



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 30, 2026 – 04:31 PM UTC

PDB ID : 6Z7T / pdb_00006z7t
Title : Nucleotide-free Myosin-II motor domain
Authors : Ewert, W.; Preller, M.
Deposited on : 2020-06-01
Resolution : 1.88 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

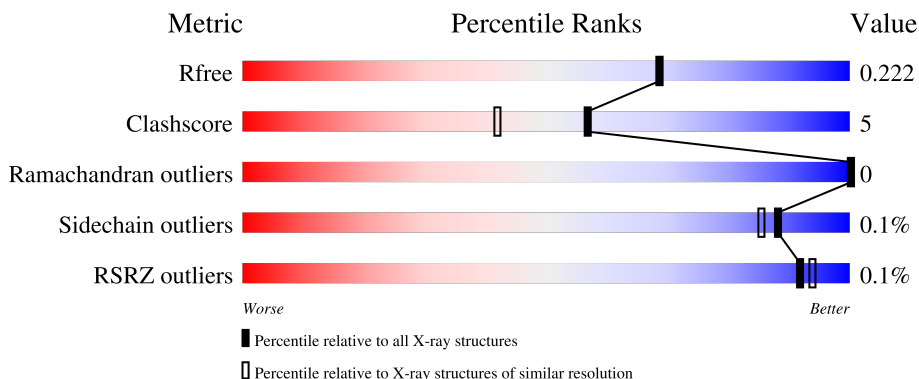
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	788	 82% 10% 8%
1	B	788	 84% 8% 7%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 24654 atoms, of which 11696 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 Myosin-2 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	726	Total	C	H	N	O	S	0	8	0
			11523	3695	5711	995	1105	17			
1	B	730	Total	C	H	N	O	S	0	4	0
			11613	3719	5763	1001	1113	17			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP P08799
A	-9	HIS	-	expression tag	UNP P08799
A	-8	HIS	-	expression tag	UNP P08799
A	-7	HIS	-	expression tag	UNP P08799
A	-6	HIS	-	expression tag	UNP P08799
A	-5	HIS	-	expression tag	UNP P08799
A	-4	HIS	-	expression tag	UNP P08799
A	-3	HIS	-	expression tag	UNP P08799
A	-2	ASP	-	expression tag	UNP P08799
A	-1	GLY	-	expression tag	UNP P08799
A	0	THR	-	expression tag	UNP P08799
A	1	GLU	-	expression tag	UNP P08799
A	762	LEU	-	expression tag	UNP P08799
A	763	GLU	-	expression tag	UNP P08799
A	764	SER	-	expression tag	UNP P08799
A	765	ASN	-	expression tag	UNP P08799
A	766	GLU	-	expression tag	UNP P08799
A	767	PRO	-	expression tag	UNP P08799
A	768	PRO	-	expression tag	UNP P08799
A	769	MET	-	expression tag	UNP P08799
A	770	ASP	-	expression tag	UNP P08799
A	771	PHE	-	expression tag	UNP P08799
A	772	ASP	-	expression tag	UNP P08799
A	773	ASP	-	expression tag	UNP P08799
A	774	ASP	-	expression tag	UNP P08799

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Chain	Residue	Modelled	Actual	Comment	Reference
A	775	ILE	-	expression tag	UNP P08799
A	776	PRO	-	expression tag	UNP P08799
A	777	PHE	-	expression tag	UNP P08799
B	-10	MET	-	initiating methionine	UNP P08799
B	-9	HIS	-	expression tag	UNP P08799
B	-8	HIS	-	expression tag	UNP P08799
B	-7	HIS	-	expression tag	UNP P08799
B	-6	HIS	-	expression tag	UNP P08799
B	-5	HIS	-	expression tag	UNP P08799
B	-4	HIS	-	expression tag	UNP P08799
B	-3	HIS	-	expression tag	UNP P08799
B	-2	ASP	-	expression tag	UNP P08799
B	-1	GLY	-	expression tag	UNP P08799
B	0	THR	-	expression tag	UNP P08799
B	1	GLU	-	expression tag	UNP P08799
B	762	LEU	-	expression tag	UNP P08799
B	763	GLU	-	expression tag	UNP P08799
B	764	SER	-	expression tag	UNP P08799
B	765	ASN	-	expression tag	UNP P08799
B	766	GLU	-	expression tag	UNP P08799
B	767	PRO	-	expression tag	UNP P08799
B	768	PRO	-	expression tag	UNP P08799
B	769	MET	-	expression tag	UNP P08799
B	770	ASP	-	expression tag	UNP P08799
B	771	PHE	-	expression tag	UNP P08799
B	772	ASP	-	expression tag	UNP P08799
B	773	ASP	-	expression tag	UNP P08799
B	774	ASP	-	expression tag	UNP P08799
B	775	ILE	-	expression tag	UNP P08799
B	776	PRO	-	expression tag	UNP P08799
B	777	PHE	-	expression tag	UNP P08799

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	0	0
2	B	2	Total Mg 2 2	0	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



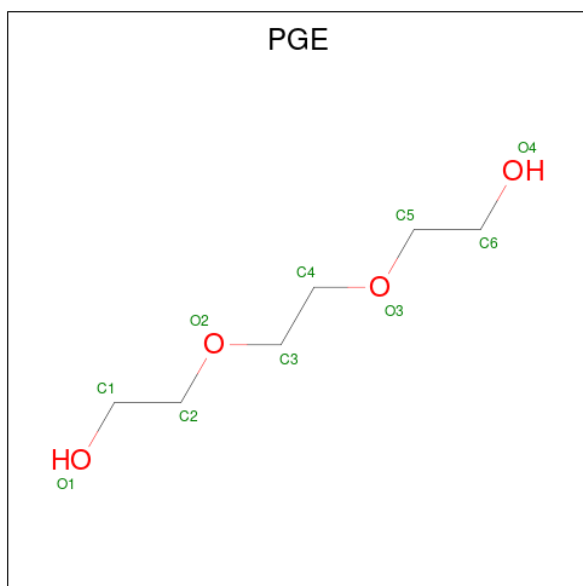
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	A	1	Total	C	H	O	0	0
			13	3	7	3		
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	A	1	Total	C	H	O	0	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	H	O	0	0
			13	3	7	3		
4	B	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	0	0
			24	6	14	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	H	O	0	0
			17	4	10	3		

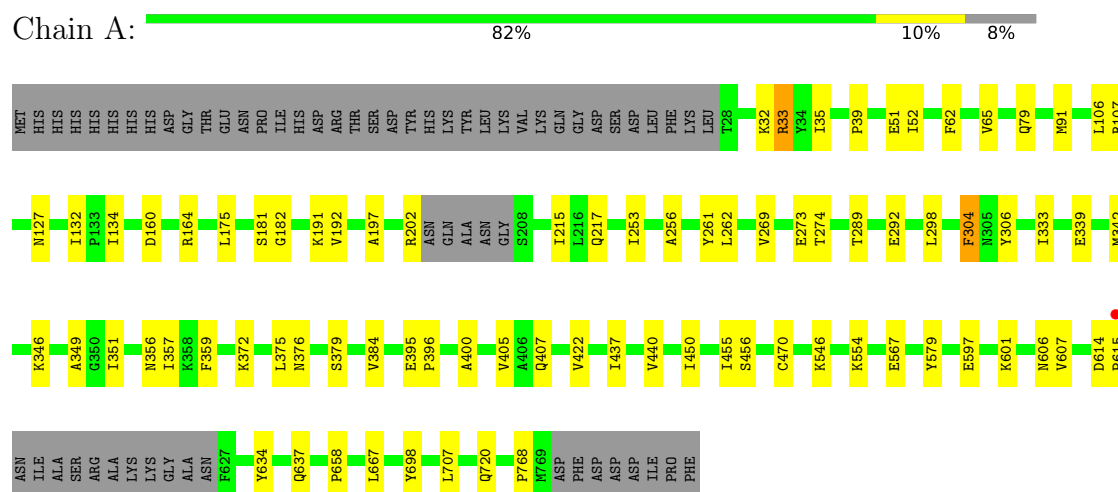
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	555	Total	O	0	0
			555	555		
7	B	580	Total	O	0	0
			580	580		

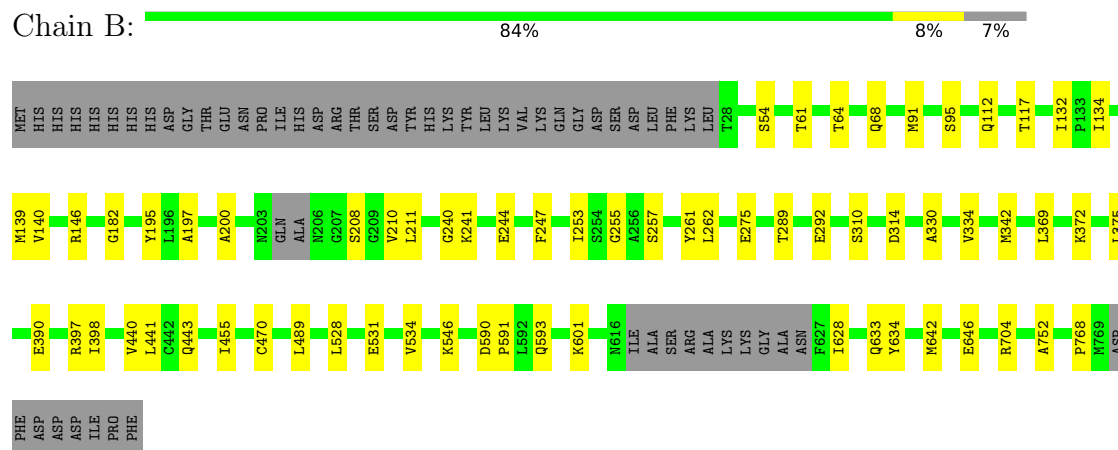
3 Residue-property plots

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: Myosin-2 heavy chain



• Molecule 1: Myosin-2 heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.68Å 174.40Å 100.25Å 90.00° 106.38° 90.00°	Depositor
Resolution (Å)	46.36 – 1.88 46.36 – 1.88	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.36-1.88) 91.8 (46.36-1.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.80 (at 1.88Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.191 , 0.217 0.193 , 0.222	Depositor DCC
R_{free} test set	2006 reflections (1.33%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.571	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.249 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	24654	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 9.53% 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: PGE, GOL, EDO, PEG, MG

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	0.53	0/5949	0.70	4/8044 (0.0%)
1	B	0.51	0/5976	0.69	1/8076 (0.0%)
All	All	0.52	0/11925	0.69	5/16120 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	304	PHE	CA-C-N	6.17	128.55	120.28
1	A	304	PHE	C-N-CA	6.17	128.55	120.28
1	A	396	PRO	O-C-N	-5.32	116.51	123.06
1	A	450	ILE	N-CA-C	-5.27	98.90	107.28
1	B	768	PRO	N-CA-C	5.12	118.66	111.33

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	A	5812	5711	5704	58	0
1	B	5850	5763	5757	50	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	40	60	60	3	0
3	B	40	60	60	1	0
4	A	30	39	37	1	0
4	B	30	39	39	3	0
5	B	10	14	14	1	0
6	B	7	10	10	0	0
7	A	555	0	0	4	0
7	B	580	0	0	5	0
All	All	12958	11696	11681	108	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 108 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:455:ILE:HD12	1:A:456:SER:O	1.83	0.77
1:A:351:ILE:HG23	1:A:422:VAL:HG13	1.66	0.76
1:B:208:SER:HB2	7:B:967:HOH:O	1.88	0.72
1:B:146:ARG:HG3	1:B:146:ARG:HH11	1.63	0.64
1:B:54:SER:HB2	1:B:61:THR:HB	1.82	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	A	728/788 (92%)	717 (98%)	11 (2%)	0	100	100
1	B	728/788 (92%)	717 (98%)	11 (2%)	0	100	100
All	All	1456/1576 (92%)	1434 (98%)	22 (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	A	627/691 (91%)	625 (100%)	2 (0%)	86	82
1	B	634/691 (92%)	634 (100%)	0	100	100
All	All	1261/1382 (91%)	1259 (100%)	2 (0%)	88	84

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33[A]	ARG
1	A	33[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	188	ASN
1	B	480	GLN
1	B	532	GLN
1	A	338	GLN
1	A	480	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 4 are monoatomic - leaving 32 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	$\# Z > 2$
4	GOL	A	815	-	5,5,5	1.27	1 (20%)	5,5,5	1.13	0
4	GOL	A	813	-	5,5,5	0.78	0	5,5,5	1.59	1 (20%)
3	EDO	A	805	-	3,3,3	0.35	0	2,2,2	0.55	0
3	EDO	B	810	-	3,3,3	0.39	0	2,2,2	0.55	0
3	EDO	A	807	-	3,3,3	0.60	0	2,2,2	0.16	0
4	GOL	B	817	-	5,5,5	0.85	0	5,5,5	1.23	0
3	EDO	B	808	-	3,3,3	0.45	0	2,2,2	0.38	0
3	EDO	B	811	-	3,3,3	0.57	0	2,2,2	0.47	0
3	EDO	B	803	-	3,3,3	0.50	0	2,2,2	0.19	0
4	GOL	A	817	-	5,5,5	0.77	0	5,5,5	0.58	0
4	GOL	B	814	-	5,5,5	0.61	0	5,5,5	1.03	0
3	EDO	A	804	-	3,3,3	0.43	0	2,2,2	0.44	0
3	EDO	B	806	-	3,3,3	0.52	0	2,2,2	0.72	0
3	EDO	A	810	-	3,3,3	0.46	0	2,2,2	0.33	0
3	EDO	A	811	-	3,3,3	0.66	0	2,2,2	0.23	0
4	GOL	A	814	-	5,5,5	1.68	2 (40%)	5,5,5	2.69	2 (40%)
4	GOL	B	816	-	5,5,5	1.22	0	5,5,5	1.52	1 (20%)
3	EDO	B	809	-	3,3,3	0.45	0	2,2,2	0.45	0
3	EDO	A	808	-	3,3,3	0.66	0	2,2,2	0.58	0
3	EDO	B	805	-	3,3,3	0.45	0	2,2,2	0.40	0
4	GOL	A	816	-	5,5,5	2.03	3 (60%)	5,5,5	2.09	1 (20%)
3	EDO	A	809	-	3,3,3	0.41	0	2,2,2	0.40	0
3	EDO	B	804	-	3,3,3	0.46	0	2,2,2	0.45	0
4	GOL	B	813	-	5,5,5	1.17	1 (20%)	5,5,5	1.18	0
4	GOL	B	815	-	5,5,5	1.12	0	5,5,5	1.36	1 (20%)
3	EDO	A	812	-	3,3,3	0.41	0	2,2,2	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PGE	B	818	-	9,9,9	0.27	0	8,8,8	0.69	0
3	EDO	A	803	-	3,3,3	0.32	0	2,2,2	0.51	0
3	EDO	B	812	-	3,3,3	0.33	0	2,2,2	0.65	0
6	PEG	B	819	-	6,6,6	0.51	0	5,5,5	0.27	0
3	EDO	A	806	-	3,3,3	0.48	0	2,2,2	0.32	0
3	EDO	B	807	-	3,3,3	0.59	0	2,2,2	0.39	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	GOL	A	815	-	-	4/4/4/4	-
4	GOL	A	813	-	-	4/4/4/4	-
3	EDO	A	805	-	-	1/1/1/1	-
3	EDO	B	810	-	-	1/1/1/1	-
3	EDO	A	807	-	-	1/1/1/1	-
4	GOL	B	817	-	-	2/4/4/4	-
3	EDO	B	808	-	-	1/1/1/1	-
3	EDO	B	811	-	-	1/1/1/1	-
3	EDO	B	803	-	-	0/1/1/1	-
4	GOL	A	817	-	-	2/4/4/4	-
4	GOL	B	814	-	-	0/4/4/4	-
3	EDO	A	804	-	-	1/1/1/1	-
3	EDO	B	806	-	-	1/1/1/1	-
3	EDO	A	810	-	-	0/1/1/1	-
3	EDO	A	811	-	-	0/1/1/1	-
4	GOL	A	814	-	-	0/4/4/4	-
4	GOL	B	816	-	-	0/4/4/4	-
3	EDO	B	809	-	-	1/1/1/1	-
3	EDO	A	808	-	-	1/1/1/1	-
3	EDO	B	805	-	-	0/1/1/1	-
4	GOL	A	816	-	-	0/4/4/4	-
3	EDO	A	809	-	-	1/1/1/1	-
3	EDO	B	804	-	-	1/1/1/1	-
4	GOL	B	813	-	-	0/4/4/4	-
4	GOL	B	815	-	-	0/4/4/4	-
3	EDO	A	812	-	-	1/1/1/1	-
5	PGE	B	818	-	-	4/7/7/7	-
3	EDO	A	803	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	812	-	-	1/1/1/1	-
6	PEG	B	819	-	-	1/4/4/4	-
3	EDO	A	806	-	-	0/1/1/1	-
3	EDO	B	807	-	-	1/1/1/1	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	816	GOL	C1-C2	2.94	1.63	1.51
4	A	814	GOL	O2-C2	-2.87	1.35	1.43
4	A	816	GOL	O2-C2	-2.65	1.35	1.43
4	B	813	GOL	O2-C2	-2.49	1.36	1.43
4	A	816	GOL	C3-C2	2.17	1.60	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	814	GOL	C3-C2-C1	-5.04	93.31	111.80
4	A	816	GOL	C3-C2-C1	-4.05	96.96	111.80
4	B	816	GOL	C3-C2-C1	-3.03	100.67	111.80
4	A	813	GOL	O1-C1-C2	-2.90	97.31	110.38
4	A	814	GOL	O2-C2-C3	2.40	119.14	109.18

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	813	GOL	O1-C1-C2-C3
4	A	813	GOL	C1-C2-C3-O3
4	A	815	GOL	O1-C1-C2-C3
4	A	815	GOL	C1-C2-C3-O3
4	B	817	GOL	O1-C1-C2-C3

There are no ring outliers.

8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	805	EDO	2	0
4	B	817	GOL	1	0
4	A	817	GOL	1	0
4	B	814	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	816	GOL	1	0
3	A	808	EDO	1	0
5	B	818	PGE	1	0
3	B	812	EDO	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	A	726/788 (92%)	-1.12	1 (0%) 92 94	13, 37, 92, 121	8 (1%)
1	B	730/788 (92%)	-1.15	0 100 100	12, 38, 77, 120	4 (0%)
All	All	1456/1576 (92%)	-1.13	1 (0%) 92 94	12, 38, 87, 121	12 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	615	PRO	2.1

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
4	GOL	A	813	6/6	0.95	0.08	44,54,65,72	0
3	EDO	A	811	4/4	0.96	0.08	29,44,56,59	0
3	EDO	B	805	4/4	0.96	0.07	31,49,66,66	0
3	EDO	B	811	4/4	0.96	0.07	47,56,60,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	801	1/1	0.96	0.12	62,62,62,62	0
3	EDO	B	803	4/4	0.97	0.06	45,54,64,69	0
3	EDO	A	810	4/4	0.97	0.07	45,60,72,80	0
3	EDO	B	808	4/4	0.97	0.06	39,56,68,79	0
3	EDO	A	806	4/4	0.97	0.06	34,42,50,58	0
3	EDO	A	812	4/4	0.97	0.08	20,20,20,20	0
4	GOL	B	816	6/6	0.97	0.05	50,73,91,92	0
2	MG	A	802	1/1	0.98	0.05	45,45,45,45	0
3	EDO	A	808	4/4	0.98	0.06	34,42,51,60	0
3	EDO	A	809	4/4	0.98	0.05	46,55,62,74	0
3	EDO	B	809	4/4	0.98	0.05	47,56,67,80	0
3	EDO	B	810	4/4	0.98	0.07	40,48,56,67	0
3	EDO	A	803	4/4	0.98	0.06	26,38,40,48	0
3	EDO	B	812	4/4	0.98	0.04	36,44,47,57	0
3	EDO	A	804	4/4	0.98	0.06	47,57,60,62	0
4	GOL	A	815	6/6	0.98	0.06	37,52,66,69	0
4	GOL	A	817	6/6	0.98	0.06	37,51,57,68	0
4	GOL	B	813	6/6	0.98	0.05	47,57,66,66	0
4	GOL	B	814	6/6	0.98	0.06	42,54,63,64	0
4	GOL	B	815	6/6	0.98	0.05	30,47,60,68	0
3	EDO	A	805	4/4	0.98	0.15	37,49,61,61	0
5	PGE	B	818	10/10	0.98	0.05	31,53,60,63	0
6	PEG	B	819	7/7	0.98	0.04	45,54,63,69	0
4	GOL	A	816	6/6	0.99	0.05	30,52,61,64	0
3	EDO	A	807	4/4	0.99	0.04	25,35,41,43	0
3	EDO	B	804	4/4	0.99	0.04	38,48,58,58	0
2	MG	B	801	1/1	0.99	0.04	53,53,53,53	0
3	EDO	B	806	4/4	0.99	0.07	27,36,44,53	0
3	EDO	B	807	4/4	0.99	0.04	27,32,44,44	0
4	GOL	B	817	6/6	0.99	0.04	32,45,57,57	0
4	GOL	A	814	6/6	0.99	0.04	30,45,51,54	0
2	MG	B	802	1/1	0.99	0.08	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.