



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 12:32 PM EDT

PDB ID : 3WA2 / pdb_00003wa2
Title : High resolution crystal structure of copper amine oxidase from arthrobacter globiformis
Authors : Murakawa, T.; Hayashi, H.; Sunami, T.; Kurihara, K.; Tamada, T.; Kuroki, R.; Suzuki, M.; Tanizawa, K.; Okajima, T.
Deposited on : 2013-04-22
Resolution : 1.08 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

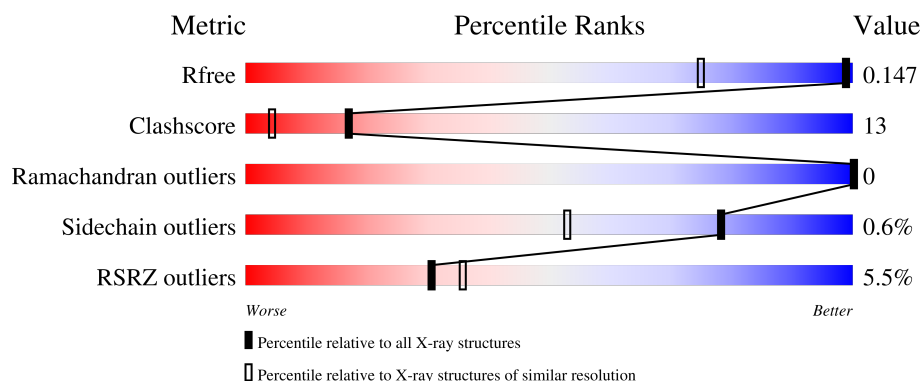
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.08 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	1687 (1.10-1.06)
Clashscore	190562	1727 (1.10-1.06)
Ramachandran outliers	187476	1679 (1.10-1.06)
Sidechain outliers	187428	1676 (1.10-1.06)
RSRZ outliers	180081	1687 (1.10-1.06)

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	X	621	5% 87% 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	X	703	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	X	711	-	-	X	-
5	PEG	X	719	-	-	X	-
5	PEG	X	721	-	-	X	-
5	PEG	X	722	-	-	X	-
6	PGE	X	724	-	-	X	-
6	PGE	X	728	-	-	X	-
8	1PE	X	730	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 12203 atoms, of which 5706 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 Phenylethylamine oxidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	X	621	Total	C	H	N	O	S	0	91	0
			10768	3422	5412	933	988	13			

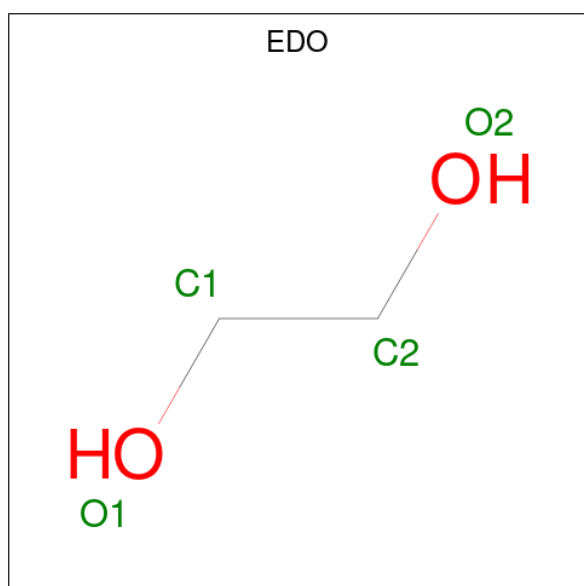
- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	X	1	Total	Cu	0	0
			1	1		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

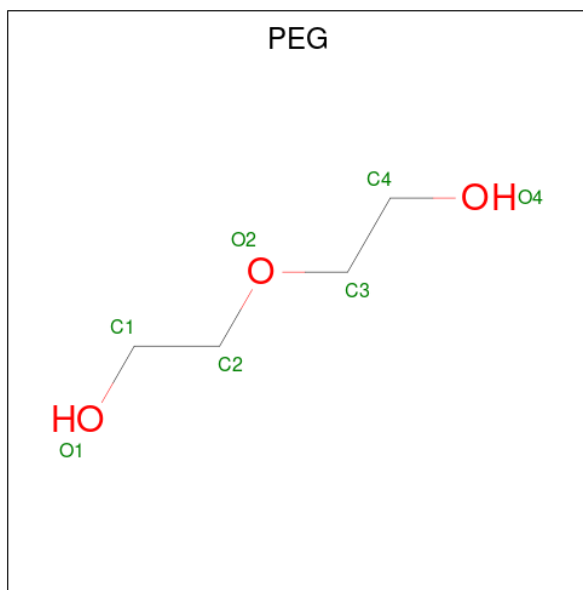
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	X	1	Total	Na	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



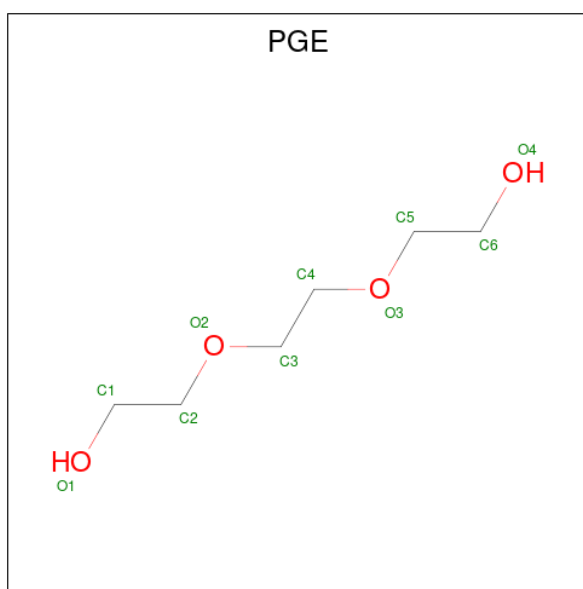
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	X	1	Total C H O 10 2 6 2	0	0
4	X	1	Total C H O 10 2 6 2	0	0
4	X	1	Total C H O 10 2 6 2	0	0
4	X	1	Total C H O 10 2 6 2	0	0
4	X	1	Total C H O 10 2 6 2	0	0
4	X	1	Total C H O 10 2 6 2	0	0
4	X	1	Total C H O 10 2 6 2	0	0
4	X	1	Total C H O 10 2 6 2	0	0
4	X	1	Total C H O 10 2 6 2	0	0
4	X	1	Total C H O 10 2 6 2	0	0
4	X	1	Total C H O 10 2 6 2	0	0
4	X	1	Total C H O 10 2 6 2	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



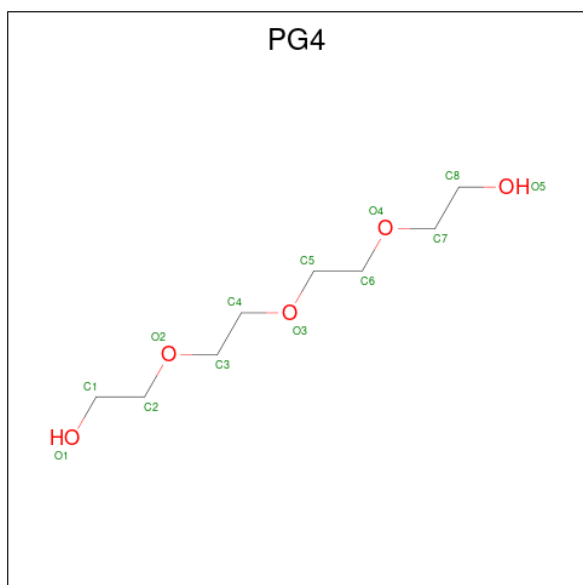
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	X	1	Total C H O 24 6 14 4	0	0
6	X	1	Total C H O 24 6 14 4	0	0
6	X	1	Total C H O 24 6 14 4	0	0

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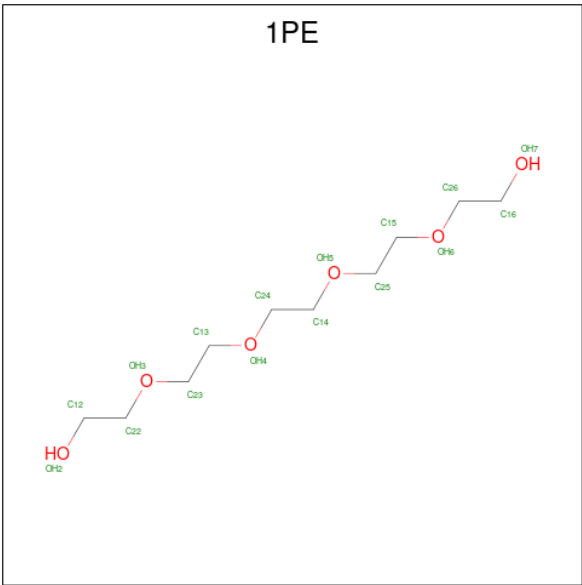
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	X	1	Total	C	H	O	0	0
			24	6	14	4		
6	X	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 7 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



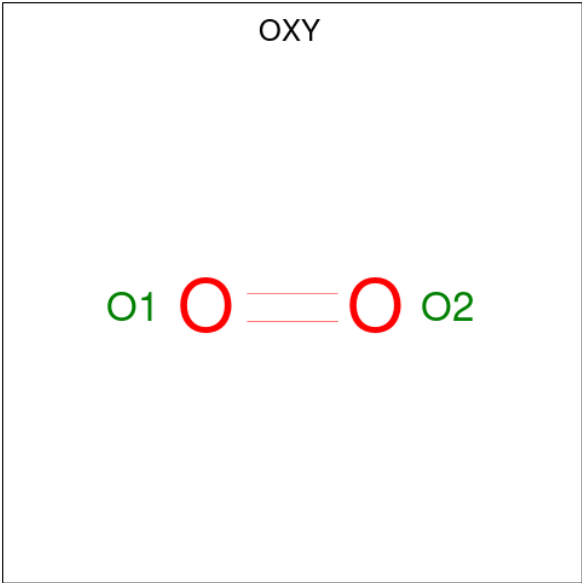
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	X	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 8 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	X	1	Total	C	H	O	0	0
			38	10	22	6		
8	X	1	Total	C	H	O	0	0
			38	10	22	6		

- Molecule 9 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	X	1	Total	O	0	0
			2	2		
9	X	1	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	X	1	Total	O	0	0
			2	2		
9	X	1	Total	O	0	0
			2	2		

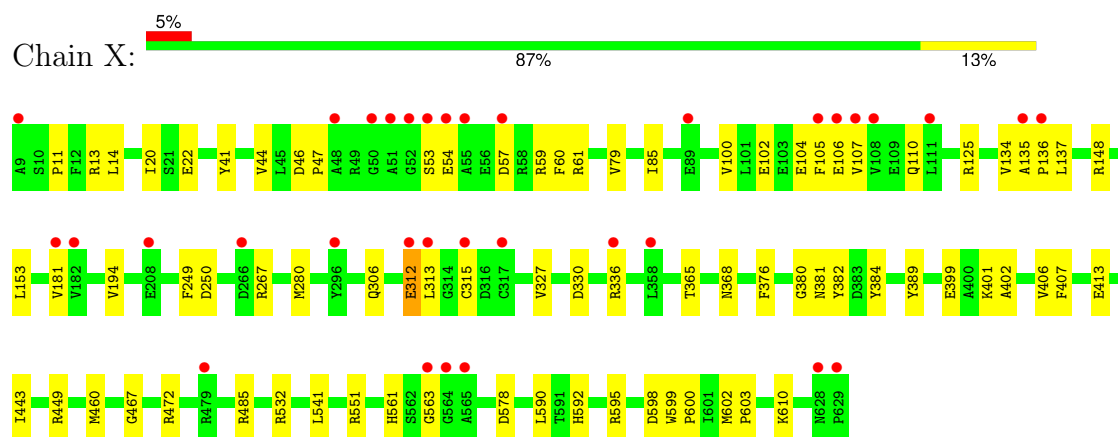
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	X	905	Total	O	0	20
			925	925		

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: Phenylethylamine oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	157.75Å 62.38Å 92.08Å 90.00° 112.10° 90.00°	Depositor
Resolution (Å)	31.97 – 1.08 31.97 – 1.08	Depositor EDS
% Data completeness (in resolution range)	86.5 (31.97-1.08) 86.6 (31.97-1.08)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.03 (at 1.08Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.130 , 0.150 0.128 , 0.147	Depositor DCC
R_{free} test set	15335 reflections (4.35%)	wwPDB-VP
Wilson B-factor (Å ²)	9.9	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 56.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	12203	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% 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: EDO, PGE, OXY, TPQ, CU, PEG, 1PE, PG4, NA

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	X	0.56	0/5741	0.73	0/7810

There are no bond length outliers.

There are no bond angle outliers.

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	X	5356	5412	5255	118	0
2	X	1	0	0	0	0
3	X	1	0	0	0	0
4	X	48	72	72	15	0
5	X	63	90	85	35	0
6	X	50	70	70	18	0
7	X	13	18	18	4	0
8	X	32	44	40	18	0
9	X	8	0	0	0	0
10	X	925	0	0	41	3
All	All	6497	5706	5540	142	3

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 13.

All (142) 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:X:595[B]:ARG:NE	8:X:730:1PE:H261	1.72	1.02
1:X:368:ASN:HD22	4:X:705:EDO:H12	1.28	0.96
5:X:719:PEG:O1	10:X:1591:HOH:O	1.88	0.91
1:X:134[A]:VAL:O	10:X:1466:HOH:O	1.88	0.90
1:X:44:VAL:HG12	4:X:711:EDO:H21	1.54	0.88
1:X:380:GLY:HA2	5:X:718:PEG:H41	1.58	0.84
1:X:368:ASN:ND2	4:X:705:EDO:H12	1.96	0.81
1:X:148[B]:ARG:NH1	10:X:1491:HOH:O	2.14	0.80
1:X:61[A]:ARG:NH1	4:X:703:EDO:O2	2.12	0.79
1:X:485[B]:ARG:NH1	10:X:1646:HOH:O	2.14	0.79
1:X:563[B]:GLY:O	10:X:947:HOH:O	2.01	0.79
4:X:705:EDO:O1	10:X:929:HOH:O	2.02	0.76
1:X:603[B]:PRO:HG2	8:X:730:1PE:OH2	1.86	0.75
1:X:135[B]:ALA:O	10:X:1478:HOH:O	2.02	0.75
1:X:399:GLU:OE1	5:X:721:PEG:C1	2.35	0.74
1:X:402:ALA:HB3	8:X:730:1PE:H131	1.72	0.71
1:X:595[B]:ARG:HE	8:X:730:1PE:H261	1.56	0.71
1:X:592[A]:HIS:CD2	8:X:730:1PE:H161	2.26	0.70
7:X:729:PG4:H42	10:X:1424:HOH:O	1.91	0.70
1:X:14:LEU:O	5:X:719:PEG:H41	1.92	0.69
1:X:41:TYR:OH	4:X:703:EDO:H12	1.93	0.69
1:X:590[B]:LEU:HD13	8:X:730:1PE:H241	1.72	0.69
1:X:399:GLU:OE1	5:X:721:PEG:H12	1.94	0.68
1:X:315:CYS:HB2	10:X:1583:HOH:O	1.93	0.68
5:X:721:PEG:H22	10:X:1695:HOH:O	1.95	0.67
1:X:104:GLU:HG2	1:X:181[A]:VAL:HG11	1.78	0.67
1:X:57[A]:ASP:OD2	10:X:1559:HOH:O	2.13	0.66
1:X:106:GLU:OE1	10:X:1185:HOH:O	2.12	0.66
1:X:595[B]:ARG:HG3	8:X:730:1PE:C16	2.26	0.66
1:X:250:ASP:OD1	4:X:711:EDO:H11	1.96	0.66
1:X:22[B]:GLU:OE2	10:X:1024:HOH:O	2.14	0.65
1:X:100:VAL:HG12	6:X:724:PGE:H1	1.78	0.64
1:X:380:GLY:H	6:X:724:PGE:H62	1.64	0.63
5:X:722:PEG:H11	10:X:1312:HOH:O	1.99	0.62
1:X:551:ARG:HG2	5:X:722:PEG:H22	1.81	0.62
1:X:135[B]:ALA:HB1	6:X:728:PGE:H6	1.81	0.61
1:X:595[B]:ARG:HG3	8:X:730:1PE:H162	1.81	0.61
1:X:102:GLU:HA	6:X:724:PGE:H22	1.83	0.60
1:X:280[B]:MET:HE1	1:X:384:TYR:CE1	2.38	0.58
1:X:599:TRP:CD2	1:X:600:PRO:HA	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:249:PHE:O	4:X:711:EDO:H22	2.02	0.58
1:X:134[B]:VAL:O	10:X:1452[B]:HOH:O	2.17	0.58
1:X:105:PHE:CA	6:X:724:PGE:H2	2.34	0.57
1:X:44:VAL:HG12	4:X:711:EDO:C2	2.32	0.57
7:X:729:PG4:H21	10:X:1424:HOH:O	2.03	0.57
1:X:401:LYS:NZ	5:X:721:PEG:H42	2.19	0.57
1:X:460[B]:MET:HG3	1:X:467:GLY:N	2.20	0.56
1:X:313[B]:LEU:HD12	1:X:313[B]:LEU:H	1.70	0.56
1:X:595[B]:ARG:CD	8:X:730:1PE:H261	2.35	0.56
1:X:59:ARG:NH2	10:X:1559:HOH:O	2.38	0.56
1:X:137:LEU:HG	10:X:1478:HOH:O	2.04	0.56
1:X:47:PRO:O	5:X:723:PEG:H12	2.06	0.55
1:X:551:ARG:HD3	5:X:722:PEG:O1	2.06	0.55
1:X:551:ARG:CG	5:X:722:PEG:H22	2.37	0.55
1:X:13:ARG:CD	5:X:719:PEG:H42	2.36	0.55
1:X:610[B]:LYS:NZ	10:X:1230:HOH:O	2.41	0.54
1:X:595[B]:ARG:HG3	8:X:730:1PE:OH7	2.07	0.54
6:X:728:PGE:C1	6:X:728:PGE:H42	2.37	0.54
1:X:136:PRO:HG3	6:X:724:PGE:H12	1.91	0.53
1:X:401:LYS:HZ3	5:X:721:PEG:H42	1.73	0.53
4:X:703:EDO:H21	10:X:1238[B]:HOH:O	2.09	0.52
1:X:148[A]:ARG:NH2	10:X:1457:HOH:O	2.43	0.52
5:X:720:PEG:H32	10:X:1701:HOH:O	2.10	0.52
1:X:136:PRO:CG	6:X:724:PGE:H12	2.40	0.52
1:X:148[B]:ARG:CZ	10:X:1491:HOH:O	2.54	0.52
1:X:389:TYR:CE2	5:X:721:PEG:H12	2.45	0.52
1:X:460[B]:MET:HG3	1:X:467:GLY:CA	2.40	0.51
1:X:592[A]:HIS:HD2	8:X:730:1PE:H161	1.75	0.51
1:X:595[B]:ARG:HE	8:X:730:1PE:C26	2.22	0.51
1:X:449[A]:ARG:HD2	1:X:578:ASP:OD1	2.12	0.50
5:X:717:PEG:H11	10:X:942:HOH:O	2.10	0.50
1:X:485[A]:ARG:CZ	10:X:1485[A]:HOH:O	2.59	0.50
1:X:46:ASP:HB2	5:X:723:PEG:H21	1.94	0.50
1:X:602[B]:MET:HG2	1:X:603[B]:PRO:O	2.12	0.49
1:X:181[A]:VAL:HG12	1:X:181[A]:VAL:O	2.12	0.49
1:X:60:PHE:CD1	1:X:79[B]:VAL:HG21	2.48	0.49
1:X:595[B]:ARG:NE	8:X:730:1PE:C26	2.60	0.49
1:X:532[A]:ARG:HB3	1:X:563[A]:GLY:HA3	1.94	0.49
1:X:61[A]:ARG:HE	4:X:703:EDO:H11	1.77	0.49
5:X:717:PEG:H12	10:X:887:HOH:O	2.13	0.49
1:X:61[A]:ARG:HE	4:X:703:EDO:C2	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:306:GLN:NE2	10:X:1392:HOH:O	2.30	0.48
1:X:148[B]:ARG:NE	10:X:1491:HOH:O	2.46	0.48
1:X:153:LEU:HD12	1:X:181[A]:VAL:HG21	1.96	0.48
1:X:125:ARG:HG2	1:X:194[A]:VAL:HG23	1.95	0.48
1:X:107[A]:VAL:HG11	1:X:181[A]:VAL:HG13	1.96	0.47
1:X:381:ASN:OD1	6:X:728:PGE:H22	2.14	0.47
1:X:551:ARG:NH2	10:X:1284:HOH:O	2.47	0.47
1:X:413:GLU:H	5:X:717:PEG:C2	2.28	0.47
1:X:136:PRO:HG3	6:X:724:PGE:C1	2.44	0.47
1:X:595[B]:ARG:NH2	8:X:730:1PE:OH2	2.48	0.46
1:X:59:ARG:CZ	1:X:85[B]:ILE:HD13	2.45	0.46
1:X:381:ASN:OD1	6:X:728:PGE:C2	2.63	0.46
1:X:399:GLU:OE1	5:X:721:PEG:H11	2.13	0.46
7:X:729:PG4:H82	10:X:1465:HOH:O	2.15	0.46
1:X:406[B]:VAL:HG22	1:X:602[B]:MET:HE2	1.98	0.46
1:X:380:GLY:HA3	6:X:728:PGE:H42	1.98	0.46
1:X:532[A]:ARG:HA	4:X:708:EDO:H12	1.98	0.46
1:X:13:ARG:NE	5:X:719:PEG:H42	2.31	0.46
1:X:105:PHE:HA	6:X:724:PGE:H2	1.97	0.45
1:X:598:ASP:OD2	8:X:730:1PE:H162	2.16	0.45
1:X:561:HIS:HD1	1:X:563[B]:GLY:H	1.64	0.45
1:X:11:PRO:HB2	1:X:47:PRO:HG3	1.98	0.45
1:X:106:GLU:HG3	1:X:110:GLN:CD	2.42	0.45
1:X:44:VAL:N	4:X:711:EDO:H12	2.31	0.45
1:X:61[B]:ARG:HB3	4:X:703:EDO:H11	1.99	0.45
1:X:134[A]:VAL:O	1:X:135[A]:ALA:CB	2.65	0.44
1:X:60:PHE:CD1	1:X:79[B]:VAL:CG2	3.01	0.44
7:X:729:PG4:H61	10:X:1424:HOH:O	2.16	0.44
1:X:20[B]:ILE:HD12	1:X:327:VAL:HG12	2.00	0.44
1:X:267[B]:ARG:NH2	10:X:1469:HOH:O	2.48	0.44
1:X:312:GLU:O	10:X:1371:HOH:O	2.21	0.43
1:X:330:ASP:OD2	1:X:336[B]:ARG:NH2	2.50	0.43
1:X:14:LEU:O	5:X:719:PEG:C4	2.65	0.43
1:X:402:ALA:HB3	8:X:730:1PE:C13	2.46	0.43
1:X:365[A]:THR:HG22	10:X:1399:HOH:O	2.18	0.43
1:X:472:ARG:NH1	5:X:715:PEG:H21	2.33	0.43
1:X:137:LEU:CD2	6:X:728:PGE:H1	2.48	0.43
8:X:731:1PE:H241	10:X:1408:HOH:O	2.18	0.42
1:X:280[A]:MET:HE1	1:X:384:TYR:CE2	2.54	0.42
1:X:563[B]:GLY:HA2	10:X:902:HOH:O	2.18	0.42
1:X:592[B]:HIS:HD2	10:X:1192:HOH:O	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:590[A]:LEU:HD21	10:X:1179:HOH:O	2.19	0.42
1:X:13:ARG:HG3	5:X:719:PEG:H42	2.02	0.42
1:X:53:SER:HA	1:X:54:GLU:HB2	2.02	0.42
1:X:407:PHE:HE2	6:X:728:PGE:H12	1.85	0.41
5:X:721:PEG:C1	10:X:1695:HOH:O	2.67	0.41
1:X:105:PHE:N	6:X:724:PGE:H2	2.35	0.41
1:X:315:CYS:HB2	10:X:1585:HOH:O	2.19	0.41
1:X:380:GLY:H	6:X:724:PGE:C6	2.32	0.41
1:X:598:ASP:OD1	8:X:730:1PE:C22	2.69	0.41
1:X:148[B]:ARG:HB3	1:X:148[B]:ARG:HH21	1.85	0.40
5:X:718:PEG:O4	6:X:728:PGE:C6	2.69	0.40
5:X:721:PEG:O4	10:X:1534:HOH:O	2.22	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:1279:HOH:O	10:X:1295:HOH:O[2_556]	1.73	0.47
10:X:1177:HOH:O	10:X:1177:HOH:O[2_555]	1.91	0.29
10:X:1534:HOH:O	10:X:1547:HOH:O[2_556]	2.08	0.12

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	X	711/621 (114%)	689 (97%)	22 (3%)	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	X	601/514 (117%)	598 (100%)	3 (0%)	81	58

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	312	GLU
1	X	376	PHE
1	X	541	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	418	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	TPQ	X	382	1	13,14,15	2.37	4 (30%)	13,19,21	1.21	1 (7%)

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
1	TPQ	X	382	1	-	1/5/22/24	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	382	TPQ	C3-C4	5.46	1.46	1.36
1	X	382	TPQ	C6-C1	4.97	1.46	1.34
1	X	382	TPQ	CB-CA	2.98	1.59	1.53
1	X	382	TPQ	C1-C2	-2.19	1.46	1.49

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	382	TPQ	C6-C1-C2	3.46	121.12	118.66

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	X	382	TPQ	N-CA-CB-C1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 35 ligands modelled in this entry, 2 are monoatomic - leaving 33 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	EDO	X	707	-	3,3,3	0.44	0	2,2,2	0.32	0
4	EDO	X	709	-	3,3,3	0.45	0	2,2,2	0.37	0
6	PGE	X	727	-	9,9,9	0.71	0	8,8,8	0.76	0
4	EDO	X	703	-	3,3,3	0.40	0	2,2,2	1.02	0
4	EDO	X	711	-	3,3,3	0.53	0	2,2,2	0.78	0
5	PEG	X	719	-	6,6,6	0.90	0	5,5,5	0.74	0
4	EDO	X	704	-	3,3,3	0.42	0	2,2,2	0.40	0
5	PEG	X	720	-	6,6,6	0.65	0	5,5,5	0.82	0
9	OXY	X	734	-	1,1,1	0.11	0	-		
9	OXY	X	733	-	1,1,1	0.15	0	-		
5	PEG	X	718	-	6,6,6	0.85	0	5,5,5	1.32	0
6	PGE	X	724	-	9,9,9	0.86	0	8,8,8	0.88	0
4	EDO	X	705	-	3,3,3	0.81	0	2,2,2	0.69	0
6	PGE	X	726	-	9,9,9	0.62	0	8,8,8	0.76	0
4	EDO	X	710	-	3,3,3	0.44	0	2,2,2	0.20	0
5	PEG	X	717	-	6,6,6	0.66	0	5,5,5	0.77	0
5	PEG	X	716	-	6,6,6	0.81	0	5,5,5	1.41	1 (20%)
8	1PE	X	730	-	15,15,15	1.19	1 (6%)	14,14,14	1.83	4 (28%)
6	PGE	X	728	-	9,9,9	0.64	0	8,8,8	1.45	1 (12%)
9	OXY	X	735	-	1,1,1	0.14	0	-		
7	PG4	X	729	-	12,12,12	0.71	0	11,11,11	1.12	1 (9%)
4	EDO	X	713	-	3,3,3	0.42	0	2,2,2	0.27	0
9	OXY	X	732	-	1,1,1	0.22	0	-		
8	1PE	X	731	-	15,15,15	0.63	0	14,14,14	1.26	3 (21%)
5	PEG	X	722	-	6,6,6	1.04	0	5,5,5	1.79	1 (20%)
4	EDO	X	706	-	3,3,3	0.34	0	2,2,2	0.58	0
4	EDO	X	708	-	3,3,3	0.35	0	2,2,2	0.16	0
6	PGE	X	725	-	9,9,9	0.71	0	8,8,8	0.78	0
5	PEG	X	715	-	6,6,6	0.72	0	5,5,5	1.19	1 (20%)
4	EDO	X	712	-	3,3,3	0.47	0	2,2,2	0.16	0
5	PEG	X	721	-	6,6,6	1.09	0	5,5,5	1.56	1 (20%)
4	EDO	X	714	-	3,3,3	0.41	0	2,2,2	0.35	0
5	PEG	X	723	-	6,6,6	0.66	0	5,5,5	0.95	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	EDO	X	707	-	-	1/1/1/1	-
4	EDO	X	709	-	-	1/1/1/1	-
6	PGE	X	727	-	-	3/7/7/7	-
4	EDO	X	703	-	-	1/1/1/1	-
4	EDO	X	711	-	-	1/1/1/1	-
5	PEG	X	719	-	-	2/4/4/4	-
4	EDO	X	704	-	-	0/1/1/1	-
5	PEG	X	720	-	-	1/4/4/4	-
5	PEG	X	718	-	-	0/4/4/4	-
6	PGE	X	724	-	-	3/7/7/7	-
4	EDO	X	705	-	-	0/1/1/1	-
6	PGE	X	726	-	-	2/7/7/7	-
4	EDO	X	710	-	-	1/1/1/1	-
5	PEG	X	717	-	-	2/4/4/4	-
5	PEG	X	716	-	-	3/4/4/4	-
8	1PE	X	730	-	-	10/13/13/13	-
6	PGE	X	728	-	-	4/7/7/7	-
7	PG4	X	729	-	-	4/10/10/10	-
4	EDO	X	713	-	-	0/1/1/1	-
8	1PE	X	731	-	-	6/13/13/13	-
5	PEG	X	722	-	-	1/4/4/4	-
4	EDO	X	706	-	-	0/1/1/1	-
4	EDO	X	708	-	-	0/1/1/1	-
6	PGE	X	725	-	-	2/7/7/7	-
5	PEG	X	715	-	-	1/4/4/4	-
4	EDO	X	712	-	-	0/1/1/1	-
5	PEG	X	721	-	-	1/4/4/4	-
4	EDO	X	714	-	-	1/1/1/1	-
5	PEG	X	723	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	X	730	1PE	OH6-C26	-2.18	1.32	1.42

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	X	730	1PE	OH7-C16-C26	-3.45	91.50	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	X	721	PEG	O2-C2-C1	3.33	124.79	110.11
8	X	730	1PE	C23-OH3-C22	3.24	127.45	113.26
5	X	722	PEG	O2-C2-C1	-3.12	96.36	110.11
6	X	728	PGE	O2-C2-C1	2.95	123.10	110.11
7	X	729	PG4	C7-O4-C6	2.92	126.03	113.26
5	X	716	PEG	C3-O2-C2	2.66	124.92	113.26
5	X	715	PEG	C3-O2-C2	2.65	124.84	113.26
8	X	730	1PE	C26-OH6-C15	-2.62	101.78	113.26
8	X	731	1PE	C25-OH5-C14	2.52	124.31	113.26
8	X	731	1PE	C26-OH6-C15	2.49	124.16	113.26
8	X	730	1PE	OH3-C23-C13	-2.45	99.20	110.35
8	X	731	1PE	C24-OH4-C13	2.03	122.16	113.26

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	X	728	PGE	C1-C2-O2-C3
7	X	729	PG4	C8-C7-O4-C6
6	X	724	PGE	C1-C2-O2-C3
8	X	731	1PE	C16-C26-OH6-C15
8	X	730	1PE	C12-C22-OH3-C23
8	X	731	1PE	OH4-C13-C23-OH3
8	X	731	1PE	OH6-C15-C25-OH5
8	X	730	1PE	C24-C14-OH5-C25
5	X	721	PEG	O2-C3-C4-O4
6	X	728	PGE	O1-C1-C2-O2
8	X	731	1PE	C23-C13-OH4-C24
8	X	730	1PE	OH4-C13-C23-OH3
5	X	723	PEG	O1-C1-C2-O2
8	X	730	1PE	OH2-C12-C22-OH3
4	X	711	EDO	O1-C1-C2-O2
4	X	714	EDO	O1-C1-C2-O2
5	X	715	PEG	O2-C3-C4-O4
6	X	726	PGE	C3-C4-O3-C5
6	X	724	PGE	C6-C5-O3-C4
4	X	709	EDO	O1-C1-C2-O2
8	X	730	1PE	OH5-C14-C24-OH4
6	X	728	PGE	O2-C3-C4-O3
8	X	731	1PE	C14-C24-OH4-C13
5	X	723	PEG	C4-C3-O2-C2
8	X	730	1PE	OH6-C15-C25-OH5

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Mol	Chain	Res	Type	Atoms
8	X	730	1PE	OH7-C16-C26-OH6
5	X	720	PEG	O1-C1-C2-O2
6	X	727	PGE	O3-C5-C6-O4
5	X	716	PEG	O1-C1-C2-O2
6	X	724	PGE	O1-C1-C2-O2
5	X	719	PEG	C1-C2-O2-C3
6	X	726	PGE	C1-C2-O2-C3
4	X	703	EDO	O1-C1-C2-O2
5	X	716	PEG	O2-C3-C4-O4
5	X	717	PEG	O1-C1-C2-O2
8	X	730	1PE	C14-C24-OH4-C13
6	X	727	PGE	C3-C4-O3-C5
4	X	707	EDO	O1-C1-C2-O2
5	X	717	PEG	C1-C2-O2-C3
6	X	728	PGE	C4-C3-O2-C2
5	X	723	PEG	C1-C2-O2-C3
7	X	729	PG4	C5-C6-O4-C7
5	X	716	PEG	C1-C2-O2-C3
8	X	730	1PE	C16-C26-OH6-C15
7	X	729	PG4	C6-C5-O3-C4
8	X	731	1PE	C25-C15-OH6-C26
6	X	725	PGE	O1-C1-C2-O2
7	X	729	PG4	O3-C5-C6-O4
4	X	710	EDO	O1-C1-C2-O2
6	X	727	PGE	O2-C3-C4-O3
5	X	719	PEG	O1-C1-C2-O2
5	X	722	PEG	O2-C3-C4-O4
5	X	723	PEG	O2-C3-C4-O4
6	X	725	PGE	C4-C3-O2-C2
8	X	730	1PE	C25-C15-OH6-C26

There are no ring outliers.

17 monomers are involved in 89 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	X	703	EDO	6	0
4	X	711	EDO	5	0
5	X	719	PEG	6	0
5	X	720	PEG	1	0
5	X	718	PEG	2	0
6	X	724	PGE	10	0
4	X	705	EDO	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	X	717	PEG	3	0
8	X	730	1PE	17	0
6	X	728	PGE	8	0
7	X	729	PG4	4	0
8	X	731	1PE	1	0
5	X	722	PEG	4	0
4	X	708	EDO	1	0
5	X	715	PEG	1	0
5	X	721	PEG	16	0
5	X	723	PEG	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	X	620/621 (99%)	0.05	34 (5%)	30 36	5, 13, 30, 148	75 (12%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	135[A]	ALA	11.7
1	X	105	PHE	10.2
1	X	55	ALA	9.3
1	X	9	ALA	6.9
1	X	564[A]	GLY	6.3
1	X	315	CYS	5.9
1	X	48	ALA	5.8
1	X	628	ASN	5.6
1	X	266	ASP	5.4
1	X	479[A]	ARG	5.3
1	X	181[A]	VAL	5.3
1	X	313[A]	LEU	5.2
1	X	51	ALA	5.0
1	X	563[A]	GLY	4.5
1	X	52	GLY	4.3
1	X	565[A]	ALA	4.2
1	X	53	SER	4.1
1	X	108	VAL	3.8
1	X	629	PRO	3.5
1	X	182[A]	VAL	3.5
1	X	50	GLY	3.5
1	X	136	PRO	3.4
1	X	54	GLU	2.8
1	X	336[A]	ARG	2.8
1	X	312	GLU	2.6
1	X	106	GLU	2.6
1	X	317	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	X	296	TYR	2.6
1	X	57[A]	ASP	2.2
1	X	89	GLU	2.2
1	X	358	LEU	2.1
1	X	111[A]	LEU	2.0
1	X	208[A]	GLU	2.0
1	X	107[A]	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	TPQ	X	382	14/15	0.95	0.09	8,12,14,14	0

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
5	PEG	X	722	7/7	0.70	0.39	10,18,39,39	17
6	PGE	X	727	10/10	0.70	0.26	21,26,36,42	24
5	PEG	X	723	7/7	0.72	0.33	10,19,32,32	17
5	PEG	X	719	7/7	0.78	0.36	16,22,33,39	17
6	PGE	X	724	10/10	0.78	0.29	31,80,109,123	24
4	EDO	X	712	4/4	0.78	0.23	21,26,29,30	10
5	PEG	X	718	7/7	0.79	0.23	9,16,24,25	17
5	PEG	X	716	7/7	0.79	0.25	20,26,35,42	17
4	EDO	X	707	4/4	0.80	0.21	57,69,88,105	0
5	PEG	X	720	7/7	0.81	0.18	17,26,31,33	17

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PEG	X	717	7/7	0.82	0.25	15,23,49,59	17
4	EDO	X	713	4/4	0.83	0.15	23,30,36,36	10
5	PEG	X	721	7/7	0.83	0.27	8,23,31,31	17
6	PGE	X	725	10/10	0.84	0.24	20,29,36,71	24
8	1PE	X	730	16/16	0.84	0.20	11,26,34,37	38
4	EDO	X	708	4/4	0.85	0.20	22,27,34,40	10
4	EDO	X	703	4/4	0.86	0.17	19,23,28,28	10
4	EDO	X	714	4/4	0.86	0.14	20,24,28,28	10
5	PEG	X	715	7/7	0.88	0.16	22,32,46,56	17
7	PG4	X	729	13/13	0.90	0.16	9,19,35,62	31
4	EDO	X	710	4/4	0.90	0.13	18,22,30,36	10
8	1PE	X	731	16/16	0.90	0.17	37,77,100,111	0
4	EDO	X	709	4/4	0.91	0.14	20,29,40,40	10
6	PGE	X	728	10/10	0.91	0.12	7,13,27,32	24
4	EDO	X	706	4/4	0.91	0.10	22,27,28,32	10
4	EDO	X	704	4/4	0.91	0.11	44,53,66,79	0
4	EDO	X	705	4/4	0.91	0.14	10,15,22,26	10
4	EDO	X	711	4/4	0.94	0.12	14,21,43,43	10
6	PGE	X	726	10/10	0.95	0.08	19,30,62,75	0
9	OXY	X	732	2/2	0.96	0.21	16,16,16,22	0
9	OXY	X	733	2/2	0.97	0.21	14,14,14,31	0
9	OXY	X	734	2/2	0.98	0.22	21,21,21,21	0
9	OXY	X	735	2/2	0.99	0.12	11,11,11,27	0
3	NA	X	702	1/1	1.00	0.06	7,7,7,7	0
2	CU	X	701	1/1	1.00	0.02	9,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.