



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 19, 2022 – 10:06 am BST

PDB ID : 7P7I
Title : Native structure of N-acetylglucosamine kinase from Plesiomonas shigelloides
Authors : Roy, S.; Isupov, M.N.; Harmer, N.J.; Ames, J.R.
Deposited on : 2021-07-19
Resolution : 1.70 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 : 2.29
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.29

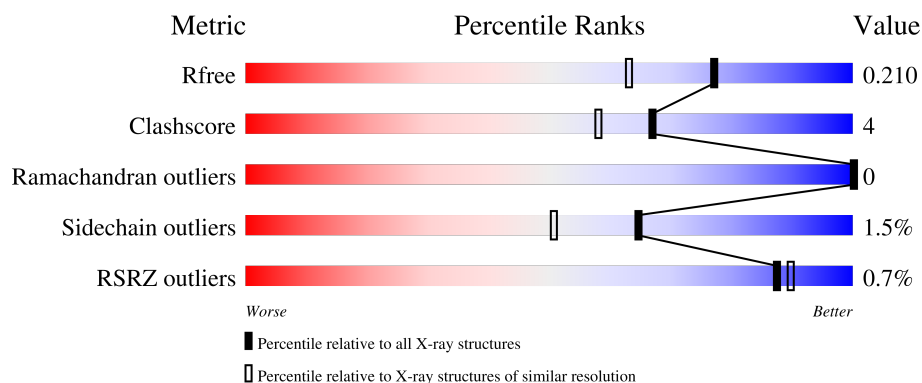
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	417	
1	BBB	417	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5488 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 Ubiquitin-like protein SMT3,N-acetyl-D-glucosamine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	304	Total	C	N	O	S	0	24	0
			2452	1575	422	442	13			
1	BBB	305	Total	C	N	O	S	0	21	0
			2439	1562	421	444	12			

There are 40 discrepancies between the modelled and reference sequences:

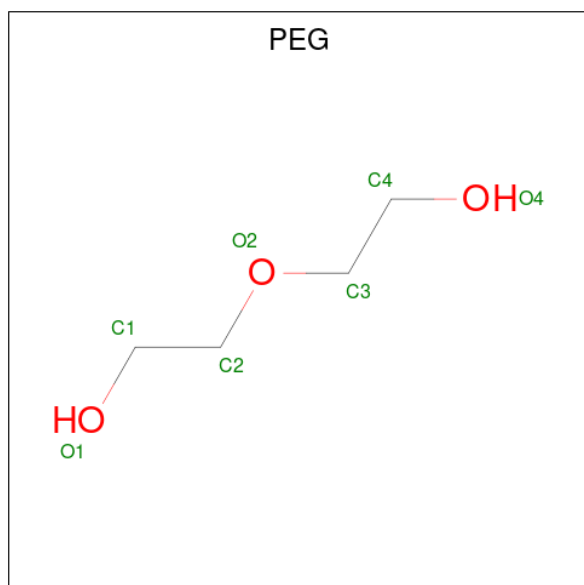
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-114	MET	-	initiating methionine	UNP Q12306
AAA	-113	ALA	-	expression tag	UNP Q12306
AAA	-112	HIS	-	expression tag	UNP Q12306
AAA	-111	HIS	-	expression tag	UNP Q12306
AAA	-110	HIS	-	expression tag	UNP Q12306
AAA	-109	HIS	-	expression tag	UNP Q12306
AAA	-108	HIS	-	expression tag	UNP Q12306
AAA	-107	HIS	-	expression tag	UNP Q12306
AAA	-106	GLY	-	expression tag	UNP Q12306
AAA	-10	SER	-	linker	UNP Q12306
AAA	-9	SER	-	linker	UNP Q12306
AAA	-8	GLY	-	linker	UNP Q12306
AAA	-7	LEU	-	linker	UNP Q12306
AAA	-6	GLU	-	linker	UNP Q12306
AAA	-5	VAL	-	linker	UNP Q12306
AAA	-4	LEU	-	linker	UNP Q12306
AAA	-3	PHE	-	linker	UNP Q12306
AAA	-2	GLN	-	linker	UNP Q12306
AAA	-1	GLY	-	linker	UNP Q12306
AAA	0	THR	-	linker	UNP Q12306
BBB	-114	MET	-	initiating methionine	UNP Q12306
BBB	-113	ALA	-	expression tag	UNP Q12306
BBB	-112	HIS	-	expression tag	UNP Q12306
BBB	-111	HIS	-	expression tag	UNP Q12306
BBB	-110	HIS	-	expression tag	UNP Q12306

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-109	HIS	-	expression tag	UNP Q12306
BBB	-108	HIS	-	expression tag	UNP Q12306
BBB	-107	HIS	-	expression tag	UNP Q12306
BBB	-106	GLY	-	expression tag	UNP Q12306
BBB	-10	SER	-	linker	UNP Q12306
BBB	-9	SER	-	linker	UNP Q12306
BBB	-8	GLY	-	linker	UNP Q12306
BBB	-7	LEU	-	linker	UNP Q12306
BBB	-6	GLU	-	linker	UNP Q12306
BBB	-5	VAL	-	linker	UNP Q12306
BBB	-4	LEU	-	linker	UNP Q12306
BBB	-3	PHE	-	linker	UNP Q12306
BBB	-2	GLN	-	linker	UNP Q12306
BBB	-1	GLY	-	linker	UNP Q12306
BBB	0	THR	-	linker	UNP Q12306

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code:

TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

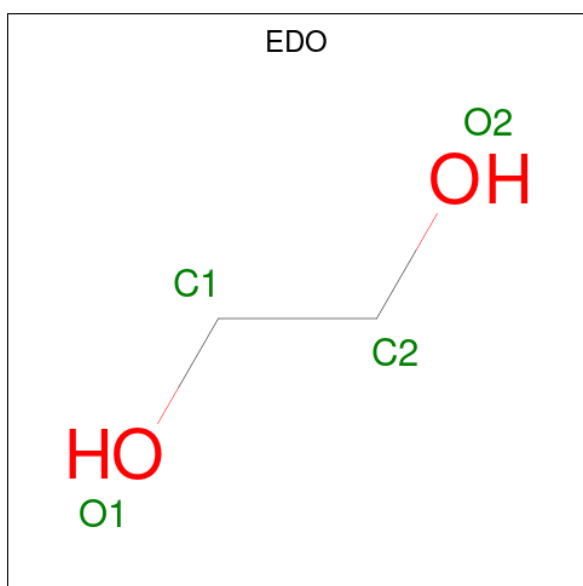
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	1	Total	Zn	0	0
			1	1		
4	BBB	1	Total	Zn	0	0
			1	1		

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



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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

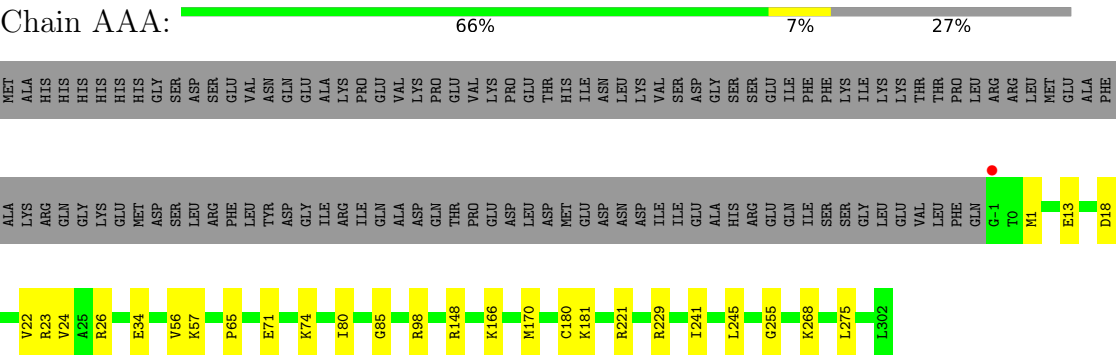
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	AAA	251	Total	O	0	0
			251	251		
8	BBB	262	Total	O	0	0
			262	262		

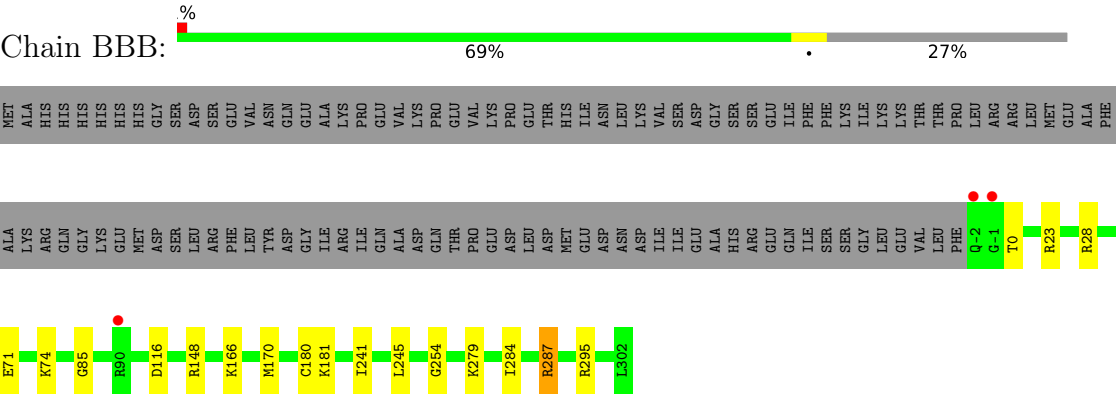
3 Residue-property plots

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: Ubiquitin-like protein SMT3,N-acetyl-D-glucosamine kinase



- Molecule 1: Ubiquitin-like protein SMT3,N-acetyl-D-glucosamine kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	95.23Å 95.23Å 180.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	60.89 – 1.70 75.02 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (60.89-1.70) 99.5 (75.02-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0267, BUSTER	Depositor
R, R_{free}	0.183 , 0.210 0.183 , 0.210	Depositor DCC
R_{free} test set	5218 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5488	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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: CL, TRS, EDO, PGE, ZN, 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	0.47	0/2571	0.79	2/3472 (0.1%)
1	BBB	0.45	0/2549	0.78	4/3442 (0.1%)
All	All	0.46	0/5120	0.79	6/6914 (0.1%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	229	ARG	NE-CZ-NH2	6.51	123.56	120.30
1	BBB	23	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	AAA	229	ARG	NE-CZ-NH1	-6.09	117.25	120.30
1	BBB	287[A]	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	BBB	287[B]	ARG	NE-CZ-NH2	-5.67	117.47	120.30

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	AAA	2452	0	2530	25	0
1	BBB	2439	0	2500	13	0
2	AAA	14	0	20	0	0
2	BBB	7	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	AAA	8	0	12	4	0
4	AAA	1	0	0	0	0
4	BBB	1	0	0	0	0
5	AAA	10	0	14	0	0
5	BBB	10	0	14	1	0
6	AAA	16	0	24	4	0
6	BBB	16	0	24	5	0
7	AAA	1	0	0	0	0
8	AAA	251	0	0	1	0
8	BBB	262	0	0	3	0
All	All	5488	0	5148	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 4.

The worst 5 of 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:AAA:23[A]:ARG:HD3	1:AAA:26:ARG:HG2	1.52	0.90
1:AAA:26:ARG:HH21	6:AAA:407:EDO:H21	1.45	0.82
6:BBB:404:EDO:H11	8:BBB:661:HOH:O	1.94	0.67
1:AAA:1[B]:MET:HE2	1:AAA:24:VAL:CG2	2.24	0.66
1:AAA:13:GLU:OE2	6:AAA:407:EDO:H22	2.00	0.61

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	326/417 (78%)	318 (98%)	8 (2%)	0	100	100
1	BBB	324/417 (78%)	316 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	650/834 (78%)	634 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	262/340 (77%)	257 (98%)	5 (2%)	57	41
1	BBB	260/340 (76%)	256 (98%)	4 (2%)	65	51
All	All	522/680 (77%)	513 (98%)	9 (2%)	65	46

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	71	GLU
1	BBB	148	ARG
1	AAA	221[A]	ARG
1	AAA	221[B]	ARG
1	BBB	0	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 3 are monoatomic - leaving 14 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	$\# Z > 2$
6	EDO	AAA	407	-	3,3,3	0.07	0	2,2,2	0.32	0
6	EDO	BBB	404	-	3,3,3	0.21	0	2,2,2	0.58	0
6	EDO	AAA	409	-	3,3,3	0.01	0	2,2,2	0.29	0
2	PEG	BBB	401	-	6,6,6	0.19	0	5,5,5	0.13	0
6	EDO	AAA	406	-	3,3,3	0.35	0	2,2,2	0.22	0
2	PEG	AAA	401	-	6,6,6	0.14	0	5,5,5	0.13	0
5	PGE	BBB	403	-	9,9,9	0.26	0	8,8,8	0.18	0
5	PGE	AAA	405	-	9,9,9	0.20	0	8,8,8	0.15	0
6	EDO	AAA	408	-	3,3,3	0.53	0	2,2,2	0.71	0
6	EDO	BBB	405	-	3,3,3	0.19	0	2,2,2	0.22	0
6	EDO	BBB	407	-	3,3,3	0.07	0	2,2,2	0.11	0
2	PEG	AAA	402	-	6,6,6	0.09	0	5,5,5	0.14	0
3	TRS	AAA	403	-	7,7,7	0.24	0	9,9,9	0.51	0
6	EDO	BBB	406	-	3,3,3	0.10	0	2,2,2	0.20	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
6	EDO	AAA	407	-	-	1/1/1/1	-
6	EDO	BBB	404	-	-	1/1/1/1	-
6	EDO	AAA	409	-	-	0/1/1/1	-
2	PEG	BBB	401	-	-	3/4/4/4	-
6	EDO	AAA	406	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	AAA	401	-	-	2/4/4/4	-
5	PGE	BBB	403	-	-	2/7/7/7	-
5	PGE	AAA	405	-	-	3/7/7/7	-
6	EDO	AAA	408	-	-	1/1/1/1	-
6	EDO	BBB	405	-	-	1/1/1/1	-
6	EDO	BBB	407	-	-	0/1/1/1	-
2	PEG	AAA	402	-	-	1/4/4/4	-
3	TRS	AAA	403	-	-	2/9/9/9	-
6	EDO	BBB	406	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	403	TRS	N-C-C1-O1
2	AAA	401	PEG	O2-C3-C4-O4
5	BBB	403	PGE	O1-C1-C2-O2
5	AAA	405	PGE	O1-C1-C2-O2
6	AAA	408	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	AAA	407	EDO	3	0
6	BBB	404	EDO	3	0
5	BBB	403	PGE	1	0
6	AAA	408	EDO	1	0
3	AAA	403	TRS	4	0
6	BBB	406	EDO	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 [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	304/417 (72%)	-0.60	1 (0%) 94 94	30, 40, 56, 86	0
1	BBB	305/417 (73%)	-0.49	3 (0%) 82 85	30, 39, 60, 104	0
All	All	609/834 (73%)	-0.55	4 (0%) 87 90	30, 39, 57, 104	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	-1	GLY	4.0
1	BBB	90[A]	ARG	3.2
1	BBB	-2	GLN	2.7
1	AAA	-1	GLY	2.5

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 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
6	EDO	AAA	409	4/4	0.63	0.22	72,78,85,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	EDO	AAA	408	4/4	0.68	0.25	57,64,81,90	0
6	EDO	AAA	406	4/4	0.74	0.11	57,64,70,71	0
2	PEG	AAA	401	7/7	0.83	0.09	79,83,99,100	0
6	EDO	BBB	404	4/4	0.83	0.15	49,66,71,94	0
6	EDO	BBB	405	4/4	0.84	0.23	65,70,77,83	0
6	EDO	BBB	407	4/4	0.84	0.13	83,87,87,118	0
6	EDO	AAA	407	4/4	0.87	0.21	71,79,81,83	0
2	PEG	AAA	402	7/7	0.88	0.21	80,82,100,101	0
2	PEG	BBB	401	7/7	0.89	0.11	75,84,92,94	0
6	EDO	BBB	406	4/4	0.93	0.21	47,60,66,80	0
5	PGE	BBB	403	10/10	0.95	0.10	49,55,61,67	0
3	TRS	AAA	403	8/8	0.95	0.22	52,68,72,87	8
5	PGE	AAA	405	10/10	0.95	0.08	51,60,66,69	0
7	CL	AAA	410	1/1	0.98	0.04	49,49,49,49	0
4	ZN	BBB	402	1/1	0.99	0.11	39,39,39,39	0
4	ZN	AAA	404	1/1	0.99	0.10	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.