



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:11 AM UTC

PDB ID : 3WA3 / pdb_00003wa3
Title : Crystal structure of copper amine oxidase from arthrobacter globiformis in N2 condition
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 : 1.55 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

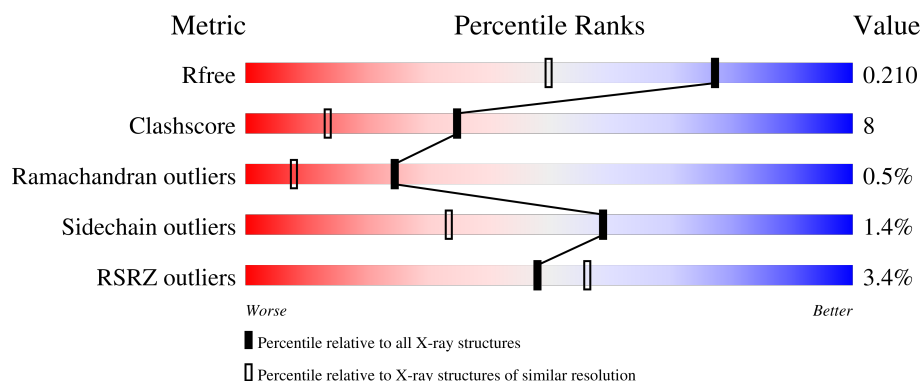
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	621	5% 90% 10%
1	B	621	2% 89% 11%

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
5	PG4	B	1007	-	-	X	-
7	EDO	A	1009	-	-	X	-
7	EDO	A	1014	-	-	X	-
7	EDO	B	1011	-	-	X	-
7	EDO	B	1014	-	-	X	-
8	PEG	A	1019	-	-	X	-
8	PEG	A	1020	-	-	X	-
8	PEG	A	1021	-	-	X	-
8	PEG	B	1019	-	-	X	-
8	PEG	B	1021	-	-	X	-
8	PEG	B	1024	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 11978 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 Phenylethylamine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	621	Total	C	N	O	S	0	22	0
			5014	3168	885	952	9			
1	B	621	Total	C	N	O	S	0	10	0
			4947	3122	875	941	9			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cu	0	0
			1	1		
2	B	1	Total	Cu	0	0
			1	1		

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

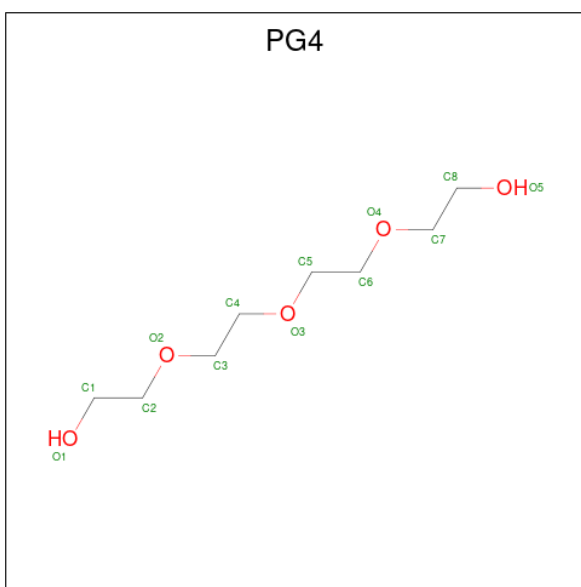
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



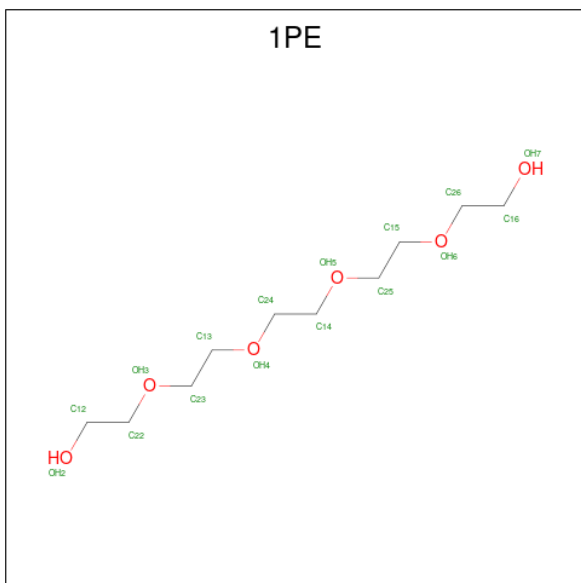
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 13	C 8	O 5	0	0
5	A	1	Total 13	C 8	O 5	0	0
5	B	1	Total 13	C 8	O 5	0	0
5	B	1	Total 13	C 8	O 5	0	0

- Molecule 6 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $\text{C}_{10}\text{H}_{22}\text{O}_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			16	10	6		
6	B	1	Total	C	O	0	0
			16	10	6		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



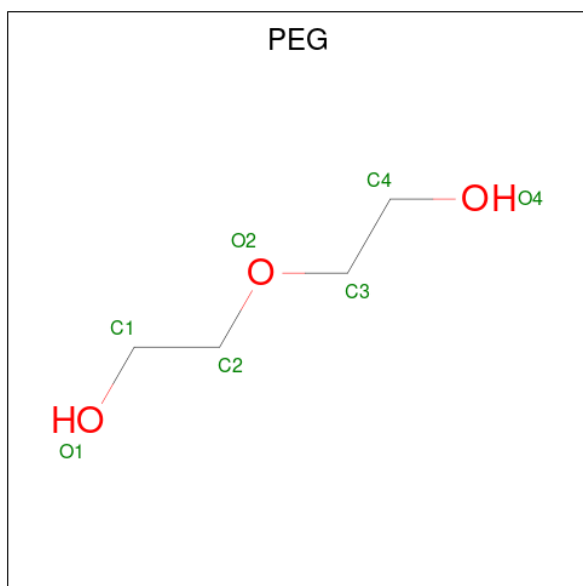
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



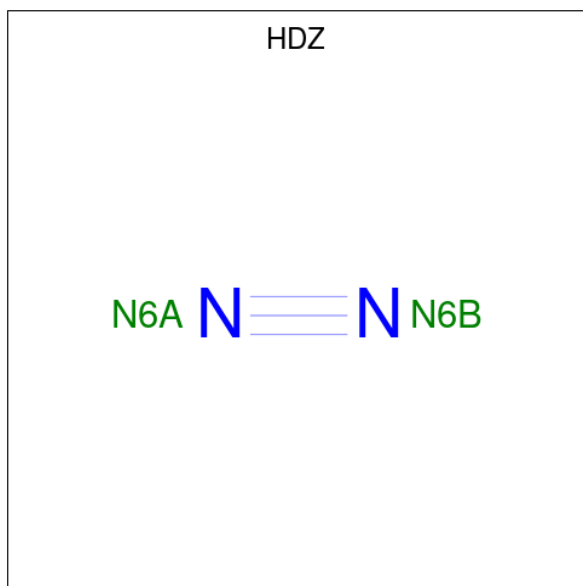
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 7 4 3	0	0
8	A	1	Total C O 7 4 3	0	0
8	A	1	Total C O 7 4 3	0	0

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

- Molecule 9 is NITROGEN MOLECULE (CCD ID: HDZ) (formula: N₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total N 2 2	0	0
9	B	1	Total N 2 2	0	0

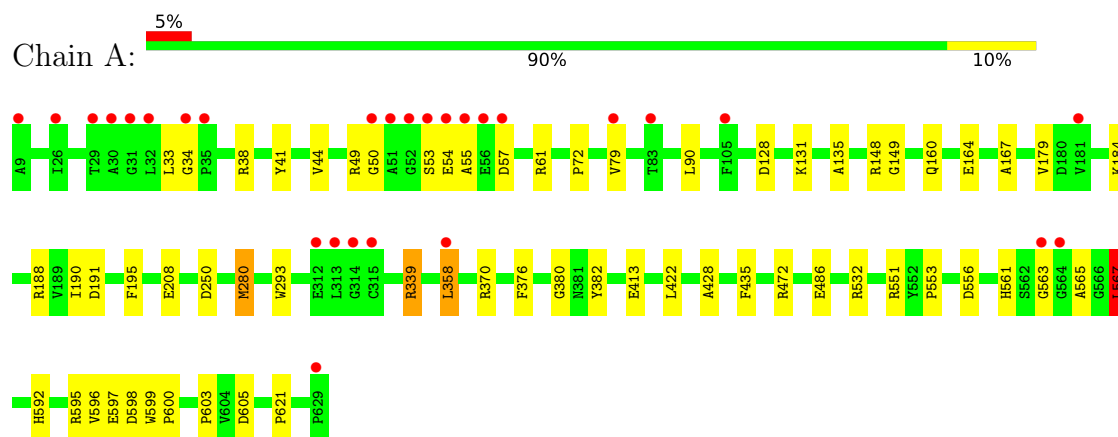
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	820	Total 820	O 820	0	0
10	B	889	Total 889	O 889	0	0

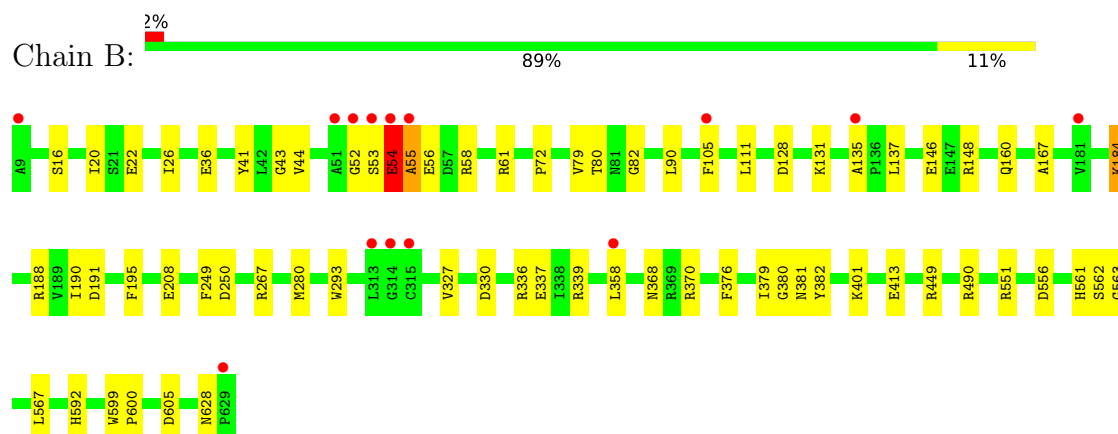
3 Residue-property plots [i](#)

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: Phenylethylamine oxidase



- 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	191.61Å 63.04Å 158.01Å 90.00° 117.44° 90.00°	Depositor
Resolution (Å)	29.93 – 1.55 29.93 – 1.55	Depositor EDS
% Data completeness (in resolution range)	94.7 (29.93-1.55) 94.8 (29.93-1.55)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 1.55Å)	Xtrriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.181 , 0.210 (Not available) , 0.210	Depositor DCC
R_{free} test set	11551 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	16.2	Xtrriage
Anisotropy	0.085	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11978	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 86.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.6872e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PG4, CU, HDZ, NA, 1PE, TPQ, PGE, PEG, EDO

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	0.72	0/5165	0.92	8/7027 (0.1%)
1	B	0.76	0/5073	0.94	3/6903 (0.0%)
All	All	0.74	0/10238	0.93	11/13930 (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	B	0	1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	34	GLY	CA-C-N	6.40	125.98	119.19
1	A	34	GLY	C-N-CA	6.40	125.98	119.19
1	B	567	LEU	CA-C-N	-6.00	112.69	119.28
1	B	567	LEU	C-N-CA	-6.00	112.69	119.28
1	B	280	MET	CG-SD-CE	-5.81	88.11	100.90
1	A	567[A]	LEU	CA-C-N	-5.78	113.72	119.56
1	A	567[A]	LEU	C-N-CA	-5.78	113.72	119.56
1	A	567[B]	LEU	CA-C-N	-5.78	113.72	119.56
1	A	567[B]	LEU	C-N-CA	-5.78	113.72	119.56
1	A	55	ALA	N-CA-C	5.75	117.41	107.93
1	A	280	MET	CG-SD-CE	-5.46	88.89	100.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	56	GLU	Peptide

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	A	5014	0	4871	65	1
1	B	4947	0	4782	69	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	30	0	42	4	0
4	B	30	0	42	6	0
5	A	26	0	35	8	0
5	B	26	0	36	13	0
6	A	16	0	22	5	0
6	B	16	0	22	3	0
7	A	32	0	48	9	0
7	B	40	0	60	17	0
8	A	42	0	60	23	0
8	B	42	0	60	16	2
9	A	2	0	0	0	0
9	B	2	0	0	0	0
10	A	820	0	0	19	6
10	B	889	0	0	17	3
All	All	11978	0	10080	153	9

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 8.

All (153) 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:B:368:ASN:HD22	7:B:1015:EDO:H12	1.13	1.08
1:B:380:GLY:HA2	5:B:1007:PG4:H82	1.40	1.01
1:B:368:ASN:ND2	7:B:1015:EDO:H12	1.83	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:GLY:HA2	5:A:1007:PG4:H72	1.53	0.88
1:B:551:ARG:HD3	4:B:1005:PGE:H5	1.56	0.87
1:A:551:ARG:HD3	8:A:1022:PEG:H11	1.60	0.83
1:B:561:HIS:ND1	1:B:562[A]:SER:O	2.11	0.82
1:A:370:ARG:HH12	8:A:1021:PEG:H11	1.44	0.81
1:A:61[A]:ARG:NH1	7:A:1009:EDO:O2	2.14	0.77
1:B:22:GLU:OE1	10:B:1920:HOH:O	2.05	0.75
1:A:44:VAL:N	7:A:1014:EDO:H12	2.02	0.75
1:A:413[B]:GLU:HB2	8:A:1019:PEG:H11	1.69	0.74
1:B:61[A]:ARG:NH1	7:B:1014:EDO:O2	2.19	0.73
1:B:131:LYS:NZ	10:B:1981:HOH:O	2.18	0.73
1:B:44:VAL:HG12	7:B:1011:EDO:H21	1.69	0.73
1:A:563[B]:GLY:O	10:A:1481:HOH:O	2.09	0.71
7:B:1015:EDO:O1	10:B:1657:HOH:O	2.10	0.69
1:B:249:PHE:O	7:B:1011:EDO:H22	1.92	0.69
1:B:208[B]:GLU:OE1	10:B:1780:HOH:O	2.10	0.69
1:A:472:ARG:O	4:A:1005:PGE:H2	1.93	0.68
5:A:1006:PG4:H21	10:A:1775:HOH:O	1.92	0.68
1:B:380:GLY:H	8:B:1019:PEG:H41	1.57	0.68
1:A:250:ASP:OD1	7:A:1014:EDO:H11	1.94	0.67
1:A:486:GLU:OE2	10:A:1650:HOH:O	2.12	0.67
5:A:1006:PG4:H42	10:A:1775:HOH:O	1.93	0.67
1:A:135:ALA:HB1	5:A:1007:PG4:H52	1.76	0.67
1:A:553:PRO:HA	1:A:567[A]:LEU:HD13	1.76	0.66
1:B:148:ARG:NH2	10:B:1601:HOH:O	2.28	0.66
1:A:250:ASP:HA	7:A:1014:EDO:H22	1.77	0.65
1:A:370:ARG:NH1	8:A:1021:PEG:H11	2.11	0.65
1:A:592:HIS:CD2	8:A:1020:PEG:H12	2.31	0.65
1:B:599:TRP:CD2	1:B:600:PRO:HA	2.32	0.65
1:B:370:ARG:HH12	8:B:1021:PEG:C1	2.10	0.65
1:B:380:GLY:HA3	5:B:1007:PG4:H42	1.80	0.64
1:A:413[B]:GLU:H	8:A:1019:PEG:H12	1.65	0.62
1:B:339:ARG:NH2	10:B:1867:HOH:O	2.34	0.61
1:B:330:ASP:OD2	1:B:336[B]:ARG:NH2	2.33	0.60
5:A:1006:PG4:H61	10:A:1775:HOH:O	2.01	0.60
1:A:603[B]:PRO:HG2	10:A:1695:HOH:O	2.03	0.59
1:A:190:ILE:HG23	6:A:1008:1PE:H232	1.85	0.58
1:B:413:GLU:H	8:B:1024:PEG:H22	1.68	0.58
1:A:131:LYS:NZ	10:A:1844:HOH:O	2.37	0.58
1:B:135:ALA:HB1	5:B:1007:PG4:H62	1.84	0.58
1:A:605:ASP:OD2	8:A:1020:PEG:H32	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:TRP:CD2	1:A:600:PRO:HA	2.39	0.57
7:B:1017:EDO:H22	10:B:1705:HOH:O	2.03	0.57
1:A:413[B]:GLU:H	8:A:1019:PEG:C1	2.18	0.56
1:A:621:PRO:HD2	10:A:1274:HOH:O	2.05	0.56
1:B:137:LEU:HD21	5:B:1007:PG4:H11	1.86	0.56
1:B:43:GLY:CA	7:B:1011:EDO:H12	2.35	0.56
1:B:327:VAL:HG23	8:B:1020:PEG:H11	1.88	0.55
4:B:1003:PGE:H6	8:B:1024:PEG:H12	1.86	0.55
1:B:449:ARG:NH1	10:B:1722:HOH:O	2.40	0.55
1:B:413:GLU:H	8:B:1024:PEG:C2	2.20	0.54
1:A:370:ARG:HH12	8:A:1021:PEG:C1	2.18	0.54
1:A:598:ASP:OD2	8:A:1020:PEG:H11	2.08	0.54
1:B:592:HIS:CE1	7:B:1017:EDO:H21	2.43	0.54
1:B:44:VAL:HG12	7:B:1011:EDO:C2	2.38	0.54
1:B:380:GLY:H	8:B:1019:PEG:C4	2.21	0.54
1:A:149:GLY:O	10:A:1459:HOH:O	2.19	0.53
1:B:20:ILE:HD12	1:B:327:VAL:HG12	1.90	0.53
1:B:128:ASP:HB2	5:B:1006:PG4:H22	1.91	0.53
1:B:490:ARG:NH1	10:B:1559:HOH:O	2.34	0.53
1:A:380:GLY:HA2	5:A:1007:PG4:C7	2.33	0.53
1:B:380:GLY:N	8:B:1019:PEG:H41	2.24	0.52
1:B:370:ARG:HH12	8:B:1021:PEG:H12	1.73	0.52
1:B:370:ARG:HH12	8:B:1021:PEG:H11	1.74	0.52
1:A:61[A]:ARG:HE	7:A:1009:EDO:H11	1.75	0.51
1:A:598:ASP:OD1	8:A:1020:PEG:H22	2.10	0.51
1:B:160:GLN:HG3	1:B:167:ALA:HB2	1.92	0.51
1:A:191:ASP:HB3	6:A:1008:1PE:H242	1.93	0.51
1:A:595[A]:ARG:HD2	1:A:597:GLU:HB2	1.91	0.51
1:A:413[A]:GLU:HG2	8:A:1019:PEG:H11	1.93	0.51
1:A:191:ASP:HB3	6:A:1008:1PE:H252	1.93	0.50
1:A:44:VAL:H	7:A:1014:EDO:H12	1.74	0.50
1:A:57:ASP:OD2	10:A:1605:HOH:O	2.19	0.50
1:A:41:TYR:CE2	7:A:1009:EDO:H12	2.46	0.49
8:A:1021:PEG:H22	10:A:1185:HOH:O	2.11	0.49
1:A:38:ARG:HD2	10:A:1894:HOH:O	2.12	0.49
1:B:250:ASP:HA	7:B:1011:EDO:H11	1.93	0.49
1:A:72:PRO:HG2	1:A:90:LEU:HB2	1.93	0.49
1:A:561:HIS:CE1	1:A:565:ALA:HB2	2.48	0.48
1:B:16:SER:HB3	8:B:1020:PEG:H31	1.94	0.48
1:B:336[A]:ARG:HD3	10:B:1870:HOH:O	2.13	0.48
1:B:551:ARG:NH2	10:B:1778:HOH:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:561:HIS:HD1	1:B:563[B]:GLY:H	1.60	0.48
1:A:380:GLY:HA3	5:A:1007:PG4:H32	1.96	0.48
1:B:41:TYR:CE2	7:B:1014:EDO:H12	2.49	0.47
1:A:370:ARG:NH1	8:A:1021:PEG:H31	2.29	0.47
1:B:250:ASP:OD1	7:B:1011:EDO:H11	2.15	0.47
1:A:208:GLU:O	4:A:1004:PGE:H22	2.13	0.47
1:B:190:ILE:HG23	6:B:1008:1PE:H222	1.97	0.46
1:A:595[B]:ARG:HE	8:A:1020:PEG:C2	2.28	0.46
1:B:293:TRP:CD1	1:B:293:TRP:H	2.33	0.46
1:A:595[B]:ARG:HE	8:A:1020:PEG:H22	1.81	0.46
1:B:43:GLY:HA3	7:B:1011:EDO:H12	1.97	0.46
1:B:105:PHE:CE2	5:B:1007:PG4:H72	2.51	0.46
1:B:36:GLU:HB3	10:B:1947:HOH:O	2.14	0.46
4:B:1005:PGE:H42	10:B:1339:HOH:O	2.16	0.45
1:B:605:ASP:HB3	7:B:1017:EDO:H11	1.99	0.45
4:B:1005:PGE:H12	10:B:1281:HOH:O	2.17	0.45
4:A:1004:PGE:H42	10:A:1900:HOH:O	2.16	0.45
1:B:137:LEU:CD2	5:B:1007:PG4:H11	2.47	0.45
1:B:370:ARG:HH22	8:B:1021:PEG:C1	2.30	0.44
4:A:1003:PGE:H3	8:A:1019:PEG:O4	2.17	0.44
1:B:551:ARG:HG2	4:B:1005:PGE:H4	1.99	0.44
1:A:595[B]:ARG:HG3	8:A:1020:PEG:O1	2.16	0.44
1:B:41:TYR:OH	7:B:1014:EDO:H12	2.17	0.44
6:A:1008:1PE:H242	6:A:1008:1PE:H252	1.76	0.44
1:B:267:ARG:NH1	10:B:1887:HOH:O	2.51	0.43
1:B:379:ILE:HG22	5:B:1007:PG4:H41	2.00	0.43
6:B:1008:1PE:H241	10:B:1707:HOH:O	2.18	0.43
1:A:595[B]:ARG:NE	8:A:1020:PEG:C2	2.81	0.43
1:A:596[A]:VAL:HG23	10:A:1156:HOH:O	2.17	0.43
1:A:280:MET:HG3	1:A:435:PHE:CE2	2.54	0.43
1:A:422:LEU:HD11	1:A:428:ALA:HB2	1.99	0.43
1:B:36:GLU:OE2	10:B:1795:HOH:O	2.21	0.43
1:A:164:GLU:HG3	10:A:1880:HOH:O	2.18	0.43
1:B:26:ILE:HD11	1:B:82:GLY:HA2	2.01	0.42
1:B:381:ASN:OD1	5:B:1007:PG4:H21	2.19	0.42
1:A:595[A]:ARG:CD	1:A:597:GLU:HB2	2.49	0.42
5:B:1006:PG4:H42	5:B:1006:PG4:H21	1.73	0.42
1:A:195:PHE:CE2	8:A:1019:PEG:H42	2.55	0.42
1:B:146:GLU:CD	1:B:188[A]:ARG:HH11	2.26	0.42
5:B:1006:PG4:H42	5:B:1006:PG4:H62	1.62	0.42
1:B:61[A]:ARG:HE	7:B:1014:EDO:H11	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LEU:HD12	1:A:33:LEU:HA	1.84	0.42
1:A:188[B]:ARG:NH1	7:A:1016:EDO:O1	2.47	0.42
1:A:195:PHE:HE2	8:A:1019:PEG:H42	1.85	0.41
1:A:358:LEU:HD22	1:A:358:LEU:HA	1.70	0.41
1:B:401:LYS:NZ	8:B:1021:PEG:H31	2.35	0.41
1:A:61[B]:ARG:HH12	1:A:556:ASP:CG	2.29	0.41
1:B:191:ASP:HB3	6:B:1008:1PE:H132	2.02	0.41
4:B:1004:PGE:H42	4:B:1004:PGE:H62	1.68	0.41
1:B:61[B]:ARG:HH12	1:B:556:ASP:CG	2.27	0.41
5:B:1007:PG4:H52	8:B:1019:PEG:H41	2.03	0.41
1:A:148[B]:ARG:HD3	1:B:80:THR:HG22	2.02	0.41
8:A:1021:PEG:H12	10:A:1259:HOH:O	2.20	0.41
1:B:111:LEU:HD21	1:B:184:LYS:HG3	2.02	0.41
1:A:128:ASP:HB2	5:A:1006:PG4:H22	2.03	0.41
1:A:160:GLN:HG3	1:A:167:ALA:HB2	2.03	0.41
1:A:293:TRP:CD1	1:A:293:TRP:H	2.37	0.41
1:B:54:GLU:HB3	1:B:55:ALA:H	1.54	0.41
1:B:72:PRO:HG2	1:B:90:LEU:HB2	2.02	0.41
5:B:1007:PG4:H82	5:B:1007:PG4:H61	1.90	0.41
1:A:49:ARG:HD3	10:A:1859:HOH:O	2.20	0.40
1:B:58:ARG:O	1:B:79:VAL:HG22	2.22	0.40
1:A:41:TYR:OH	7:A:1009:EDO:H12	2.21	0.40
1:A:339:ARG:NH2	10:A:1548:HOH:O	2.55	0.40
6:A:1008:1PE:H262	10:A:1404:HOH:O	2.21	0.40
1:B:195:PHE:CD2	8:B:1024:PEG:H11	2.57	0.40
1:B:413:GLU:N	8:B:1024:PEG:H22	2.34	0.40
1:A:370:ARG:HH22	8:A:1021:PEG:H11	1.86	0.40

All (9) 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:A:1262:HOH:O	10:A:1262:HOH:O[2_756]	2.07	0.13
8:B:1022:PEG:O4	10:B:1566:HOH:O[2_755]	2.11	0.09
10:A:1815:HOH:O	10:A:1819:HOH:O[2_756]	2.12	0.08
1:A:532[B]:ARG:NH1	10:A:1648:HOH:O[2_756]	2.13	0.07
10:A:1619:HOH:O	10:A:1622:HOH:O[2_756]	2.13	0.07
8:B:1021:PEG:O4	10:B:1657:HOH:O[2_755]	2.13	0.07
10:A:1806:HOH:O	10:A:1811:HOH:O[2_756]	2.15	0.05
10:B:1854:HOH:O	10:B:1857:HOH:O[2_755]	2.18	0.02
10:A:1883:HOH:O	10:A:1895:HOH:O[2_756]	2.19	0.01

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	640/621 (103%)	612 (96%)	26 (4%)	2 (0%)	36	18
1	B	628/621 (101%)	607 (97%)	17 (3%)	4 (1%)	21	6
All	All	1268/1242 (102%)	1219 (96%)	43 (3%)	6 (0%)	24	8

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	53	SER
1	A	54	GLU
1	B	55	ALA
1	B	52	GLY
1	B	54	GLU
1	A	50	GLY

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	534/514 (104%)	525 (98%)	9 (2%)	53	25
1	B	523/514 (102%)	517 (99%)	6 (1%)	65	43
All	All	1057/1028 (103%)	1042 (99%)	15 (1%)	59	33

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	SER
1	A	79	VAL
1	A	179	VAL
1	A	184	LYS
1	A	339	ARG
1	A	358	LEU
1	A	376	PHE
1	A	567[A]	LEU
1	A	567[B]	LEU
1	B	54	GLU
1	B	184	LYS
1	B	337	GLU
1	B	358	LEU
1	B	376	PHE
1	B	628	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	340	ASN
1	A	418	ASN
1	A	518	ASN
1	A	519	GLN
1	B	81	ASN
1	B	368	ASN
1	B	418	ASN
1	B	518	ASN
1	B	573	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	TPQ	B	382	1	13,14,15	2.54	2 (15%)	13,19,21	1.75	3 (23%)
1	TPQ	A	382	1	13,14,15	2.63	2 (15%)	13,19,21	1.39	3 (23%)

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	B	382	1	-	1/5/22/24	0/1/1/1
1	TPQ	A	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	B	382	TPQ	C3-C4	6.86	1.48	1.36
1	A	382	TPQ	C3-C4	6.56	1.48	1.36
1	A	382	TPQ	C6-C1	6.12	1.49	1.34
1	B	382	TPQ	C6-C1	5.37	1.47	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	382	TPQ	C6-C1-C2	4.53	121.88	118.66
1	B	382	TPQ	C1-C6-C5	-2.60	118.22	122.59
1	A	382	TPQ	C1-C6-C5	-2.43	118.51	122.59
1	A	382	TPQ	C6-C1-C2	2.17	120.20	118.66
1	A	382	TPQ	C6-C5-C4	2.17	120.59	116.80
1	B	382	TPQ	C6-C5-C4	2.13	120.52	116.80

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 48 ligands modelled in this entry, 4 are monoatomic - leaving 44 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	$\# Z > 2$
7	EDO	B	1014	-	3,3,3	0.30	0	2,2,2	0.09	0
7	EDO	B	1013	-	3,3,3	0.41	0	2,2,2	0.30	0
5	PG4	A	1006	-	12,12,12	0.71	0	11,11,11	0.90	0
8	PEG	A	1019	-	6,6,6	0.70	0	5,5,5	0.98	1 (20%)
7	EDO	B	1012	-	3,3,3	0.48	0	2,2,2	0.23	0
8	PEG	A	1018	-	6,6,6	0.62	0	5,5,5	1.04	1 (20%)
8	PEG	B	1023	-	6,6,6	0.58	0	5,5,5	0.78	0
8	PEG	A	1017	-	6,6,6	0.53	0	5,5,5	0.76	0
4	PGE	A	1004	-	9,9,9	0.62	0	8,8,8	0.76	0
4	PGE	B	1003	-	9,9,9	0.67	0	8,8,8	0.70	0
8	PEG	B	1020	-	6,6,6	0.65	0	5,5,5	0.74	0
7	EDO	B	1010	-	3,3,3	0.41	0	2,2,2	0.37	0
8	PEG	B	1019	-	6,6,6	0.62	0	5,5,5	0.84	0
4	PGE	B	1005	-	9,9,9	0.64	0	8,8,8	0.82	0
7	EDO	B	1015	-	3,3,3	0.64	0	2,2,2	1.00	0
7	EDO	B	1018	-	3,3,3	0.44	0	2,2,2	0.33	0
4	PGE	B	1004	-	9,9,9	0.69	0	8,8,8	0.81	0
8	PEG	B	1022	-	6,6,6	0.62	0	5,5,5	0.91	0
7	EDO	A	1009	-	3,3,3	0.41	0	2,2,2	0.11	0
7	EDO	A	1012	-	3,3,3	0.42	0	2,2,2	0.42	0
5	PG4	A	1007	-	12,12,12	0.66	0	11,11,11	0.76	0
7	EDO	A	1016	-	3,3,3	0.55	0	2,2,2	0.12	0
9	HDZ	B	1025	-	1,1,1	0.67	0	-	-	-
6	1PE	B	1008	-	15,15,15	0.66	0	14,14,14	1.04	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PG4	B	1007	-	12,12,12	0.55	0	11,11,11	1.06	2 (18%)
7	EDO	B	1009	-	3,3,3	0.51	0	2,2,2	0.52	0
7	EDO	B	1017	-	3,3,3	0.48	0	2,2,2	0.15	0
7	EDO	A	1011	-	3,3,3	0.53	0	2,2,2	0.26	0
6	1PE	A	1008	-	15,15,15	0.71	0	14,14,14	0.88	0
5	PG4	B	1006	-	12,12,12	0.77	0	11,11,11	0.75	0
8	PEG	B	1021	-	6,6,6	0.90	0	5,5,5	0.75	0
4	PGE	A	1005	-	9,9,9	0.78	0	8,8,8	1.02	1 (12%)
7	EDO	A	1015	-	3,3,3	0.70	0	2,2,2	0.07	0
9	HDZ	A	1023	-	1,1,1	0.70	0	-		
8	PEG	A	1022	-	6,6,6	0.52	0	5,5,5	0.75	0
7	EDO	A	1013	-	3,3,3	0.37	0	2,2,2	0.39	0
8	PEG	A	1020	-	6,6,6	1.17	0	5,5,5	0.86	0
7	EDO	A	1010	-	3,3,3	0.39	0	2,2,2	0.40	0
8	PEG	B	1024	-	6,6,6	0.79	0	5,5,5	0.78	0
7	EDO	B	1016	-	3,3,3	0.45	0	2,2,2	0.45	0
7	EDO	B	1011	-	3,3,3	0.49	0	2,2,2	0.66	0
4	PGE	A	1003	-	9,9,9	0.69	0	8,8,8	0.78	0
8	PEG	A	1021	-	6,6,6	0.73	0	5,5,5	0.86	0
7	EDO	A	1014	-	3,3,3	0.53	0	2,2,2	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
7	EDO	B	1014	-	-	1/1/1/1	-
7	EDO	B	1013	-	-	1/1/1/1	-
5	PG4	A	1006	-	-	4/10/10/10	-
8	PEG	A	1019	-	-	3/4/4/4	-
7	EDO	B	1012	-	-	1/1/1/1	-
8	PEG	A	1018	-	-	1/4/4/4	-
8	PEG	B	1023	-	-	0/4/4/4	-
8	PEG	A	1017	-	-	2/4/4/4	-
4	PGE	A	1004	-	-	5/7/7/7	-
4	PGE	B	1003	-	-	4/7/7/7	-
8	PEG	B	1020	-	-	0/4/4/4	-
7	EDO	B	1010	-	-	0/1/1/1	-
8	PEG	B	1019	-	-	2/4/4/4	-
4	PGE	B	1005	-	-	6/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	B	1015	-	-	0/1/1/1	-
7	EDO	B	1018	-	-	0/1/1/1	-
4	PGE	B	1004	-	-	6/7/7/7	-
8	PEG	B	1022	-	-	2/4/4/4	-
7	EDO	A	1009	-	-	1/1/1/1	-
7	EDO	A	1012	-	-	1/1/1/1	-
5	PG4	A	1007	-	-	3/10/10/10	-
7	EDO	A	1016	-	-	0/1/1/1	-
6	1PE	B	1008	-	-	6/13/13/13	-
5	PG4	B	1007	-	-	6/10/10/10	-
7	EDO	B	1009	-	-	1/1/1/1	-
7	EDO	B	1017	-	-	0/1/1/1	-
7	EDO	A	1011	-	-	0/1/1/1	-
6	1PE	A	1008	-	-	6/13/13/13	-
5	PG4	B	1006	-	-	6/10/10/10	-
8	PEG	B	1021	-	-	2/4/4/4	-
4	PGE	A	1005	-	-	3/7/7/7	-
7	EDO	A	1015	-	-	0/1/1/1	-
8	PEG	A	1022	-	-	1/4/4/4	-
7	EDO	A	1013	-	-	1/1/1/1	-
8	PEG	A	1020	-	-	3/4/4/4	-
7	EDO	A	1010	-	-	0/1/1/1	-
8	PEG	B	1024	-	-	1/4/4/4	-
7	EDO	B	1016	-	-	0/1/1/1	-
7	EDO	B	1011	-	-	1/1/1/1	-
4	PGE	A	1003	-	-	4/7/7/7	-
8	PEG	A	1021	-	-	3/4/4/4	-
7	EDO	A	1014	-	-	1/1/1/1	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1007	PG4	O2-C2-C1	2.50	121.14	110.11
8	A	1018	PEG	C3-O2-C2	2.22	123.00	113.26
6	B	1008	1PE	C25-OH5-C14	2.16	122.70	113.26
4	A	1005	PGE	C3-O2-C2	2.09	122.43	113.26
8	A	1019	PEG	C3-O2-C2	2.09	122.42	113.26
5	B	1007	PG4	C3-O2-C2	2.04	122.18	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1008	1PE	C23-OH3-C22	2.04	122.18	113.26

There are no chirality outliers.

All (88) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1019	PEG	C4-C3-O2-C2
5	B	1007	PG4	C1-C2-O2-C3
5	B	1006	PG4	C6-C5-O3-C4
5	B	1006	PG4	O3-C5-C6-O4
8	A	1021	PEG	C1-C2-O2-C3
4	B	1005	PGE	O2-C3-C4-O3
6	B	1008	1PE	OH4-C13-C23-OH3
4	A	1005	PGE	C1-C2-O2-C3
8	A	1020	PEG	O1-C1-C2-O2
5	B	1007	PG4	O2-C3-C4-O3
6	B	1008	1PE	OH5-C14-C24-OH4
4	B	1003	PGE	C3-C4-O3-C5
4	B	1003	PGE	C1-C2-O2-C3
4	B	1005	PGE	C1-C2-O2-C3
4	A	1004	PGE	O3-C5-C6-O4
5	A	1006	PG4	O4-C7-C8-O5
8	B	1022	PEG	O2-C3-C4-O4
4	A	1005	PGE	O2-C3-C4-O3
6	A	1008	1PE	OH6-C15-C25-OH5
4	A	1003	PGE	O1-C1-C2-O2
4	A	1004	PGE	O1-C1-C2-O2
5	A	1007	PG4	O4-C7-C8-O5
5	B	1007	PG4	O1-C1-C2-O2
8	B	1021	PEG	O1-C1-C2-O2
5	B	1007	PG4	C4-C3-O2-C2
4	B	1005	PGE	O1-C1-C2-O2
8	A	1017	PEG	O1-C1-C2-O2
8	A	1019	PEG	O2-C3-C4-O4
7	B	1011	EDO	O1-C1-C2-O2
8	B	1019	PEG	O1-C1-C2-O2
4	A	1003	PGE	C1-C2-O2-C3
4	B	1003	PGE	O3-C5-C6-O4
4	B	1004	PGE	O3-C5-C6-O4
5	B	1007	PG4	O4-C7-C8-O5
4	B	1004	PGE	C1-C2-O2-C3
6	A	1008	1PE	OH5-C14-C24-OH4

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Mol	Chain	Res	Type	Atoms
7	A	1014	EDO	O1-C1-C2-O2
8	A	1020	PEG	C1-C2-O2-C3
6	B	1008	1PE	OH6-C15-C25-OH5
8	A	1017	PEG	O2-C3-C4-O4
4	A	1004	PGE	C6-C5-O3-C4
4	B	1004	PGE	C6-C5-O3-C4
4	A	1003	PGE	C3-C4-O3-C5
7	A	1012	EDO	O1-C1-C2-O2
7	A	1013	EDO	O1-C1-C2-O2
4	B	1004	PGE	O1-C1-C2-O2
8	B	1019	PEG	O2-C3-C4-O4
8	B	1021	PEG	C1-C2-O2-C3
6	A	1008	1PE	C12-C22-OH3-C23
8	B	1022	PEG	O1-C1-C2-O2
8	A	1019	PEG	O1-C1-C2-O2
6	B	1008	1PE	C12-C22-OH3-C23
4	A	1003	PGE	O2-C3-C4-O3
8	B	1024	PEG	C1-C2-O2-C3
4	B	1004	PGE	C4-C3-O2-C2
8	A	1022	PEG	O2-C3-C4-O4
4	A	1005	PGE	O3-C5-C6-O4
6	A	1008	1PE	C24-C14-OH5-C25
5	A	1007	PG4	O3-C5-C6-O4
5	A	1006	PG4	C8-C7-O4-C6
7	B	1012	EDO	O1-C1-C2-O2
7	B	1013	EDO	O1-C1-C2-O2
4	A	1004	PGE	O2-C3-C4-O3
8	A	1020	PEG	C4-C3-O2-C2
5	B	1006	PG4	O2-C3-C4-O3
4	B	1005	PGE	C4-C3-O2-C2
4	A	1004	PGE	C1-C2-O2-C3
5	B	1006	PG4	C5-C6-O4-C7
7	B	1014	EDO	O1-C1-C2-O2
6	B	1008	1PE	OH7-C16-C26-OH6
8	A	1021	PEG	C4-C3-O2-C2
5	B	1006	PG4	C8-C7-O4-C6
5	B	1006	PG4	C4-C3-O2-C2
4	B	1003	PGE	O2-C3-C4-O3
6	B	1008	1PE	C23-C13-OH4-C24
7	A	1009	EDO	O1-C1-C2-O2
7	B	1009	EDO	O1-C1-C2-O2
6	A	1008	1PE	C25-C15-OH6-C26

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Mol	Chain	Res	Type	Atoms
5	A	1006	PG4	O3-C5-C6-O4
8	A	1018	PEG	O1-C1-C2-O2
5	A	1006	PG4	O2-C3-C4-O3
8	A	1021	PEG	O1-C1-C2-O2
5	B	1007	PG4	O3-C5-C6-O4
4	B	1005	PGE	O3-C5-C6-O4
4	B	1004	PGE	O2-C3-C4-O3
6	A	1008	1PE	C13-C23-OH3-C22
5	A	1007	PG4	O2-C3-C4-O3
4	B	1005	PGE	C6-C5-O3-C4

There are no ring outliers.

28 monomers are involved in 103 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1014	EDO	4	0
5	A	1006	PG4	4	0
8	A	1019	PEG	7	0
4	A	1004	PGE	2	0
4	B	1003	PGE	1	0
8	B	1020	PEG	2	0
8	B	1019	PEG	4	0
4	B	1005	PGE	4	0
7	B	1015	EDO	3	0
4	B	1004	PGE	1	0
8	B	1022	PEG	0	1
7	A	1009	EDO	4	0
5	A	1007	PG4	4	0
7	A	1016	EDO	1	0
6	B	1008	1PE	3	0
5	B	1007	PG4	10	0
7	B	1017	EDO	3	0
6	A	1008	1PE	5	0
5	B	1006	PG4	3	0
8	B	1021	PEG	5	1
4	A	1005	PGE	1	0
8	A	1022	PEG	1	0
8	A	1020	PEG	8	0
8	B	1024	PEG	5	0
7	B	1011	EDO	7	0
4	A	1003	PGE	1	0
8	A	1021	PEG	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1014	EDO	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

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	620/621 (99%)	-0.03	28 (4%)	38 46	7, 18, 39, 110	22 (3%)
1	B	620/621 (99%)	-0.21	14 (2%)	61 69	9, 17, 33, 96	11 (1%)
All	All	1240/1242 (99%)	-0.12	42 (3%)	48 56	7, 17, 36, 110	33 (2%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	55	ALA	7.2
1	B	52	GLY	5.8
1	B	55	ALA	5.2
1	A	53	SER	5.0
1	B	105	PHE	4.8
1	B	53	SER	4.6
1	B	9	ALA	4.6
1	A	51	ALA	4.5
1	A	52	GLY	4.4
1	A	105	PHE	4.1
1	A	29	THR	3.5
1	A	9	ALA	3.2
1	A	30	ALA	3.2
1	A	313	LEU	3.2
1	B	629	PRO	3.1
1	A	315	CYS	3.0
1	B	358	LEU	3.0
1	A	31	GLY	2.8
1	B	315	CYS	2.8
1	B	51	ALA	2.7
1	A	56	GLU	2.7
1	A	50	GLY	2.7
1	A	358	LEU	2.7
1	B	313	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	35	PRO	2.7
1	A	314	GLY	2.5
1	B	54	GLU	2.5
1	A	563[A]	GLY	2.5
1	A	54	GLU	2.5
1	A	26	ILE	2.5
1	B	135	ALA	2.4
1	A	79	VAL	2.3
1	B	181	VAL	2.3
1	A	57	ASP	2.3
1	A	32	LEU	2.2
1	A	629	PRO	2.2
1	A	34	GLY	2.2
1	A	564[A]	GLY	2.1
1	A	312	GLU	2.1
1	A	181	VAL	2.1
1	B	314	GLY	2.1
1	A	83	THR	2.1

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	A	382	14/15	0.94	0.08	10,14,18,18	0
1	TPQ	B	382	14/15	0.95	0.07	9,14,17,18	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($\text{\AA}^2$)	Q<0.9
8	PEG	A	1018	7/7	0.68	0.22	38,38,42,44	7
4	PGE	A	1004	10/10	0.76	0.20	54,57,62,63	0
7	EDO	A	1012	4/4	0.77	0.16	62,62,62,63	0
7	EDO	A	1016	4/4	0.77	0.19	38,45,46,48	0
7	EDO	B	1018	4/4	0.77	0.23	61,62,63,64	0
7	EDO	A	1010	4/4	0.77	0.22	43,44,45,48	0
6	1PE	A	1008	16/16	0.78	0.18	38,45,53,53	16
8	PEG	A	1022	7/7	0.78	0.18	37,43,49,50	0
8	PEG	B	1022	7/7	0.78	0.20	27,29,34,39	7
8	PEG	B	1019	7/7	0.80	0.17	28,38,40,43	0
4	PGE	B	1005	10/10	0.80	0.20	36,38,43,45	10
7	EDO	B	1009	4/4	0.81	0.16	31,36,42,45	0
6	1PE	B	1008	16/16	0.82	0.16	36,42,45,46	16
7	EDO	A	1015	4/4	0.82	0.18	34,35,36,37	0
8	PEG	B	1021	7/7	0.82	0.18	9,22,26,27	7
4	PGE	B	1004	10/10	0.82	0.18	55,60,64,66	0
4	PGE	B	1003	10/10	0.83	0.15	44,51,58,60	0
8	PEG	B	1020	7/7	0.83	0.18	27,29,31,35	7
4	PGE	A	1005	10/10	0.84	0.16	23,30,36,36	0
7	EDO	A	1014	4/4	0.84	0.15	23,24,25,28	4
7	EDO	B	1010	4/4	0.85	0.14	37,39,42,45	0
8	PEG	A	1019	7/7	0.86	0.17	20,22,29,31	7
4	PGE	A	1003	10/10	0.86	0.12	31,40,46,48	0
8	PEG	B	1024	7/7	0.86	0.19	22,24,26,30	7
7	EDO	B	1013	4/4	0.87	0.15	27,32,35,37	4
7	EDO	B	1016	4/4	0.87	0.13	35,35,38,41	0
7	EDO	B	1017	4/4	0.87	0.17	14,18,20,21	4
5	PG4	B	1007	13/13	0.88	0.12	9,23,31,36	0
8	PEG	A	1017	7/7	0.88	0.13	26,33,37,41	7
8	PEG	A	1021	7/7	0.88	0.17	15,26,33,35	7
7	EDO	B	1014	4/4	0.89	0.16	22,23,27,29	4
7	EDO	B	1015	4/4	0.89	0.11	8,11,14,17	4
5	PG4	A	1006	13/13	0.89	0.13	17,29,38,43	0
5	PG4	A	1007	13/13	0.90	0.11	8,21,30,37	0
7	EDO	A	1009	4/4	0.90	0.15	23,26,27,34	4
7	EDO	A	1013	4/4	0.90	0.11	30,33,34,34	4
7	EDO	A	1011	4/4	0.91	0.10	28,31,34,37	0
5	PG4	B	1006	13/13	0.91	0.11	15,23,39,39	0
8	PEG	A	1020	7/7	0.92	0.14	9,19,28,37	7
8	PEG	B	1023	7/7	0.92	0.09	27,32,33,35	0
7	EDO	B	1011	4/4	0.92	0.12	20,20,21,28	4
7	EDO	B	1012	4/4	0.94	0.09	27,32,35,39	0
9	HDZ	A	1023	2/2	0.94	0.20	26,26,26,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	HDZ	B	1025	2/2	0.96	0.15	25,25,25,27	0
3	NA	B	1002	1/1	0.99	0.04	11,11,11,11	0
2	CU	B	1001	1/1	0.99	0.02	12,12,12,12	0
3	NA	A	1002	1/1	0.99	0.05	12,12,12,12	0
2	CU	A	1001	1/1	1.00	0.02	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.