



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 10:42 pm BST

PDB ID : 6Q62
Title : Xanthomonas albilineans Dihydropteroate synthase in complex with (indole-2-carboxylic acid) and (6-chloroguanine)
Authors : Oliveira, A.A.; Hyvonen, M.; Guido, R.V.C.
Deposited on : 2018-12-10
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

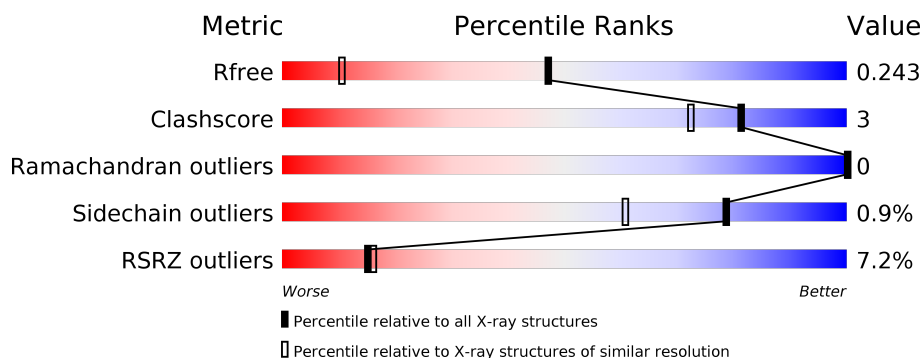
1 Overall quality at a glance

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	300	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>5%</div> <div>10%</div> </div> </div>
1	B	300	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>5%</div> <div>11%</div> </div> </div>
1	C	300	<div> <div>12%</div> <div> <div></div> <div>85%</div> <div>•</div> <div>11%</div> </div> </div>
1	D	300	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>6%</div> <div>13%</div> </div> </div>

2 Entry composition [i](#)

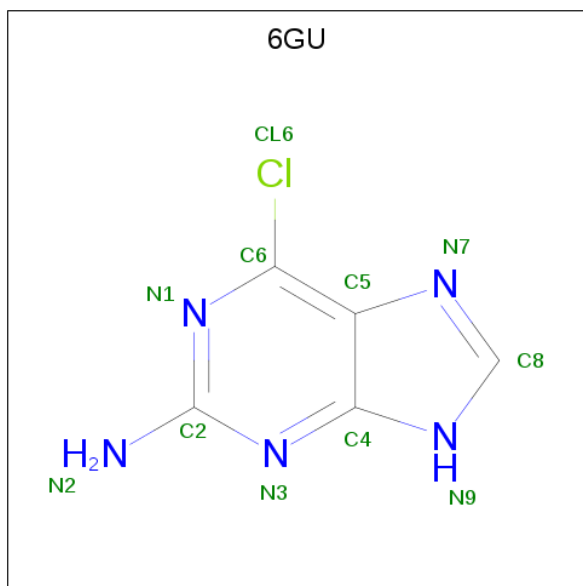
There are 7 unique types of molecules in this entry. The entry contains 8745 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dihydropteroate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	2	0
			1996	1257	366	365	8			
1	C	268	Total	C	N	O	S	0	0	0
			1913	1210	352	344	7			
1	B	266	Total	C	N	O	S	0	3	0
			1982	1253	359	362	8			
1	D	261	Total	C	N	O	S	0	1	0
			1926	1219	349	350	8			

- Molecule 2 is 6-chloroguanine (three-letter code: 6GU) (formula: C₅H₄ClN₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	0	0
			11	5	1	5		
2	C	1	Total	C	Cl	N	0	0
			11	5	1	5		

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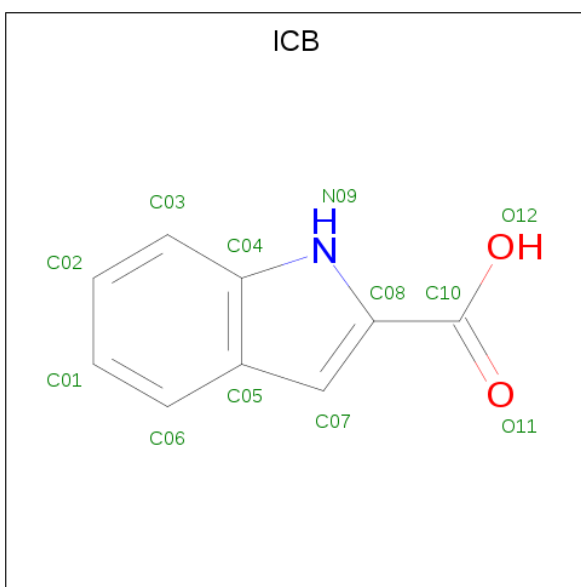
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	Cl	N	0	0
			11	5	1	5		
2	D	1	Total	C	Cl	N	0	0
			11	5	1	5		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is 1H-indole-2-carboxylic acid (three-letter code: ICB) (formula: C₉H₇NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			12	9	1	2		
4	C	1	Total	C	N	O	0	0
			12	9	1	2		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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

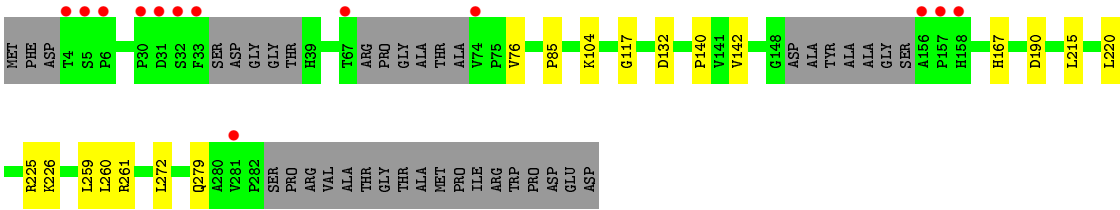
- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			7	4	3		
6	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	241	Total 241	O 241	0	0
7	C	131	Total 131	O 131	0	0
7	B	240	Total 240	O 240	0	0
7	D	169	Total 169	O 169	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.38Å 74.55Å 89.30Å 90.00° 101.21° 90.00°	Depositor
Resolution (Å)	42.09 – 1.50 42.09 – 1.50	Depositor EDS
% Data completeness (in resolution range)	71.7 (42.09-1.50) 71.7 (42.09-1.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 1.50Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.211 , 0.239 0.215 , 0.243	Depositor DCC
R_{free} test set	6098 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	14.9	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8745	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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 67.87 % 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 4.7959e-06. 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ICB, PEG, 6GU, EDO, SO4

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	0.50	0/2027	0.59	0/2762
1	B	0.51	0/2011	0.61	0/2738
1	C	0.46	0/1942	0.58	0/2653
1	D	0.48	0/1954	0.58	0/2662
All	All	0.49	0/7934	0.59	0/10815

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	1996	0	2036	11	0
1	B	1982	0	2020	9	0
1	C	1913	0	1932	9	0
1	D	1926	0	1972	13	0
2	A	11	0	4	1	0
2	B	11	0	4	1	0
2	C	11	0	4	1	0
2	D	11	0	4	1	0
3	A	4	0	6	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	4	0	6	2	0
3	C	4	0	6	0	0
3	D	8	0	12	0	0
4	A	12	0	0	0	0
4	C	12	0	0	0	0
5	A	10	0	0	0	0
5	B	15	0	0	0	0
5	C	10	0	0	0	0
5	D	10	0	0	0	0
6	D	14	0	20	2	0
7	A	241	0	0	1	0
7	B	240	0	0	1	0
7	C	131	0	0	0	0
7	D	169	0	0	0	0
All	All	8745	0	8026	42	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 (42) 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:227:ARG:H	3:B:402:EDO:H22	1.28	0.96
1:A:227:ARG:H	3:A:402:EDO:H12	1.31	0.92
1:B:190:ASP:OD2	1:B:220[B]:LEU:HD22	1.90	0.71
1:A:220[B]:LEU:HD13	1:A:259:LEU:HB3	1.79	0.64
1:D:190:ASP:OD2	1:D:220[A]:LEU:HD22	1.96	0.64
1:A:190:ASP:OD2	1:A:220[A]:LEU:HD22	1.97	0.64
1:B:227:ARG:N	3:B:402:EDO:H22	2.09	0.62
1:D:220[B]:LEU:HD13	1:D:259:LEU:HB3	1.81	0.62
1:A:276:GLN:HG2	7:A:660:HOH:O	2.00	0.60
1:C:59:LEU:HD21	1:C:259:LEU:HD21	1.86	0.57
1:B:226:LYS:NZ	2:B:401:6GU:CL6	2.75	0.55
1:D:226:LYS:NZ	2:D:401:6GU:CL6	2.77	0.55
1:B:51:ARG:HD2	7:B:559:HOH:O	2.09	0.53
1:C:226:LYS:NZ	2:C:401:6GU:CL6	2.79	0.52
1:D:225:ARG:HD2	6:D:402:PEG:H11	1.92	0.51
1:A:226:LYS:NZ	2:A:401:6GU:CL6	2.81	0.50
1:C:190:ASP:OD2	1:C:220:LEU:HD22	2.12	0.50
1:B:138:ARG:HA	1:B:186:ARG:CZ	2.43	0.49
1:D:117:GLY:O	1:D:140:PRO:HD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:PRO:HG3	6:D:403:PEG:H41	1.95	0.48
1:D:76:VAL:CG2	1:D:104:LYS:HD3	2.43	0.48
1:A:227:ARG:N	3:A:402:EDO:H12	2.14	0.47
1:B:117:GLY:O	1:B:140:PRO:HD2	2.15	0.47
1:C:117:GLY:O	1:C:140:PRO:HD2	2.15	0.47
1:B:167:HIS:NE2	1:B:215:LEU:HD21	2.30	0.47
1:D:76:VAL:HG23	1:D:104:LYS:HD3	1.96	0.46
1:A:117:GLY:O	1:A:140:PRO:HD2	2.16	0.46
1:D:260:LEU:HD12	1:D:272:LEU:HD11	1.98	0.46
1:C:162:VAL:HG21	1:C:201:ASP:HB3	1.97	0.46
1:B:146:MET:HG3	1:B:195:PHE:HB3	2.00	0.44
1:A:220[B]:LEU:CD1	1:A:259:LEU:HB3	2.48	0.44
1:D:167:HIS:NE2	1:D:215:LEU:HD21	2.32	0.44
1:D:259:LEU:HD23	1:D:259:LEU:HA	1.96	0.42
1:A:167:HIS:NE2	1:A:215:LEU:HD21	2.34	0.42
1:D:142:VAL:HG11	1:D:220[B]:LEU:HD23	2.01	0.41
1:D:220[B]:LEU:HD11	1:D:261:ARG:HB2	2.02	0.41
1:C:59:LEU:HD21	1:C:259:LEU:CD2	2.50	0.41
1:A:260:LEU:HD12	1:A:272:LEU:HD11	2.03	0.41
1:C:220:LEU:HD23	1:C:221:ALA:N	2.35	0.41
1:A:220[B]:LEU:HD11	1:A:261:ARG:HB2	2.03	0.40
1:C:220:LEU:HD21	1:C:261:ARG:HB2	2.04	0.40
1:C:259:LEU:HD23	1:C:259:LEU:HA	1.93	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	265/300 (88%)	260 (98%)	5 (2%)	0	100	100
1	B	261/300 (87%)	256 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	262/300 (87%)	258 (98%)	4 (2%)	0	100	100
1	D	254/300 (85%)	249 (98%)	5 (2%)	0	100	100
All	All	1042/1200 (87%)	1023 (98%)	19 (2%)	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	A	205/232 (88%)	203 (99%)	2 (1%)	76	57
1	B	204/232 (88%)	203 (100%)	1 (0%)	88	78
1	C	187/232 (81%)	185 (99%)	2 (1%)	73	53
1	D	198/232 (85%)	196 (99%)	2 (1%)	76	57
All	All	794/928 (86%)	787 (99%)	7 (1%)	78	61

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	GLU
1	A	279	GLN
1	C	43	GLU
1	C	223	LEU
1	B	74	VAL
1	D	132	ASP
1	D	279	GLN

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

Mol	Chain	Res	Type
1	D	93	GLN

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 ⓘ

22 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$
5	SO4	C	404	-	4,4,4	0.30	0	6,6,6	0.19	0
2	6GU	A	401	-	10,12,12	2.82	4 (40%)	8,17,17	1.46	2 (25%)
3	EDO	D	404	-	3,3,3	0.46	0	2,2,2	0.60	0
5	SO4	D	407	-	4,4,4	0.15	0	6,6,6	0.12	0
2	6GU	B	401	-	10,12,12	2.73	4 (40%)	8,17,17	1.55	2 (25%)
2	6GU	D	401	-	10,12,12	2.75	4 (40%)	8,17,17	1.39	1 (12%)
5	SO4	C	405	-	4,4,4	0.11	0	6,6,6	0.10	0
4	ICB	A	403	-	9,13,13	0.97	0	10,18,18	0.85	0
3	EDO	A	402	-	3,3,3	0.45	0	2,2,2	0.36	0
5	SO4	D	406	-	4,4,4	0.10	0	6,6,6	0.20	0
6	PEG	D	402	-	6,6,6	0.21	0	5,5,5	0.29	0
5	SO4	A	405	-	4,4,4	0.20	0	6,6,6	0.24	0
2	6GU	C	401	-	10,12,12	2.86	4 (40%)	8,17,17	1.41	1 (12%)
4	ICB	C	403	-	9,13,13	1.19	0	10,18,18	0.96	1 (10%)
5	SO4	A	404	-	4,4,4	0.32	0	6,6,6	0.24	0
5	SO4	B	405	-	4,4,4	0.13	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	D	405	-	3,3,3	0.42	0	2,2,2	0.34	0
3	EDO	C	402	-	3,3,3	0.40	0	2,2,2	0.53	0
6	PEG	D	403	-	6,6,6	0.06	0	5,5,5	0.03	0
3	EDO	B	402	-	3,3,3	0.34	0	2,2,2	0.44	0
5	SO4	B	403	-	4,4,4	0.14	0	6,6,6	0.14	0
5	SO4	B	404	-	4,4,4	0.42	0	6,6,6	0.37	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
6	PEG	D	403	-	-	1/4/4/4	-
6	PEG	D	402	-	-	1/4/4/4	-
3	EDO	C	402	-	-	1/1/1/1	-
2	6GU	B	401	-	-	-	0/2/2/2
2	6GU	A	401	-	-	-	0/2/2/2
3	EDO	B	402	-	-	1/1/1/1	-
2	6GU	D	401	-	-	-	0/2/2/2
2	6GU	C	401	-	-	-	0/2/2/2
3	EDO	D	404	-	-	0/1/1/1	-
4	ICB	C	403	-	-	0/0/4/4	0/2/2/2
4	ICB	A	403	-	-	0/0/4/4	0/2/2/2
3	EDO	D	405	-	-	0/1/1/1	-
3	EDO	A	402	-	-	0/1/1/1	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	6GU	C6-C5	-5.79	1.36	1.43
2	A	401	6GU	C6-C5	-5.69	1.36	1.43
2	A	401	6GU	C6-CL6	-5.68	1.60	1.74
2	D	401	6GU	C6-CL6	-5.67	1.60	1.74
2	B	401	6GU	C6-CL6	-5.41	1.61	1.74
2	C	401	6GU	C6-CL6	-5.35	1.61	1.74
2	B	401	6GU	C6-C5	-4.99	1.37	1.43
2	D	401	6GU	C6-C5	-4.59	1.37	1.43
2	D	401	6GU	C2-N1	3.37	1.41	1.35
2	C	401	6GU	C4-N9	3.03	1.40	1.34
2	B	401	6GU	C2-N1	3.02	1.40	1.35
2	B	401	6GU	C4-N9	2.97	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	6GU	C4-N9	2.88	1.40	1.34
2	C	401	6GU	C2-N1	2.72	1.40	1.35
2	A	401	6GU	C2-N1	2.54	1.39	1.35
2	A	401	6GU	C4-N9	2.46	1.39	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	6GU	N2-C2-N1	-2.68	113.08	117.25
2	D	401	6GU	N2-C2-N1	-2.34	113.61	117.25
2	A	401	6GU	C5-C6-CL6	-2.31	117.01	121.04
2	B	401	6GU	N2-C2-N3	2.23	121.43	117.79
2	A	401	6GU	N2-C2-N1	-2.22	113.79	117.25
2	C	401	6GU	C5-C6-CL6	-2.17	117.26	121.04
4	C	403	ICB	C08-N09-C04	2.01	108.64	104.45

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	403	PEG	C1-C2-O2-C3
6	D	402	PEG	C1-C2-O2-C3
3	B	402	EDO	O1-C1-C2-O2
3	C	402	EDO	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	6GU	1	0
2	B	401	6GU	1	0
2	D	401	6GU	1	0
3	A	402	EDO	2	0
6	D	402	PEG	1	0
2	C	401	6GU	1	0
6	D	403	PEG	1	0
3	B	402	EDO	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 ⓘ

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, 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	269/300 (89%)	0.08	13 (4%)	30 33	8, 15, 41, 70	0
1	B	266/300 (88%)	0.13	15 (5%)	24 26	7, 14, 39, 69	0
1	C	268/300 (89%)	0.78	36 (13%)	3 3	10, 25, 50, 75	0
1	D	261/300 (87%)	0.36	13 (4%)	28 31	9, 20, 45, 72	0
All	All	1064/1200 (88%)	0.34	77 (7%)	15 16	7, 18, 45, 75	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	69	PRO	11.1
1	C	69	PRO	10.0
1	A	67	THR	7.9
1	D	5	SER	7.8
1	B	32	SER	6.1
1	C	68	ARG	5.3
1	C	70	GLY	5.0
1	A	70	GLY	4.8
1	D	32	SER	4.5
1	C	71	ALA	4.5
1	A	68	ARG	4.5
1	B	2	PHE	4.4
1	C	164	ALA	4.4
1	D	74	VAL	4.4
1	B	33	PHE	4.1
1	B	73	ALA	4.0
1	C	212	LEU	4.0
1	C	217	VAL	3.9
1	B	30	PRO	3.9
1	D	158	HIS	3.9
1	B	148	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	156	ALA	3.6
1	D	30	PRO	3.6
1	B	31	ASP	3.5
1	D	4	THR	3.5
1	C	157	PRO	3.4
1	D	33	PHE	3.4
1	C	175	PHE	3.4
1	B	3	ASP	3.3
1	C	92	ALA	3.3
1	C	34	SER	3.3
1	C	8	LEU	3.2
1	C	187	LEU	3.2
1	C	160	ASP	3.2
1	B	4	THR	3.2
1	D	67	THR	3.1
1	A	175	PHE	3.0
1	C	7	ARG	2.9
1	B	160	ASP	2.9
1	C	214	GLU	2.9
1	C	176	ALA	2.8
1	B	175	PHE	2.8
1	C	170	LEU	2.8
1	C	12	GLY	2.7
1	C	167	HIS	2.7
1	C	215	LEU	2.7
1	D	156	ALA	2.7
1	D	31	ASP	2.7
1	C	183	ASP	2.6
1	A	71	ALA	2.6
1	C	281	VAL	2.6
1	C	216	GLY	2.6
1	A	216	GLY	2.5
1	A	215	LEU	2.5
1	B	67	THR	2.5
1	B	74	VAL	2.5
1	B	38	THR	2.5
1	C	182	ILE	2.5
1	A	158	HIS	2.4
1	A	212	LEU	2.4
1	C	143	LEU	2.4
1	A	282	PRO	2.4
1	C	205	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	163	VAL	2.3
1	C	174	ILE	2.3
1	B	66	SER	2.3
1	A	6	PRO	2.2
1	C	169	PHE	2.2
1	D	281	VAL	2.2
1	D	6	PRO	2.2
1	A	5	SER	2.1
1	C	10	CYS	2.1
1	C	282	PRO	2.1
1	C	14	ILE	2.1
1	C	134	VAL	2.1
1	D	157	PRO	2.0
1	C	179	MET	2.0

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

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

6.3 Carbohydrates ⓘ

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
6	PEG	D	403	7/7	0.72	0.26	68,69,69,70	0
5	SO4	B	404	5/5	0.78	0.14	40,44,47,50	0
6	PEG	D	402	7/7	0.83	0.21	21,31,43,44	0
4	ICB	C	403	12/12	0.83	0.18	39,41,47,50	0
3	EDO	A	402	4/4	0.85	0.12	27,27,28,32	0
3	EDO	C	402	4/4	0.86	0.12	37,37,38,39	0
5	SO4	B	405	5/5	0.88	0.13	86,86,86,86	0
3	EDO	D	404	4/4	0.88	0.15	31,34,35,36	0
3	EDO	B	402	4/4	0.89	0.15	24,26,27,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	6GU	C	401	11/11	0.89	0.09	22,24,29,39	0
4	ICB	A	403	12/12	0.89	0.12	32,33,42,42	0
2	6GU	B	401	11/11	0.90	0.09	13,16,23,34	0
2	6GU	D	401	11/11	0.90	0.09	15,19,27,36	0
2	6GU	A	401	11/11	0.90	0.09	12,18,21,32	0
5	SO4	D	406	5/5	0.91	0.12	40,44,45,47	0
5	SO4	D	407	5/5	0.92	0.10	69,69,69,70	0
3	EDO	D	405	4/4	0.92	0.17	24,32,35,40	0
5	SO4	C	405	5/5	0.92	0.24	60,61,62,63	0
5	SO4	C	404	5/5	0.93	0.12	36,40,42,43	0
5	SO4	A	405	5/5	0.94	0.14	57,58,58,59	0
5	SO4	B	403	5/5	0.94	0.10	55,56,56,58	0
5	SO4	A	404	5/5	0.96	0.11	26,31,32,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.