



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 07:21 AM UTC

PDB ID : 8OFB / pdb_00008ofb
Title : Crystal Structure of T. maritima reverse gyrase with a minimal latch, hexagonal form
Authors : Klostermeier, D.; Rasche, R.; Mhaindarkar, V.; Kummel, D.; Rudolph, M.G.
Deposited on : 2023-03-15
Resolution : 2.39 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 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

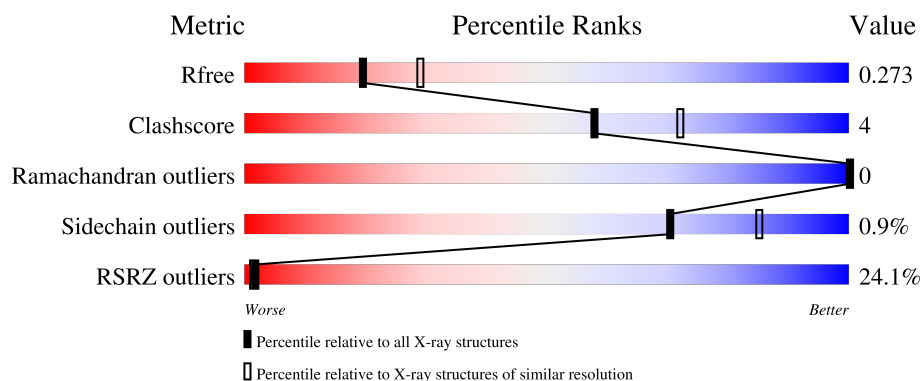
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	1043	24% 86% 14%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8679 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 Reverse gyrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1040	Total	C	N	O	S	0	0	0
			8521	5434	1475	1588	24			

There are 61 discrepancies between the modelled and reference sequences:

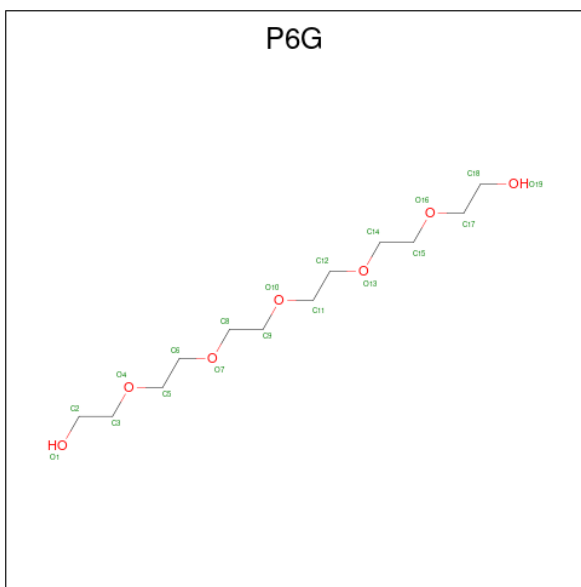
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	deletion	UNP O51934
A	?	-	ASP	deletion	UNP O51934
A	?	-	LYS	deletion	UNP O51934
A	?	-	ALA	deletion	UNP O51934
A	?	-	PRO	deletion	UNP O51934
A	?	-	ARG	deletion	UNP O51934
A	?	-	PHE	deletion	UNP O51934
A	?	-	VAL	deletion	UNP O51934
A	?	-	LEU	deletion	UNP O51934
A	?	-	ALA	deletion	UNP O51934
A	?	-	ARG	deletion	UNP O51934
A	?	-	VAL	deletion	UNP O51934
A	?	-	LEU	deletion	UNP O51934
A	?	-	LYS	deletion	UNP O51934
A	?	-	GLU	deletion	UNP O51934
A	?	-	MET	deletion	UNP O51934
A	?	-	GLY	deletion	UNP O51934
A	?	-	LEU	deletion	UNP O51934
A	?	-	ILE	deletion	UNP O51934
A	?	-	LYS	deletion	UNP O51934
A	?	-	ALA	deletion	UNP O51934
A	?	-	GLN	deletion	UNP O51934
A	?	-	GLU	deletion	UNP O51934
A	?	-	ASN	deletion	UNP O51934
A	?	-	PRO	deletion	UNP O51934
A	?	-	ASP	deletion	UNP O51934
A	?	-	VAL	deletion	UNP O51934

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP O51934
A	?	-	GLU	deletion	UNP O51934
A	?	-	LEU	deletion	UNP O51934
A	?	-	ARG	deletion	UNP O51934
A	?	-	LYS	deletion	UNP O51934
A	?	-	ILE	deletion	UNP O51934
A	?	-	ALA	deletion	UNP O51934
A	?	-	LYS	deletion	UNP O51934
A	?	-	GLU	deletion	UNP O51934
A	?	-	HIS	deletion	UNP O51934
A	?	-	LEU	deletion	UNP O51934
A	?	-	THR	deletion	UNP O51934
A	?	-	GLN	deletion	UNP O51934
A	?	-	LYS	deletion	UNP O51934
A	?	-	GLU	deletion	UNP O51934
A	?	-	PHE	deletion	UNP O51934
A	?	-	VAL	deletion	UNP O51934
A	?	-	GLU	deletion	UNP O51934
A	?	-	LYS	deletion	UNP O51934
A	?	-	VAL	deletion	UNP O51934
A	?	-	LYS	deletion	UNP O51934
A	?	-	GLU	deletion	UNP O51934
A	?	-	MET	deletion	UNP O51934
A	?	-	PHE	deletion	UNP O51934
A	?	-	ARG	deletion	UNP O51934
A	?	-	GLY	deletion	UNP O51934
A	?	-	VAL	deletion	UNP O51934
A	?	-	VAL	deletion	UNP O51934
A	?	-	VAL	deletion	UNP O51934
A	?	-	LYS	deletion	UNP O51934
A	?	-	ASP	deletion	UNP O51934
A	?	-	GLU	deletion	UNP O51934
A	?	-	ASP	deletion	UNP O51934
A	?	-	LEU	deletion	UNP O51934

- Molecule 2 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: C₁₂H₂₆O₇).

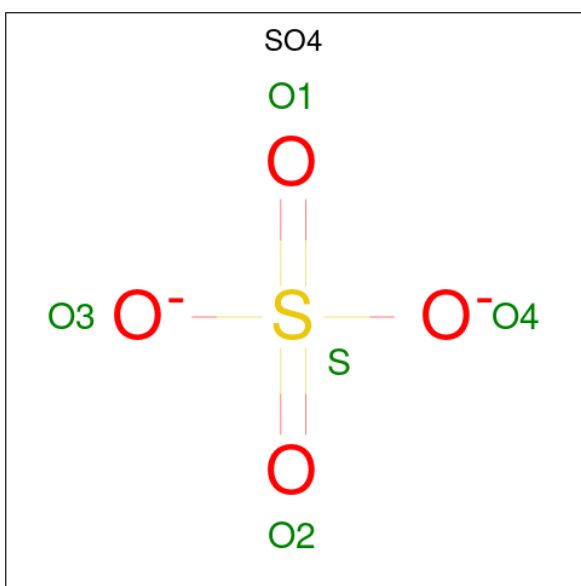


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			19	12	7		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Zn	0	0
			2	2		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Cl 2 2	0	0

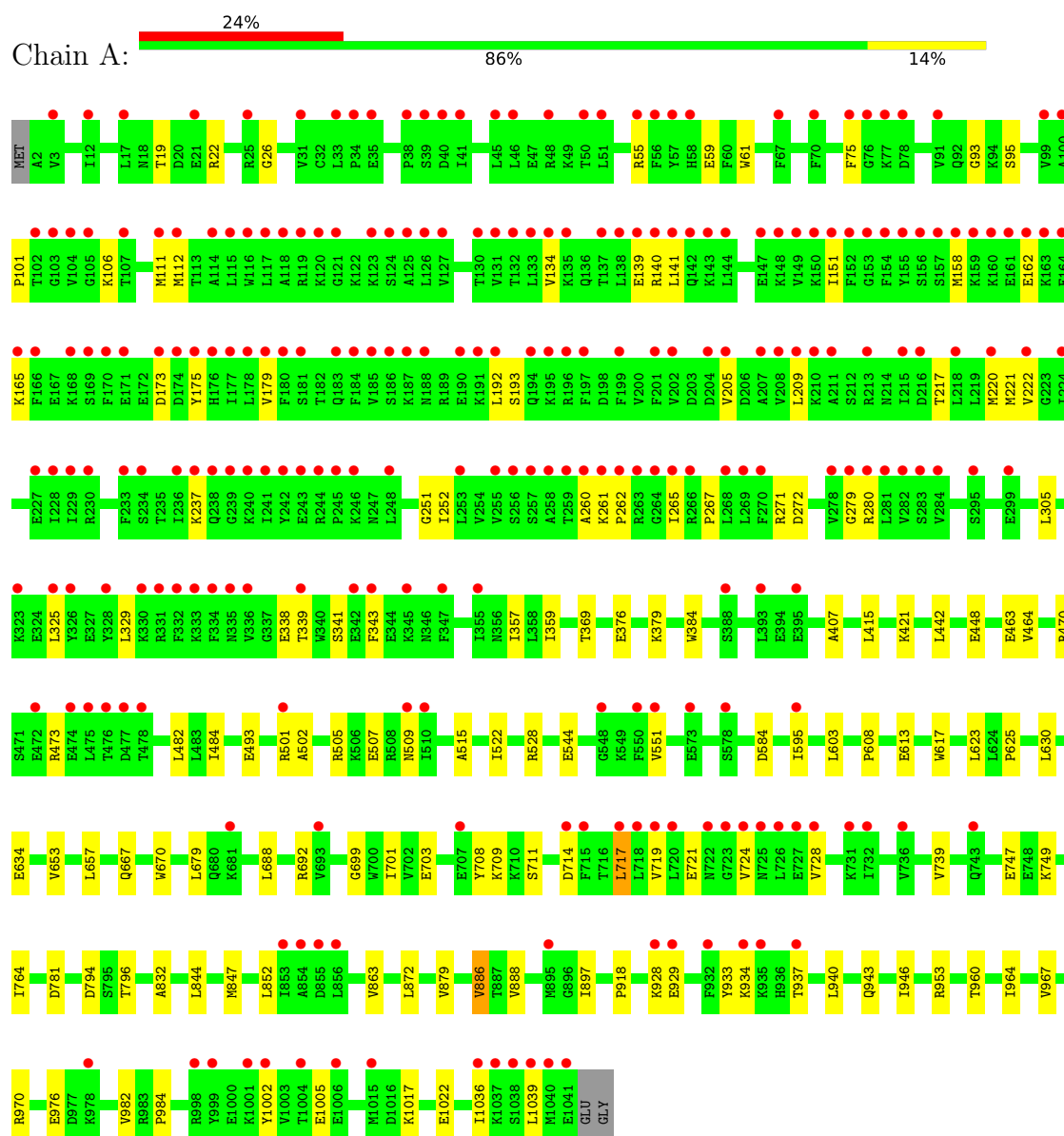
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	110	Total O 110 110	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: Reverse gyrase



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	90.83Å 90.83Å 571.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	75.85 – 2.39 75.85 – 2.39	Depositor EDS
% Data completeness (in resolution range)	79.4 (75.85-2.39) 75.9 (75.85-2.39)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.243 , 0.272 0.243 , 0.273	Depositor DCC
R_{free} test set	2279 reflections (3.98%)	wwPDB-VP
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.5	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	0.91	EDS
Total number of atoms	8679	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, P6G, ZN, 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	0.08	0/8676	0.22	0/11668

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

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	8521	0	8649	77	0
2	A	19	0	26	1	0
3	A	2	0	0	0	0
4	A	25	0	0	0	0
5	A	2	0	0	0	0
6	A	110	0	0	1	0
All	All	8679	0	8675	77	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 4.

All (77) 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:608:PRO:HB3	1:A:634:GLU:HB2	1.64	0.78
1:A:711:SER:HB2	1:A:937:THR:HB	1.78	0.65
1:A:95:SER:O	1:A:505:ARG:NH1	2.31	0.64
1:A:509:ASN:HB3	1:A:528:ARG:HH22	1.61	0.64
1:A:75:PHE:HB2	1:A:112:MET:HE3	1.80	0.63
1:A:670:TRP:HB3	1:A:1036:ILE:HG21	1.80	0.62
1:A:613:GLU:HG2	1:A:657:LEU:HB2	1.80	0.62
1:A:139:GLU:OE2	1:A:140:ARG:NH1	2.33	0.61
1:A:946:ILE:HD11	1:A:982:VAL:HG21	1.82	0.61
1:A:717:LEU:HB2	1:A:933:TYR:HE2	1.65	0.60
1:A:724:VAL:HG12	1:A:918:PRO:HD2	1.83	0.58
1:A:193:SER:OG	1:A:220:MET:SD	2.60	0.58
1:A:493:GLU:HG3	1:A:501:ARG:HH22	1.67	0.58
1:A:544:GLU:HB2	1:A:551:VAL:HG23	1.87	0.56
1:A:1017:LYS:HB3	1:A:1022:GLU:HB2	1.87	0.55
1:A:369:THR:HG23	1:A:407:ALA:HB2	1.90	0.54
1:A:376:GLU:HG3	1:A:415:LEU:HD21	1.89	0.54
1:A:260:ALA:HA	1:A:280:ARG:HA	1.90	0.53
1:A:886:VAL:HG13	1:A:897:ILE:HB	1.89	0.53
1:A:55:ARG:O	1:A:59:GLU:HG2	2.09	0.52
1:A:719:VAL:HG23	1:A:928:LYS:HB2	1.91	0.52
1:A:134:VAL:HG13	1:A:179:VAL:HG12	1.92	0.51
1:A:623:LEU:HB2	1:A:630:LEU:HD11	1.92	0.51
1:A:442:LEU:HD21	1:A:448:GLU:HG2	1.93	0.50
1:A:714:ASP:OD2	1:A:934:LYS:NZ	2.36	0.50
1:A:111:MET:HE1	1:A:140:ARG:HB3	1.94	0.49
1:A:960:THR:O	1:A:964:ILE:HG12	2.12	0.49
1:A:261:LYS:N	1:A:262:PRO:HD2	2.27	0.49
1:A:701:ILE:HG22	1:A:984:PRO:HD3	1.93	0.48
1:A:338:GLU:OE2	1:A:341:SER:OG	2.32	0.48
1:A:379:LYS:HB3	1:A:464:VAL:HG11	1.96	0.48
1:A:325:LEU:HD11	1:A:384:TRP:CG	2.50	0.47
1:A:329:LEU:HD12	1:A:359:ILE:HD11	1.97	0.47
1:A:667:GLN:OE1	1:A:692:ARG:NH1	2.47	0.47
1:A:796:THR:HA	1:A:832:ALA:HB2	1.96	0.47
1:A:421:LYS:HG3	1:A:463:GLU:HG2	1.96	0.47
1:A:470:ARG:HG2	1:A:473:ARG:NH1	2.29	0.47
1:A:747:GLU:OE1	1:A:749:LYS:NZ	2.48	0.46
1:A:237:LYS:HD2	1:A:265:ILE:HD13	1.98	0.46
1:A:739:VAL:HG22	1:A:888:VAL:HG12	1.98	0.45
1:A:484:ILE:HD13	1:A:603:LEU:HB2	1.98	0.45
1:A:222:VAL:HB	1:A:251:GLY:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:943:GLN:NE2	1:A:976:GLU:OE2	2.51	0.44
1:A:617:TRP:HB2	1:A:653:VAL:HG11	1.98	0.44
1:A:1036:ILE:HA	1:A:1039:LEU:HG	1.98	0.44
1:A:93:GLY:HA2	1:A:252:ILE:HD11	1.99	0.44
1:A:305:LEU:HD13	1:A:357:ILE:HD13	1.99	0.44
1:A:192:LEU:HB3	1:A:221:MET:HE2	1.99	0.44
1:A:158:MET:HB2	1:A:162:GLU:HB2	1.99	0.43
1:A:19:THR:HG23	1:A:22:ARG:H	1.84	0.43
1:A:967:VAL:HG22	1:A:970:ARG:HH21	1.83	0.43
1:A:482:LEU:HD11	1:A:603:LEU:HG	1.99	0.43
1:A:719:VAL:HG22	1:A:929:GLU:O	2.18	0.43
1:A:141:LEU:HB3	1:A:151:ILE:HD13	2.01	0.43
1:A:699:GLY:O	1:A:703:GLU:HG2	2.18	0.43
1:A:847:MET:HG3	1:A:852:LEU:HD22	2.00	0.43
1:A:26:GLY:HA2	1:A:625:PRO:HA	2.01	0.42
1:A:209:LEU:HD22	1:A:267:PRO:HG3	2.00	0.42
1:A:679:LEU:HB3	1:A:688:LEU:HD12	2.02	0.42
1:A:708:TYR:CD1	1:A:940:LEU:HG	2.54	0.42
1:A:515:ALA:HB3	1:A:522:ILE:HG23	2.01	0.42
1:A:162:GLU:HA	1:A:165:LYS:HE2	2.02	0.42
1:A:271:ARG:HD2	1:A:272:ASP:OD1	2.20	0.42
1:A:1002:TYR:CZ	1:A:1039:LEU:HB3	2.54	0.42
1:A:339:THR:HB	1:A:343:PHE:CD2	2.55	0.41
1:A:794:ASP:OD1	6:A:1201:HOH:O	2.22	0.41
1:A:217:THR:O	1:A:221:MET:HG3	2.21	0.41
1:A:101:PRO:O	1:A:106:LYS:HD2	2.21	0.41
1:A:279:GLY:HA3	1:A:502:ALA:O	2.21	0.41
1:A:509:ASN:ND2	1:A:584:ASP:O	2.54	0.41
1:A:764:ILE:HD13	1:A:863:VAL:HG13	2.03	0.41
1:A:507:GLU:HG3	1:A:595:ILE:HD11	2.03	0.40
1:A:173:ASP:HA	1:A:175:TYR:CE2	2.56	0.40
1:A:61:TRP:CG	2:A:1101:P6G:H32	2.56	0.40
1:A:205:VAL:O	1:A:209:LEU:HG	2.21	0.40
1:A:844:LEU:HD23	1:A:844:LEU:HA	1.91	0.40
1:A:953:ARG:HD3	1:A:1005:GLU:OE2	2.20	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	1038/1043 (100%)	1020 (98%)	18 (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	936/938 (100%)	928 (99%)	8 (1%)	70	85

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	709	LYS
1	A	717	LEU
1	A	721	GLU
1	A	728	VAL
1	A	781	ASP
1	A	872	LEU
1	A	879	VAL
1	A	886	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	287	ASN
1	A	346	ASN
1	A	513	HIS
1	A	530	HIS
1	A	743	GLN
1	A	780	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](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	SO4	A	1105	-	4,4,4	0.25	0	6,6,6	0.08	0
4	SO4	A	1104	-	4,4,4	0.24	0	6,6,6	0.06	0
2	P6G	A	1101	-	18,18,18	0.55	0	17,17,17	0.37	0
4	SO4	A	1108	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	A	1107	-	4,4,4	0.24	0	6,6,6	0.06	0
4	SO4	A	1106	-	4,4,4	0.24	0	6,6,6	0.08	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	P6G	A	1101	-	-	6/16/16/16	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

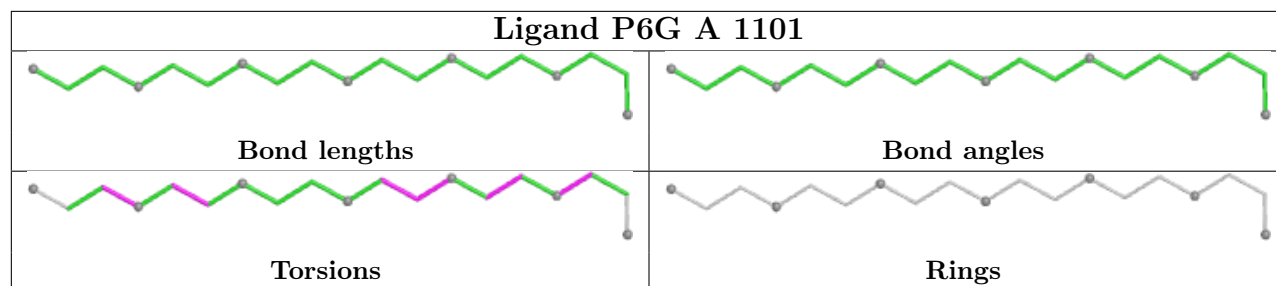
Mol	Chain	Res	Type	Atoms
2	A	1101	P6G	O7-C8-C9-O10
2	A	1101	P6G	O4-C5-C6-O7
2	A	1101	P6G	C9-C8-O7-C6
2	A	1101	P6G	C2-C3-O4-C5
2	A	1101	P6G	O13-C14-C15-O16
2	A	1101	P6G	C18-C17-O16-C15

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	P6G	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	1040/1043 (99%)	1.18	251 (24%) 2 1	23, 54, 133, 207	0

All (251) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	104	VAL	7.0
1	A	262	PRO	6.7
1	A	724	VAL	6.5
1	A	932	PHE	6.4
1	A	282	VAL	6.1
1	A	170	PHE	5.9
1	A	151	ILE	5.9
1	A	175	TYR	5.7
1	A	722	ASN	5.5
1	A	278	VAL	5.5
1	A	854	ALA	5.4
1	A	152	PHE	5.4
1	A	166	PHE	5.4
1	A	103	GLY	5.3
1	A	164	GLU	5.2
1	A	260	ALA	5.1
1	A	155	TYR	5.0
1	A	236	ILE	5.0
1	A	258	ALA	5.0
1	A	475	LEU	4.9
1	A	743	GLN	4.9
1	A	159	LYS	4.8
1	A	248	LEU	4.8
1	A	1039	LEU	4.8
1	A	39	SER	4.8
1	A	131	VAL	4.8
1	A	256	SER	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	132	THR	4.7
1	A	178	LEU	4.7
1	A	118	ALA	4.7
1	A	257	SER	4.7
1	A	265	ILE	4.6
1	A	263	ARG	4.5
1	A	160	LYS	4.5
1	A	205	VAL	4.5
1	A	476	THR	4.5
1	A	184	PHE	4.4
1	A	233	PHE	4.4
1	A	149	VAL	4.4
1	A	1002	TYR	4.3
1	A	855	ASP	4.3
1	A	177	ILE	4.2
1	A	125	ALA	4.2
1	A	154	PHE	4.2
1	A	197	PHE	4.2
1	A	161	GLU	4.2
1	A	723	GLY	4.1
1	A	207	ALA	4.1
1	A	153	GLY	4.1
1	A	157	SER	4.1
1	A	1036	ILE	4.1
1	A	731	LYS	4.0
1	A	245	PRO	4.0
1	A	213	ARG	3.9
1	A	156	SER	3.8
1	A	283	SER	3.8
1	A	215	ILE	3.7
1	A	168	LYS	3.7
1	A	115	LEU	3.7
1	A	195	LYS	3.7
1	A	133	LEU	3.7
1	A	201	PHE	3.6
1	A	141	LEU	3.6
1	A	253	LEU	3.6
1	A	726	LEU	3.6
1	A	224	ILE	3.6
1	A	509	ASN	3.6
1	A	259	THR	3.6
1	A	929	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	1006	GLU	3.6
1	A	135	LYS	3.5
1	A	138	LEU	3.5
1	A	268	LEU	3.5
1	A	332	PHE	3.5
1	A	165	LYS	3.5
1	A	181	SER	3.5
1	A	243	GLU	3.5
1	A	727	GLU	3.4
1	A	1041	GLU	3.4
1	A	239	GLY	3.4
1	A	142	GLN	3.4
1	A	264	GLY	3.4
1	A	102	THR	3.3
1	A	169	SER	3.3
1	A	176	HIS	3.3
1	A	185	VAL	3.3
1	A	501	ARG	3.3
1	A	218	LEU	3.2
1	A	148	LYS	3.2
1	A	237	LYS	3.2
1	A	279	GLY	3.2
1	A	158	MET	3.2
1	A	127	VAL	3.2
1	A	202	VAL	3.2
1	A	246	LYS	3.2
1	A	718	LEU	3.2
1	A	55	ARG	3.2
1	A	299	GLU	3.2
1	A	393	LEU	3.2
1	A	194	GLN	3.2
1	A	1038	SER	3.1
1	A	179	VAL	3.1
1	A	192	LEU	3.1
1	A	41	ILE	3.1
1	A	999	TYR	3.1
1	A	56	PHE	3.1
1	A	99	VAL	3.1
1	A	187	LYS	3.1
1	A	144	LEU	3.1
1	A	228	ILE	3.0
1	A	334	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	342	GLU	3.0
1	A	112	MET	3.0
1	A	143	LYS	3.0
1	A	137	THR	3.0
1	A	242	TYR	2.9
1	A	343	PHE	2.9
1	A	209	LEU	2.9
1	A	229	ILE	2.9
1	A	477	ASP	2.9
1	A	934	LYS	2.9
1	A	269	LEU	2.9
1	A	328	TYR	2.9
1	A	241	ILE	2.9
1	A	33	LEU	2.8
1	A	35	GLU	2.8
1	A	355	ILE	2.8
1	A	78	ASP	2.8
1	A	57	TYR	2.8
1	A	67	PHE	2.8
1	A	147	GLU	2.8
1	A	717	LEU	2.8
1	A	331	ARG	2.8
1	A	222	VAL	2.8
1	A	719	VAL	2.8
1	A	38	PRO	2.7
1	A	1001	LYS	2.7
1	A	725	ASN	2.7
1	A	126	LEU	2.7
1	A	183	GLN	2.7
1	A	174	ASP	2.7
1	A	333	LYS	2.7
1	A	728	VAL	2.6
1	A	40	ASP	2.6
1	A	70	PHE	2.6
1	A	270	PHE	2.6
1	A	208	VAL	2.6
1	A	111	MET	2.6
1	A	17	LEU	2.6
1	A	196	ARG	2.6
1	A	280	ARG	2.6
1	A	107	THR	2.6
1	A	121	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	45	LEU	2.6
1	A	230	ARG	2.6
1	A	240	LYS	2.6
1	A	1037	LYS	2.6
1	A	707	GLU	2.5
1	A	173	ASP	2.5
1	A	578	SER	2.5
1	A	978	LYS	2.5
1	A	140	ARG	2.5
1	A	117	LEU	2.5
1	A	75	PHE	2.5
1	A	124	SER	2.5
1	A	284	VAL	2.5
1	A	295	SER	2.5
1	A	853	ILE	2.5
1	A	21	GLU	2.5
1	A	266	ARG	2.5
1	A	120	LYS	2.5
1	A	150	LYS	2.5
1	A	163	LYS	2.5
1	A	330	LYS	2.5
1	A	548	GLY	2.5
1	A	119	ARG	2.5
1	A	325	LEU	2.5
1	A	123	LYS	2.4
1	A	1015	MET	2.4
1	A	34	PRO	2.4
1	A	244	ARG	2.4
1	A	937	THR	2.4
1	A	336	VAL	2.4
1	A	261	LYS	2.4
1	A	3	VAL	2.4
1	A	255	VAL	2.4
1	A	732	ILE	2.4
1	A	188	ASN	2.4
1	A	180	PHE	2.4
1	A	46	LEU	2.4
1	A	51	LEU	2.4
1	A	573	GLU	2.4
1	A	323	LYS	2.3
1	A	895	MET	2.3
1	A	12	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	134	VAL	2.3
1	A	736	VAL	2.3
1	A	139	GLU	2.3
1	A	395	GLU	2.3
1	A	191	LYS	2.3
1	A	76	GLY	2.3
1	A	105	GLY	2.3
1	A	100	ALA	2.3
1	A	130	THR	2.3
1	A	347	PHE	2.3
1	A	935	LYS	2.3
1	A	1040	MET	2.3
1	A	550	PHE	2.2
1	A	551	VAL	2.3
1	A	478	THR	2.2
1	A	856	LEU	2.2
1	A	715	PHE	2.2
1	A	216	ASP	2.2
1	A	58	HIS	2.2
1	A	227	GLU	2.2
1	A	234	SER	2.2
1	A	116	TRP	2.2
1	A	114	ALA	2.2
1	A	474	GLU	2.2
1	A	720	LEU	2.1
1	A	199	PHE	2.1
1	A	50	THR	2.1
1	A	339	THR	2.1
1	A	388	SER	2.1
1	A	998	ARG	2.1
1	A	220	MET	2.1
1	A	510	ILE	2.1
1	A	681	LYS	2.1
1	A	928	LYS	2.1
1	A	335	ASN	2.1
1	A	91	VAL	2.1
1	A	238	GLN	2.1
1	A	186	SER	2.1
1	A	1004	THR	2.1
1	A	714	ASP	2.1
1	A	31	VAL	2.1
1	A	693	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	210	LYS	2.1
1	A	345	LYS	2.1
1	A	171	GLU	2.1
1	A	190	GLU	2.1
1	A	472	GLU	2.1
1	A	281	LEU	2.1
1	A	595	ILE	2.1
1	A	211	ALA	2.0
1	A	204	ASP	2.0
1	A	326	TYR	2.0
1	A	162	GLU	2.0
1	A	25	ARG	2.0
1	A	48	ARG	2.0
1	A	77	LYS	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.

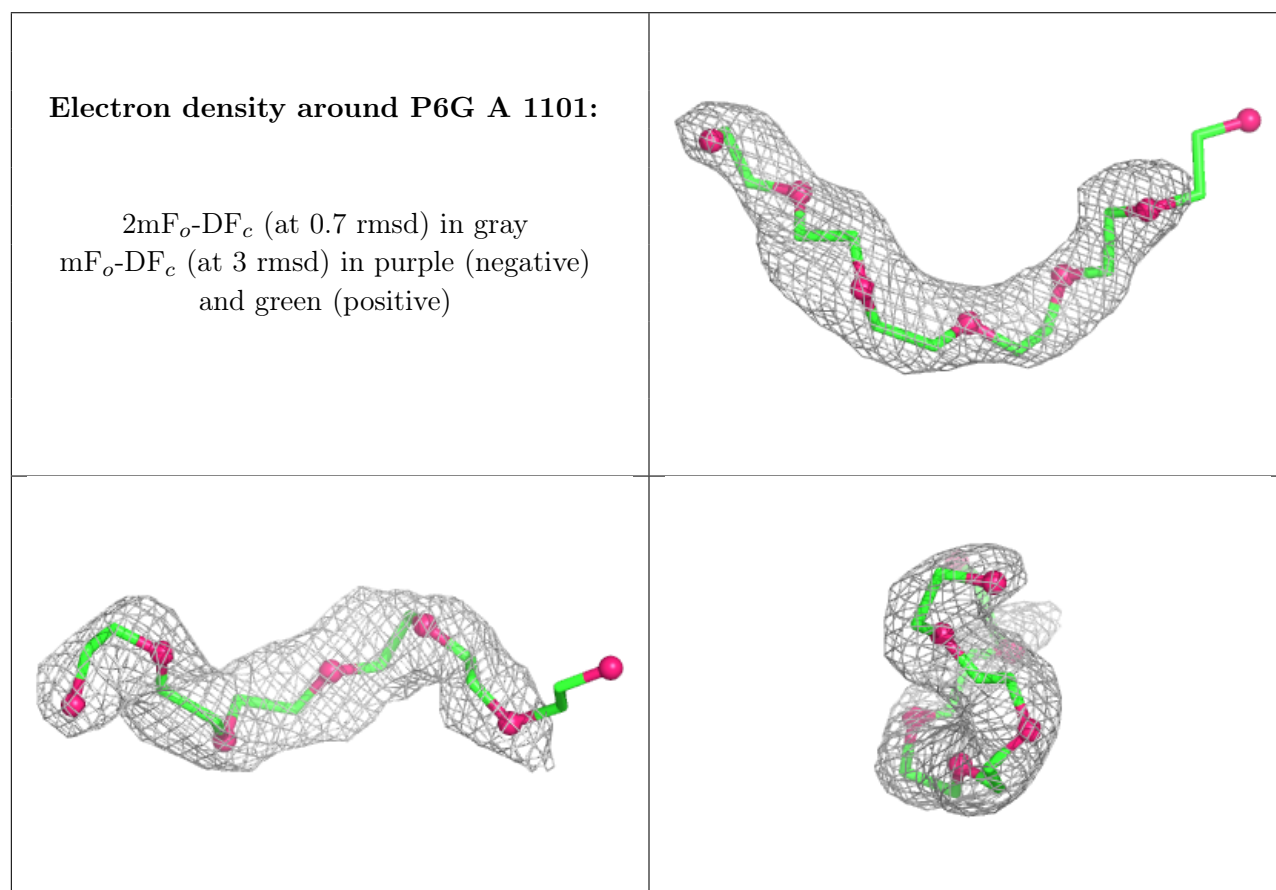
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	A	1108	5/5	0.66	0.12	85,91,94,113	0
4	SO4	A	1105	5/5	0.77	0.12	63,79,94,108	0
4	SO4	A	1107	5/5	0.79	0.16	65,70,95,113	0
2	P6G	A	1101	19/19	0.79	0.17	59,72,88,95	0
4	SO4	A	1104	5/5	0.83	0.19	53,63,79,91	0
4	SO4	A	1106	5/5	0.89	0.15	48,53,69,75	0
5	CL	A	1109	1/1	0.89	0.10	46,46,46,46	0
5	CL	A	1110	1/1	0.94	0.07	53,53,53,53	0
3	ZN	A	1102	1/1	0.98	0.04	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	A	1103	1/1	0.99	0.05	52,52,52,52	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.