



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:47 PM UTC

PDB ID : 4WAC / pdb_00004wac
Title : Crystal Structure of TarM
Authors : Koc, C.; Stehle, T.; Xia, G.; Peschel, A.
Deposited on : 2014-08-29
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

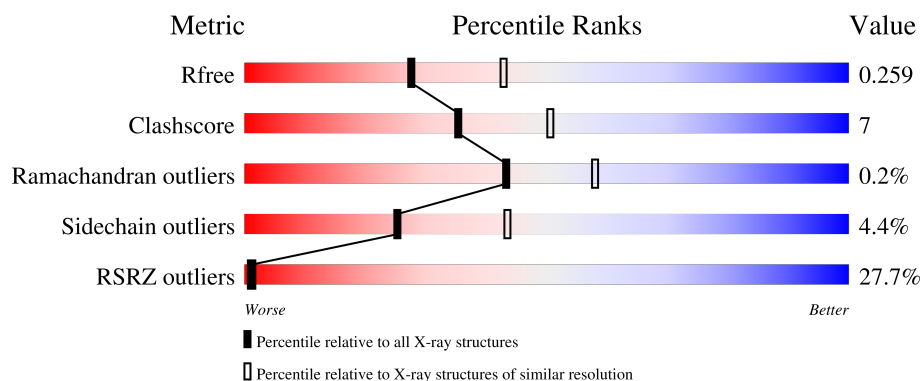
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	498	28% 79% 18% .

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4194 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.

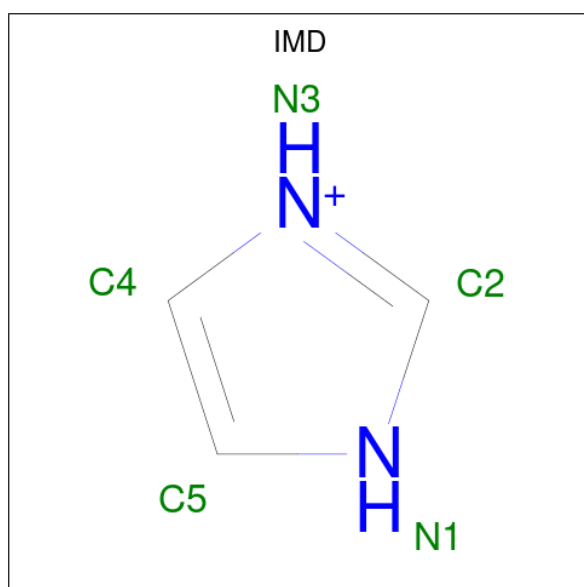
- Molecule 1 is a protein called Glycosyl transferase, group 1 family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	498	4079	2612	687	761	19	0	1	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	ILE	-	expression tag	UNP Q2FI41
A	-3	ASP	-	expression tag	UNP Q2FI41
A	-2	PRO	-	expression tag	UNP Q2FI41
A	-1	PHE	-	expression tag	UNP Q2FI41
A	0	THR	-	expression tag	UNP Q2FI41

- Molecule 2 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



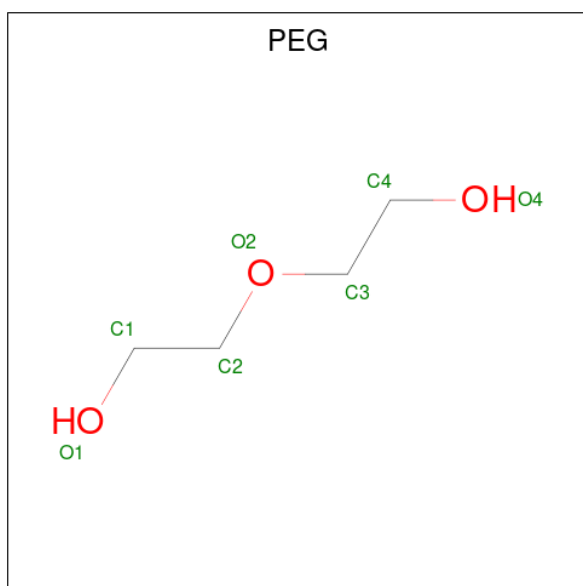
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
2	A	1	5	3	2	0	0

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $\text{C}_4\text{H}_{10}\text{O}_3$).



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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

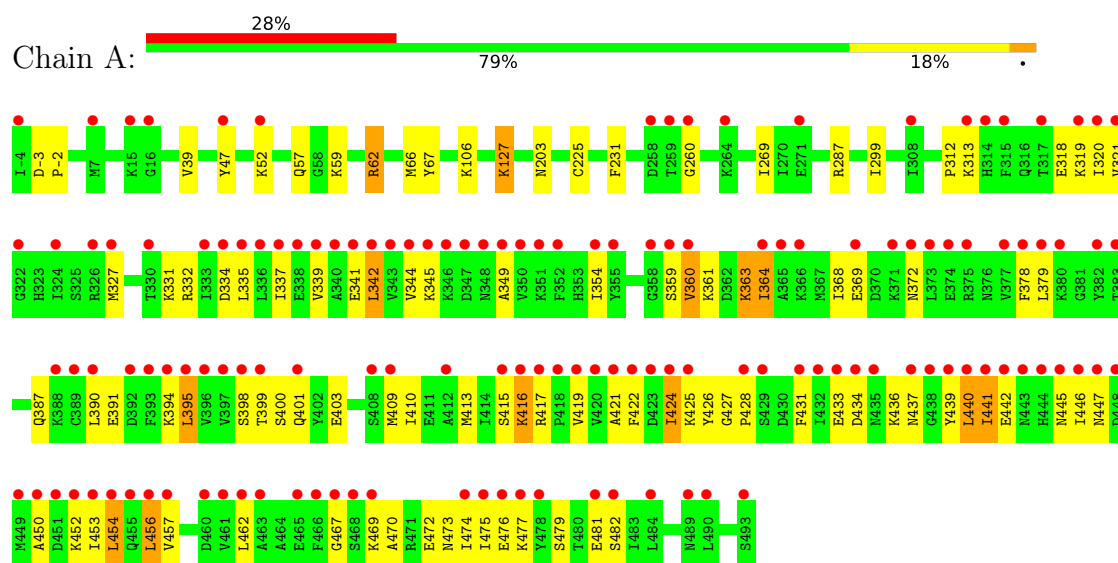
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	87	Total	O	0	0
			87	87		

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: Glycosyl transferase, group 1 family protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	124.75Å 124.75Å 223.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.62 – 2.40 48.62 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.62-2.40) 99.6 (48.62-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.215 , 0.252 0.224 , 0.259	Depositor DCC
R_{free} test set	2036 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	47.6	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.5	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	0.93	EDS
Total number of atoms	4194	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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, EDO, ACT, IMD

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	0.68	0/4161	0.96	4/5587 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	260	GLY	N-CA-C	-5.44	107.02	115.67
1	A	427	GLY	CA-C-N	5.28	125.09	119.28
1	A	427	GLY	C-N-CA	5.28	125.09	119.28
1	A	342	LEU	N-CA-C	5.00	116.42	111.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	442	GLU	Peptide

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	4079	0	4101	60	0
2	A	5	0	5	0	0
3	A	8	0	6	0	0
4	A	7	0	10	0	0
5	A	8	0	12	2	0
6	A	87	0	0	1	0
All	All	4194	0	4134	61	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.

All (61) 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:312:PRO:HB3	1:A:391:GLU:HG3	1.59	0.83
1:A:339:VAL:HG22	1:A:446:ILE:HB	1.61	0.83
1:A:409:MET:HE1	1:A:428:PRO:HG3	1.65	0.78
1:A:203:ASN:HB3	5:A:506:EDO:H11	1.66	0.75
1:A:409:MET:HG2	1:A:419:VAL:HG11	1.70	0.74
1:A:401:GLN:HA	1:A:424:ILE:HG21	1.68	0.73
1:A:57:GLN:OE1	1:A:59:LYS:NZ	2.24	0.70
1:A:472:GLU:HA	1:A:475:ILE:HD12	1.75	0.68
5:A:506:EDO:O1	6:A:601:HOH:O	2.12	0.68
1:A:334:ASP:OD1	1:A:335:LEU:N	2.29	0.65
1:A:62:ARG:HG2	1:A:62:ARG:HH21	1.63	0.62
1:A:395:LEU:HD21	1:A:457:VAL:HG12	1.82	0.61
1:A:361:LYS:HG3	1:A:379:LEU:HD21	1.83	0.59
1:A:331:LYS:NZ	1:A:403:GLU:OE2	2.37	0.58
1:A:453:ILE:O	1:A:457:VAL:HG13	2.04	0.58
1:A:337:ILE:HD11	1:A:364:ILE:HG23	1.86	0.58
1:A:341:GLU:HG3	1:A:345:LYS:HE2	1.87	0.56
1:A:332:ARG:HB2	1:A:399:THR:O	2.07	0.55
1:A:454:LEU:HA	1:A:457:VAL:HG22	1.88	0.54
1:A:364:ILE:O	1:A:368:ILE:HG13	2.08	0.53
1:A:434:ASP:HB2	1:A:440:LEU:CD2	2.39	0.53
1:A:341:GLU:O	1:A:345:LYS:HG2	2.09	0.52
1:A:359:SER:C	1:A:363:LYS:HZ1	2.19	0.51
1:A:473:ASN:O	1:A:477:LYS:HG2	2.10	0.51
1:A:327:MET:HB3	1:A:360:VAL:HG12	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:ILE:HD12	1:A:445:ASN:O	2.10	0.51
1:A:439:TYR:CD2	1:A:452:LYS:HB3	2.47	0.50
1:A:342:LEU:HD21	1:A:447:ASN:OD1	2.12	0.50
1:A:415:SER:O	1:A:417:ARG:NH1	2.45	0.49
1:A:470:ALA:O	1:A:474:ILE:HG12	2.11	0.49
1:A:416:LYS:O	1:A:467:GLY:HA3	2.12	0.49
1:A:433:GLU:OE2	1:A:437:ASN:ND2	2.46	0.49
1:A:361:LYS:CG	1:A:379:LEU:HD21	2.43	0.49
1:A:400:SER:O	1:A:424:ILE:HG12	2.13	0.49
1:A:335:LEU:O	1:A:339:VAL:HG23	2.13	0.49
1:A:425:LYS:HA	1:A:426:TYR:HA	1.55	0.48
1:A:231:PHE:CG	1:A:269:ILE:HG12	2.48	0.48
1:A:354:ILE:N	1:A:378:PHE:O	2.44	0.47
1:A:425:LYS:HB2	1:A:426:TYR:CD2	2.49	0.47
1:A:318:GLU:O	1:A:320:ILE:N	2.46	0.47
1:A:450:ALA:O	1:A:454:LEU:HG	2.15	0.46
1:A:410:ILE:HG13	1:A:431:PHE:CZ	2.51	0.46
1:A:473:ASN:O	1:A:476:GLU:HG2	2.17	0.45
1:A:47:TYR:CD1	1:A:66:MET:HE1	2.52	0.45
1:A:398:SER:HB3	1:A:421:ALA:HB2	1.98	0.45
1:A:364:ILE:O	1:A:368:ILE:N	2.47	0.44
1:A:369:GLU:C	1:A:372:ASN:H	2.25	0.44
1:A:287:ARG:HG3	1:A:299:ILE:HG22	1.99	0.43
1:A:106:LYS:O	1:A:106:LYS:HG2	2.17	0.43
1:A:360:VAL:HG13	1:A:364:ILE:HD12	2.01	0.43
1:A:39:VAL:HA	1:A:67:TYR:O	2.19	0.42
1:A:413:MET:HE1	1:A:431:PHE:O	2.19	0.42
1:A:456:LEU:HD11	1:A:462:LEU:HB2	2.02	0.42
1:A:327:MET:HE2	1:A:379:LEU:HD11	2.01	0.42
1:A:319:LYS:HE2	1:A:349:ALA:HB3	2.01	0.42
1:A:479:SER:O	1:A:482:SER:OG	2.29	0.42
1:A:456:LEU:HA	1:A:456:LEU:HD12	1.59	0.41
1:A:-3:ASP:HA	1:A:-2:PRO:HD2	1.88	0.41
1:A:387:GLN:HA	1:A:390:LEU:HD12	2.03	0.41
1:A:422:PHE:CE1	1:A:441:ILE:HD11	2.56	0.41
1:A:225:CYS:SG	1:A:231:PHE:HA	2.61	0.40

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	497/498 (100%)	473 (95%)	23 (5%)	1 (0%)	43	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	LYS

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	A	455/454 (100%)	435 (96%)	20 (4%)	25	43

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LYS
1	A	62	ARG
1	A	127	LYS
1	A	313	LYS
1	A	321	VAL
1	A	344	VAL
1	A	360	VAL
1	A	363	LYS
1	A	364	ILE
1	A	394	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	395	LEU
1	A	416	LYS
1	A	424	ILE
1	A	436	LYS
1	A	440	LEU
1	A	441	ILE
1	A	454	LEU
1	A	456	LEU
1	A	469	LYS
1	A	481	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	68	ASN
1	A	79	ASN
1	A	81	HIS
1	A	98	ASN
1	A	138	ASN
1	A	149	ASN
1	A	203	ASN
1	A	255	ASN
1	A	304	ASN
1	A	405	GLN
1	A	458	ASN

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

6 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
3	ACT	A	505	-	3,3,3	1.10	0	3,3,3	1.11	0
5	EDO	A	506	-	3,3,3	0.14	0	2,2,2	0.81	0
3	ACT	A	502	-	3,3,3	0.83	0	3,3,3	1.77	2 (66%)
2	IMD	A	501	-	5,5,5	0.65	0	5,5,5	0.79	0
4	PEG	A	503	-	6,6,6	0.50	0	5,5,5	0.90	0
5	EDO	A	504	-	3,3,3	0.49	0	2,2,2	0.22	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	IMD	A	501	-	-	-	0/1/1/1
5	EDO	A	504	-	-	0/1/1/1	-
5	EDO	A	506	-	-	1/1/1/1	-
4	PEG	A	503	-	-	1/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	ACT	OXT-C-O	-2.21	113.83	122.03
3	A	502	ACT	OXT-C-CH3	2.11	123.91	115.05

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	PEG	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	506	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	506	EDO	2	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

6.1 Protein, DNA and RNA chains

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	498/498 (100%)	1.05	138 (27%) 1 1	28, 69, 106, 124	1 (0%)

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	451	ASP	8.7
1	A	462	LEU	7.5
1	A	453	ILE	6.9
1	A	337	ILE	6.8
1	A	340	ALA	6.7
1	A	454	LEU	6.7
1	A	441	ILE	6.4
1	A	419	VAL	6.2
1	A	440	LEU	6.1
1	A	373	LEU	5.9
1	A	418	PRO	5.7
1	A	449	MET	5.7
1	A	439	TYR	5.4
1	A	336	LEU	5.4
1	A	374	GLU	5.2
1	A	352	PHE	5.2
1	A	397	VAL	5.1
1	A	344	VAL	5.0
1	A	447	ASN	5.0
1	A	435	ASN	4.9
1	A	461	VAL	4.9
1	A	457	VAL	4.9
1	A	455	GLN	4.9
1	A	398	SER	4.8
1	A	432	ILE	4.7
1	A	343	VAL	4.7
1	A	450	ALA	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	456	LEU	4.6
1	A	342	LEU	4.4
1	A	377	VAL	4.4
1	A	444	HIS	4.3
1	A	345	LYS	4.2
1	A	468	SER	4.2
1	A	379	LEU	4.1
1	A	382	TYR	4.1
1	A	446	ILE	4.1
1	A	319	LYS	4.1
1	A	452	LYS	4.0
1	A	333	ILE	4.0
1	A	421	ALA	3.8
1	A	416	LYS	3.8
1	A	395	LEU	3.8
1	A	424	ILE	3.8
1	A	438	GLY	3.8
1	A	339	VAL	3.7
1	A	347	ASP	3.7
1	A	478	TYR	3.7
1	A	360	VAL	3.6
1	A	433	GLU	3.6
1	A	315	PHE	3.6
1	A	422	PHE	3.6
1	A	399	THR	3.5
1	A	16	GLY	3.5
1	A	431	PHE	3.5
1	A	409	MET	3.4
1	A	322	GLY	3.4
1	A	334	ASP	3.4
1	A	321	VAL	3.4
1	A	415	SER	3.4
1	A	474	ILE	3.3
1	A	359	SER	3.3
1	A	380	LYS	3.3
1	A	434	ASP	3.3
1	A	348	ASN	3.3
1	A	437	ASN	3.2
1	A	350	VAL	3.2
1	A	358	GLY	3.2
1	A	375	ARG	3.2
1	A	392	ASP	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	324	ILE	3.2
1	A	320	ILE	3.2
1	A	448	ASP	3.1
1	A	378	PHE	3.1
1	A	412	ALA	3.1
1	A	338	GLU	3.1
1	A	314	HIS	3.1
1	A	493	SER	3.1
1	A	-4	ILE	3.1
1	A	420	VAL	3.1
1	A	341	GLU	3.0
1	A	465	GLU	3.0
1	A	443	ASN	3.0
1	A	466	PHE	3.0
1	A	365	ALA	3.0
1	A	463	ALA	3.0
1	A	346	LYS	3.0
1	A	475	ILE	2.9
1	A	259	THR	2.9
1	A	349	ALA	2.8
1	A	423	ASP	2.7
1	A	372	ASN	2.7
1	A	425	LYS	2.7
1	A	330	THR	2.7
1	A	354	ILE	2.6
1	A	7	MET	2.6
1	A	442	GLU	2.6
1	A	482	SER	2.6
1	A	351	LYS	2.6
1	A	388	LYS	2.6
1	A	327	MET	2.6
1	A	469	LYS	2.6
1	A	260	GLY	2.5
1	A	383	THR	2.5
1	A	408	SER	2.5
1	A	308	ILE	2.5
1	A	317	THR	2.5
1	A	313	LYS	2.4
1	A	258	ASP	2.4
1	A	490	LEU	2.4
1	A	393	PHE	2.4
1	A	417	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	445	ASN	2.4
1	A	396	VAL	2.3
1	A	467	GLY	2.3
1	A	460	ASP	2.3
1	A	389	CYS	2.3
1	A	428	PRO	2.3
1	A	489	ASN	2.3
1	A	484	LEU	2.3
1	A	264	LYS	2.3
1	A	47	TYR	2.2
1	A	429	SER	2.2
1	A	476	GLU	2.2
1	A	15	LYS	2.2
1	A	477	LYS	2.2
1	A	335	LEU	2.2
1	A	390	LEU	2.2
1	A	364	ILE	2.2
1	A	369	GLU	2.2
1	A	394	LYS	2.2
1	A	401	GLN	2.1
1	A	271	GLU	2.1
1	A	355	TYR	2.1
1	A	481	GLU	2.1
1	A	326	ARG	2.1
1	A	366	LYS	2.1
1	A	52	LYS	2.1
1	A	371	LYS	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
3	ACT	A	505	4/4	0.63	0.27	48,52,54,82	0
5	EDO	A	504	4/4	0.67	0.27	73,78,81,91	0
4	PEG	A	503	7/7	0.75	0.22	60,77,89,100	0
5	EDO	A	506	4/4	0.92	0.17	48,48,60,76	0
3	ACT	A	502	4/4	0.95	0.12	41,53,60,65	0
2	IMD	A	501	5/5	0.97	0.16	38,38,39,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.