



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 10:34 PM UTC

PDB ID : 6Q62 / pdb_00006q62
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.

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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

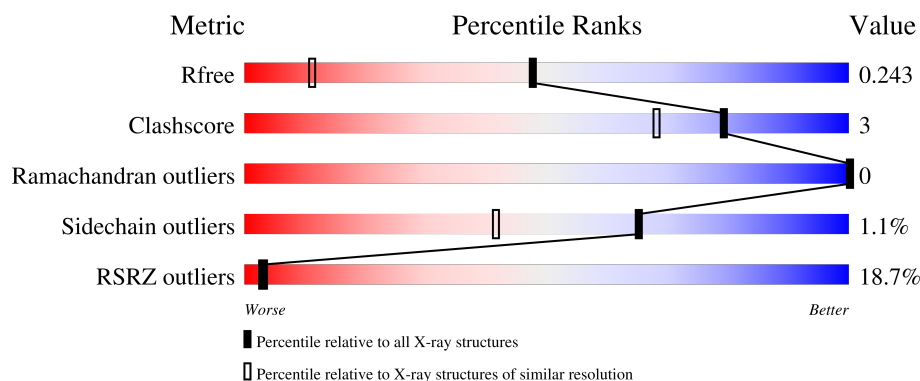
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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}	180053	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (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 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	300	8% 84% 5% 10%
1	B	300	9% 83% 5% 11%
1	C	300	35% 84% 6% 11%
1	D	300	14% 81% 6% 13%

2 Entry composition [i](#)

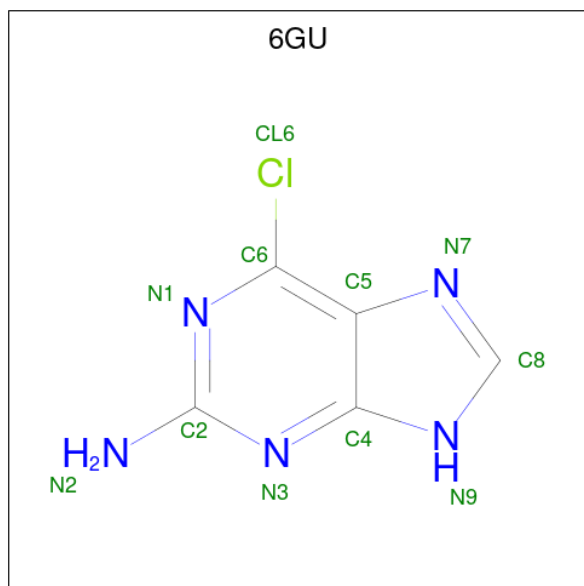
There are 7 unique types of molecules in this entry. The entry contains 8745 atoms, of which 0 are hydrogens and 0 are deuteriums.

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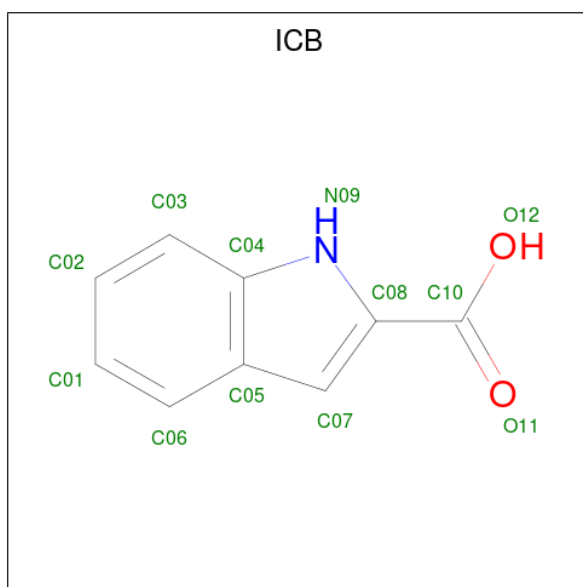
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	Cl	N	0	0
			11	5	1	5		
2	D	1	Total	C	Cl	N	0	0
			11	5	1	5		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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 (CCD ID: ICB) (formula: $C_9H_7NO_2$).



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 (CCD ID: 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 (CCD ID: 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		

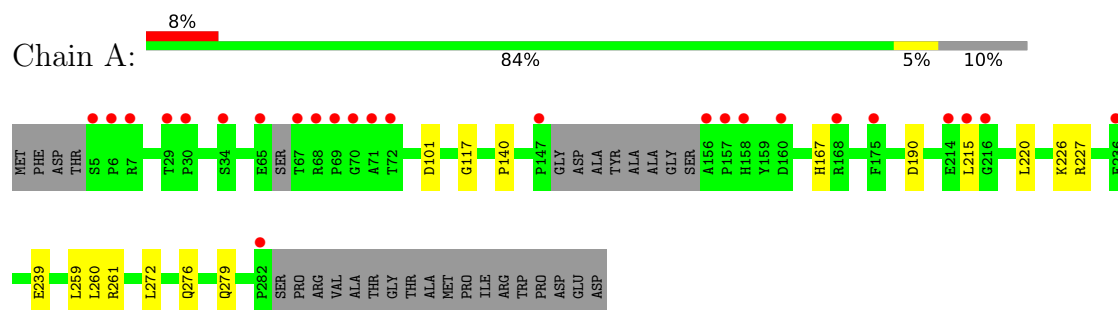
- Molecule 7 is water.

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

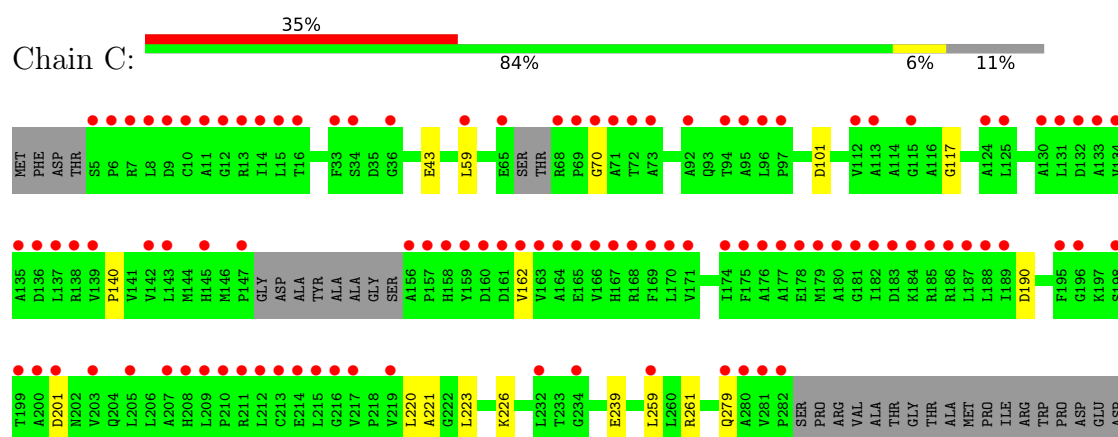
3 Residue-property plots [i](#)

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.

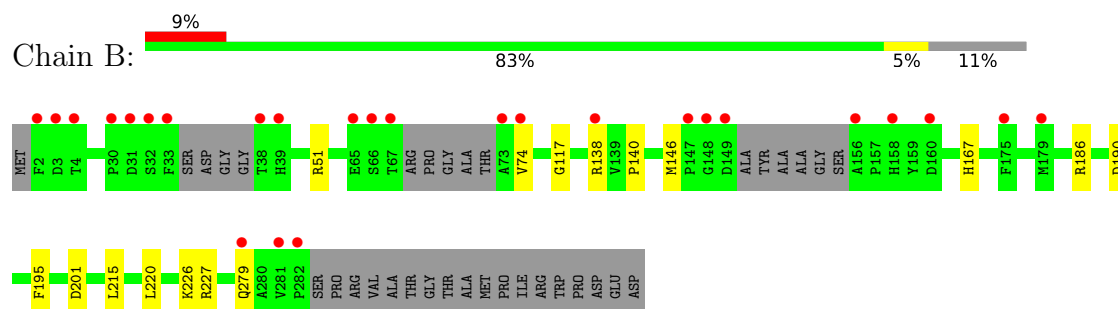
• Molecule 1: Dihydropteroate synthase



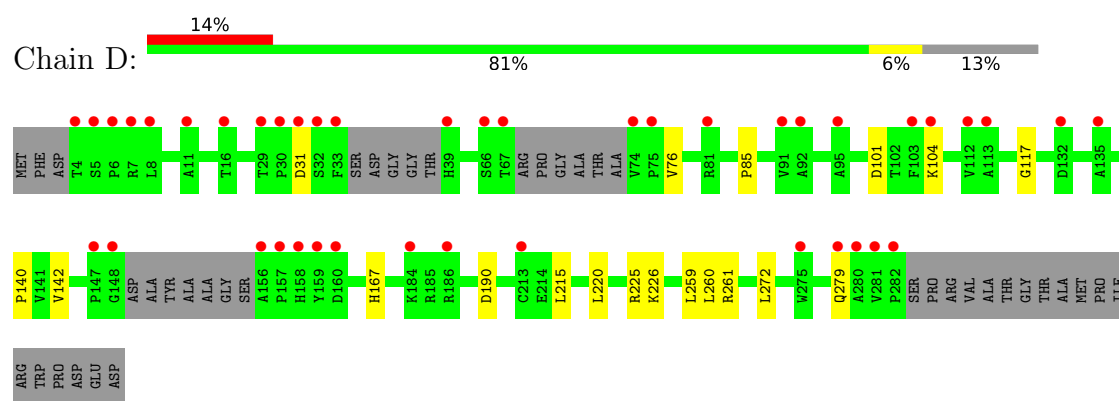
• Molecule 1: Dihydropteroate synthase



• Molecule 1: Dihydropteroate synthase



• Molecule 1: Dihydropteroate synthase



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)	Xtrriage
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	Xtrriage
Anisotropy	0.012	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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.*

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

5.1 Standard geometry

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

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	0.82	0/2027	1.02	1/2762 (0.0%)
1	B	0.83	0/2011	1.03	1/2738 (0.0%)
1	C	0.79	0/1942	1.08	3/2653 (0.1%)
1	D	0.81	0/1954	1.02	2/2662 (0.1%)
All	All	0.81	0/7934	1.04	7/10815 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	201	ASP	CA-CB-CG	6.03	118.63	112.60
1	A	101	ASP	CA-CB-CG	5.79	118.39	112.60
1	D	101	ASP	CA-CB-CG	5.54	118.14	112.60
1	D	31	ASP	CA-CB-CG	5.26	117.86	112.60
1	C	101	ASP	CA-CB-CG	5.22	117.82	112.60
1	C	70	GLY	CA-C-N	5.14	128.14	120.90
1	C	70	GLY	C-N-CA	5.14	128.14	120.90

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	1996	0	2036	11	0
1	B	1982	0	2020	10	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
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	43	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 (43) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:117:GLY:O	1:C:140:PRO:HD2	2.15	0.47
1:B:117:GLY:O	1:B: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
1:B:220[B]:LEU:HD23	1:B:220[B]:LEU:C	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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
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%)	68	45
1	B	204/232 (88%)	202 (99%)	2 (1%)	68	45
1	C	187/232 (81%)	183 (98%)	4 (2%)	47	19
1	D	198/232 (85%)	197 (100%)	1 (0%)	81	66
All	All	794/928 (86%)	785 (99%)	9 (1%)	65	41

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	239	GLU
1	A	279	GLN
1	C	43	GLU
1	C	223	LEU
1	C	239	GLU
1	C	279	GLN
1	B	74	VAL
1	B	279	GLN

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Mol	Chain	Res	Type
1	D	279	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	123	GLN
1	C	123	GLN
1	B	123	GLN
1	D	123	GLN

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](#)

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	A	404	-	4,4,4	0.41	0	6,6,6	0.26	0
5	SO4	B	403	-	4,4,4	0.22	0	6,6,6	0.12	0
6	PEG	D	402	-	6,6,6	0.22	0	5,5,5	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	B	402	-	3,3,3	0.32	0	2,2,2	0.47	0
6	PEG	D	403	-	6,6,6	0.06	0	5,5,5	0.04	0
2	6GU	D	401	-	12,12,12	2.91	7 (58%)	17,17,17	1.99	5 (29%)
3	EDO	C	402	-	3,3,3	0.37	0	2,2,2	0.56	0
5	SO4	C	404	-	4,4,4	0.39	0	6,6,6	0.18	0
2	6GU	A	401	-	12,12,12	2.77	5 (41%)	17,17,17	2.01	5 (29%)
5	SO4	C	405	-	4,4,4	0.23	0	6,6,6	0.13	0
3	EDO	D	405	-	3,3,3	0.38	0	2,2,2	0.39	0
5	SO4	B	405	-	4,4,4	0.23	0	6,6,6	0.13	0
2	6GU	B	401	-	12,12,12	2.82	6 (50%)	17,17,17	2.19	5 (29%)
4	ICB	A	403	-	13,13,13	1.14	2 (15%)	16,18,18	0.63	0
4	ICB	C	403	-	13,13,13	1.05	0	16,18,18	1.02	1 (6%)
5	SO4	A	405	-	4,4,4	0.30	0	6,6,6	0.26	0
5	SO4	D	406	-	4,4,4	0.22	0	6,6,6	0.17	0
3	EDO	A	402	-	3,3,3	0.42	0	2,2,2	0.40	0
5	SO4	B	404	-	4,4,4	0.52	0	6,6,6	0.33	0
2	6GU	C	401	-	12,12,12	2.90	7 (58%)	17,17,17	2.00	4 (23%)
3	EDO	D	404	-	3,3,3	0.42	0	2,2,2	0.63	0
5	SO4	D	407	-	4,4,4	0.24	0	6,6,6	0.11	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
2	6GU	A	401	-	-	-	0/2/2/2
2	6GU	B	401	-	-	-	0/2/2/2
4	ICB	A	403	-	-	0/4/4/4	0/2/2/2
2	6GU	C	401	-	-	-	0/2/2/2
4	ICB	C	403	-	-	0/4/4/4	0/2/2/2
3	EDO	D	404	-	-	0/1/1/1	-
6	PEG	D	402	-	-	1/4/4/4	-
3	EDO	B	402	-	-	1/1/1/1	-
6	PEG	D	403	-	-	1/4/4/4	-
2	6GU	D	401	-	-	-	0/2/2/2
3	EDO	C	402	-	-	1/1/1/1	-
3	EDO	A	402	-	-	0/1/1/1	-
3	EDO	D	405	-	-	0/1/1/1	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	6GU	C6-CL6	-7.27	1.60	1.74
2	D	401	6GU	C6-CL6	-7.25	1.60	1.74
2	B	401	6GU	C6-CL6	-6.90	1.61	1.74
2	C	401	6GU	C6-CL6	-6.81	1.61	1.74
2	C	401	6GU	C8-N7	3.96	1.40	1.32
2	D	401	6GU	C8-N7	3.72	1.39	1.32
2	A	401	6GU	C8-N7	3.63	1.39	1.32
2	B	401	6GU	C8-N7	3.61	1.39	1.32
2	D	401	6GU	C2-N1	3.47	1.41	1.35
2	B	401	6GU	C2-N1	3.11	1.40	1.35
2	C	401	6GU	C2-N3	2.91	1.40	1.35
2	C	401	6GU	C2-N1	2.80	1.40	1.35
2	A	401	6GU	C2-N1	2.62	1.39	1.35
2	B	401	6GU	C5-C4	2.51	1.43	1.39
2	C	401	6GU	C4-N9	2.44	1.40	1.36
2	D	401	6GU	C5-C4	2.38	1.43	1.39
2	B	401	6GU	C4-N9	2.37	1.40	1.36
2	C	401	6GU	C5-C4	2.29	1.42	1.39
2	D	401	6GU	C4-N9	2.26	1.40	1.36
2	D	401	6GU	C4-N3	2.24	1.38	1.34
2	D	401	6GU	C2-N3	2.14	1.39	1.35
2	C	401	6GU	C4-N3	2.12	1.38	1.34
2	B	401	6GU	C4-N3	2.12	1.38	1.34
4	A	403	ICB	O12-C10	-2.10	1.24	1.30
4	A	403	ICB	C05-C04	2.09	1.44	1.41
2	A	401	6GU	C5-C4	2.09	1.42	1.39
2	A	401	6GU	C4-N3	2.05	1.38	1.34

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	6GU	C5-C6-N1	4.98	127.07	122.14
2	B	401	6GU	C5-C6-N1	4.96	127.05	122.14
2	C	401	6GU	C5-C6-N1	4.96	127.05	122.14
2	A	401	6GU	C5-C6-N1	4.72	126.80	122.14
2	A	401	6GU	C5-C6-CL6	-4.33	117.01	120.76
2	C	401	6GU	C5-C6-CL6	-4.04	117.26	120.76
2	B	401	6GU	C5-C4-N3	-3.96	122.67	126.55
2	B	401	6GU	C5-C6-CL6	-3.68	117.57	120.76
2	D	401	6GU	C5-C6-CL6	-3.44	117.78	120.76
2	C	401	6GU	C5-C4-N3	-3.23	123.38	126.55
2	A	401	6GU	C5-C4-N3	-3.23	123.39	126.55
2	D	401	6GU	C5-C4-N3	-3.17	123.44	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	403	ICB	O11-C10-C08	-2.96	115.01	121.01
2	B	401	6GU	N2-C2-N3	2.81	121.43	117.22
2	B	401	6GU	N2-C2-N1	-2.76	113.08	117.22
2	D	401	6GU	N2-C2-N1	-2.41	113.61	117.22
2	A	401	6GU	N2-C2-N1	-2.29	113.79	117.22
2	D	401	6GU	N2-C2-N3	2.17	120.47	117.22
2	A	401	6GU	N2-C2-N3	2.09	120.36	117.22
2	C	401	6GU	N2-C2-N3	2.02	120.25	117.22

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
6	D	402	PEG	1	0
3	B	402	EDO	2	0
6	D	403	PEG	1	0
2	D	401	6GU	1	0
2	A	401	6GU	1	0
2	B	401	6GU	1	0
3	A	402	EDO	2	0
2	C	401	6GU	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

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%)	0.41	25 (9%) 14 15	5, 15, 41, 70	2 (0%)
1	B	266/300 (88%)	0.37	26 (9%) 13 13	4, 14, 39, 69	3 (1%)
1	C	268/300 (89%)	1.81	106 (39%) 1 0	10, 25, 50, 75	0
1	D	261/300 (87%)	0.96	42 (16%) 4 4	5, 20, 45, 72	1 (0%)
All	All	1064/1200 (88%)	0.89	199 (18%) 3 3	4, 18, 45, 75	6 (0%)

All (199) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	4	THR	8.2
1	D	148	GLY	7.9
1	D	67	THR	7.6
1	C	164	ALA	7.5
1	A	67	THR	6.4
1	C	174	ILE	6.1
1	C	217	VAL	6.1
1	D	5	SER	6.0
1	C	175	PHE	5.9
1	D	74	VAL	5.9
1	A	69	PRO	5.8
1	C	157	PRO	5.8
1	C	14	ILE	5.7
1	C	161	ASP	5.7
1	B	67	THR	5.6
1	C	216	GLY	5.5
1	C	156	ALA	5.5
1	B	73	ALA	5.5
1	C	8	LEU	5.5
1	C	69	PRO	5.4
1	C	182	ILE	5.3

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Mol	Chain	Res	Type	RSRZ
1	C	134	VAL	5.2
1	B	2	PHE	5.2
1	B	149	ASP	5.1
1	D	6	PRO	5.1
1	C	282	PRO	5.1
1	C	160	ASP	5.0
1	D	156	ALA	5.0
1	C	170	LEU	5.0
1	C	159	TYR	4.9
1	C	12	GLY	4.9
1	C	163	VAL	4.9
1	C	158	HIS	4.9
1	D	282	PRO	4.9
1	B	282	PRO	4.8
1	C	169	PHE	4.7
1	C	214	GLU	4.7
1	B	32	SER	4.7
1	C	171	VAL	4.7
1	C	212	LEU	4.6
1	C	135	ALA	4.5
1	B	33	PHE	4.5
1	A	156	ALA	4.5
1	C	70	GLY	4.4
1	C	162	VAL	4.4
1	C	95	ALA	4.4
1	C	215	LEU	4.3
1	B	4	THR	4.3
1	A	282	PRO	4.3
1	C	176	ALA	4.3
1	D	157	PRO	4.2
1	B	74	VAL	4.2
1	A	216	GLY	4.2
1	C	131	LEU	4.1
1	C	92	ALA	4.1
1	C	136	ASP	4.0
1	C	187	LEU	4.0
1	C	11	ALA	3.9
1	A	70	GLY	3.9
1	D	33	PHE	3.8
1	C	71	ALA	3.8
1	C	124	ALA	3.7
1	C	7	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	168	ARG	3.7
1	A	157	PRO	3.7
1	C	125	LEU	3.7
1	D	158	HIS	3.7
1	C	180	ALA	3.7
1	A	71	ALA	3.6
1	A	5	SER	3.6
1	C	132	ASP	3.6
1	A	158	HIS	3.5
1	C	34	SER	3.5
1	D	32	SER	3.5
1	B	148	GLY	3.5
1	D	8	LEU	3.5
1	C	177	ALA	3.5
1	D	135	ALA	3.4
1	C	181	GLY	3.4
1	C	6	PRO	3.3
1	C	211	ARG	3.3
1	C	183	ASP	3.2
1	C	184	LYS	3.2
1	C	166	VAL	3.2
1	D	11	ALA	3.2
1	A	236	GLU	3.2
1	C	96	LEU	3.2
1	D	30	PRO	3.2
1	D	31	ASP	3.2
1	C	94	THR	3.2
1	C	68	ARG	3.2
1	B	38	THR	3.1
1	C	147	PRO	3.1
1	B	156	ALA	3.1
1	B	30	PRO	3.1
1	B	31	ASP	3.1
1	C	143	LEU	3.0
1	B	3	ASP	3.0
1	C	72	THR	3.0
1	C	186	ARG	3.0
1	D	92	ALA	3.0
1	C	185	ARG	3.0
1	C	16	THR	3.0
1	C	178	GLU	2.9
1	C	200	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	167	HIS	2.9
1	D	280	ALA	2.9
1	B	66	SER	2.9
1	D	279	GLN	2.9
1	C	137	LEU	2.9
1	C	139	VAL	2.8
1	C	205	LEU	2.8
1	C	113	ALA	2.8
1	C	210	PRO	2.8
1	C	179	MET	2.8
1	A	68	ARG	2.8
1	D	29	THR	2.8
1	C	234	GLY	2.8
1	C	10	CYS	2.8
1	C	15	LEU	2.7
1	B	160	ASP	2.7
1	C	280	ALA	2.7
1	D	16	THR	2.7
1	C	195	PHE	2.7
1	D	281	VAL	2.7
1	A	65	GLU	2.7
1	D	75	PRO	2.7
1	D	147	PRO	2.7
1	C	5	SER	2.6
1	C	213	CYS	2.6
1	B	65	GLU	2.6
1	B	158	HIS	2.6
1	C	209	LEU	2.6
1	A	6	PRO	2.6
1	B	279	GLN	2.6
1	C	133	ALA	2.6
1	A	7	ARG	2.6
1	D	7	ARG	2.6
1	A	72	THR	2.6
1	D	66	SER	2.6
1	C	65	GLU	2.5
1	C	279	GLN	2.5
1	A	168	ARG	2.5
1	A	147	PRO	2.5
1	B	39	HIS	2.5
1	D	39	HIS	2.5
1	D	95	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	281	VAL	2.4
1	D	184	LYS	2.4
1	C	138	ARG	2.4
1	C	73	ALA	2.4
1	D	91	VAL	2.4
1	C	201	ASP	2.3
1	C	36	GLY	2.3
1	C	189	ILE	2.3
1	B	138	ARG	2.3
1	A	30	PRO	2.3
1	C	9	ASP	2.3
1	C	115	GLY	2.3
1	D	275	TRP	2.3
1	C	188	LEU	2.3
1	D	113	ALA	2.2
1	D	104	LYS	2.2
1	C	232	LEU	2.2
1	D	159	TYR	2.2
1	B	147	PRO	2.2
1	B	179	MET	2.2
1	B	281	VAL	2.2
1	A	214	GLU	2.2
1	C	130	ALA	2.2
1	A	34	SER	2.2
1	C	112	VAL	2.2
1	C	219	VAL	2.2
1	C	145	HIS	2.2
1	A	215	LEU	2.1
1	C	259	LEU	2.1
1	C	142	VAL	2.1
1	D	112	VAL	2.1
1	A	29	THR	2.1
1	C	208	HIS	2.1
1	D	186	ARG	2.1
1	A	175	PHE	2.1
1	C	198	SER	2.1
1	C	203	VAL	2.1
1	C	97	PRO	2.1
1	D	132	ASP	2.1
1	D	160	ASP	2.1
1	C	207	ALA	2.1
1	C	13	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	81	ARG	2.1
1	C	33	PHE	2.0
1	C	199	THR	2.0
1	D	103	PHE	2.0
1	C	59	LEU	2.0
1	C	196	GLY	2.0
1	C	165	GLU	2.0
1	B	175	PHE	2.0
1	D	213	CYS	2.0
1	A	160	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 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
6	PEG	D	403	7/7	0.68	0.17	68,69,69,70	0
5	SO4	B	405	5/5	0.73	0.20	86,86,86,86	0
6	PEG	D	402	7/7	0.77	0.17	21,31,43,44	0
5	SO4	B	404	5/5	0.77	0.14	40,44,47,50	0
4	ICB	C	403	12/12	0.79	0.18	39,41,47,50	0
3	EDO	C	402	4/4	0.81	0.14	37,37,38,39	0
5	SO4	D	406	5/5	0.82	0.13	40,44,45,47	0
3	EDO	D	404	4/4	0.82	0.15	31,34,35,36	0
5	SO4	C	405	5/5	0.82	0.13	60,61,62,63	0
3	EDO	A	402	4/4	0.83	0.12	27,27,28,32	0
3	EDO	B	402	4/4	0.84	0.16	24,26,27,32	0
5	SO4	B	403	5/5	0.85	0.12	55,56,56,58	0
5	SO4	D	407	5/5	0.85	0.14	69,69,69,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	A	405	5/5	0.85	0.12	57,58,58,59	0
4	ICB	A	403	12/12	0.85	0.14	32,33,42,42	0
2	6GU	C	401	11/11	0.86	0.10	22,24,29,39	0
5	SO4	C	404	5/5	0.87	0.11	36,40,42,43	0
2	6GU	A	401	11/11	0.88	0.10	12,18,21,32	0
2	6GU	B	401	11/11	0.89	0.09	13,16,23,34	0
2	6GU	D	401	11/11	0.90	0.09	15,19,27,36	0
3	EDO	D	405	4/4	0.91	0.12	24,32,35,40	0
5	SO4	A	404	5/5	0.91	0.09	26,31,32,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.