



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 11:42 PM UTC

PDB ID : 7P7I / pdb_00007p7i
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

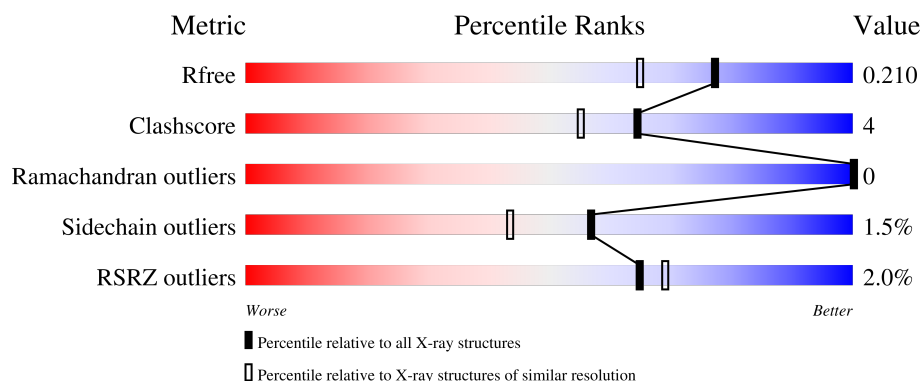
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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:

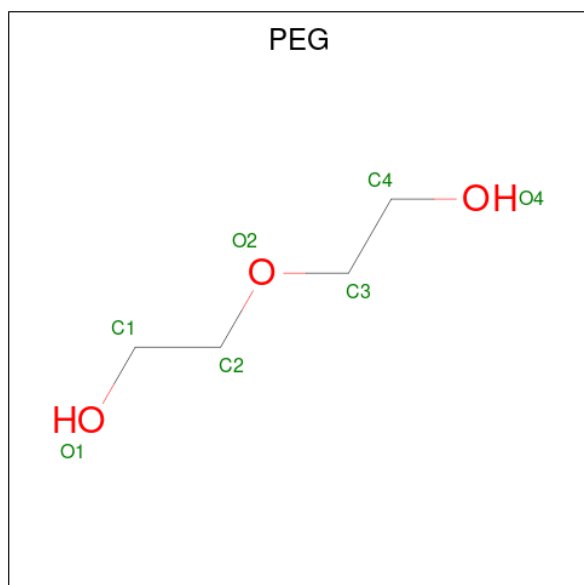
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-114	MET	-	initiating methionine	UNP Q12306
AAA	-113	ALA	-	expression tag	UNP Q12306
AAA	-112	HIS	-	expression tag	UNP Q12306
AAA	-111	HIS	-	expression tag	UNP Q12306
AAA	-110	HIS	-	expression tag	UNP Q12306
AAA	-109	HIS	-	expression tag	UNP Q12306
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

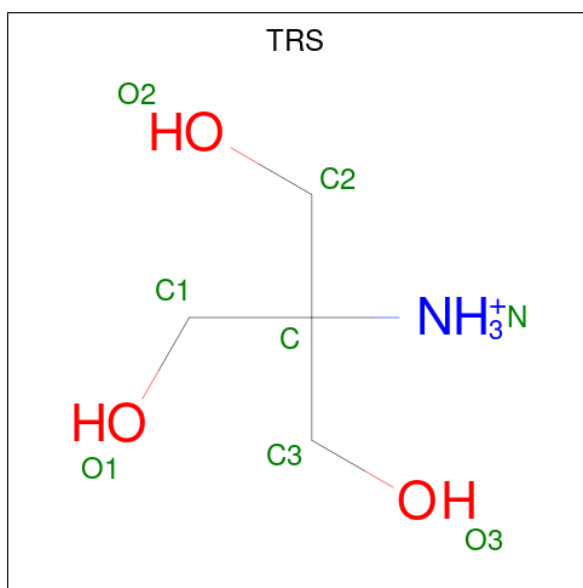
- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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 (CCD ID: TRS)

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

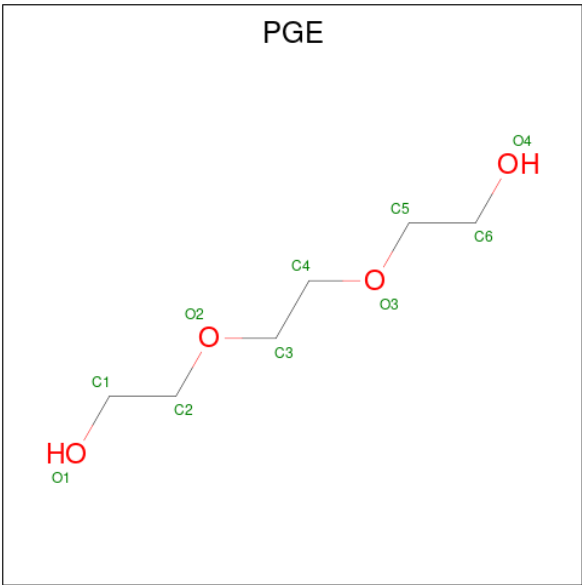


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

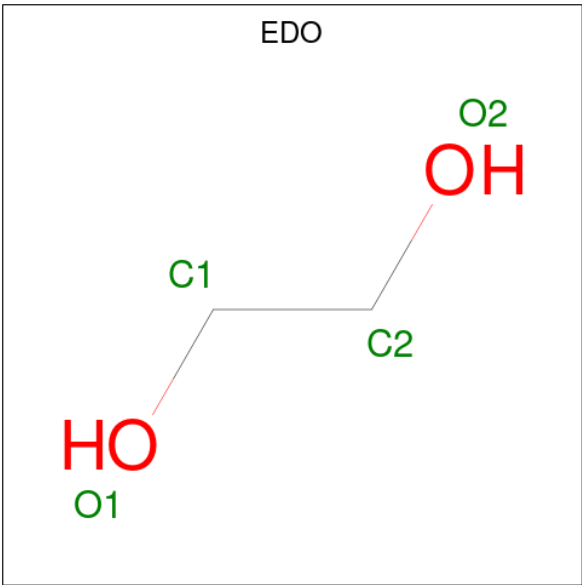
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	1	Total	Zn	0	0
			1	1		
4	BBB	1	Total	Zn	0	0
			1	1		

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: 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 (CCD ID: EDO) (formula: C₂H₆O₂).



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 4 2 2	0	0
6	AAA	1	Total C O 4 2 2	0	0
6	BBB	1	Total C O 4 2 2	0	0
6	BBB	1	Total C O 4 2 2	0	0
6	BBB	1	Total C O 4 2 2	0	0
6	BBB	1	Total C O 4 2 2	0	0

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

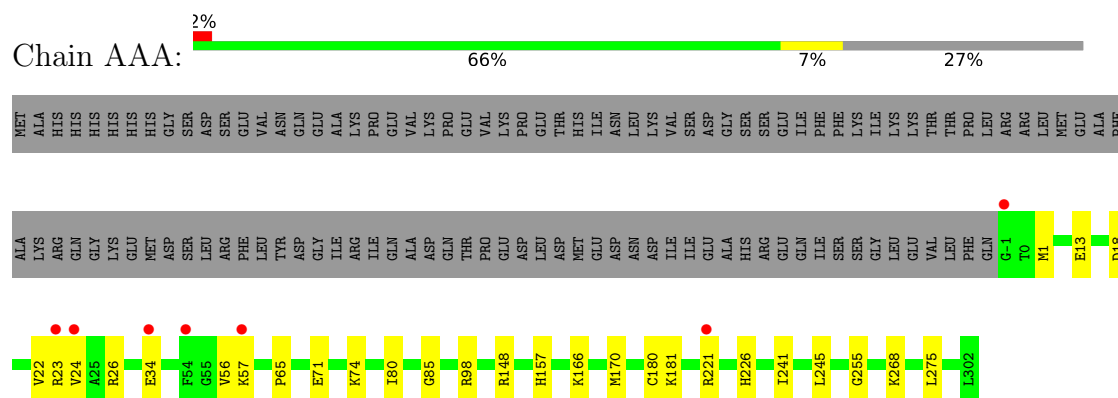
- Molecule 8 is water.

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

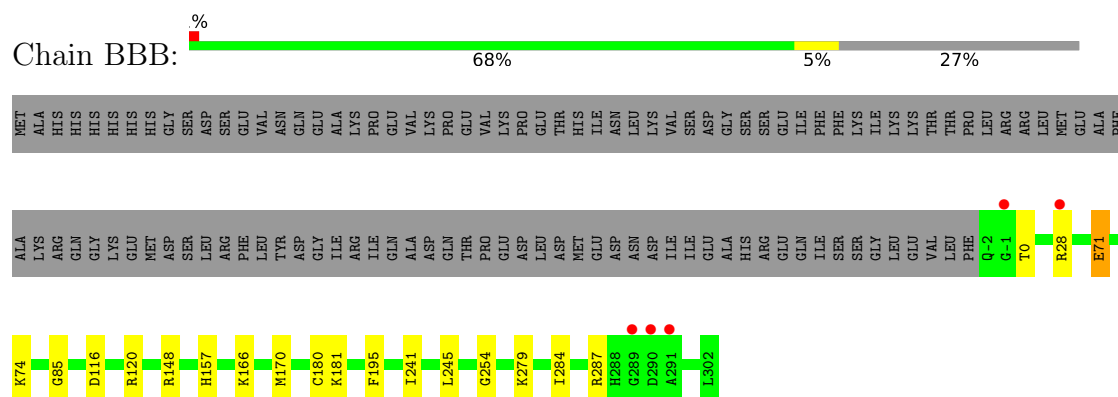
3 Residue-property plots [i](#)

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: 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 60.89 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (60.89-1.70) 99.5 (60.89-1.70)	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	5219 reflections (4.98%)	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)	0.34 , 49.6	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	0.98	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: ZN, EDO, CL, PEG, PGE, TRS

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	0.65	1/2571 (0.0%)	0.99	1/3472 (0.0%)
1	BBB	0.64	0/2549	1.00	5/3442 (0.1%)
All	All	0.65	1/5120 (0.0%)	0.99	6/6914 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	226	HIS	CE1-NE2	5.38	1.38	1.32

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	120	ARG	CA-C-N	-6.46	113.03	122.46
1	BBB	120	ARG	C-N-CA	-6.46	113.03	122.46
1	BBB	71	GLU	CB-CG-CD	6.12	123.00	112.60
1	BBB	157	HIS	CA-CB-CG	-5.50	108.31	113.80
1	AAA	157	HIS	CA-CB-CG	-5.24	108.56	113.80
1	BBB	195	PHE	CA-CB-CG	5.24	119.04	113.80

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
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.

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: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:13:GLU:OE2	6:AAA:407:EDO:H22	2.00	0.61
1:BBB:284[B]:ILE:HD13	1:BBB:284[B]:ILE:H	1.67	0.60
1:BBB:180:CYS:O	1:BBB:181:LYS:HB2	2.03	0.57
1:AAA:255:GLY:O	6:AAA:408:EDO:H21	2.05	0.56
1:AAA:1[B]:MET:HE2	1:AAA:24:VAL:CG2	2.36	0.55
1:AAA:1[B]:MET:CE	1:AAA:24:VAL:HG21	2.37	0.55
1:AAA:18:ASP:OD2	1:AAA:22[B]:VAL:HG22	2.06	0.55
1:AAA:1[B]:MET:HE1	1:AAA:24:VAL:HG21	1.90	0.54
6:BBB:404:EDO:H22	8:BBB:556:HOH:O	2.08	0.54
1:AAA:245:LEU:HD21	1:BBB:245:LEU:HD21	1.91	0.53
1:AAA:275:LEU:HD13	5:BBB:403:PGE:H32	1.90	0.53
1:AAA:65:PRO:HD2	1:AAA:80[A]:ILE:HD11	1.90	0.52
1:AAA:180:CYS:O	1:AAA:181:LYS:HB2	2.10	0.51
1:BBB:74:LYS:HE3	1:BBB:85:GLY:O	2.10	0.51
1:AAA:241[A]:ILE:HA	3:AAA:403:TRS:H21	1.94	0.50
1:AAA:1[B]:MET:HB2	1:AAA:56:VAL:HG21	1.94	0.49
1:AAA:166[B]:LYS:HG2	1:AAA:170[B]:MET:SD	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:74:LYS:HE3	1:AAA:85:GLY:O	2.13	0.48
1:AAA:18:ASP:CG	1:AAA:22[B]:VAL:HG22	2.39	0.47
1:AAA:1[B]:MET:CE	1:AAA:24:VAL:CG2	2.93	0.47
1:AAA:71:GLU:HG2	1:BBB:279:LYS:HE3	1.96	0.46
1:AAA:268[B]:LYS:HE2	8:AAA:528:HOH:O	2.15	0.46
1:BBB:254:GLY:H	6:BBB:406:EDO:C1	2.28	0.46
1:AAA:245:LEU:CD2	1:BBB:245:LEU:HD21	2.45	0.46
1:BBB:254:GLY:H	6:BBB:406:EDO:C2	2.30	0.45
1:AAA:241[B]:ILE:HA	3:AAA:403:TRS:H21	1.99	0.44
1:BBB:116:ASP:OD2	1:BBB:287[A]:ARG:HD3	2.18	0.44
1:BBB:166[B]:LYS:HG2	1:BBB:170[B]:MET:SD	2.57	0.44
3:AAA:403:TRS:O3	3:AAA:403:TRS:O1	2.33	0.43
6:BBB:404:EDO:C2	8:BBB:556:HOH:O	2.63	0.43
3:AAA:403:TRS:H12	1:BBB:241:ILE:HA	1.99	0.43
1:AAA:23[B]:ARG:NH2	6:AAA:407:EDO:O2	2.46	0.42
1:AAA:23[B]:ARG:NE	1:AAA:26:ARG:HG2	2.35	0.41
1:AAA:57[B]:LYS:HE3	1:AAA:98:ARG:HB3	2.03	0.41

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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
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%)	50	34
1	BBB	260/340 (76%)	256 (98%)	4 (2%)	57	43
All	All	522/680 (77%)	513 (98%)	9 (2%)	57	38

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	34[A]	GLU
1	AAA	34[B]	GLU
1	AAA	148	ARG
1	AAA	221[A]	ARG
1	AAA	221[B]	ARG
1	BBB	0	THR
1	BBB	28	ARG
1	BBB	71	GLU
1	BBB	148	ARG

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	$\# Z > 2$
2	PEG	BBB	401	-	6,6,6	0.19	0	5,5,5	0.13	0
6	EDO	AAA	409	-	3,3,3	0.02	0	2,2,2	0.21	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
6	EDO	AAA	408	-	3,3,3	0.51	0	2,2,2	0.61	0
6	EDO	BBB	404	-	3,3,3	0.22	0	2,2,2	0.54	0
6	EDO	BBB	407	-	3,3,3	0.08	0	2,2,2	0.16	0
6	EDO	BBB	406	-	3,3,3	0.10	0	2,2,2	0.23	0
6	EDO	AAA	406	-	3,3,3	0.35	0	2,2,2	0.22	0
2	PEG	AAA	402	-	6,6,6	0.09	0	5,5,5	0.14	0
5	PGE	AAA	405	-	9,9,9	0.19	0	8,8,8	0.15	0
6	EDO	AAA	407	-	3,3,3	0.07	0	2,2,2	0.27	0
6	EDO	BBB	405	-	3,3,3	0.18	0	2,2,2	0.17	0
3	TRS	AAA	403	-	7,7,7	0.26	0	9,9,9	0.54	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	PEG	BBB	401	-	-	3/4/4/4	-
6	EDO	AAA	409	-	-	0/1/1/1	-
2	PEG	AAA	401	-	-	2/4/4/4	-
5	PGE	BBB	403	-	-	2/7/7/7	-
6	EDO	AAA	408	-	-	1/1/1/1	-
6	EDO	BBB	404	-	-	1/1/1/1	-
6	EDO	BBB	407	-	-	0/1/1/1	-
6	EDO	BBB	406	-	-	0/1/1/1	-
6	EDO	AAA	406	-	-	0/1/1/1	-
2	PEG	AAA	402	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PGE	AAA	405	-	-	3/7/7/7	-
6	EDO	AAA	407	-	-	1/1/1/1	-
6	EDO	BBB	405	-	-	1/1/1/1	-
3	TRS	AAA	403	-	-	2/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (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
2	BBB	401	PEG	O2-C3-C4-O4
5	AAA	405	PGE	O3-C5-C6-O4
6	BBB	404	EDO	O1-C1-C2-O2
6	BBB	405	EDO	O1-C1-C2-O2
2	BBB	401	PEG	C1-C2-O2-C3
5	BBB	403	PGE	C3-C4-O3-C5
3	AAA	403	TRS	C3-C-C1-O1
6	AAA	407	EDO	O1-C1-C2-O2
2	BBB	401	PEG	C4-C3-O2-C2
2	AAA	401	PEG	C1-C2-O2-C3
5	AAA	405	PGE	C3-C4-O3-C5
2	AAA	402	PEG	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	BBB	403	PGE	1	0
6	AAA	408	EDO	1	0
6	BBB	404	EDO	3	0
6	BBB	406	EDO	2	0
6	AAA	407	EDO	3	0
3	AAA	403	TRS	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	304/417 (72%)	0.02	7 (2%) 61 65	19, 38, 54, 86	24 (7%)
1	BBB	305/417 (73%)	0.02	5 (1%) 70 75	20, 38, 56, 104	21 (6%)
All	All	609/834 (73%)	0.02	12 (1%) 65 69	19, 38, 55, 104	45 (7%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	289	GLY	5.7
1	BBB	290	ASP	4.0
1	AAA	57[A]	LYS	3.2
1	AAA	23[A]	ARG	3.0
1	BBB	-1	GLY	2.9
1	AAA	54	PHE	2.7
1	AAA	24	VAL	2.7
1	BBB	291	ALA	2.4
1	AAA	-1	GLY	2.4
1	BBB	28	ARG	2.1
1	AAA	34[A]	GLU	2.0
1	AAA	221[A]	ARG	2.0

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
6	EDO	AAA	406	4/4	0.72	0.23	57,64,70,71	0
6	EDO	BBB	407	4/4	0.78	0.17	83,87,87,118	0
6	EDO	BBB	406	4/4	0.80	0.17	47,60,66,80	0
6	EDO	BBB	404	4/4	0.80	0.18	49,66,71,94	0
2	PEG	BBB	401	7/7	0.85	0.17	75,84,92,94	0
6	EDO	BBB	405	4/4	0.86	0.15	65,70,77,83	0
6	EDO	AAA	408	4/4	0.87	0.19	57,64,81,90	0
2	PEG	AAA	402	7/7	0.88	0.15	80,82,100,101	0
2	PEG	AAA	401	7/7	0.89	0.15	79,83,99,100	0
6	EDO	AAA	409	4/4	0.90	0.16	72,78,85,92	0
3	TRS	AAA	403	8/8	0.92	0.27	52,68,72,87	8
6	EDO	AAA	407	4/4	0.93	0.16	71,79,81,83	0
5	PGE	AAA	405	10/10	0.94	0.11	51,60,66,69	0
5	PGE	BBB	403	10/10	0.94	0.10	49,55,61,67	0
4	ZN	AAA	404	1/1	0.99	0.03	38,38,38,38	0
7	CL	AAA	410	1/1	0.99	0.14	49,49,49,49	0
4	ZN	BBB	402	1/1	1.00	0.02	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.