



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 10:23 pm BST

PDB ID : 3EF8
Title : Crystal structure of Putative Scytalone Dehydratase (YP_496742.1) from NOVOSPHINGOBIUM AROMATICIVORANS DSM 12444 at 1.50 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2008-09-08
Resolution : 1.50 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 following versions of software and data (see [references ⓘ](#)) 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	:	2.11
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)	:	2.11

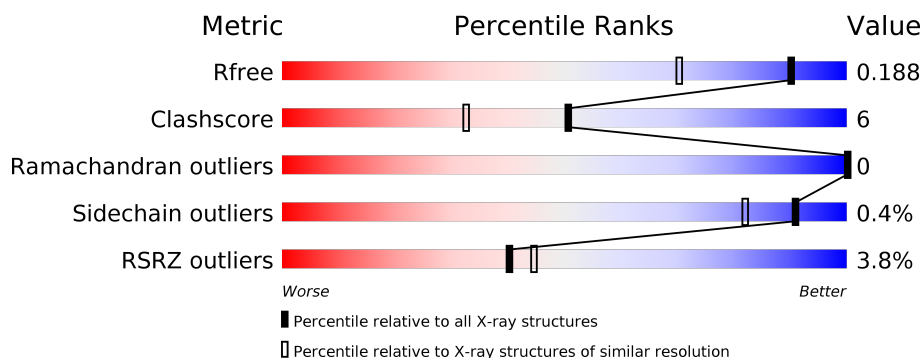
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 on 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	150	<div> <div>3%</div> <div> <div></div> <div>91%</div> <div>8%</div> <div>.</div> </div> </div>
1	B	150	<div> <div>4%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div>..</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2797 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 Putative Scyalone Dehydratase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	Se	0	6	0
			1223	768	217	230	2	6			
1	B	149	Total	C	N	O	S	Se	0	4	0
			1212	764	215	225	2	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	leader sequence	UNP Q2G8B5
B	0	GLY	-	leader sequence	UNP Q2G8B5

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

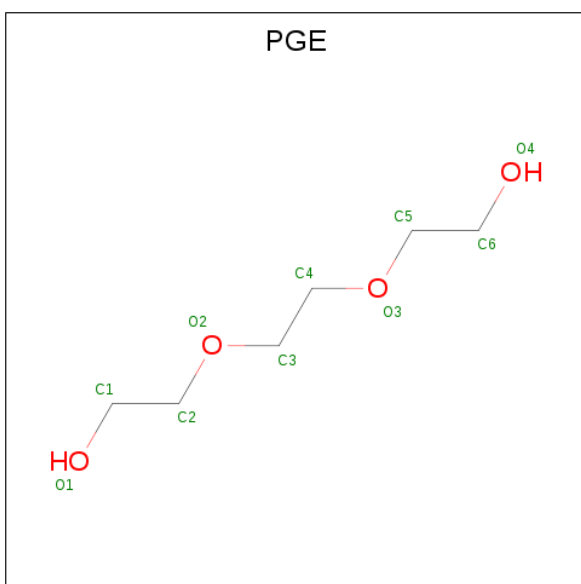
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



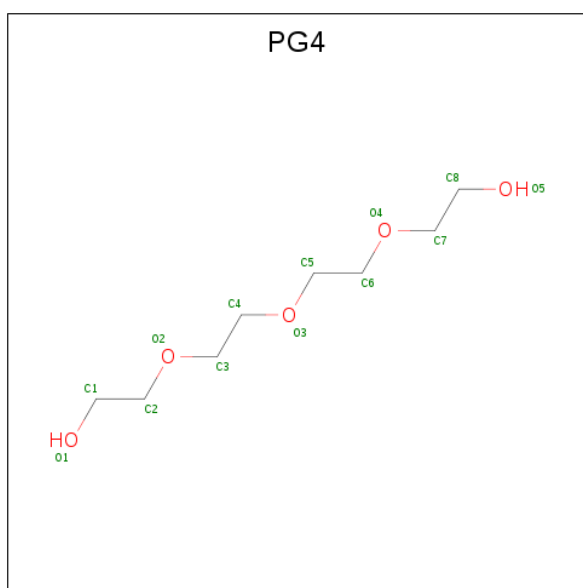
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



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

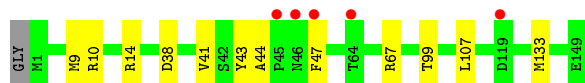
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	121	Total	O	0	1
			122	122		
6	B	111	Total	O	0	1
			112	112		

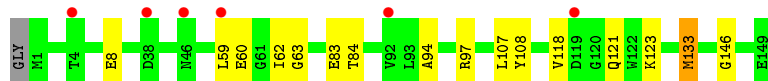
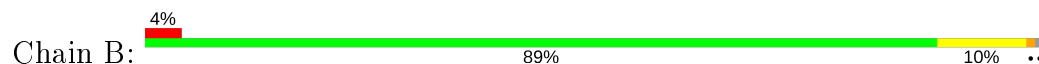
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Putative Scyalone Dehydratase



• Molecule 1: Putative Scyalone Dehydratase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	59.85Å 59.85Å 237.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.92 – 1.50 29.93 – 1.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.92-1.50) 100.0 (29.93-1.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.98 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.4.0067, PHENIX	Depositor
R, R_{free}	0.163 , 0.188 0.161 , 0.188	Depositor DCC
R_{free} test set	2579 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	11.5	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 68.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.032 for -h-k,k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2797	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.48 % 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 2.7186e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: MG, PG4, PEG, 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	0.76	0/1244	0.87	3/1675 (0.2%)
1	B	0.73	0/1233	0.91	2/1659 (0.1%)
All	All	0.74	0/2477	0.89	5/3334 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	97	ARG	NE-CZ-NH1	9.69	125.14	120.30
1	A	10	ARG	NE-CZ-NH1	-8.31	116.14	120.30
1	B	97	ARG	NE-CZ-NH2	-8.16	116.22	120.30
1	A	107	LEU	CB-CG-CD1	-5.52	101.61	111.00
1	A	14	ARG	NE-CZ-NH2	-5.21	117.69	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	A	1223	0	1147	10	0
1	B	1212	0	1153	15	0
2	A	1	0	0	0	0
3	A	21	0	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	14	0	20	3	0
4	A	40	0	56	2	0
5	A	13	0	18	0	0
5	B	39	0	54	7	0
6	A	122	0	0	0	0
6	B	112	0	0	2	0
All	All	2797	0	2478	29	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 6.

All (29) 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:8:GLU:HG3	3:B:151:PEG:H41	1.68	0.75
1:A:67[B]:ARG:NH2	1:A:99[B]:THR:O	2.23	0.71
1:A:9:MSE:HE1	4:A:157:PGE:H1	1.73	0.71
5:B:152:PG4:H22	5:B:152:PG4:O3	1.90	0.70
1:B:108:TYR:CD2	1:B:133[A]:MSE:HG2	2.27	0.69
1:B:83:GLU:O	3:B:151:PEG:H42	1.94	0.68
5:B:152:PG4:H22	6:B:180:HOH:O	2.00	0.60
1:A:9:MSE:CE	4:A:157:PGE:H1	2.32	0.60
1:A:38[B]:ASP:O	1:A:38[B]:ASP:CG	2.47	0.51
1:B:146:GLY:HA2	5:B:153:PG4:H42	1.94	0.50
1:B:121:GLN:HG2	1:B:123:LYS:NZ	2.31	0.46
1:A:133[B]:MSE:HA	3:A:151:PEG:H22	1.98	0.46
1:A:41:VAL:HG11	1:A:43:TYR:CZ	2.51	0.45
1:B:62:ILE:HG23	1:B:63:GLY:N	2.32	0.45
1:B:121:GLN:HG2	1:B:123:LYS:HZ3	1.81	0.44
1:A:44:ALA:HB3	1:A:47:PHE:HB3	1.99	0.44
1:A:38[B]:ASP:O	1:A:38[B]:ASP:OD1	2.36	0.43
1:A:41:VAL:CG1	1:A:43:TYR:CZ	3.01	0.43
1:B:83:GLU:O	3:B:151:PEG:C4	2.65	0.43
1:B:146:GLY:HA2	5:B:153:PG4:H51	2.00	0.43
1:B:108:TYR:CD2	1:B:133[B]:MSE:HG3	2.53	0.43
1:B:94:ALA:HB3	1:B:107[B]:LEU:HB3	2.01	0.42
5:B:153:PG4:H22	6:B:175:HOH:O	2.20	0.42
1:B:118:VAL:O	1:B:118:VAL:HG23	2.17	0.42
1:B:59:LEU:O	1:B:60:GLU:C	2.58	0.42
1:A:133[A]:MSE:HA	3:A:151:PEG:H22	2.01	0.42
1:B:83:GLU:HG2	1:B:84:THR:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:GLY:HA2	5:B:153:PG4:C5	2.51	0.41
5:B:152:PG4:O3	5:B:152:PG4:C2	2.66	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	153/150 (102%)	153 (100%)	0	0	100	100
1	B	151/150 (101%)	147 (97%)	4 (3%)	0	100	100
All	All	304/300 (101%)	300 (99%)	4 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	124/123 (101%)	124 (100%)	0	100	100
1	B	123/123 (100%)	121 (98%)	2 (2%)	62	36
All	All	247/246 (100%)	245 (99%)	2 (1%)	91	66

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

Mol	Chain	Res	Type
1	B	133[A]	MSE
1	B	133[B]	MSE

Some 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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 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	$\# Z > 2$
3	PEG	A	152	-	6,6,6	0.44	0	5,5,5	0.47	0
5	PG4	B	154	-	12,12,12	0.47	0	11,11,11	0.72	0
4	PGE	A	157	-	9,9,9	0.51	0	8,8,8	0.59	0
3	PEG	A	153	-	6,6,6	0.30	0	5,5,5	0.53	0
3	PEG	B	151	-	6,6,6	0.55	0	5,5,5	1.19	0
4	PGE	A	154	-	9,9,9	0.46	0	8,8,8	0.47	0
5	PG4	B	153	-	12,12,12	0.94	0	11,11,11	1.71	3 (27%)
3	PEG	B	150	-	6,6,6	0.42	0	5,5,5	0.89	0
5	PG4	B	152	-	12,12,12	0.25	0	11,11,11	1.24	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PG4	A	158	-	12,12,12	0.48	0	11,11,11	0.70	0
4	PGE	A	155	-	9,9,9	0.43	0	8,8,8	0.39	0
4	PGE	A	156	-	9,9,9	0.37	0	8,8,8	0.39	0
3	PEG	A	151	-	6,6,6	0.61	0	5,5,5	0.56	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
3	PEG	A	152	-	-	1/4/4/4	-
5	PG4	B	154	-	-	3/10/10/10	-
4	PGE	A	157	-	-	3/7/7/7	-
3	PEG	A	153	-	-	2/4/4/4	-
3	PEG	B	151	-	-	2/4/4/4	-
4	PGE	A	154	-	-	2/7/7/7	-
5	PG4	B	153	-	-	6/10/10/10	-
3	PEG	B	150	-	-	1/4/4/4	-
5	PG4	B	152	-	-	2/10/10/10	-
5	PG4	A	158	-	-	3/10/10/10	-
4	PGE	A	155	-	-	3/7/7/7	-
4	PGE	A	156	-	-	4/7/7/7	-
3	PEG	A	151	-	-	0/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	153	PG4	C3-O2-C2	3.05	126.53	113.29
5	B	153	PG4	O2-C3-C4	2.99	123.90	110.39
5	B	152	PG4	C5-O3-C4	-2.74	101.43	113.29
5	B	153	PG4	O3-C5-C6	2.57	121.98	110.39

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	153	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
5	B	153	PG4	C4-C3-O2-C2
5	B	153	PG4	O2-C3-C4-O3
5	B	153	PG4	O1-C1-C2-O2
5	B	154	PG4	O1-C1-C2-O2
3	B	150	PEG	O1-C1-C2-O2
5	A	158	PG4	O1-C1-C2-O2
4	A	156	PGE	O3-C5-C6-O4
4	A	157	PGE	O2-C3-C4-O3
4	A	157	PGE	O3-C5-C6-O4
3	A	153	PEG	O2-C3-C4-O4
3	A	152	PEG	O1-C1-C2-O2
5	B	154	PG4	C4-C3-O2-C2
5	B	153	PG4	C1-C2-O2-C3
4	A	154	PGE	O1-C1-C2-O2
4	A	156	PGE	C3-C4-O3-C5
4	A	155	PGE	O1-C1-C2-O2
5	B	154	PG4	O2-C3-C4-O3
5	B	153	PG4	C3-C4-O3-C5
4	A	155	PGE	O3-C5-C6-O4
4	A	154	PGE	O2-C3-C4-O3
4	A	156	PGE	C4-C3-O2-C2
3	B	151	PEG	C4-C3-O2-C2
4	A	157	PGE	C3-C4-O3-C5
5	A	158	PG4	O2-C3-C4-O3
5	A	158	PG4	C1-C2-O2-C3
3	B	151	PEG	C1-C2-O2-C3
4	A	155	PGE	O2-C3-C4-O3
4	A	156	PGE	O2-C3-C4-O3
5	B	152	PG4	O1-C1-C2-O2
5	B	152	PG4	C8-C7-O4-C6
5	B	153	PG4	O3-C5-C6-O4

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	157	PGE	2	0
3	B	151	PEG	3	0
5	B	153	PG4	4	0
5	B	152	PG4	3	0
3	A	151	PEG	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	143/150 (95%)	0.07	5 (3%) 44 48	6, 14, 29, 43	0
1	B	143/150 (95%)	0.13	6 (4%) 36 40	6, 14, 31, 37	0
All	All	286/300 (95%)	0.10	11 (3%) 40 44	6, 14, 31, 43	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	45	PRO	4.3
1	A	46	ASN	4.1
1	B	46	ASN	3.4
1	B	59	LEU	2.9
1	A	47	PHE	2.8
1	B	4	THR	2.2
1	B	92	VAL	2.2
1	B	119	ASP	2.1
1	A	64	THR	2.1
1	A	119[A]	ASP	2.0
1	B	38	ASP	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 carbohydrates 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PEG	A	152	7/7	0.61	0.20	50,51,54,56	0
5	PG4	B	153	13/13	0.62	0.28	23,40,45,45	0
3	PEG	B	151	7/7	0.72	0.28	27,33,35,41	0
3	PEG	B	150	7/7	0.74	0.17	25,35,40,44	0
3	PEG	A	153	7/7	0.79	0.14	39,42,48,51	0
4	PGE	A	155	10/10	0.79	0.18	35,42,47,51	0
3	PEG	A	151	7/7	0.83	0.13	34,38,42,43	0
4	PGE	A	156	10/10	0.87	0.20	21,37,49,54	0
5	PG4	B	154	13/13	0.88	0.16	21,33,53,61	0
5	PG4	A	158	13/13	0.90	0.18	18,35,50,51	0
4	PGE	A	157	10/10	0.90	0.14	11,39,48,54	0
5	PG4	B	152	13/13	0.91	0.18	24,33,45,49	0
4	PGE	A	154	10/10	0.95	0.14	16,30,38,39	0
2	MG	A	150	1/1	0.99	0.06	18,18,18,18	1

6.5 Other polymers

There are no such residues in this entry.