



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 12:23 PM UTC

PDB ID : 5AG3 / pdb_00005ag3
Title : Chorismatase mechanisms reveal fundamentally different types of reaction in a single conserved protein fold
Authors : Hubrich, F.; Juneja, P.; Mueller, M.; Diederichs, K.; Welte, W.; Andexer, J.N.
Deposited on : 2015-01-28
Resolution : 1.90 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 ⓘ 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

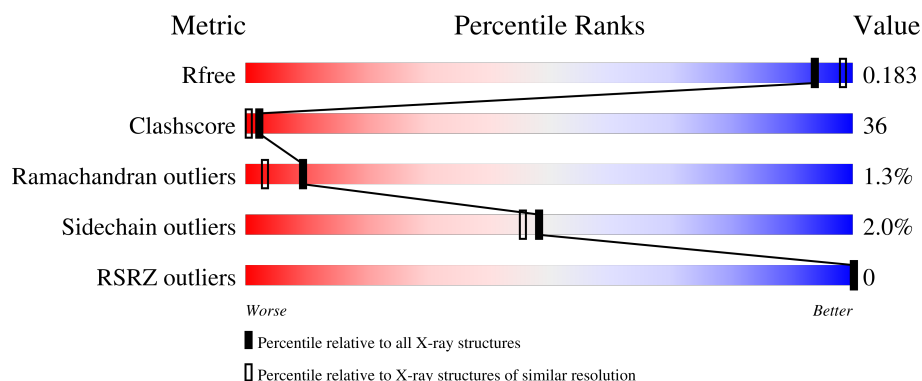
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	340	
1	B	340	
1	C	340	

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	PEG	C	1345	-	-	X	-

2 Entry composition [i](#)

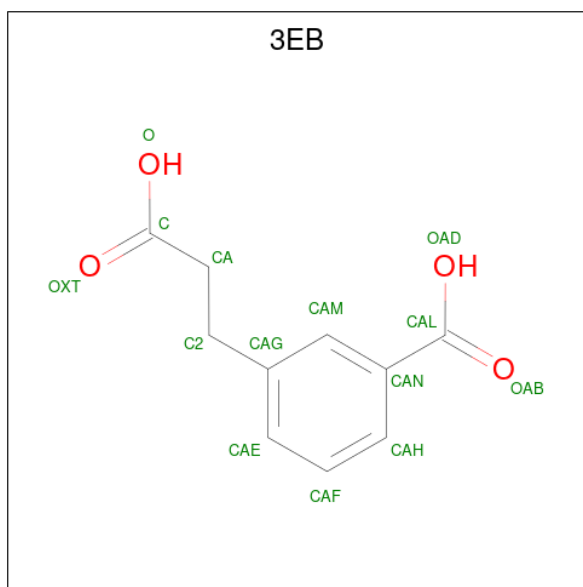
There are 5 unique types of molecules in this entry. The entry contains 8694 atoms, of which 130 are hydrogens and 0 are deuteriums.

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 PTERIDINE-DEPENDENT DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	1	0
			2592	1633	459	486	14			
1	B	332	Total	C	N	O	S	0	0	0
			2579	1623	458	485	13			
1	C	335	Total	C	N	O	S	0	0	0
			2602	1640	461	488	13			

- Molecule 2 is 3-(2-CARBOXYETHYL)BENZOIC ACID (CCD ID: 3EB) (formula: C₁₀H₁₀O₄).



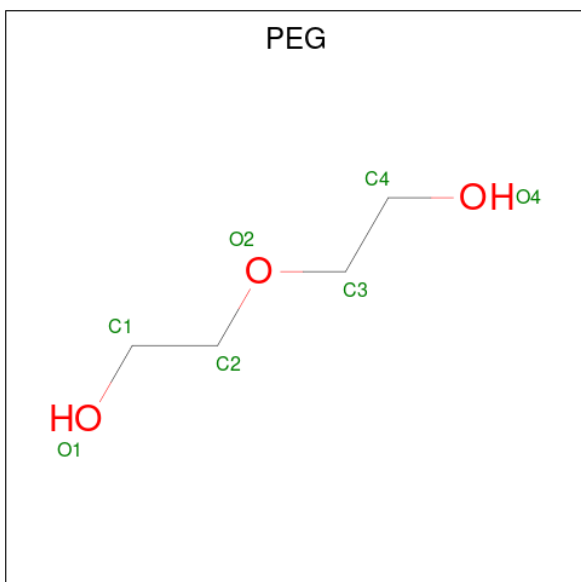
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			14	10	4		
2	B	1	Total	C	O	0	0
			14	10	4		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

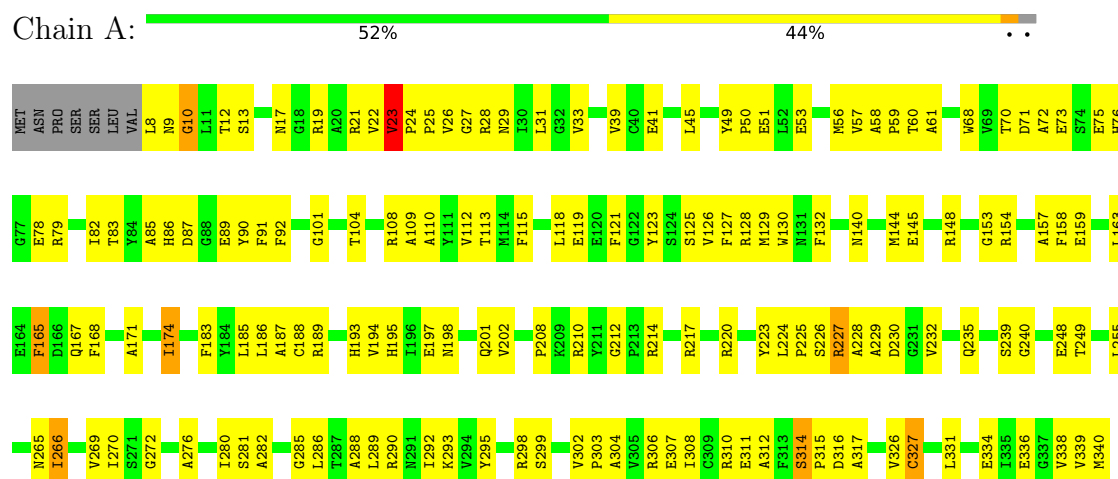
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	222	Total O 222 222	0	0
5	B	198	Total O 198 198	0	0
5	C	227	Total O 227 227	0	0

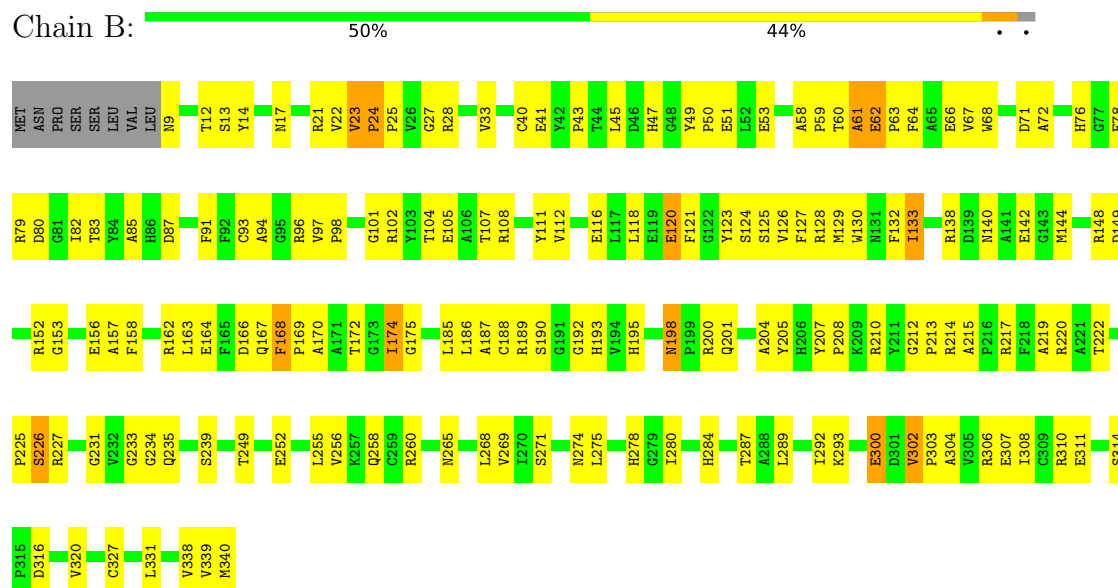
3 Residue-property plots

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: PUTATIVE PTERIDINE-DEPENDENT DIOXYGENASE



• Molecule 1: PUTATIVE PTERIDINE-DEPENDENT DIOXYGENASE



• Molecule 1: PUTATIVE PTERIDINE-DEPENDENT DIOXYGENASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	116.17Å 116.17Å 70.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.81 – 1.90 44.81 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.81-1.90) 99.8 (44.81-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 1.89Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.149 , 0.184 0.151 , 0.183	Depositor DCC
R_{free} test set	4184 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	34.1	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 32.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.479 for -h,-k,l 0.128 for h,-h-k,-l 0.129 for -k,-h,-l	Xtriage
Reported twinning fraction	0.500 for -h,-k,l	Depositor
Outliers	0 of 83807 reflections	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	8694	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% of the height of the origin peak. No significant pseudotranslation is detected.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, SO4, 3EB

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	0.62	0/2658	1.05	10/3608 (0.3%)
1	B	0.58	0/2642	1.02	9/3587 (0.3%)
1	C	0.66	0/2665	1.06	23/3619 (0.6%)
All	All	0.62	0/7965	1.04	42/10814 (0.4%)

There are no bond length outliers.

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	VAL	CA-C-N	-13.24	110.12	119.66
1	A	23	VAL	C-N-CA	-13.24	110.12	119.66
1	A	314	SER	CA-C-N	11.21	131.62	119.28
1	A	314	SER	C-N-CA	11.21	131.62	119.28
1	B	168	PHE	CA-C-N	-9.58	110.51	120.85

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	2592	0	2486	182	1
1	B	2579	0	2466	174	0
1	C	2602	0	2497	207	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	14	0	8	0	0
2	B	14	0	8	1	0
3	A	10	0	0	0	0
3	B	5	0	0	0	0
3	C	10	0	0	0	0
4	A	49	70	67	3	0
4	B	14	20	20	0	0
4	C	28	40	38	6	0
5	A	222	0	0	21	2
5	B	198	0	0	22	2
5	C	227	0	0	20	3
All	All	8564	130	7590	563	5

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 36.

The worst 5 of 563 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:8:LEU:HD13	1:A:227:ARG:HG2	1.25	1.17
1:C:338:VAL:HG11	1:C:340:MET:HE3	1.26	1.09
1:C:129:MET:HE3	1:C:169:PRO:HG3	1.36	1.07
1:C:163:LEU:HD11	1:C:167:GLN:HG3	1.32	1.05
1:C:155:ALA:HB3	1:C:214:ARG:HG3	1.33	1.05

All (5) 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)
5:A:2183:HOH:O	5:C:2165:HOH:O[1_556]	2.06	0.14
5:A:2044:HOH:O	5:C:2181:HOH:O[2_555]	2.09	0.11
1:A:73:GLU:OE2	1:C:195:HIS:N[2_555]	2.13	0.07
5:B:2092:HOH:O	5:C:2258:HOH:O[2_555]	2.18	0.02
5:B:2093:HOH:O	5:B:3263:HOH:O[3_445]	2.18	0.02

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	332/340 (98%)	314 (95%)	15 (4%)	3 (1%)	14	6
1	B	330/340 (97%)	316 (96%)	11 (3%)	3 (1%)	14	6
1	C	333/340 (98%)	311 (93%)	15 (4%)	7 (2%)	5	1
All	All	995/1020 (98%)	941 (95%)	41 (4%)	13 (1%)	9	3

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	VAL
1	A	227	ARG
1	C	22	VAL
1	C	228	ALA
1	C	231	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	266/272 (98%)	263 (99%)	3 (1%)	65	67
1	B	264/272 (97%)	257 (97%)	7 (3%)	39	34
1	C	267/272 (98%)	261 (98%)	6 (2%)	45	42
All	All	797/816 (98%)	781 (98%)	16 (2%)	48	46

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	300	GLU
1	C	224	LEU
1	B	226	SER
1	C	222	THR
1	B	174	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	193	HIS
1	C	131	ASN
1	B	167	GLN
1	A	274	ASN
1	B	284	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

20 ligands 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
4	PEG	C	1343	-	6,6,6	0.83	0	5,5,5	0.50	0
3	SO4	A	1342	-	4,4,4	0.24	0	6,6,6	0.11	0
4	PEG	B	1344	-	6,6,6	0.79	0	5,5,5	0.26	0
3	SO4	B	1342	-	4,4,4	0.23	0	6,6,6	0.17	0
4	PEG	B	1343	-	6,6,6	0.76	0	5,5,5	0.41	0
4	PEG	A	1345	-	6,6,6	0.81	0	5,5,5	0.32	0
4	PEG	A	1348	-	6,6,6	0.78	0	5,5,5	0.21	0
3	SO4	C	1342	-	4,4,4	0.23	0	6,6,6	0.19	0
4	PEG	C	1345	-	6,6,6	0.81	0	5,5,5	0.40	0
3	SO4	C	1341	-	4,4,4	0.22	0	6,6,6	0.26	0
4	PEG	A	1344	-	6,6,6	0.77	0	5,5,5	0.29	0
2	3EB	B	1341	-	14,14,14	0.99	2 (14%)	18,18,18	1.15	2 (11%)
4	PEG	A	1349	-	6,6,6	0.79	0	5,5,5	0.50	0
4	PEG	C	1346	-	6,6,6	0.82	0	5,5,5	0.44	0
2	3EB	A	1341	-	14,14,14	1.18	2 (14%)	18,18,18	0.88	2 (11%)
4	PEG	A	1347	-	6,6,6	0.81	0	5,5,5	0.28	0
4	PEG	C	1344	-	6,6,6	0.78	0	5,5,5	0.20	0
4	PEG	A	1350	-	6,6,6	0.81	0	5,5,5	0.31	0
3	SO4	A	1343	-	4,4,4	0.25	0	6,6,6	0.31	0
4	PEG	A	1346	-	6,6,6	0.79	0	5,5,5	0.31	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	1347	-	-	2/4/4/4	-
4	PEG	C	1344	-	-	3/4/4/4	-
4	PEG	C	1343	-	-	2/4/4/4	-
2	3EB	A	1341	-	-	2/9/9/9	0/1/1/1
4	PEG	B	1344	-	-	3/4/4/4	-
4	PEG	A	1344	-	-	2/4/4/4	-
2	3EB	B	1341	-	-	3/9/9/9	0/1/1/1
4	PEG	A	1349	-	-	2/4/4/4	-
4	PEG	A	1350	-	-	2/4/4/4	-
4	PEG	C	1345	-	-	2/4/4/4	-
4	PEG	B	1343	-	-	2/4/4/4	-
4	PEG	A	1345	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	A	1348	-	-	3/4/4/4	-
4	PEG	C	1346	-	-	3/4/4/4	-
4	PEG	A	1346	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1341	3EB	OXT-C	3.11	1.32	1.22
2	A	1341	3EB	O-C	-2.96	1.21	1.30
2	B	1341	3EB	OXT-C	2.64	1.30	1.22
2	B	1341	3EB	O-C	-2.52	1.22	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1341	3EB	OXT-C-CA	-3.42	112.24	123.09
2	B	1341	3EB	O-C-CA	3.31	124.46	114.00
2	A	1341	3EB	OXT-C-CA	-2.50	115.17	123.09
2	A	1341	3EB	O-C-CA	2.42	121.64	114.00

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1347	PEG	O2-C3-C4-O4
4	A	1348	PEG	O1-C1-C2-O2
4	C	1344	PEG	O2-C3-C4-O4
4	A	1346	PEG	O2-C3-C4-O4
4	A	1350	PEG	O2-C3-C4-O4

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1345	PEG	1	0
4	C	1345	PEG	4	0
2	B	1341	3EB	1	0
4	A	1349	PEG	2	0
4	C	1344	PEG	2	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	333/340 (97%)	-1.59	0 100 100	16, 32, 55, 120	1 (0%)
1	B	332/340 (97%)	-1.54	0 100 100	22, 37, 65, 119	0
1	C	335/340 (98%)	-1.51	0 100 100	20, 31, 77, 132	0
All	All	1000/1020 (98%)	-1.54	0 100 100	16, 34, 68, 132	1 (0%)

There are no RSRZ outliers to report.

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 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(Å ²)	Q<0.9
3	SO4	A	1342	5/5	0.99	0.02	54,58,64,65	0
4	PEG	A	1344	7/7	0.99	0.04	49,75,96,100	0
4	PEG	A	1345	7/7	0.99	0.03	51,67,80,80	0
4	PEG	A	1346	7/7	0.99	0.03	51,61,67,68	0
4	PEG	A	1347	7/7	0.99	0.02	38,56,75,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PEG	A	1348	7/7	0.99	0.04	73,87,93,93	0
4	PEG	A	1349	7/7	0.99	0.03	47,58,71,75	0
4	PEG	A	1350	7/7	0.99	0.03	32,54,66,66	0
4	PEG	B	1343	7/7	0.99	0.02	42,57,68,68	0
4	PEG	B	1344	7/7	0.99	0.03	56,70,88,88	0
4	PEG	C	1343	7/7	0.99	0.03	40,56,75,75	0
4	PEG	C	1344	7/7	0.99	0.03	49,66,82,82	0
4	PEG	C	1345	7/7	0.99	0.02	34,43,53,53	0
4	PEG	C	1346	7/7	0.99	0.03	45,56,64,68	0
2	3EB	A	1341	14/14	1.00	0.01	20,26,31,35	0
3	SO4	A	1343	5/5	1.00	0.02	32,35,43,49	0
3	SO4	B	1342	5/5	1.00	0.01	29,30,36,42	0
3	SO4	C	1341	5/5	1.00	0.02	42,54,59,63	0
3	SO4	C	1342	5/5	1.00	0.02	27,35,41,44	0
2	3EB	B	1341	14/14	1.00	0.02	22,28,33,37	0

6.5 Other polymers ⓘ

There are no such residues in this entry.