



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 04:37 AM UTC

PDB ID : 8ORK / pdb_00008ork
Title : cyclic 2,3-diphosphoglycerate synthetase from the hyperthermophilic archaeon
Methanothermus fervidus
Authors : De Rose, S.A.; Isupov, M.
Deposited on : 2023-04-14
Resolution : 1.64 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	:	4-5-2 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

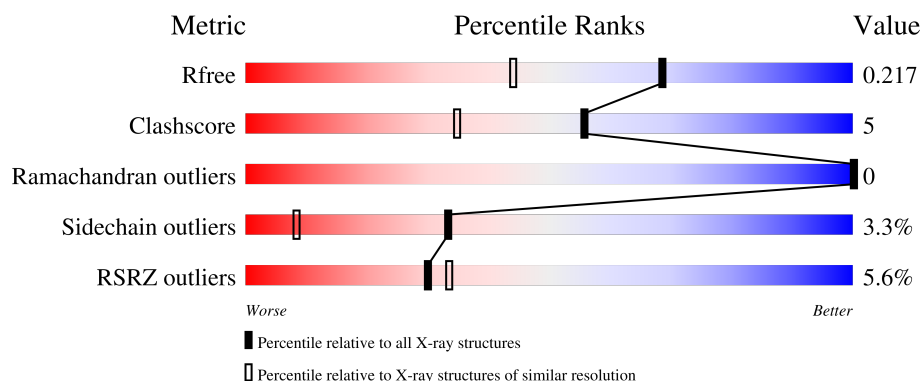
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.64 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	1141 (1.64-1.64)
Clashscore	190562	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)
RSRZ outliers	180081	1141 (1.64-1.64)

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	460	5% 89% 10%

2 Entry composition [i](#)

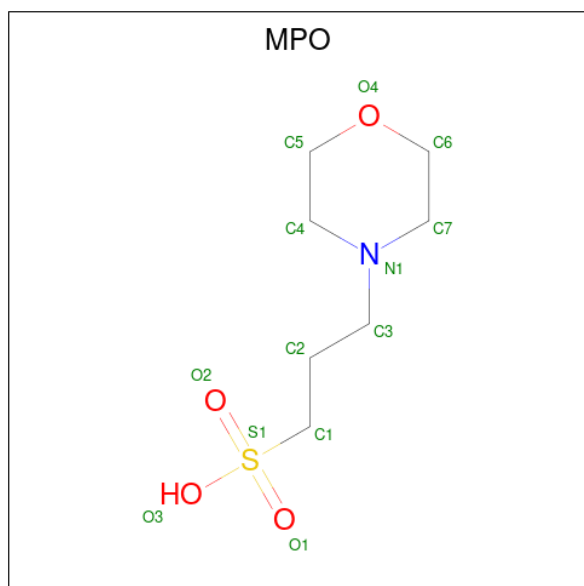
There are 7 unique types of molecules in this entry. The entry contains 8415 atoms, of which 4183 are hydrogens and 0 are deuteriums.

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 Cyclic 2,3-diphosphoglycerate synthetase.

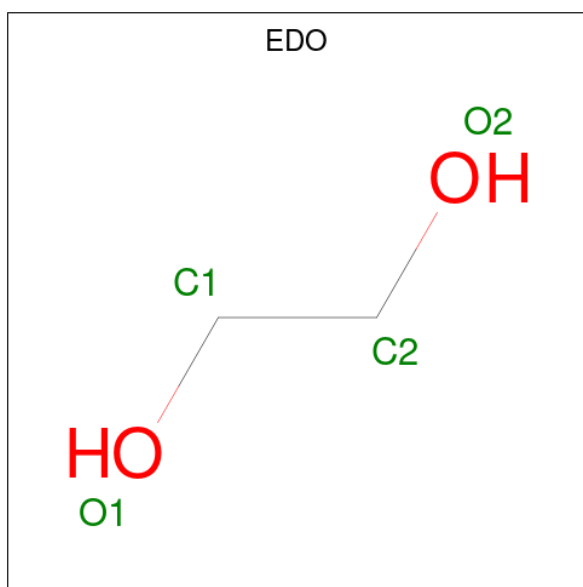
Mol	Chain	Residues	Atoms								ZeroOcc	AltConf	Trace
1	AAA	460	Total	C	H	N	O	S	Se		78	45	0
			7824	2464	4008	625	700	10	17				

- Molecule 2 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (CCD ID: MPO) (formula: $C_7H_{15}NO_4S$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	AAA	1	Total	C	H	N	O	S		1	0
			28	7	15	1	4	1			

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



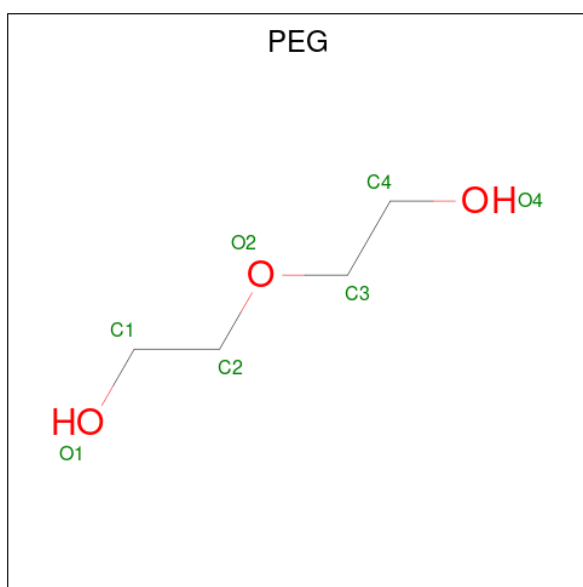
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
3	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
3	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
3	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
3	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
3	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
3	AAA	1	Total	C	H	O	1	0
			10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

Continued on next page...

Continued from previous page...

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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	1	Total	Na	0	0
			1	1		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	1	Total	Cl	0	0
			1	1		

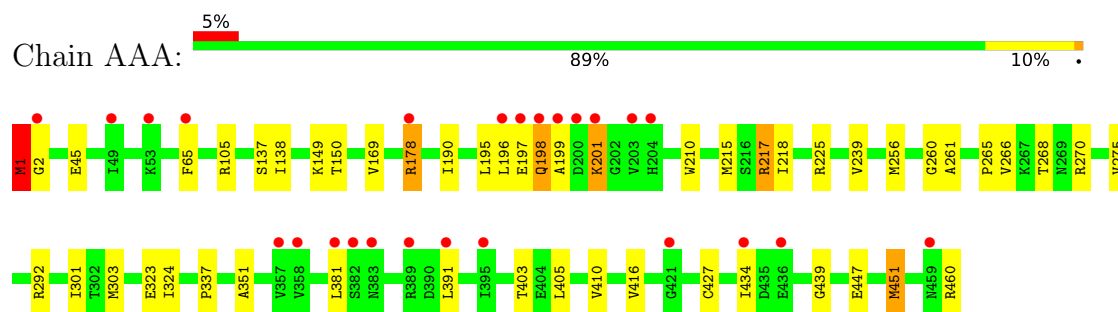
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AAA	294	Total	O	0	0
			294	294		

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: Cyclic 2,3-diphosphoglycerate synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	74.26Å 105.61Å 156.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.71 – 1.64 42.71 – 1.64	Depositor EDS
% Data completeness (in resolution range)	96.0 (42.71-1.64) 96.0 (42.71-1.64)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 1.64Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.177 , 0.213 0.180 , 0.217	Depositor DCC
R_{free} test set	3734 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	28.0	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8415	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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: CL, NA, EDO, MPO, PEG

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	1.01	0/3991	1.24	3/5361 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	451	MSE	CG-SE-CE	7.08	114.50	98.92
1	AAA	65	PHE	CA-CB-CG	5.30	119.10	113.80
1	AAA	1	MSE	CG-SE-CE	5.04	110.01	98.92

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	3816	4008	4049	37	0
2	AAA	13	15	15	0	0
3	AAA	100	150	150	2	0
4	AAA	7	10	10	1	0
5	AAA	1	0	0	0	0
6	AAA	1	0	0	0	0
7	AAA	294	0	0	2	0
All	All	4232	4183	4224	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 5.

The worst 5 of 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:AAA:169:VAL:HG23	1:AAA:218:ILE:HD11	1.69	0.74
1:AAA:1:MSE:H1	1:AAA:1:MSE:SE	2.27	0.68
1:AAA:337:PRO:HB2	1:AAA:427[A]:CYS:SG	2.36	0.66
1:AAA:197:GLU:OE1	1:AAA:197:GLU:N	2.29	0.65
1:AAA:256[B]:MSE:HG3	1:AAA:268:THR:HG21	1.80	0.62

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	503/460 (109%)	494 (98%)	9 (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	436/380 (115%)	419 (96%)	17 (4%)	28	5

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	416	VAL
1	AAA	460	ARG
1	AAA	201[B]	LYS
1	AAA	217	ARG
1	AAA	225	ARG

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 2 are monoatomic - leaving 27 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	EDO	AAA	503	-	3,3,3	0.23	0	2,2,2	0.30	0
3	EDO	AAA	508	-	3,3,3	0.16	0	2,2,2	0.12	0
3	EDO	AAA	514	-	3,3,3	0.07	0	2,2,2	0.10	0
3	EDO	AAA	520	-	3,3,3	0.22	0	2,2,2	0.15	0
3	EDO	AAA	518	-	3,3,3	0.20	0	2,2,2	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	AAA	505	-	3,3,3	0.22	0	2,2,2	0.25	0
3	EDO	AAA	521	-	3,3,3	0.05	0	2,2,2	0.04	0
3	EDO	AAA	525	-	3,3,3	0.21	0	2,2,2	0.16	0
3	EDO	AAA	526	-	3,3,3	0.07	0	2,2,2	0.19	0
3	EDO	AAA	513	-	3,3,3	0.27	0	2,2,2	0.11	0
3	EDO	AAA	512	-	3,3,3	0.05	0	2,2,2	0.13	0
3	EDO	AAA	504	-	3,3,3	0.26	0	2,2,2	0.21	0
2	MPO	AAA	501	-	13,13,13	0.59	0	17,17,17	1.25	2 (11%)
3	EDO	AAA	510	-	3,3,3	0.06	0	2,2,2	0.25	0
3	EDO	AAA	519	-	3,3,3	0.15	0	2,2,2	0.08	0
3	EDO	AAA	509	-	3,3,3	0.28	0	2,2,2	0.27	0
3	EDO	AAA	507	-	3,3,3	0.13	0	2,2,2	0.21	0
3	EDO	AAA	502	-	3,3,3	0.09	0	2,2,2	0.08	0
3	EDO	AAA	516	-	3,3,3	0.19	0	2,2,2	0.30	0
3	EDO	AAA	506	-	3,3,3	0.13	0	2,2,2	0.02	0
3	EDO	AAA	522	-	3,3,3	0.09	0	2,2,2	0.07	0
3	EDO	AAA	517	-	3,3,3	0.37	0	2,2,2	0.22	0
4	PEG	AAA	527	-	6,6,6	0.31	0	5,5,5	0.16	0
3	EDO	AAA	523	-	3,3,3	0.16	0	2,2,2	0.15	0
3	EDO	AAA	524	-	3,3,3	0.07	0	2,2,2	0.16	0
3	EDO	AAA	515	-	3,3,3	0.07	0	2,2,2	0.08	0
3	EDO	AAA	511	-	3,3,3	0.10	0	2,2,2	0.17	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	EDO	AAA	503	-	-	1/1/1/1	-
3	EDO	AAA	508	-	-	0/1/1/1	-
3	EDO	AAA	514	-	-	1/1/1/1	-
3	EDO	AAA	520	-	-	1/1/1/1	-
3	EDO	AAA	518	-	-	1/1/1/1	-
3	EDO	AAA	505	-	-	1/1/1/1	-
3	EDO	AAA	521	-	-	1/1/1/1	-
3	EDO	AAA	525	-	-	0/1/1/1	-
3	EDO	AAA	526	-	-	1/1/1/1	-
3	EDO	AAA	513	-	-	1/1/1/1	-
3	EDO	AAA	512	-	-	0/1/1/1	-
3	EDO	AAA	504	-	-	1/1/1/1	-
2	MPO	AAA	501	-	-	0/7/15/15	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	AAA	510	-	-	1/1/1/1	-
3	EDO	AAA	519	-	-	1/1/1/1	-
3	EDO	AAA	509	-	-	0/1/1/1	-
3	EDO	AAA	507	-	-	1/1/1/1	-
3	EDO	AAA	502	-	-	0/1/1/1	-
3	EDO	AAA	516	-	-	1/1/1/1	-
3	EDO	AAA	506	-	-	1/1/1/1	-
3	EDO	AAA	522	-	-	1/1/1/1	-
3	EDO	AAA	517	-	-	1/1/1/1	-
4	PEG	AAA	527	-	-	1/4/4/4	-
3	EDO	AAA	523	-	-	0/1/1/1	-
3	EDO	AAA	524	-	-	0/1/1/1	-
3	EDO	AAA	515	-	-	1/1/1/1	-
3	EDO	AAA	511	-	-	1/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	501	MPO	O2-S1-O1	3.47	125.10	113.82
2	AAA	501	MPO	O3-S1-O1	-3.27	103.23	111.40

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	510	EDO	O1-C1-C2-O2
3	AAA	511	EDO	O1-C1-C2-O2
3	AAA	518	EDO	O1-C1-C2-O2
3	AAA	519	EDO	O1-C1-C2-O2
3	AAA	526	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	503	EDO	1	0
3	AAA	521	EDO	1	0
3	AAA	525	EDO	1	0
4	AAA	527	PEG	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	AAA	448/460 (97%)	0.01	25 (5%) 30 33	12, 30, 66, 104	40 (8%)

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	196	LEU	5.1
1	AAA	65	PHE	4.4
1	AAA	436[A]	GLU	4.2
1	AAA	381	LEU	3.6
1	AAA	2	GLY	3.5

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 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
3	EDO	AAA	504	4/4	0.78	0.37	38,53,74,80	10
3	EDO	AAA	519	4/4	0.78	0.33	53,55,63,63	10

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	AAA	525	4/4	0.79	0.26	46,54,59,66	10
3	EDO	AAA	517	4/4	0.80	0.19	47,50,66,71	10
3	EDO	AAA	523	4/4	0.81	0.25	37,54,57,57	10
3	EDO	AAA	511	4/4	0.82	0.21	39,48,64,73	10
3	EDO	AAA	507	4/4	0.83	0.21	46,59,61,67	10
3	EDO	AAA	514	4/4	0.85	0.20	48,56,59,60	10
3	EDO	AAA	522	4/4	0.85	0.21	49,54,63,64	10
3	EDO	AAA	520	4/4	0.86	0.20	32,48,61,62	10
3	EDO	AAA	509	4/4	0.86	0.20	39,54,70,73	1
3	EDO	AAA	508	4/4	0.87	0.15	54,60,63,67	1
3	EDO	AAA	524	4/4	0.87	0.23	49,54,60,60	10
3	EDO	AAA	515	4/4	0.87	0.17	48,55,71,71	10
3	EDO	AAA	526	4/4	0.87	0.25	42,45,59,60	10
4	PEG	AAA	527	7/7	0.87	0.21	35,49,81,87	17
3	EDO	AAA	516	4/4	0.88	0.17	31,42,62,62	10
3	EDO	AAA	521	4/4	0.88	0.18	32,44,68,72	10
3	EDO	AAA	506	4/4	0.88	0.21	30,46,63,65	10
3	EDO	AAA	513	4/4	0.88	0.14	43,49,61,63	1
3	EDO	AAA	510	4/4	0.90	0.21	38,49,55,56	10
3	EDO	AAA	505	4/4	0.90	0.13	48,51,53,57	1
3	EDO	AAA	503	4/4	0.91	0.12	27,43,54,64	1
3	EDO	AAA	518	4/4	0.92	0.11	27,40,44,49	10
3	EDO	AAA	512	4/4	0.93	0.13	52,57,68,68	10
3	EDO	AAA	502	4/4	0.93	0.12	46,54,62,65	10
6	CL	AAA	529	1/1	0.95	0.12	47,47,47,47	0
2	MPO	AAA	501	13/13	0.98	0.06	24,40,49,54	1
5	NA	AAA	528	1/1	1.00	0.03	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.