	0
2	EDO	BBB	503	4/4	0.68	0.16	51,58,59,60	0
2	EDO	AAA	409	4/4	0.71	0.20	57,58,58,59	0
2	EDO	BBB	505	4/4	0.76	0.22	47,53,54,62	0
2	EDO	AAA	403	4/4	0.76	0.14	64,66,67,67	0
2	EDO	AAA	408	4/4	0.78	0.14	60,62,62,64	0
3	PEG	BBB	501	7/7	0.80	0.14	47,49,54,58	0
3	PEG	AAA	404	7/7	0.81	0.33	31,37,49,51	0
3	PEG	BBB	506	7/7	0.81	0.18	51,52,61,64	0
2	EDO	BBB	507	4/4	0.82	0.16	46,50,52,52	0
2	EDO	AAA	406	4/4	0.83	0.12	58,59,63,63	0
2	EDO	AAA	407	4/4	0.86	0.19	48,50,53,57	0
4	SO4	BBB	510	5/5	0.88	0.48	92,93,104,116	0
3	PEG	AAA	405	7/7	0.89	0.17	55,58,61,67	0
2	EDO	BBB	502	4/4	0.89	0.11	50,51,51,55	0
2	EDO	AAA	411	4/4	0.91	0.26	56,57,58,60	0
2	EDO	AAA	412	4/4	0.92	0.17	35,38,41,42	0
4	SO4	AAA	413	5/5	0.93	0.17	32,47,58,60	0
2	EDO	BBB	504	4/4	0.95	0.15	42,45,47,49	0
2	EDO	AAA	401	4/4	0.95	0.13	29,30,33,34	0
2	EDO	AAA	402	4/4	0.97	0.14	31,34,36,37	0
2	EDO	AAA	410	4/4	0.97	0.51	49,53,56,59	0
4	SO4	BBB	509	5/5	0.99	0.05	33,36,41,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.