Full wwPDB X-ray Structure Validation Report (i)

May 17, 2020 – 02:45 pm BST

PDB ID	:	6QYH
Title	:	Structure of Apo HPAB from E.coli
Authors	:	Pecqueur, L.; Lombard, M.; Deng, Y.; Fontecave, M.
Deposited on	:	2019-03-09
Resolution	:	1.94 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.
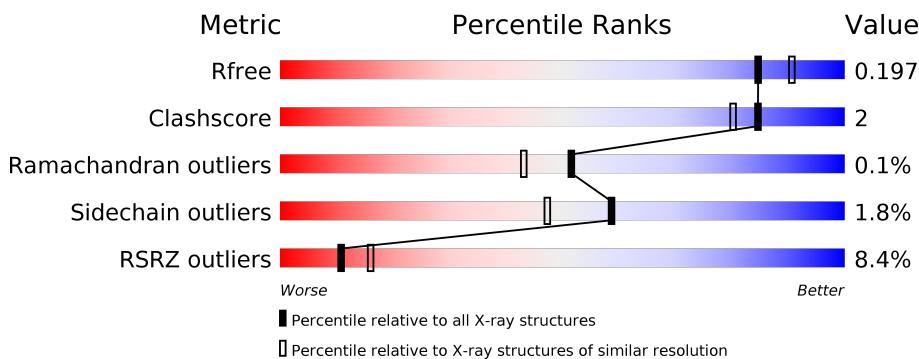
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
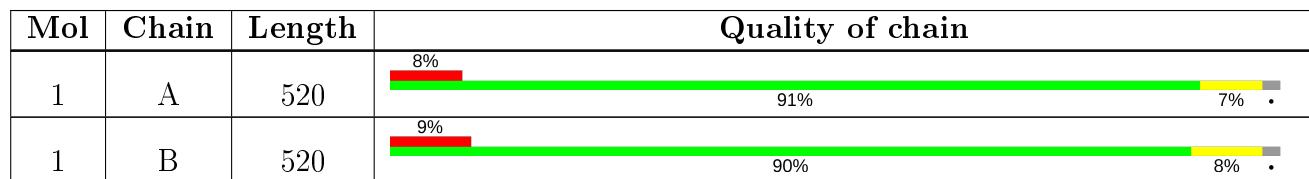
The reported resolution of this entry is 1.94 Å.

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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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 <=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	520	8% 91% 7% ·
1	B	520	9% 90% 8% ·

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8811 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.
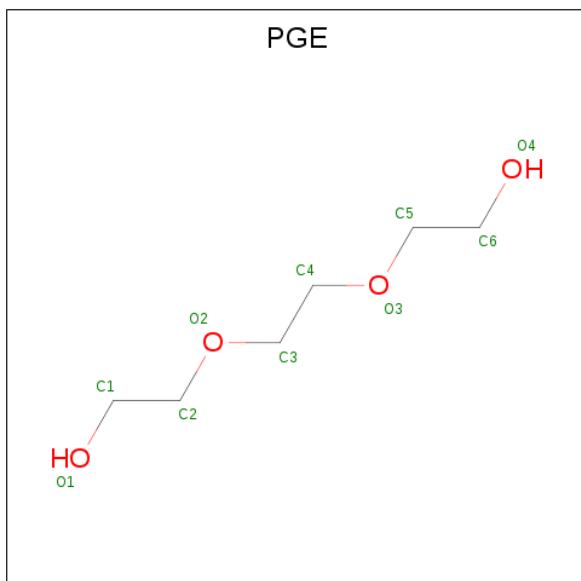
- Molecule 1 is a protein called 4-hydroxyphenylacetate 3-monooxygenase oxygenase component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	511	Total	C	N	O	S	0	8	0
			4095	2591	709	766	29			
1	B	512	Total	C	N	O	S	0	8	0
			4107	2599	714	765	29			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).
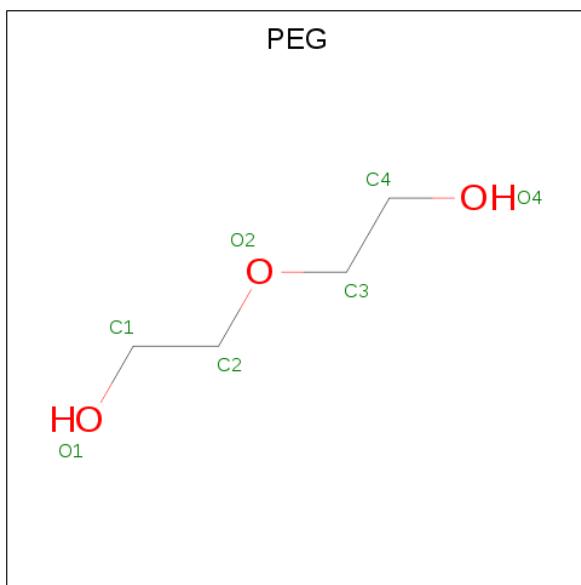
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Ca	0	0
			2	2		
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 10	C 6	O 4	0	0
3	A	1	Total 10	C 6	O 4	0	0
3	A	1	Total 10	C 6	O 4	0	0
3	B	1	Total 10	C 6	O 4	0	0
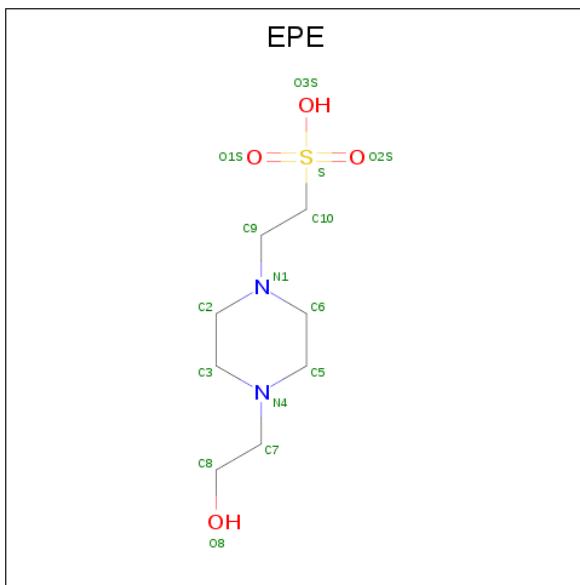
- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

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

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID

(three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
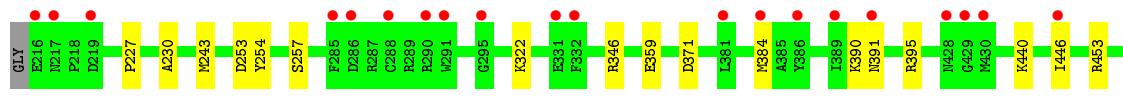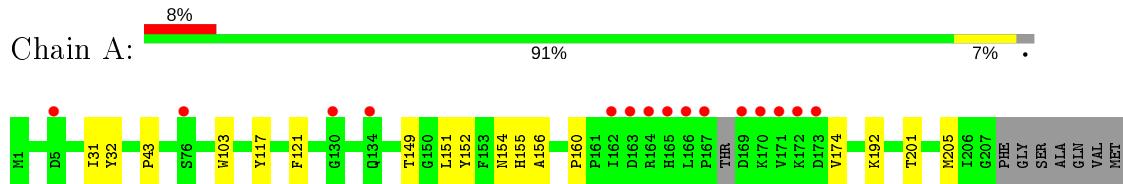
• Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	271	Total	O	0	0
			271	271		
6	B	231	Total	O	0	0
			231	231		
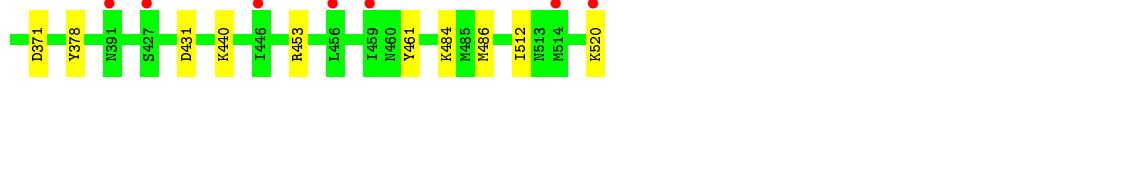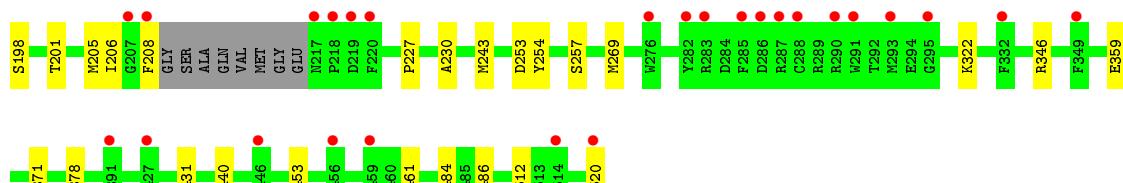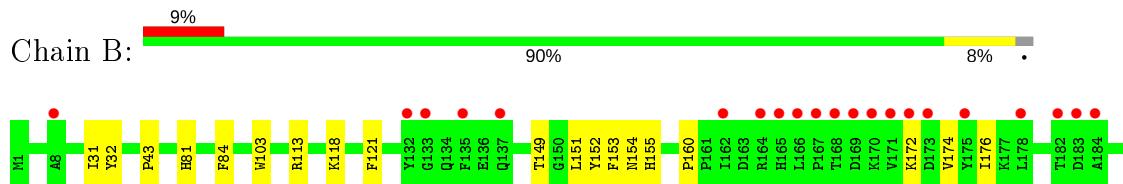
3 Residue-property plots ⓘ

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: 4-hydroxyphenylacetate 3-monooxygenase oxygenase component

- Molecule 1: 4-hydroxyphenylacetate 3-monooxygenase oxygenase component

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	189.28Å 189.28Å 163.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.45 – 1.94 49.38 – 1.94	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.45-1.94) 99.9 (49.38-1.94)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.44 (at 1.94Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.166 , 0.184 0.174 , 0.197	Depositor DCC
R_{free} test set	2220 reflections (1.74%)	wwPDB-VP
Wilson B-factor (Å^2)	39.6	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 61.2	EDS
L-test for twinning[2]	$<|L|>=0.47, <L^2>=0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8811	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: EPE, CA, 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	0.52	0/4196	0.60	0/5689
1	B	0.51	0/4204	0.61	0/5702
All	All	0.52	0/8400	0.61	0/11391

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	4095	0	3920	20	0
1	B	4107	0	3929	22	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
3	A	30	0	42	2	0
3	B	10	0	14	0	0
4	A	42	0	60	0	0
4	B	7	0	10	0	0
5	B	15	0	17	0	0
6	A	271	0	0	1	0
6	B	231	0	0	0	0
All	All	8811	0	7992	38	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 2.

All (38) 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:154:ASN:HB2	1:A:201:THR:HG21	1.78	0.65
1:B:154:ASN:HD22	1:B:201:THR:HG21	1.68	0.59
1:A:149:THR:OG1	1:A:151:LEU:HG	2.04	0.57
1:A:391[B]:ASN:ND2	1:A:395:ARG:HH11	2.04	0.56
1:B:149:THR:OG1	1:B:151:LEU:HG	2.05	0.56
1:A:390:LYS:HE2	1:A:446:ILE:O	2.06	0.55
1:A:486:MET:SD	1:B:322:LYS:HG3	2.49	0.52
1:B:154:ASN:HB2	1:B:201:THR:HG21	1.91	0.52
1:B:160:PRO:HG2	1:B:174:VAL:HG12	1.92	0.51
1:B:113[B]:ARG:HH12	1:B:461[B]:TYR:HE1	1.57	0.51
1:A:227:PRO:HG2	1:A:230:ALA:HB2	1.93	0.51
1:A:160:PRO:HG2	1:A:174:VAL:HG12	1.93	0.51
3:A:602:PGE:H52	1:B:484:LYS:HB3	1.93	0.51
1:A:322:LYS:HG3	1:B:486:MET:SD	2.50	0.50
1:B:227:PRO:HG2	1:B:230:ALA:HB2	1.93	0.49
1:B:176:ILE:HD12	1:B:269:MET:HE3	1.96	0.48
1:B:253:ASP:HA	1:B:440:LYS:HD3	1.95	0.48
1:A:359:GLU:HB2	1:A:371:ASP:HB2	1.95	0.47
1:B:81:HIS:HB3	1:B:84:PHE:CD2	2.49	0.47
1:B:118[B]:LYS:HG2	1:B:153:PHE:HB3	1.97	0.47
1:B:359:GLU:HB2	1:B:371:ASP:HB2	1.97	0.46
1:A:253:ASP:HA	1:A:440:LYS:HD3	1.97	0.46
1:A:465:GLN:HG3	3:A:603:PGE:H32	1.97	0.46
1:A:512:ILE:HG21	1:B:43:PRO:HB3	1.99	0.45
1:B:254:TYR:HB3	1:B:257:SER:HB2	1.99	0.45
1:A:43:PRO:HB2	1:A:243:MET:HG3	1.99	0.45
1:A:117:TYR:HE1	1:A:461:TYR:OH	1.99	0.45
1:A:254:TYR:HB3	1:A:257:SER:HB2	1.98	0.44
1:B:118[A]:LYS:HG3	1:B:154:ASN:HA	2.00	0.43
1:B:43:PRO:HB2	1:B:243:MET:HG3	2.00	0.43
1:A:384[A]:MET:HG3	6:A:734:HOH:O	2.19	0.43
1:A:43:PRO:HB3	1:B:512:ILE:HG21	2.00	0.42
1:B:206:ILE:HG12	1:B:269:MET:HE1	2.00	0.42
1:A:31:ILE:HG12	1:A:32:TYR:CD2	2.55	0.42
1:A:121:PHE:CZ	1:A:205:MET:HG3	2.54	0.41
1:B:121:PHE:CZ	1:B:205:MET:HG3	2.55	0.41
1:A:156:ALA:HB1	1:A:192:LYS:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:ILE:HG12	1:B:32:TYR:CD2	2.56	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	513/520 (99%)	500 (98%)	13 (2%)	0	100	100
1	B	516/520 (99%)	503 (98%)	12 (2%)	1 (0%)	47	39
All	All	1029/1040 (99%)	1003 (98%)	25 (2%)	1 (0%)	51	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	172	LYS

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	423/436 (97%)	418 (99%)	5 (1%)	71	64
1	B	423/436 (97%)	413 (98%)	10 (2%)	49	36
All	All	846/872 (97%)	831 (98%)	15 (2%)	59	47

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

Mol	Chain	Res	Type
1	A	103	TRP
1	A	152	TYR
1	A	155	HIS
1	A	346	ARG
1	A	453	ARG
1	B	103	TRP
1	B	152	TYR
1	B	155	HIS
1	B	198	SER
1	B	208	PHE
1	B	346	ARG
1	B	378	TYR
1	B	431	ASP
1	B	453	ARG
1	B	520	LYS

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

Mol	Chain	Res	Type
1	A	71	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	PEG	A	608	-	6,6,6	0.11	0	5,5,5	0.08	0
4	PEG	B	604	-	6,6,6	0.22	0	5,5,5	0.22	0
5	EPE	B	605	-	15,15,15	1.27	1 (6%)	18,20,20	0.44	0
4	PEG	A	609	-	6,6,6	0.12	0	5,5,5	0.05	0
3	PGE	B	603	-	9,9,9	0.18	0	8,8,8	0.19	0
3	PGE	A	603	-	9,9,9	0.13	0	8,8,8	0.19	0
4	PEG	A	610	-	6,6,6	0.11	0	5,5,5	0.08	0
4	PEG	A	605	-	6,6,6	0.06	0	5,5,5	0.06	0
3	PGE	A	604	-	9,9,9	0.18	0	8,8,8	0.18	0
4	PEG	A	607	-	6,6,6	0.10	0	5,5,5	0.05	0
4	PEG	A	606	-	6,6,6	0.18	0	5,5,5	0.16	0
3	PGE	A	602	-	9,9,9	0.19	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
4	PEG	A	608	-	-	4/4/4/4	-
4	PEG	B	604	-	-	3/4/4/4	-
5	EPE	B	605	-	-	4/9/19/19	0/1/1/1
4	PEG	A	609	-	-	3/4/4/4	-
3	PGE	B	603	-	-	1/7/7/7	-
3	PGE	A	603	-	-	5/7/7/7	-
4	PEG	A	610	-	-	0/4/4/4	-
4	PEG	A	605	-	-	2/4/4/4	-
3	PGE	A	604	-	-	4/7/7/7	-
4	PEG	A	607	-	-	1/4/4/4	-
4	PEG	A	606	-	-	0/4/4/4	-
3	PGE	A	602	-	-	3/7/7/7	-

All (1) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	605	EPE	C10-S	-4.81	1.70	1.77

There are no bond angle outliers.

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	605	EPE	C9-C10-S-O2S
5	B	605	EPE	C9-C10-S-O3S
3	A	603	PGE	O1-C1-C2-O2
3	A	602	PGE	O2-C3-C4-O3
4	B	604	PEG	O2-C3-C4-O4
3	A	602	PGE	O3-C5-C6-O4
5	B	605	EPE	S-C10-C9-N1
3	A	604	PGE	O2-C3-C4-O3
4	B	604	PEG	C4-C3-O2-C2
3	B	603	PGE	C1-C2-O2-C3
4	A	608	PEG	C1-C2-O2-C3
4	A	609	PEG	C1-C2-O2-C3
4	A	609	PEG	C4-C3-O2-C2
4	A	608	PEG	C4-C3-O2-C2
4	A	605	PEG	C4-C3-O2-C2
4	A	607	PEG	C4-C3-O2-C2
3	A	603	PGE	C6-C5-O3-C4
5	B	605	EPE	C9-C10-S-O1S
3	A	603	PGE	C1-C2-O2-C3
3	A	604	PGE	C1-C2-O2-C3
4	A	605	PEG	O1-C1-C2-O2
4	A	609	PEG	O2-C3-C4-O4
3	A	604	PGE	C6-C5-O3-C4
3	A	602	PGE	C3-C4-O3-C5
4	A	608	PEG	O2-C3-C4-O4
3	A	603	PGE	C4-C3-O2-C2
3	A	603	PGE	O2-C3-C4-O3
4	B	604	PEG	C1-C2-O2-C3
3	A	604	PGE	O1-C1-C2-O2
4	A	608	PEG	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	603	PGE	1	0
3	A	602	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	511/520 (98%)	0.29	39 (7%)	13 19	30, 43, 67, 99	0
1	B	512/520 (98%)	0.37	47 (9%)	9 13	30, 46, 78, 111	0
All	All	1023/1040 (98%)	0.33	86 (8%)	11 16	30, 44, 74, 111	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	168	THR	7.2
1	B	171	VAL	7.1
1	A	167	PRO	6.0
1	B	208	PHE	5.8
1	B	166	LEU	5.6
1	A	165	HIS	5.5
1	A	162	ILE	5.3
1	B	520	LYS	5.2
1	A	285	PHE	5.2
1	B	288	CYS	5.0
1	A	166	LEU	4.6
1	B	164	ARG	4.5
1	A	172	LYS	4.3
1	B	218	PRO	4.2
1	A	171	VAL	4.0
1	B	165	HIS	4.0
1	B	167	PRO	4.0
1	B	219	ASP	3.8
1	B	285	PHE	3.8
1	B	286	ASP	3.7
1	B	184	ALA	3.7
1	B	282	TYR	3.6
1	A	286	ASP	3.5
1	A	216	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	332	PHE	3.4
1	A	332	PHE	3.4
1	B	220	PHE	3.4
1	B	169	ASP	3.3
1	A	288	CYS	3.2
1	B	283	ARG	3.2
1	B	133	GLY	3.2
1	B	293	MET	3.2
1	A	461	TYR	3.2
1	B	207	GLY	3.1
1	B	135	PHE	3.1
1	B	183	ASP	3.0
1	B	172	LYS	3.0
1	A	169	ASP	2.9
1	B	162	ILE	2.9
1	B	175	TYR	2.9
1	B	182	THR	2.9
1	B	178	LEU	2.9
1	B	391[A]	ASN	2.9
1	B	459	ILE	2.8
1	A	428	ASN	2.8
1	A	446	ILE	2.8
1	A	384[A]	MET	2.8
1	A	134	GLN	2.8
1	A	391[A]	ASN	2.8
1	B	8	ALA	2.7
1	A	459	ILE	2.7
1	A	217	ASN	2.7
1	B	173	ASP	2.7
1	A	429	GLY	2.7
1	B	276	TRP	2.6
1	A	456	LEU	2.6
1	A	290	ARG	2.6
1	A	164	ARG	2.6
1	B	290	ARG	2.6
1	B	170	LYS	2.5
1	A	331	GLU	2.5
1	A	291	TRP	2.5
1	B	456	LEU	2.5
1	A	520	LYS	2.5
1	A	130	GLY	2.5
1	A	386	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	137	GLN	2.4
1	A	173	ASP	2.4
1	A	430	MET	2.3
1	B	217	ASN	2.3
1	A	219	ASP	2.3
1	A	76	SER	2.3
1	A	170	LYS	2.3
1	B	291	TRP	2.2
1	A	295	GLY	2.2
1	B	446	ILE	2.2
1	B	427	SER	2.1
1	B	514[A]	MET	2.1
1	B	132	TYR	2.1
1	A	389	ILE	2.1
1	A	381	LEU	2.1
1	A	163	ASP	2.1
1	B	287	ARG	2.0
1	B	295	GLY	2.0
1	B	349	PHE	2.0
1	A	5	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 (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
3	PGE	A	602	10/10	0.72	0.22	70,78,80,80	0
4	PEG	A	606	7/7	0.77	0.19	67,68,70,72	0
5	EPE	B	605	15/15	0.81	0.22	76,77,81,82	15

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PGE	B	603	10/10	0.81	0.18	62,64,64,65	0
4	PEG	A	609	7/7	0.83	0.14	69,70,73,75	0
3	PGE	A	604	10/10	0.84	0.18	71,76,83,85	0
4	PEG	B	604	7/7	0.84	0.20	74,75,77,77	0
3	PGE	A	603	10/10	0.84	0.28	63,71,82,83	0
4	PEG	A	610	7/7	0.86	0.16	69,70,75,75	0
4	PEG	A	608	7/7	0.86	0.16	84,85,87,88	0
4	PEG	A	607	7/7	0.87	0.14	76,76,80,80	0
2	CA	B	602	1/1	0.90	0.09	45,45,45,45	1
2	CA	B	601	1/1	0.93	0.23	45,45,45,45	1
2	CA	A	601	1/1	0.93	0.16	44,44,44,44	1
4	PEG	A	605	7/7	0.95	0.13	74,74,75,77	0

6.5 Other polymers (i)

There are no such residues in this entry.