



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 06:25 AM UTC

PDB ID : 7I2W / pdb_00007i2w
Title : Group deposition for crystallographic fragment screening of the NS5 RNA-dependent RNA polymerase from Dengue virus serotype 2 – Crystal structure of the NS5 RNA-dependent RNA polymerase from Dengue virus serotype 2 in complex with POB0015 (DNV2_NS5A-x0866)
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Deposited on : 2025-03-06
Resolution : 1.75 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)

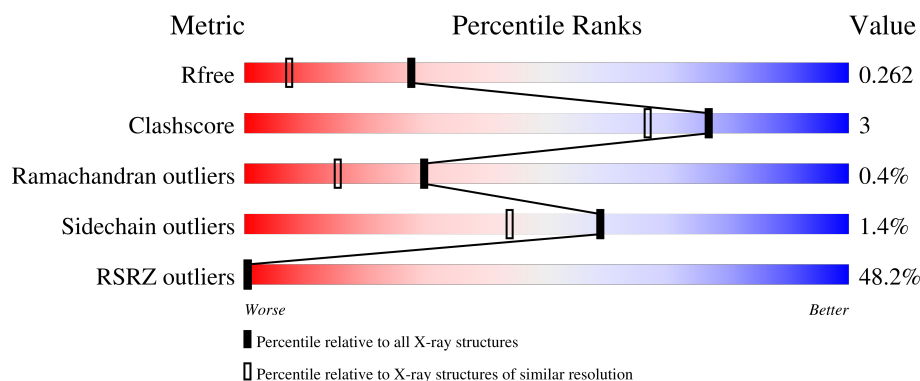
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	637	43% 83% 7% 10%

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:

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PO4	A	1006	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5144 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 NS5 RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	571	4702	2962	841	865	34	0	5	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	264	GLY	-	expression tag	UNP Q91H74
A	265	PRO	-	expression tag	UNP Q91H74

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



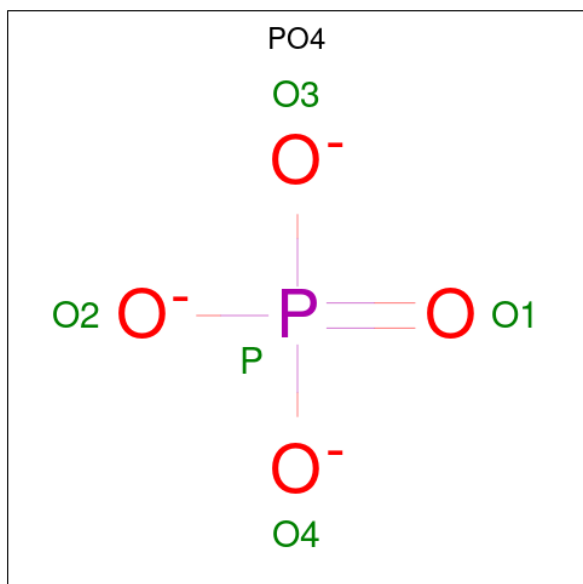
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	1
			24	12	2	8	2		

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).

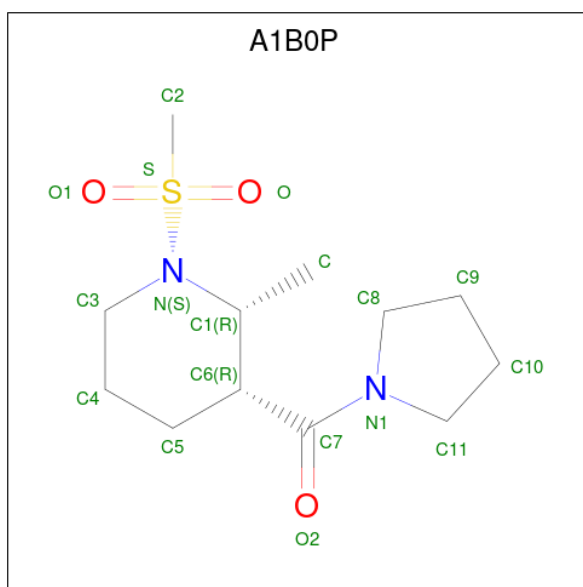


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		

- Molecule 8 is [(2R,3R)-1-(methanesulfonyl)-2-methylpiperidin-3-yl](pyrrolidin-1-yl)methanone (CCD ID: A1B0P) (formula: C₁₂H₂₂N₂O₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	S	0	0
			18	12	2	3	1		

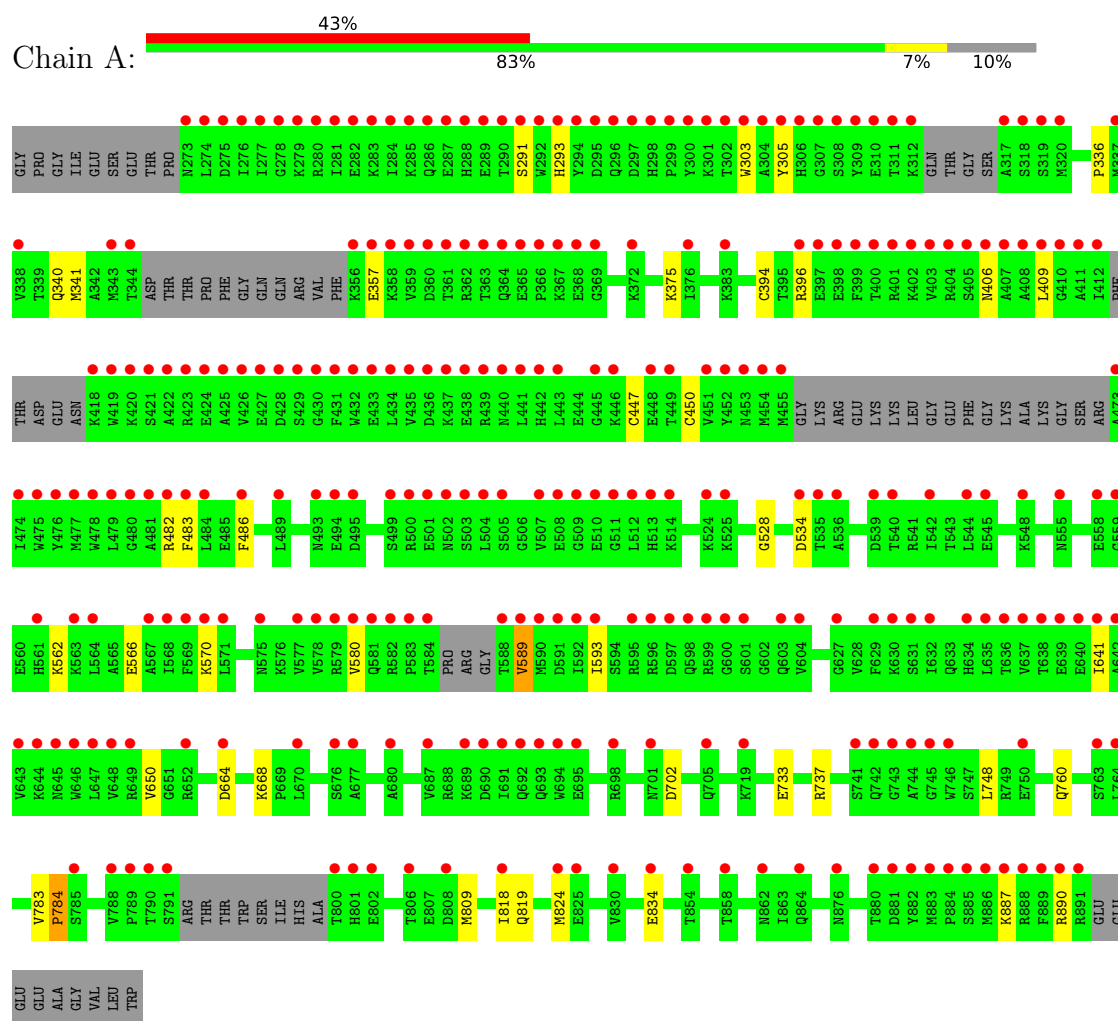
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	372	Total	O	0	0
			372	372		

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: NS5 RNA-dependent RNA polymerase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	82.30Å 116.05Å 147.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.30 – 1.75 91.30 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.9 (91.30-1.75) 98.9 (91.30-1.75)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.201 , 0.239 0.241 , 0.262	Depositor DCC
R_{free} test set	3668 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 130.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5144	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.31% 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: PO4, DMS, MES, CL, A1B0P, ZN, PEG

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	1.04	0/4806	1.31	2/6479 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	650	VAL	CA-C-O	-5.62	115.07	119.46
1	A	702	ASP	CB-CA-C	5.18	118.43	110.14

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	784	PRO	Mainchain

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	4702	0	4610	24	0
2	A	2	0	0	0	0
3	A	24	0	26	1	0
4	A	8	0	12	3	0
5	A	10	0	0	4	0
6	A	7	0	10	0	0
7	A	1	0	0	0	0
8	A	18	0	0	0	0
9	A	372	0	0	5	2
All	All	5144	0	4658	27	2

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 (27) 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:664:ASP:OD1	5:A:1006:PO4:O4	1.93	0.86
4:A:1004:DMS:H11	9:A:1253:HOH:O	1.88	0.74
1:A:664:ASP:OD1	5:A:1006:PO4:P	2.59	0.61
4:A:1004:DMS:H12	9:A:1245:HOH:O	2.01	0.60
1:A:534:ASP:OD1	5:A:1006:PO4:O4	2.26	0.53
1:A:336:PRO:O	1:A:340:GLN:HG2	2.10	0.51
1:A:396:ARG:HG2	1:A:483:PHE:CZ	2.45	0.50
1:A:562:LYS:HE3	1:A:566:GLU:OE2	2.11	0.50
1:A:834:GLU:OE2	1:A:890:ARG:NE	2.37	0.47
4:A:1004:DMS:C1	9:A:1253:HOH:O	2.53	0.47
1:A:562:LYS:O	1:A:566:GLU:HG3	2.14	0.47
1:A:409:LEU:O	1:A:482:ARG:HG2	2.14	0.47
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.55	0.46
1:A:748:LEU:HD13	3:A:1003[B]:MES:H61	1.98	0.46
1:A:534:ASP:OD1	5:A:1006:PO4:P	2.75	0.45
1:A:528:GLY:O	1:A:668:LYS:HE3	2.17	0.44
1:A:818:ILE:HD13	1:A:824:MET:HE3	2.00	0.44
1:A:783:VAL:O	1:A:784:PRO:C	2.60	0.44
1:A:303:TRP:CE3	1:A:593:ILE:HD12	2.53	0.43
1:A:562:LYS:NZ	9:A:1120:HOH:O	2.50	0.43
1:A:293:HIS:NE2	1:A:589:VAL:HG11	2.33	0.43
1:A:305:TYR:HA	1:A:593:ILE:HG22	2.01	0.43
1:A:341:MET:HE2	1:A:341:MET:HB3	1.84	0.43
1:A:760:GLN:NE2	1:A:809:MET:HE3	2.34	0.43
1:A:733:GLU:O	1:A:737:ARG:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:819:GLN:NE2	9:A:1114:HOH:O	2.42	0.42
1:A:394:CYS:HB3	1:A:486:PHE:CE2	2.56	0.41

All (2) 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)
9:A:1138:HOH:O	9:A:1138:HOH:O[2_445]	1.65	0.55
9:A:1311:HOH:O	9:A:1392:HOH:O[2_545]	1.92	0.28

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	562/637 (88%)	546 (97%)	14 (2%)	2 (0%)	30 15

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	291	SER
1	A	406	ASN

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	505/554 (91%)	498 (99%)	7 (1%)	59 44

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

Mol	Chain	Res	Type
1	A	357	GLU
1	A	375	LYS
1	A	570	LYS
1	A	580	VAL
1	A	589	VAL
1	A	641	ILE
1	A	887	LYS

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

Mol	Chain	Res	Type
1	A	786	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](#)

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 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	$\# Z > 2$
5	PO4	A	1006	-	4,4,4	4.06	3 (75%)	6,6,6	0.69	0
4	DMS	A	1005	-	3,3,3	0.24	0	3,3,3	0.05	0
3	MES	A	1003[B]	-	12,12,12	0.74	0	15,16,16	0.73	0
5	PO4	A	1007	-	4,4,4	1.09	1 (25%)	6,6,6	0.45	0
3	MES	A	1003[A]	-	12,12,12	0.76	0	15,16,16	0.41	0
8	A1B0P	A	1010	-	18,19,19	0.33	0	23,28,28	0.38	0
6	PEG	A	1008	-	6,6,6	0.13	0	5,5,5	0.10	0
4	DMS	A	1004	-	3,3,3	0.46	0	3,3,3	0.52	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	A	1008	-	-	2/4/4/4	-
3	MES	A	1003[A]	-	-	3/6/14/14	0/1/1/1
3	MES	A	1003[B]	-	-	3/6/14/14	0/1/1/1
8	A1B0P	A	1010	-	-	10/14/35/35	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1006	PO4	P-O1	6.61	1.65	1.50
5	A	1006	PO4	P-O4	-3.18	1.45	1.54
5	A	1006	PO4	P-O2	2.94	1.63	1.54
5	A	1007	PO4	P-O1	2.11	1.55	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1003[A]	MES	C7-C8-S-O1S
3	A	1003[A]	MES	C7-C8-S-O3S
3	A	1003[B]	MES	C8-C7-N4-C3
8	A	1010	A1B0P	C6-C7-N1-C8

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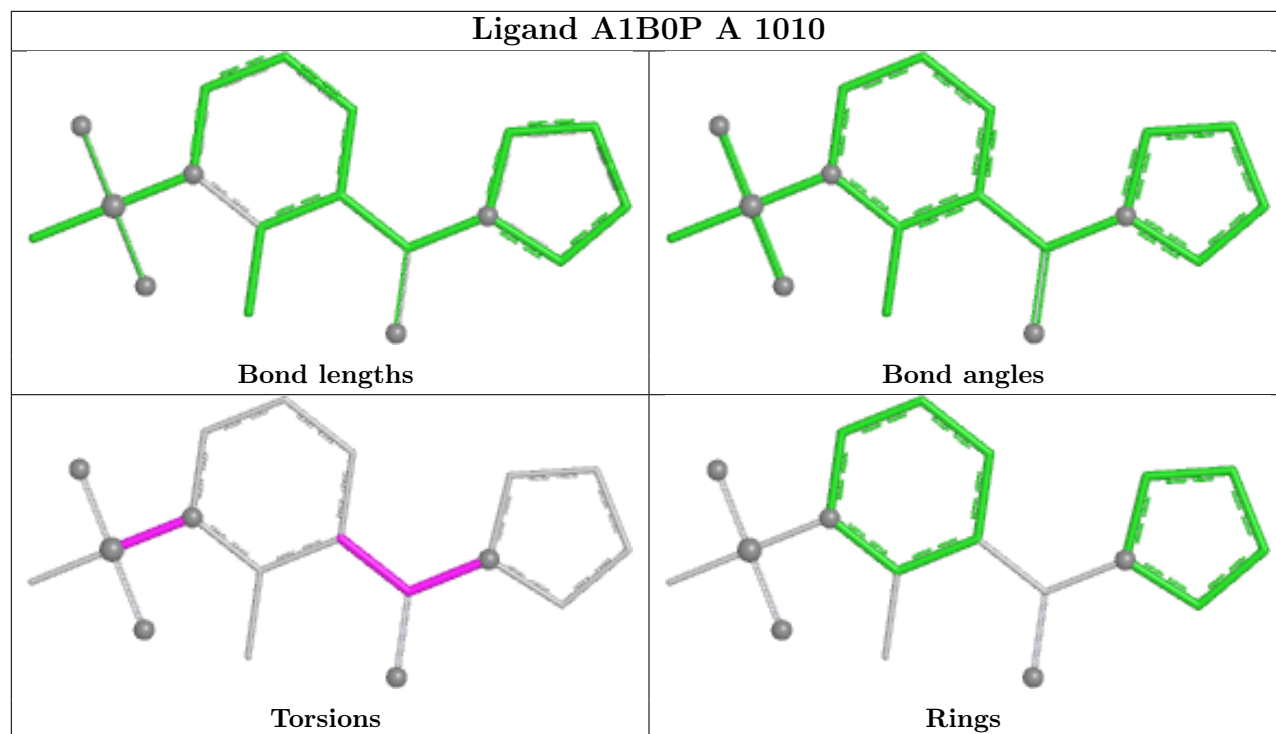
Mol	Chain	Res	Type	Atoms
8	A	1010	A1B0P	O2-C7-N1-C8
8	A	1010	A1B0P	C6-C7-N1-C11
8	A	1010	A1B0P	O2-C7-N1-C11
8	A	1010	A1B0P	C1-N-S-C2
8	A	1010	A1B0P	C1-N-S-O1
8	A	1010	A1B0P	C3-N-S-C2
8	A	1010	A1B0P	C3-N-S-O1
6	A	1008	PEG	O2-C3-C4-O4
3	A	1003[A]	MES	C7-C8-S-O2S
6	A	1008	PEG	C4-C3-O2-C2
3	A	1003[B]	MES	C8-C7-N4-C5
3	A	1003[B]	MES	C7-C8-S-O3S
8	A	1010	A1B0P	C1-C6-C7-O2
8	A	1010	A1B0P	C1-C6-C7-N1

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1006	PO4	4	0
3	A	1003[B]	MES	1	0
4	A	1004	DMS	3	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	571/637 (89%)	3.10	275 (48%) 0 0	6, 35, 72, 120	157 (27%)

All (275) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	411	ALA	15.7
1	A	589	VAL	14.2
1	A	475	TRP	12.5
1	A	292	TRP	12.2
1	A	412	ILE	11.8
1	A	431	PHE	10.9
1	A	435	VAL	10.9
1	A	512	LEU	10.7
1	A	409	LEU	10.7
1	A	637	VAL	10.7
1	A	359	VAL	10.5
1	A	293	HIS	10.5
1	A	294	TYR	10.4
1	A	274	LEU	10.3
1	A	474	ILE	10.3
1	A	694	TRP	10.3
1	A	399	PHE	10.2
1	A	363	THR	10.2
1	A	806	THR	10.2
1	A	504	LEU	10.2
1	A	284	ILE	10.0
1	A	744	ALA	10.0
1	A	425	ALA	9.8
1	A	788	VAL	9.7
1	A	434	LEU	9.7
1	A	426	VAL	9.6
1	A	600	GLY	9.5

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Mol	Chain	Res	Type	RSRZ
1	A	407	ALA	9.4
1	A	507	VAL	9.4
1	A	276	ILE	9.4
1	A	691	ILE	9.3
1	A	635	LEU	9.3
1	A	476	TYR	9.2
1	A	366	PRO	9.1
1	A	422	ALA	9.1
1	A	643	VAL	9.1
1	A	281	ILE	9.1
1	A	410	GLY	9.0
1	A	505	SER	9.0
1	A	525	LYS	9.0
1	A	403	VAL	9.0
1	A	369	GLY	8.9
1	A	408	ALA	8.9
1	A	642	ALA	8.6
1	A	719[A]	LYS	8.5
1	A	584	THR	8.4
1	A	277	ILE	8.4
1	A	319	SER	8.4
1	A	641	ILE	8.3
1	A	791	SER	8.3
1	A	741[A]	SER	8.2
1	A	367	LYS	8.2
1	A	636	THR	8.2
1	A	288	HIS	8.1
1	A	291	SER	8.1
1	A	745	GLY	8.0
1	A	800	THR	8.0
1	A	317	ALA	8.0
1	A	477	MET	7.9
1	A	361	THR	7.8
1	A	789	PRO	7.8
1	A	763[A]	SER	7.8
1	A	638	THR	7.7
1	A	295	ASP	7.7
1	A	438	GLU	7.7
1	A	785[A]	SER	7.7
1	A	885	SER	7.6
1	A	790	THR	7.6
1	A	439	ARG	7.6

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Mol	Chain	Res	Type	RSRZ
1	A	889	PHE	7.6
1	A	311	THR	7.6
1	A	473	ALA	7.6
1	A	419	TRP	7.6
1	A	405	SER	7.5
1	A	298	HIS	7.5
1	A	429	SER	7.4
1	A	499	SER	7.4
1	A	509	GLY	7.3
1	A	535	THR	7.3
1	A	430	GLY	7.2
1	A	596	ARG	7.0
1	A	649	ARG	7.0
1	A	300	TYR	7.0
1	A	536	ALA	6.9
1	A	421	SER	6.9
1	A	280	ARG	6.9
1	A	400	THR	6.8
1	A	743	GLY	6.8
1	A	595	ARG	6.8
1	A	801	HIS	6.7
1	A	599	ARG	6.7
1	A	511	GLY	6.7
1	A	358	LYS	6.7
1	A	598	GLN	6.6
1	A	597	ASP	6.6
1	A	320	MET	6.6
1	A	481	ALA	6.6
1	A	705	GLN	6.6
1	A	864[A]	GLN	6.6
1	A	514	LYS	6.5
1	A	631	SER	6.5
1	A	513	HIS	6.4
1	A	428	ASP	6.4
1	A	484	LEU	6.4
1	A	273	ASN	6.4
1	A	423	ARG	6.4
1	A	406	ASN	6.3
1	A	500	ARG	6.3
1	A	539	ASP	6.3
1	A	437	LYS	6.2
1	A	886	MET	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	534	ASP	6.2
1	A	640	GLU	6.1
1	A	692	GLN	6.1
1	A	746	TRP	6.1
1	A	312	LYS	6.1
1	A	644	LYS	6.1
1	A	278	GLY	6.1
1	A	279	LYS	6.1
1	A	451	VAL	6.0
1	A	639	GLU	6.0
1	A	360	ASP	6.0
1	A	301	LYS	6.0
1	A	884	PRO	6.0
1	A	397	GLU	6.0
1	A	452	TYR	5.9
1	A	302	THR	5.9
1	A	318	SER	5.9
1	A	588	THR	5.8
1	A	645	ASN	5.8
1	A	441	LEU	5.8
1	A	887	LYS	5.8
1	A	404	ARG	5.8
1	A	283	LYS	5.8
1	A	502	ASN	5.7
1	A	634	HIS	5.7
1	A	290	THR	5.7
1	A	580	VAL	5.7
1	A	440	ASN	5.7
1	A	503	SER	5.6
1	A	398	GLU	5.6
1	A	802	GLU	5.6
1	A	285	LYS	5.6
1	A	445	GLY	5.5
1	A	436	ASP	5.5
1	A	693	GLN	5.5
1	A	508	GLU	5.5
1	A	689	LYS	5.4
1	A	418	LYS	5.4
1	A	296	GLN	5.4
1	A	309	TYR	5.3
1	A	286	GLN	5.3
1	A	368	GLU	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	424	GLU	5.3
1	A	583	PRO	5.3
1	A	401	ARG	5.3
1	A	299	PRO	5.2
1	A	356	LYS	5.2
1	A	742	GLN	5.2
1	A	402	LYS	5.2
1	A	275	ASP	5.0
1	A	630	LYS	5.0
1	A	764	LEU	5.0
1	A	442	HIS	5.0
1	A	289	GLU	4.9
1	A	698	ARG	4.9
1	A	365	GLU	4.9
1	A	479	LEU	4.9
1	A	287	GLU	4.9
1	A	581	GLN	4.9
1	A	591	ASP	4.9
1	A	310	GLU	4.8
1	A	544	LEU	4.8
1	A	582	ARG	4.8
1	A	695	GLU	4.7
1	A	357	GLU	4.6
1	A	453	ASN	4.6
1	A	888	ARG	4.5
1	A	303	TRP	4.5
1	A	593	ILE	4.5
1	A	510	GLU	4.5
1	A	364	GLN	4.5
1	A	454	MET	4.5
1	A	297	ASP	4.5
1	A	427	GLU	4.4
1	A	305	TYR	4.4
1	A	448	GLU	4.4
1	A	420	LYS	4.4
1	A	575	ASN	4.3
1	A	478	TRP	4.2
1	A	282	GLU	4.2
1	A	344	THR	4.2
1	A	690	ASP	4.2
1	A	501	GLU	4.1
1	A	455	MET	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	449	THR	4.0
1	A	446	LYS	4.0
1	A	592	ILE	3.8
1	A	396	ARG	3.8
1	A	648	VAL	3.8
1	A	433	GLU	3.7
1	A	891	ARG	3.7
1	A	882	TYR	3.7
1	A	670	LEU	3.6
1	A	568	ILE	3.6
1	A	590	MET	3.6
1	A	577	VAL	3.6
1	A	443	LEU	3.6
1	A	578	VAL	3.5
1	A	563	LYS	3.5
1	A	680	ALA	3.5
1	A	881	ASP	3.4
1	A	482	ARG	3.4
1	A	629	PHE	3.4
1	A	750	GLU	3.3
1	A	524	LYS	3.2
1	A	304	ALA	3.2
1	A	701	ASN	3.2
1	A	307	GLY	3.2
1	A	558	GLU	3.1
1	A	677	ALA	3.1
1	A	540	THR	3.1
1	A	830	VAL	3.1
1	A	542	ILE	3.1
1	A	559	GLY	3.0
1	A	652	ARG	3.0
1	A	308	SER	3.0
1	A	876	ASN	3.0
1	A	890	ARG	2.9
1	A	647	LEU	2.9
1	A	306	HIS	2.9
1	A	579	ARG	2.8
1	A	818	ILE	2.8
1	A	880	THR	2.8
1	A	632	ILE	2.7
1	A	601	SER	2.7
1	A	372	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	604	VAL	2.7
1	A	489	LEU	2.7
1	A	676	SER	2.7
1	A	571	LEU	2.7
1	A	603	GLN	2.6
1	A	432	TRP	2.6
1	A	567	ALA	2.6
1	A	824	MET	2.5
1	A	480	GLY	2.5
1	A	570	LYS	2.5
1	A	555	ASN	2.4
1	A	808	ASP	2.4
1	A	854	THR	2.4
1	A	664	ASP	2.4
1	A	545	GLU	2.4
1	A	883	MET	2.4
1	A	862	ASN	2.4
1	A	564	LEU	2.4
1	A	362	ARG	2.4
1	A	383	LYS	2.4
1	A	825	GLU	2.3
1	A	561	HIS	2.3
1	A	338	VAL	2.3
1	A	548	LYS	2.2
1	A	495	ASP	2.2
1	A	337	MET	2.2
1	A	627	GLY	2.2
1	A	483	PHE	2.2
1	A	569	PHE	2.2
1	A	494	GLU	2.1
1	A	646	TRP	2.1
1	A	834	GLU	2.1
1	A	858	THR	2.1
1	A	493	ASN	2.0
1	A	687	VAL	2.0
1	A	343	MET	2.0
1	A	376	ILE	2.0
1	A	486	PHE	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

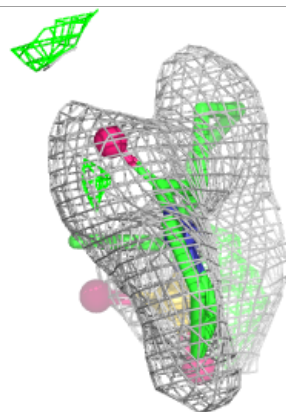
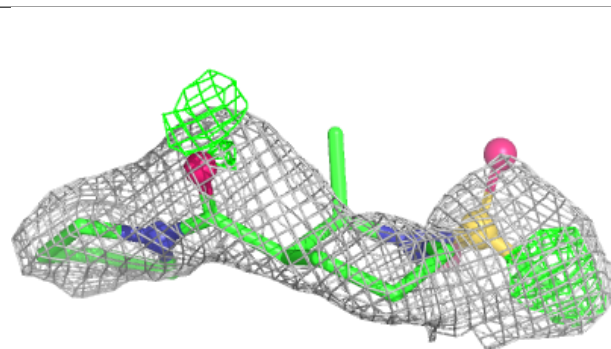
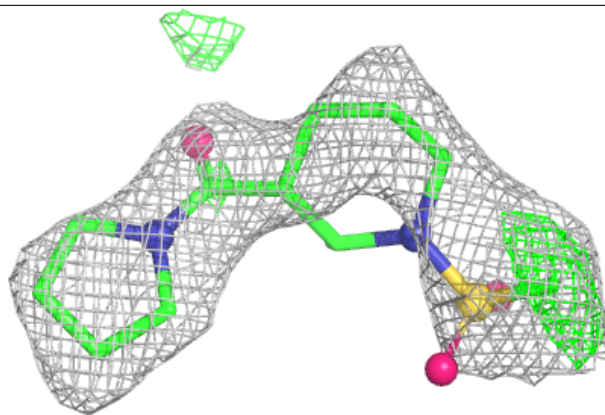
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	PO4	A	1007	5/5	0.63	0.18	64,78,84,104	0
8	A1B0P	A	1010	18/18	0.72	0.33	55,63,75,77	18
5	PO4	A	1006	5/5	0.77	0.17	34,36,53,58	0
6	PEG	A	1008	7/7	0.81	0.19	61,68,75,77	0
4	DMS	A	1005	4/4	0.82	0.25	85,91,93,97	0
4	DMS	A	1004	4/4	0.94	0.13	40,41,42,43	0
3	MES	A	1003[A]	12/12	0.95	0.23	709,715,747,747	12
3	MES	A	1003[B]	12/12	0.95	0.23	22,25,28,28	12
7	CL	A	1009	1/1	0.98	0.06	39,39,39,39	0
2	ZN	A	1002	1/1	0.99	0.04	53,53,53,53	0
2	ZN	A	1001	1/1	1.00	0.03	22,22,22,22	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.

Electron density around A1B0P A 1010:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.