wwPDB X-ray Structure Validation Summary Report (i)

Nov 2, 2023 – 10:00 PM EDT

PDB ID	:	3WA2
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 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 (i) 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 (i)) were used in the production of this report:

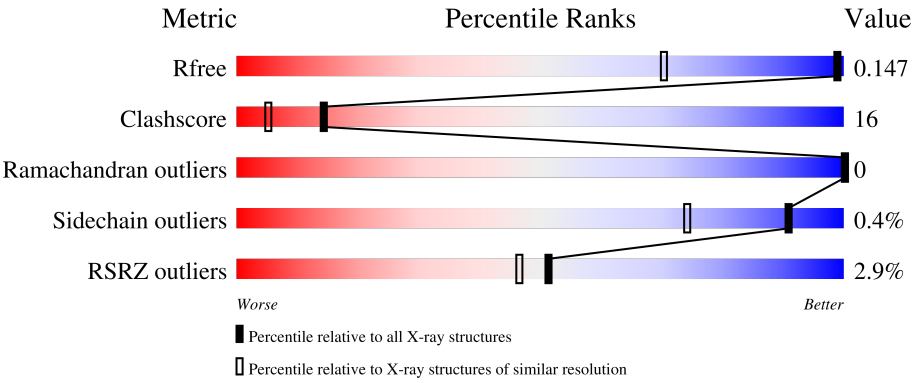
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	1386 (1.12-1.04)
Clashscore	141614	1021 (1.10-1.06)
Ramachandran outliers	138981	1381 (1.12-1.04)
Sidechain outliers	138945	1379 (1.12-1.04)
RSRZ outliers	127900	1359 (1.12-1.04)

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 <=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	3% 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	708	-	-	X	-
4	EDO	X	711	-	-	X	-
5	PEG	X	717	-	-	X	-
5	PEG	X	719	-	-	X	X
5	PEG	X	721	-	-	X	-
5	PEG	X	722	-	-	X	X
5	PEG	X	723	-	-	X	X
6	PGE	X	724	-	-	X	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
			Total	C	H	N	O	S			
1	X	621	10768	3422	5412	933	988	13	0	91	0

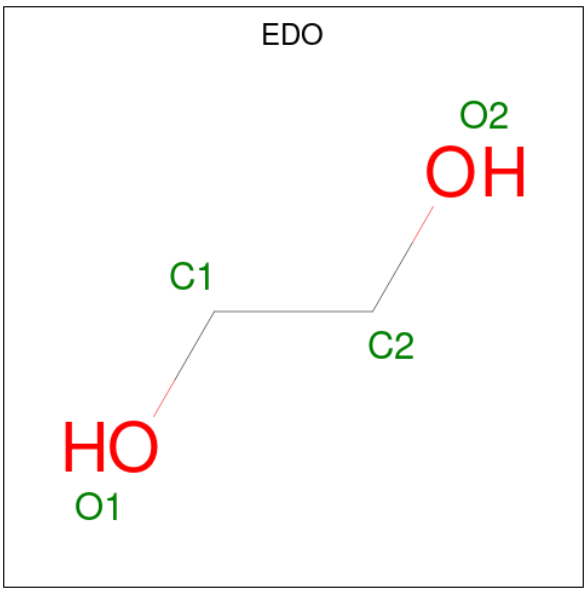
- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

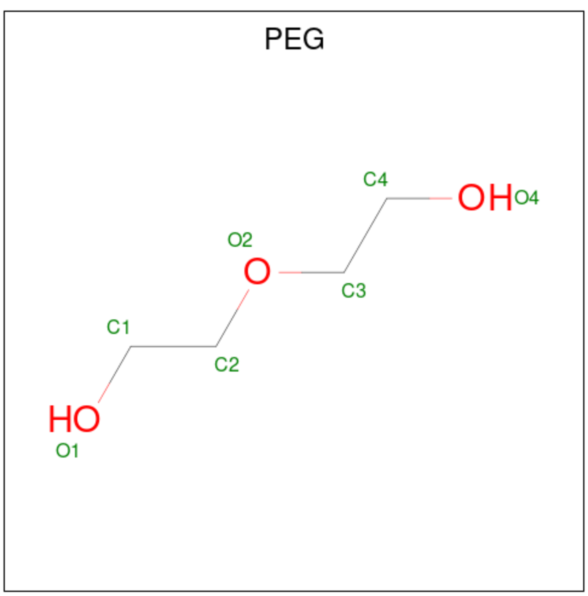
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
3	X	1	1	1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



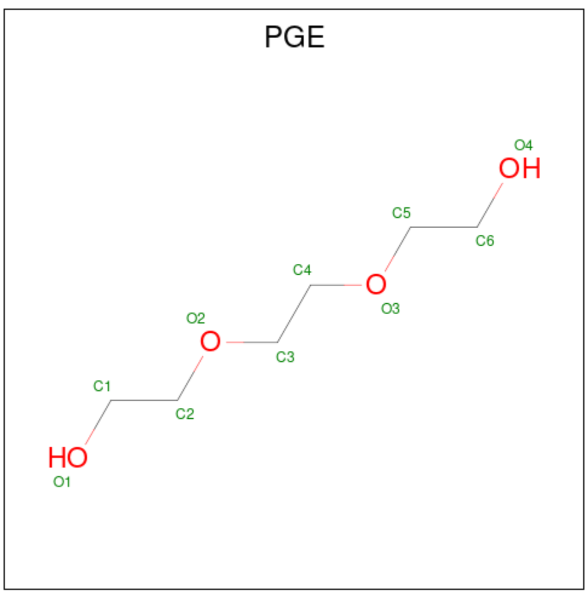
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	X	1	Total C H O 10 2 6 2	0	0
4	X	1	Total C H O 10 2 6 2	0	0
4	X	1	Total C H O 10 2 6 2	0	0
4	X	1	Total C H O 10 2 6 2	0	0
4	X	1	Total C H O 10 2 6 2	0	0
4	X	1	Total C H O 10 2 6 2	0	0
4	X	1	Total C H O 10 2 6 2	0	0
4	X	1	Total C H O 10 2 6 2	0	0
4	X	1	Total 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 (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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

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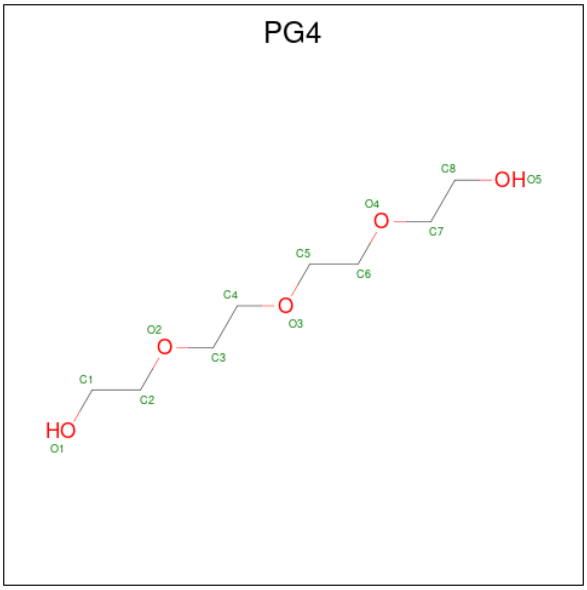
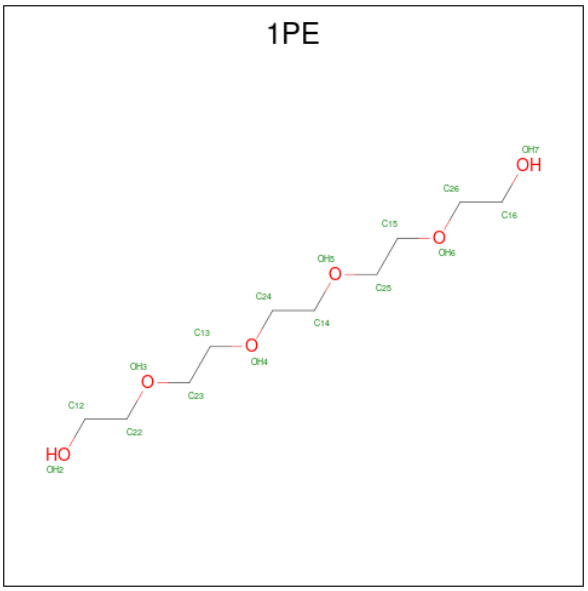
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	X	1	Total	C	H	O	0	0
			24	6	14	4		
6	X	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



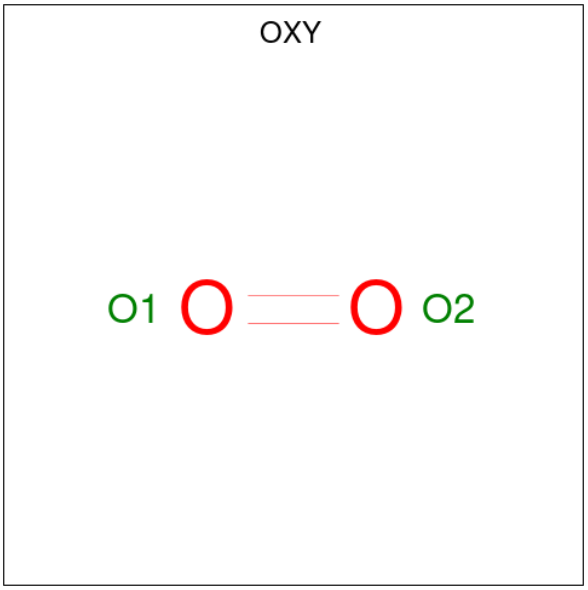
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	X	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 8 is PENTAETHYLENE GLYCOL (three-letter code: 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 (three-letter code: OXY) (formula: O_2).



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 2 2	0	0
9	X	1	Total O 2 2	0	0

- Molecule 10 is water.

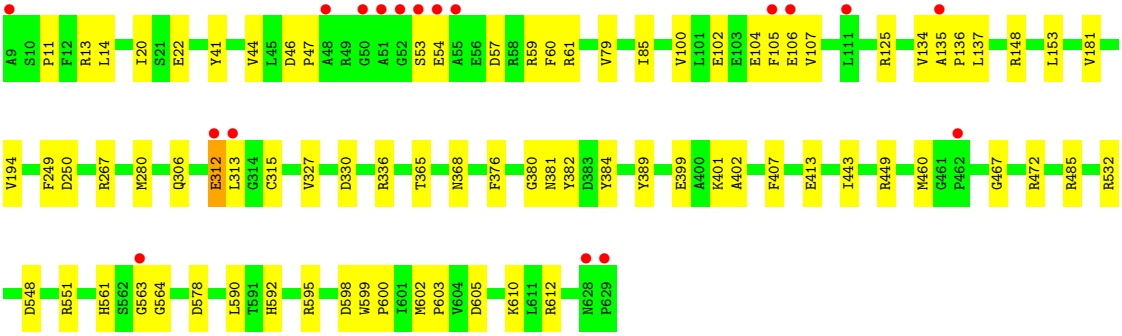
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	X	905	Total O 925 925	0	20

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

Chain X:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	5.03 (at 1.08Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.130 , 0.150 0.127 , 0.147	Depositor DCC
R_{free} test set	15335 reflections (5.02%)	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)	0.42 , 57.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 1PE, OXY, NA, EDO, PGE, PEG, PG4, TPQ, CU

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	0.49	0/5741	0.72	1/7810 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	612	ARG	NE-CZ-NH1	5.25	122.92	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	5356	5412	5255	139	0
2	X	1	0	0	0	0
3	X	1	0	0	0	0
4	X	48	72	72	20	0
5	X	63	90	85	42	0
6	X	50	70	70	19	0
7	X	13	18	18	4	0
8	X	32	44	40	40	0
9	X	8	0	0	0	0
10	X	925	0	0	44	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6497	5706	5540	174	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 16.

The worst 5 of 174 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:602[B]:MET:HG3	8:X:730:1PE:H221	1.40	1.04
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
1:X:602[B]:MET:CG	8:X:730:1PE:H221	1.95	0.94
5:X:719:PEG:O1	10:X:1591:HOH:O	1.88	0.91

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%)	599 (100%)	2 (0%)	92 75

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

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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	2.57	4 (30%)	15,19,21	1.42	2 (13%)

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	6.80	1.46	1.35
1	X	382	TPQ	C6-C1	4.74	1.46	1.34
1	X	382	TPQ	CB-CA	2.88	1.59	1.53
1	X	382	TPQ	C1-C2	-2.05	1.46	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	382	TPQ	CB-CA-C	-3.61	104.70	111.47
1	X	382	TPQ	C6-C1-C2	3.23	121.12	118.64

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 monosaccharides 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	$\#\|Z\| > 2$
5	PEG	X	722	-	6,6,6	1.03	0	5,5,5	1.79	1 (20%)
4	EDO	X	712	-	3,3,3	0.50	0	2,2,2	0.11	0
5	PEG	X	720	-	6,6,6	0.64	0	5,5,5	0.82	0
4	EDO	X	711	-	3,3,3	0.56	0	2,2,2	0.89	0
6	PGE	X	725	-	9,9,9	0.70	0	8,8,8	0.79	0
4	EDO	X	703	-	3,3,3	0.42	0	2,2,2	1.08	0
4	EDO	X	706	-	3,3,3	0.36	0	2,2,2	0.55	0
4	EDO	X	713	-	3,3,3	0.45	0	2,2,2	0.22	0
9	OXY	X	732	-	1,1,1	0.21	0	-		
9	OXY	X	735	-	1,1,1	0.12	0	-		
8	1PE	X	731	-	15,15,15	0.62	0	14,14,14	1.27	3 (21%)
6	PGE	X	724	-	9,9,9	0.85	0	8,8,8	0.89	0
9	OXY	X	734	-	1,1,1	0.08	0	-		
4	EDO	X	714	-	3,3,3	0.45	0	2,2,2	0.34	0
6	PGE	X	727	-	9,9,9	0.70	0	8,8,8	0.76	0
4	EDO	X	704	-	3,3,3	0.45	0	2,2,2	0.36	0
5	PEG	X	719	-	6,6,6	0.89	0	5,5,5	0.75	0
6	PGE	X	726	-	9,9,9	0.60	0	8,8,8	0.76	0
5	PEG	X	721	-	6,6,6	1.08	0	5,5,5	1.57	1 (20%)
5	PEG	X	716	-	6,6,6	0.80	0	5,5,5	1.41	1 (20%)
8	1PE	X	730	-	15,15,15	1.17	1 (6%)	14,14,14	1.84	4 (28%)
4	EDO	X	707	-	3,3,3	0.47	0	2,2,2	0.27	0
9	OXY	X	733	-	1,1,1	0.13	0	-		
7	PG4	X	729	-	12,12,12	0.70	0	11,11,11	1.13	1 (9%)
5	PEG	X	715	-	6,6,6	0.71	0	5,5,5	1.20	1 (20%)
6	PGE	X	728	-	9,9,9	0.63	0	8,8,8	1.46	1 (12%)
4	EDO	X	709	-	3,3,3	0.47	0	2,2,2	0.33	0
5	PEG	X	717	-	6,6,6	0.65	0	5,5,5	0.77	0
5	PEG	X	718	-	6,6,6	0.84	0	5,5,5	1.33	1 (20%)
4	EDO	X	708	-	3,3,3	0.38	0	2,2,2	0.13	0
5	PEG	X	723	-	6,6,6	0.65	0	5,5,5	0.96	0
4	EDO	X	705	-	3,3,3	0.86	0	2,2,2	0.76	0
4	EDO	X	710	-	3,3,3	0.47	0	2,2,2	0.15	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
5	PEG	X	722	-	-	1/4/4/4	-
4	EDO	X	712	-	-	0/1/1/1	-
5	PEG	X	720	-	-	1/4/4/4	-
4	EDO	X	711	-	-	1/1/1/1	-
6	PGE	X	725	-	-	2/7/7/7	-
4	EDO	X	703	-	-	1/1/1/1	-
4	EDO	X	706	-	-	0/1/1/1	-
4	EDO	X	713	-	-	0/1/1/1	-
8	1PE	X	731	-	-	6/13/13/13	-
6	PGE	X	724	-	-	4/7/7/7	-
4	EDO	X	714	-	-	1/1/1/1	-
6	PGE	X	727	-	-	3/7/7/7	-
4	EDO	X	704	-	-	0/1/1/1	-
5	PEG	X	719	-	-	2/4/4/4	-
6	PGE	X	726	-	-	3/7/7/7	-
5	PEG	X	721	-	-	1/4/4/4	-
5	PEG	X	716	-	-	3/4/4/4	-
8	1PE	X	730	-	-	9/13/13/13	-
4	EDO	X	707	-	-	1/1/1/1	-
7	PG4	X	729	-	-	5/10/10/10	-
5	PEG	X	715	-	-	1/4/4/4	-
6	PGE	X	728	-	-	4/7/7/7	-
4	EDO	X	709	-	-	1/1/1/1	-
5	PEG	X	717	-	-	2/4/4/4	-
5	PEG	X	718	-	-	1/4/4/4	-
4	EDO	X	708	-	-	0/1/1/1	-
5	PEG	X	723	-	-	4/4/4/4	-
4	EDO	X	705	-	-	0/1/1/1	-
4	EDO	X	710	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	X	730	1PE	OH6-C26	-2.16	1.32	1.42

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	X	730	1PE	OH7-C16-C26	-3.50	91.50	111.81
5	X	721	PEG	O2-C2-C1	3.35	124.79	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	X	730	1PE	C23-OH3-C22	3.27	127.45	113.29
5	X	722	PEG	O2-C2-C1	-3.12	96.36	110.07
6	X	728	PGE	O2-C2-C1	2.97	123.10	110.07

There are no chirality outliers.

5 of 58 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

There are no ring outliers.

18 monomers are involved in 123 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	X	722	PEG	9	0
5	X	720	PEG	1	0
4	X	711	EDO	5	0
4	X	703	EDO	6	0
8	X	731	1PE	1	0
6	X	724	PGE	10	0
5	X	719	PEG	6	0
6	X	726	PGE	1	0
5	X	721	PEG	16	0
8	X	730	1PE	39	0
7	X	729	PG4	4	0
5	X	715	PEG	1	0
6	X	728	PGE	8	0
5	X	717	PEG	4	0
5	X	718	PEG	2	0
4	X	708	EDO	6	0
5	X	723	PEG	6	0
4	X	705	EDO	3	0

5.7 Other polymers

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, 95^{th} 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%)	-0.21	18 (2%) 51 46	6, 13, 33, 144	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	53	SER	12.1
1	X	54	GLU	8.1
1	X	52	GLY	8.0
1	X	105	PHE	6.2
1	X	55	ALA	4.3

6.2 Non-standard residues in protein, DNA, RNA chains

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, 95^{th} 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	0.08	8,12,14,14	0

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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, 95^{th} 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	719	7/7	0.65	0.59	16,22,33,39	17
6	PGE	X	724	10/10	0.65	0.43	31,80,109,123	24
5	PEG	X	723	7/7	0.67	0.44	10,19,32,32	17
5	PEG	X	716	7/7	0.69	0.35	20,26,35,42	17
5	PEG	X	722	7/7	0.70	0.55	10,18,39,39	17
6	PGE	X	727	10/10	0.71	0.25	21,26,36,42	24
5	PEG	X	718	7/7	0.73	0.29	9,16,24,25	17
4	EDO	X	712	4/4	0.74	0.14	21,26,29,30	10
5	PEG	X	720	7/7	0.74	0.22	17,26,31,33	17
4	EDO	X	713	4/4	0.76	0.13	23,30,36,36	10
5	PEG	X	721	7/7	0.77	0.40	8,23,31,31	17
4	EDO	X	707	4/4	0.80	0.20	57,69,88,105	0
4	EDO	X	703	4/4	0.80	0.27	19,23,28,28	10
5	PEG	X	717	7/7	0.81	0.28	15,23,49,59	17
4	EDO	X	708	4/4	0.82	0.28	22,27,34,40	10
8	1PE	X	730	16/16	0.83	0.28	11,26,34,37	38
6	PGE	X	725	10/10	0.84	0.25	20,29,36,71	24
4	EDO	X	706	4/4	0.85	0.12	22,27,28,32	10
4	EDO	X	710	4/4	0.85	0.11	18,22,30,36	10
4	EDO	X	714	4/4	0.86	0.13	20,24,28,28	10
5	PEG	X	715	7/7	0.87	0.14	22,32,46,56	17
8	1PE	X	731	16/16	0.87	0.17	37,77,100,111	0
4	EDO	X	705	4/4	0.88	0.24	10,15,22,26	10
6	PGE	X	728	10/10	0.89	0.19	7,13,27,32	24
4	EDO	X	709	4/4	0.90	0.25	20,29,40,40	10
7	PG4	X	729	13/13	0.90	0.13	9,19,35,62	31
4	EDO	X	704	4/4	0.91	0.16	44,53,66,79	0
4	EDO	X	711	4/4	0.93	0.13	14,21,43,43	10
6	PGE	X	726	10/10	0.95	0.10	19,30,62,75	0
9	OXY	X	732	2/2	0.98	0.12	16,16,16,22	0
9	OXY	X	733	2/2	0.98	0.10	14,14,14,31	0
9	OXY	X	734	2/2	0.99	0.28	21,21,21,21	0
9	OXY	X	735	2/2	0.99	0.14	11,11,11,27	0
3	NA	X	702	1/1	1.00	0.10	7,7,7,7	0
2	CU	X	701	1/1	1.00	0.03	9,9,9,9	0

6.5 Other polymers (i)

There are no such residues in this entry.