Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 07:48 PM EDT

PDB ID	:	2Y9W
Title	:	Crystal structure of PPO3, a tyrosinase from Agaricus bisporus, in deoxy-form that contains additional unknown lectin-like subunit
Authors	:	Ismaya, W.T.; Rozeboom, H.J.; Weijn, A.; Mes, J.J.; Fusetti, F.; Wichers, H.J.; Dijkstra, B.W.
Deposited on	:	2011-02-17
Resolution	:	2.30 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 (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:

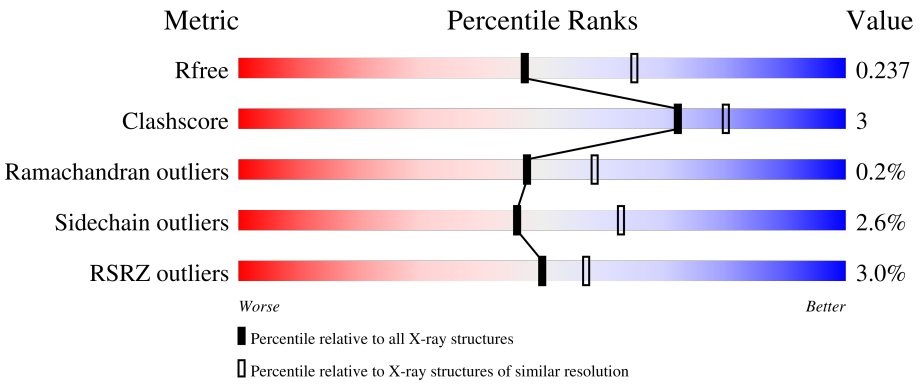
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	A	391	3% 91% 8% •
1	B	391	% 88% 11% •
2	C	150	5% 81% 9% 9%
2	D	150	6% 79% 10% • 10%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8962 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 POLYPHENOL OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	391	3213	2073	535	593	12	0	1	0
1	B	391	3215	2074	537	592	12	0	1	0

- Molecule 2 is a protein called LECTIN-LIKE FOLD PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	136	1056	666	183	205	2	0	0	0
2	D	135	1048	660	182	204	2	0	0	0

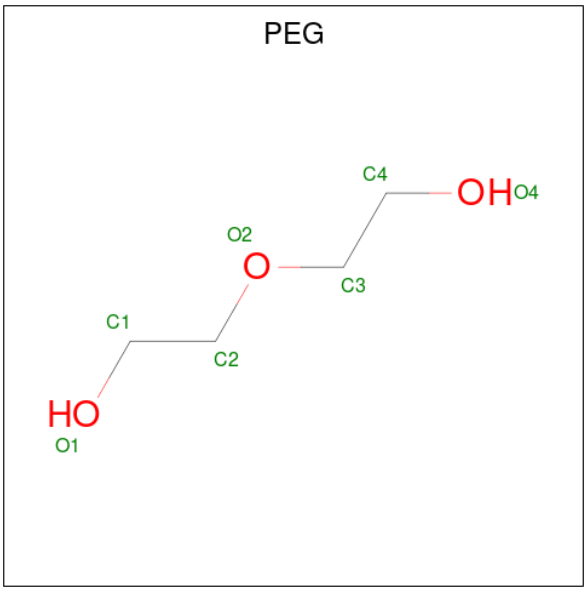
- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 4 is HOLMIUM ATOM (three-letter code: HO) (formula: Ho).

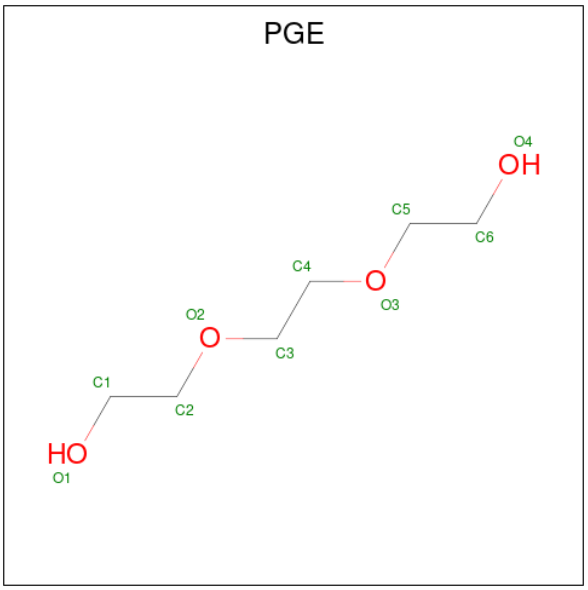
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ho		
4	A	3	3	3	0	0
4	B	3	3	3	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

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



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

- Molecule 7 is water.

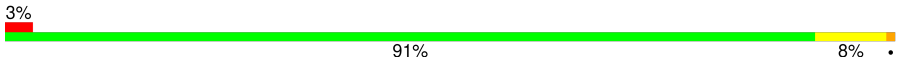
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	149	149	149	0	0
			Total	O		
7	B	160	160	160	0	0
			Total	O		
7	C	42	42	42	0	0
			Total	O		
7	D	38	38	38	0	0

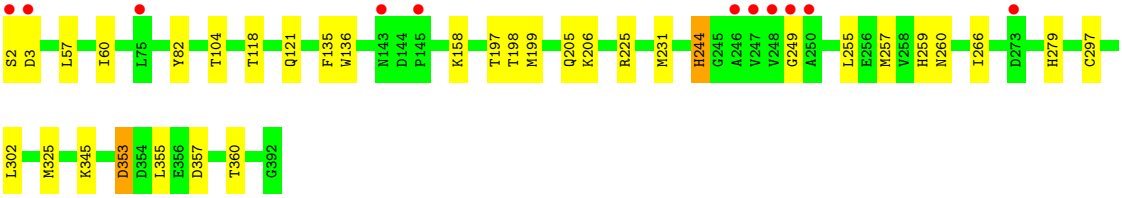
3 Residue-property plots (i)

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: POLYPHENOL OXIDASE

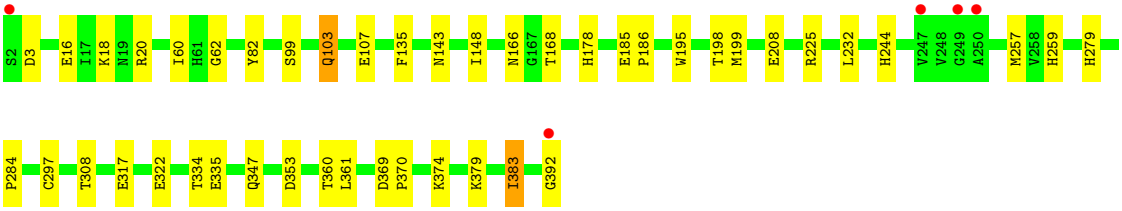
Chain A:





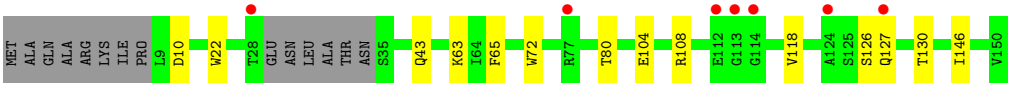
• Molecule 1: POLYPHENOL OXIDASE

Chain B:



• Molecule 2: LECTIN-LIKE FOLD PROTEIN

Chain C:



• Molecule 2: LECTIN-LIKE FOLD PROTEIN

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	104.06Å 104.52Å 109.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.13 – 2.30 47.13 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.13-2.30) 99.1 (47.13-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.181 , 0.237 0.182 , 0.237	Depositor DCC
R_{free} test set	2699 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	30.0	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.033 for -h,l,k 0.035 for -l,-k,-h 0.047 for k,h,-l 0.022 for k,l,h 0.022 for l,h,k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8962	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, CU, HO, PGE

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	0.52	0/3326	0.56	0/4538
1	B	0.52	0/3328	0.57	0/4540
2	C	0.45	0/1082	0.57	0/1470
2	D	0.46	0/1074	0.57	0/1459
All	All	0.51	0/8810	0.57	0/12007

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	A	3213	0	3028	20	0
1	B	3215	0	3033	23	0
2	C	1056	0	1004	8	0
2	D	1048	0	993	7	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
5	A	7	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	7	0	10	0	0
5	C	7	0	10	3	0
6	D	10	0	14	1	0
7	A	149	0	0	2	0
7	B	160	0	0	1	0
7	C	42	0	0	0	0
7	D	38	0	0	1	0
All	All	8962	0	8102	57	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (57) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ASP:O	1:A:360:THR:HG22	1.63	0.97
1:B:335:GLU:HG2	1:B:353:ASP:HB3	1.53	0.91
1:A:244:HIS:HB2	1:A:257:MET:HE2	1.70	0.71
1:B:308:THR:HG21	1:B:383:ILE:HD13	1.76	0.67
2:C:63:LYS:HZ2	5:C:1151:PEG:H21	1.60	0.65
1:B:225[B]:ARG:NH2	1:B:392:GLY:O	2.30	0.65
1:B:317:GLU:HG2	1:B:334:THR:HG22	1.79	0.64
2:C:63:LYS:HZ3	5:C:1151:PEG:H32	1.63	0.62
1:B:103:GLN:O	1:B:107:GLU:HG2	1.99	0.62
1:B:166:ASN:OD1	1:B:168:THR:HG22	2.02	0.60
1:A:244:HIS:HD2	1:A:260:ASN:HD21	1.52	0.57
2:D:103:GLU:HG2	7:D:2011:HOH:O	2.05	0.55
1:A:135:PHE:HB3	1:A:297:CYS:SG	2.45	0.55
1:B:20:ARG:HD3	1:B:297:CYS:SG	2.47	0.54
2:D:18:ASN:HB2	2:D:121:ILE:HD13	1.90	0.54
2:C:63:LYS:NZ	5:C:1151:PEG:H32	2.23	0.53
1:A:266:ILE:HD12	1:A:266:ILE:N	2.23	0.53
1:B:244:HIS:HB2	1:B:257:MET:HE1	1.90	0.53
1:A:249:GLY:HA2	1:A:257:MET:HE3	1.89	0.53
1:A:118:THR:O	1:A:121:GLN:NE2	2.35	0.53
1:A:199:MET:HE1	7:A:2081:HOH:O	2.09	0.52
1:A:249:GLY:HA2	1:A:257:MET:CE	2.39	0.52
1:B:369:ASP:HB2	1:B:370:PRO:HD3	1.91	0.52
1:B:225[B]:ARG:NH2	7:B:2092:HOH:O	2.38	0.52
1:B:178:HIS:HE1	1:B:208:GLU:OE1	1.93	0.51
1:A:198:THR:O	1:A:199:MET:HE3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:THR:OG1	1:A:199:MET:HE3	2.10	0.51
1:B:198:THR:HA	1:B:279:HIS:CE1	2.46	0.50
1:A:60:ILE:O	1:A:82:TYR:HB2	2.12	0.49
2:C:104:GLU:HA	2:C:146:ILE:O	2.12	0.48
2:C:108:ARG:HG3	2:C:118:VAL:HG12	1.95	0.48
1:B:308:THR:HG21	1:B:383:ILE:CD1	2.45	0.46
2:C:65:PHE:HB2	2:C:72:TRP:CZ3	2.50	0.46
1:B:135:PHE:HB3	1:B:297:CYS:SG	2.57	0.45
1:B:60:ILE:O	1:B:82:TYR:HB2	2.16	0.45
1:A:353:ASP:OD2	7:A:2124:HOH:O	2.21	0.45
2:D:58:TYR:HD1	6:D:1151:PGE:H32	1.81	0.45
1:A:136:TRP:CZ3	1:A:266:ILE:HD11	2.52	0.45
1:B:99:SER:OG	1:B:361:LEU:HD13	2.18	0.44
1:B:62:GLY:HA3	1:B:284:PRO:HA	2.00	0.44
2:C:22:TRP:CZ3	2:C:43:GLN:HG2	2.53	0.44
1:A:198:THR:HA	1:A:279:HIS:CE1	2.52	0.43
2:D:12:PRO:O	2:D:52:ARG:HD2	2.18	0.43
2:D:125:SER:C	2:D:127:GLN:H	2.22	0.43
1:A:2:SER:O	1:A:3:ASP:HB2	2.19	0.43
1:B:198:THR:O	1:B:199:MET:HE2	2.19	0.42
1:A:57:LEU:HD11	1:A:104:THR:HG21	2.01	0.42
2:C:126:SER:O	2:C:127:GLN:HB2	2.20	0.42
1:B:16:GLU:HB3	1:B:18:LYS:HE2	2.00	0.41
1:B:185:GLU:HA	1:B:186:PRO:HD3	1.89	0.41
1:B:374:LYS:O	1:B:379:LYS:HE3	2.20	0.41
2:D:17:LEU:HD23	2:D:22:TRP:HB3	2.02	0.41
1:B:195:TRP:CG	1:B:199:MET:HG3	2.55	0.41
1:A:121:GLN:OE1	1:B:347:GLN:HG3	2.21	0.41
2:D:69:SER:O	2:D:70:ASN:HB2	2.20	0.41
1:A:205:GLN:O	1:A:206:LYS:HB2	2.20	0.41
1:A:231:MET:HE1	1:A:302:LEU:HD13	2.01	0.41

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	390/391 (100%)	377 (97%)	12 (3%)	1 (0%)	41	50
1	B	390/391 (100%)	374 (96%)	16 (4%)	0	100	100
2	C	132/150 (88%)	128 (97%)	4 (3%)	0	100	100
2	D	131/150 (87%)	123 (94%)	7 (5%)	1 (1%)	19	23
All	All	1043/1082 (96%)	1002 (96%)	39 (4%)	2 (0%)	47	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	325	MET
2	D	126	SER

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	343/342 (100%)	335 (98%)	8 (2%)	50	67
1	B	343/342 (100%)	334 (97%)	9 (3%)	46	63
2	C	112/123 (91%)	109 (97%)	3 (3%)	44	61
2	D	111/123 (90%)	107 (96%)	4 (4%)	35	49
All	All	909/930 (98%)	885 (97%)	24 (3%)	46	63

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	LYS
1	A	225	ARG
1	A	244	HIS
1	A	255	LEU
1	A	259	HIS
1	A	345	LYS

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Mol	Chain	Res	Type
1	A	353	ASP
1	A	355	LEU
1	B	3	ASP
1	B	103	GLN
1	B	143	ASN
1	B	148	ILE
1	B	232	LEU
1	B	259	HIS
1	B	322	GLU
1	B	360	THR
1	B	383	ILE
2	C	10	ASP
2	C	80	THR
2	C	130	THR
2	D	17	LEU
2	D	85	SER
2	D	136	LEU
2	D	140	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	244	HIS
1	A	253	ASN
1	A	390	HIS
1	B	126	GLN
1	B	178	HIS
2	C	43	GLN
2	C	70	ASN
2	C	143	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 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	A	1393	-	6,6,6	0.45	0	5,5,5	0.39	0
5	PEG	B	1393	-	6,6,6	0.43	0	5,5,5	0.34	0
5	PEG	C	1151	-	6,6,6	0.44	0	5,5,5	0.44	0
6	PGE	D	1151	-	9,9,9	0.53	0	8,8,8	0.25	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	A	1393	-	-	3/4/4/4	-
5	PEG	B	1393	-	-	2/4/4/4	-
5	PEG	C	1151	-	-	3/4/4/4	-
6	PGE	D	1151	-	-	3/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1393	PEG	O1-C1-C2-O2
5	C	1151	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	D	1151	PGE	O3-C5-C6-O4
6	D	1151	PGE	O2-C3-C4-O3
5	C	1151	PEG	O2-C3-C4-O4
5	B	1393	PEG	O2-C3-C4-O4
5	B	1393	PEG	C4-C3-O2-C2
5	A	1393	PEG	C4-C3-O2-C2
5	C	1151	PEG	C4-C3-O2-C2
5	A	1393	PEG	C1-C2-O2-C3
6	D	1151	PGE	C6-C5-O3-C4

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1151	PEG	3	0
6	D	1151	PGE	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	391/391 (100%)	-0.22	11 (2%)	53	60	18, 31, 51, 64	0
1	B	391/391 (100%)	-0.23	5 (1%)	77	81	17, 30, 51, 63	0
2	C	136/150 (90%)	-0.02	7 (5%)	28	35	22, 36, 66, 87	0
2	D	135/150 (90%)	-0.05	9 (6%)	17	23	20, 33, 59, 85	0
All	All	1053/1082 (97%)	-0.18	32 (3%)	50	57	17, 31, 54, 87	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	248	VAL	5.1
2	D	126	SER	4.9
2	C	127	GLN	4.6
2	D	125	SER	4.5
1	A	2	SER	4.4
2	D	127	GLN	3.4
1	A	250	ALA	3.3
1	A	249	GLY	3.2
1	B	2	SER	3.2
1	A	247	VAL	3.2
2	C	28	THR	3.1
2	C	114	GLY	3.1
1	A	145	PRO	3.1
2	C	113	GLY	3.0
2	D	124	ALA	3.0
1	A	3	ASP	3.0
2	C	124	ALA	2.9
2	C	77	ARG	2.9
1	A	246	ALA	2.9
2	D	128	GLY	2.9
2	D	28	THR	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	112	GLU	2.6
2	D	77	ARG	2.5
1	A	75	LEU	2.5
1	A	143	ASN	2.4
1	B	249	GLY	2.3
1	A	273	ASP	2.3
1	B	392	GLY	2.3
1	B	247	VAL	2.3
1	B	250	ALA	2.2
2	D	136	LEU	2.1
2	D	112	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides 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	A	1393	7/7	0.89	0.23	39,39,41,42	0
6	PGE	D	1151	10/10	0.90	0.17	39,41,47,48	0
5	PEG	C	1151	7/7	0.91	0.19	39,40,41,42	0
4	HO	B	404	1/1	0.92	0.18	39,39,39,39	1
5	PEG	B	1393	7/7	0.93	0.18	33,35,37,40	0
4	HO	A	403	1/1	0.94	0.12	49,49,49,49	1
4	HO	A	404	1/1	0.96	0.05	61,61,61,61	1
4	HO	B	403	1/1	0.97	0.05	47,47,47,47	1
3	CU	A	401	1/1	0.98	0.05	34,34,34,34	0
3	CU	B	401	1/1	0.98	0.07	29,29,29,29	0
3	CU	B	400	1/1	0.99	0.06	31,31,31,31	0
3	CU	A	400	1/1	1.00	0.04	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	HO	A	402	1/1	1.00	0.09	38,38,38,38	0
4	HO	B	402	1/1	1.00	0.12	32,32,32,32	1

6.5 Other polymers (i)

There are no such residues in this entry.