



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2025 – 10:54 AM EDT

PDB ID : 7I2W
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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

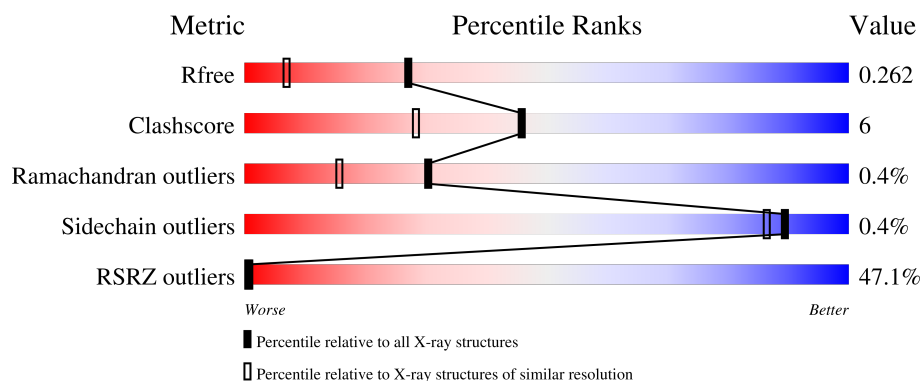
1 Overall quality at a glance

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}	164625	2888 (1.76-1.76)
Clashscore	180529	3097 (1.76-1.76)
Ramachandran outliers	177936	3072 (1.76-1.76)
Sidechain outliers	177891	3072 (1.76-1.76)
RSRZ outliers	164620	2887 (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	

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) : 2.41.4

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DMS	A	1004	-	-	X	-
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
1	A	571	Total	C	N	O	S	0	5	0
			4702	2962	841	865	34			

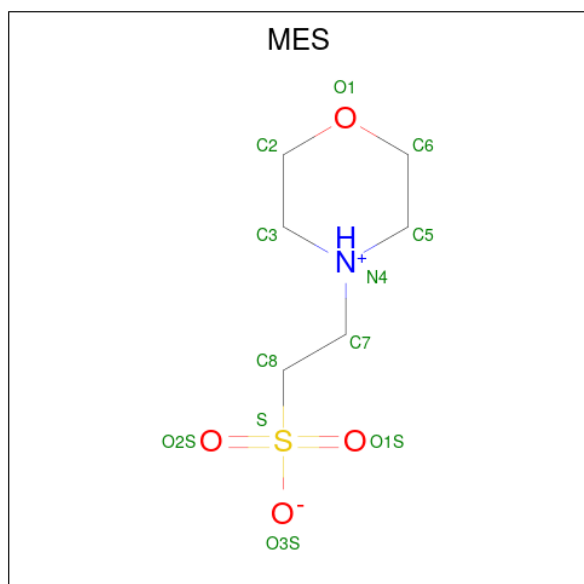
There are 2 discrepancies between the modelled and reference sequences:

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 (three-letter code: ZN) (formula: Zn).

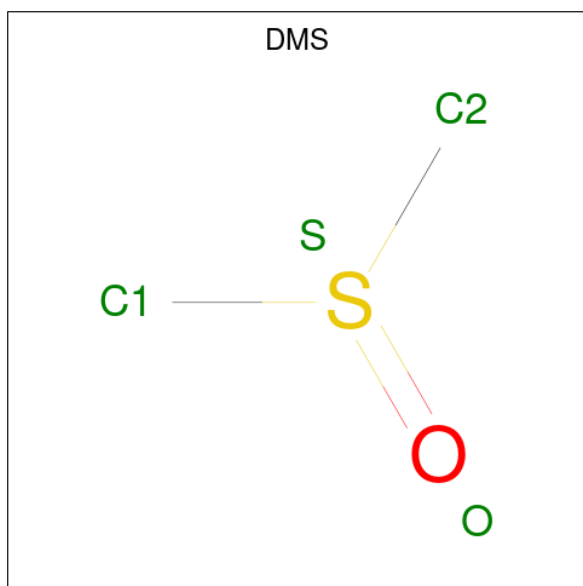
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



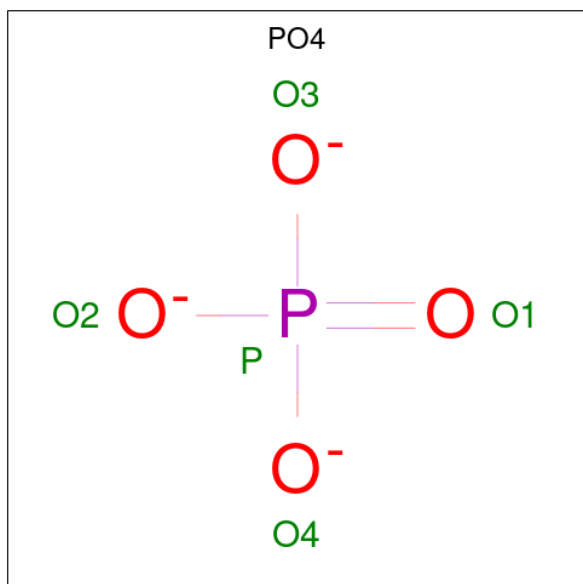
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	1
			24	12	2	8	2		

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



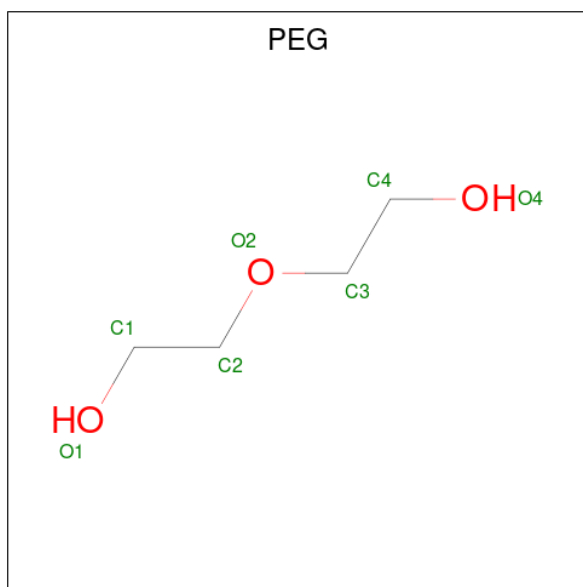
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: 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 (three-letter code: PEG) (formula: C₄H₁₀O₃).

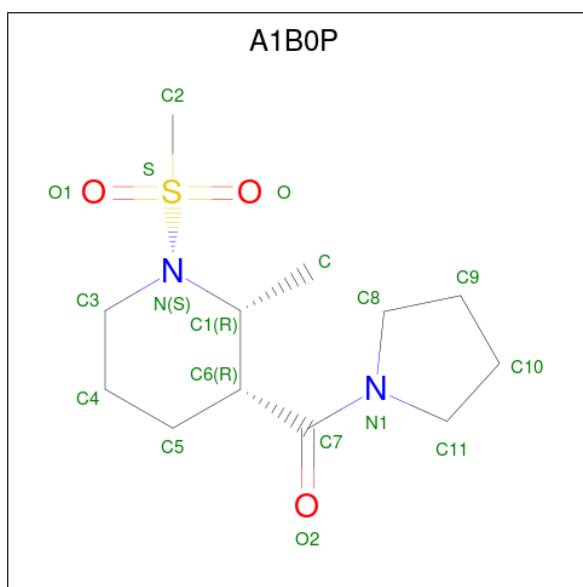


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is CHLORIDE ION (three-letter code: 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 (three-letter code: 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		

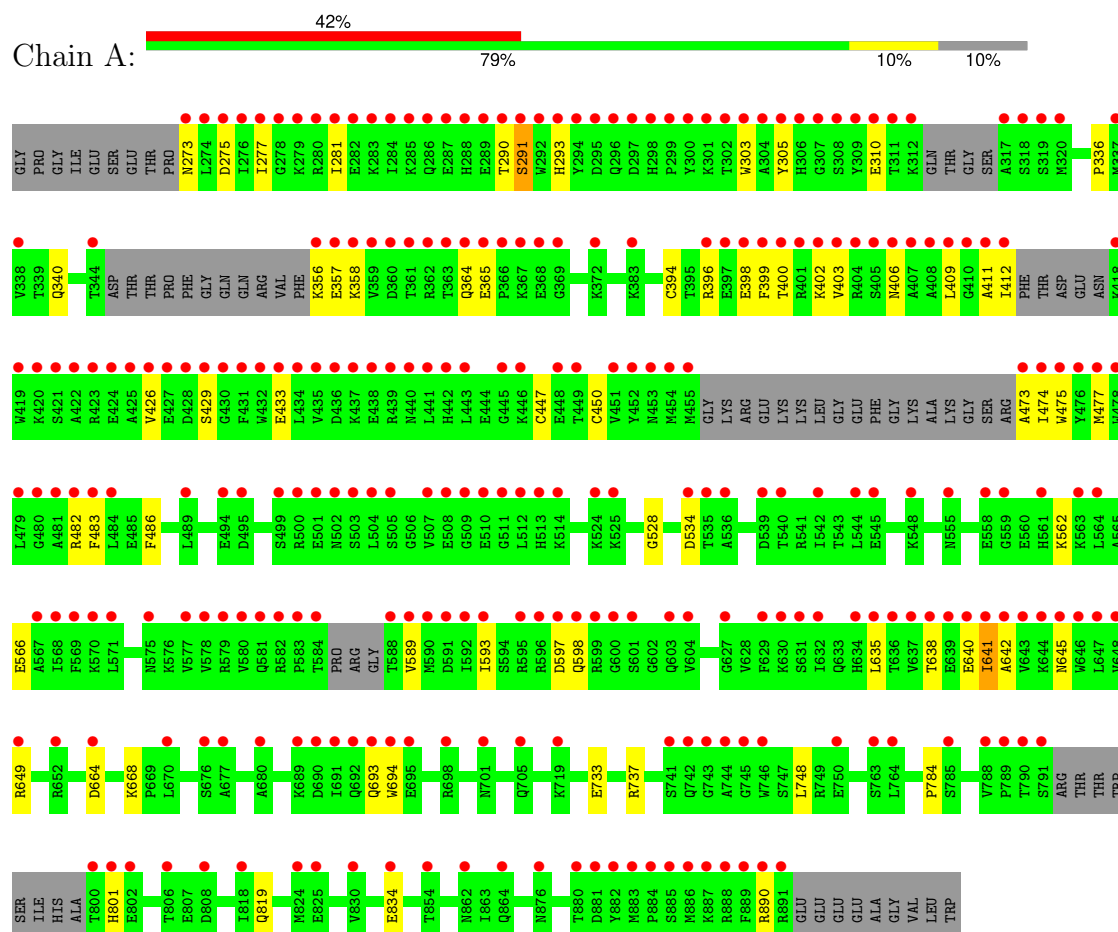
- Molecule 9 is water.

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 (5.12%)	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: ZN, PO4, MES, DMS, PEG, CL, A1B0P

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	0.70	0/4806	0.79	0/6479

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.

There are no bond angle outliers.

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	50	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	24	0	26	1	0
4	A	8	0	12	4	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	54	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 6.

All (54) 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:412:ILE:O	1:A:412:ILE:HG13	1.62	0.94
1:A:400:THR:O	1:A:403:VAL:HG22	1.74	0.87
1:A:664:ASP:OD1	5:A:1006:PO4:O4	1.93	0.86
1:A:399:PHE:O	1:A:403:VAL:HG13	1.83	0.78
1:A:638:THR:O	1:A:641:ILE:HG22	1.84	0.77
1:A:357:GLU:N	1:A:357:GLU:OE2	2.18	0.76
1:A:412:ILE:O	1:A:412:ILE:CG1	2.36	0.73
1:A:635:LEU:HD23	1:A:640:GLU:HG2	1.81	0.63
1:A:356:LYS:HE3	1:A:358:LYS:CB	2.29	0.62
1:A:664:ASP:OD1	5:A:1006:PO4:P	2.59	0.61
1:A:356:LYS:HE3	1:A:358:LYS:HB2	1.83	0.59
1:A:474:ILE:HD12	1:A:474:ILE:N	2.17	0.58
1:A:364:GLN:HG2	1:A:365:GLU:N	2.19	0.56
4:A:1004:DMS:C1	9:A:1253:HOH:O	2.53	0.56
1:A:398:GLU:O	1:A:402:LYS:HG3	2.06	0.54
1:A:534:ASP:OD1	5:A:1006:PO4:O4	2.26	0.53
1:A:641:ILE:CG2	1:A:642:ALA:N	2.71	0.53
1:A:364:GLN:HG2	1:A:365:GLU:H	1.72	0.53
1:A:475:TRP:CD1	1:A:475:TRP:N	2.75	0.53
1:A:597:ASP:O	1:A:598:GLN:HB2	2.08	0.53
1:A:336:PRO:O	1:A:340:GLN:HG2	2.10	0.51
1:A:645:ASN:O	1:A:649:ARG:HB2	2.11	0.51
1:A:429:SER:O	1:A:433:GLU:HG3	2.11	0.50
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:290:THR:O	1:A:291:SER:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:834:GLU:OE2	1:A:890:ARG:NE	2.37	0.47
1:A:411:ALA:HA	1:A:477:MET:O	2.14	0.47
1:A:290:THR:O	1:A:291:SER:CB	2.62	0.47
1:A:641:ILE:HG22	1:A:642:ALA:N	2.30	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:400:THR:HA	1:A:426:VAL:HG21	1.97	0.47
4:A:1004:DMS:H11	9:A:1253:HOH:O	2.12	0.46
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.55	0.46
1:A:356:LYS:HG3	1:A:358:LYS:H	1.81	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:291:SER:HB3	1:A:310:GLU:HG3	1.98	0.44
1:A:528:GLY:O	1:A:668:LYS:HE3	2.17	0.44
1:A:303:TRP:CE3	1:A:593:ILE:HD12	2.53	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:475:TRP:N	1:A:475:TRP:HD1	2.16	0.43
4:A:1004:DMS:H12	9:A:1245:HOH:O	2.18	0.43
4:A:1004:DMS:H13	9:A:1253:HOH:O	2.15	0.43
1:A:733:GLU:O	1:A:737:ARG:HG3	2.20	0.42
1:A:277:ILE:O	1:A:281:ILE:HG13	2.18	0.42
1:A:819:GLN:NE2	9:A:1114:HOH:O	2.42	0.42
1:A:356:LYS:HE3	1:A:358:LYS:HB3	2.01	0.42
1:A:273:ASN:N	1:A:275:ASP:OD1	2.53	0.41
1:A:693:GLN:OE1	1:A:694:TRP:NE1	2.54	0.41
1:A:473:ALA:C	1:A:474:ILE:HD12	2.41	0.41
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	16

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%)	503 (100%)	2 (0%)	89	86

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	641	ILE
1	A	801	HIS

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 ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
3	MES	A	1003[B]	-	12,12,12	0.74	0	15,16,16	0.73	0
4	DMS	A	1005	-	3,3,3	0.24	0	3,3,3	0.05	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
4	DMS	A	1004	-	3,3,3	0.46	0	3,3,3	0.52	0
6	PEG	A	1008	-	6,6,6	0.13	0	5,5,5	0.10	0
5	PO4	A	1006	-	4,4,4	4.06	3 (75%)	6,6,6	0.69	0
5	PO4	A	1007	-	4,4,4	1.09	1 (25%)	6,6,6	0.45	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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MES	A	1003[A]	-	-	3/6/14/14	0/1/1/1
8	A1B0P	A	1010	-	-	10/14/35/35	0/2/2/2
3	MES	A	1003[B]	-	-	3/6/14/14	0/1/1/1

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:

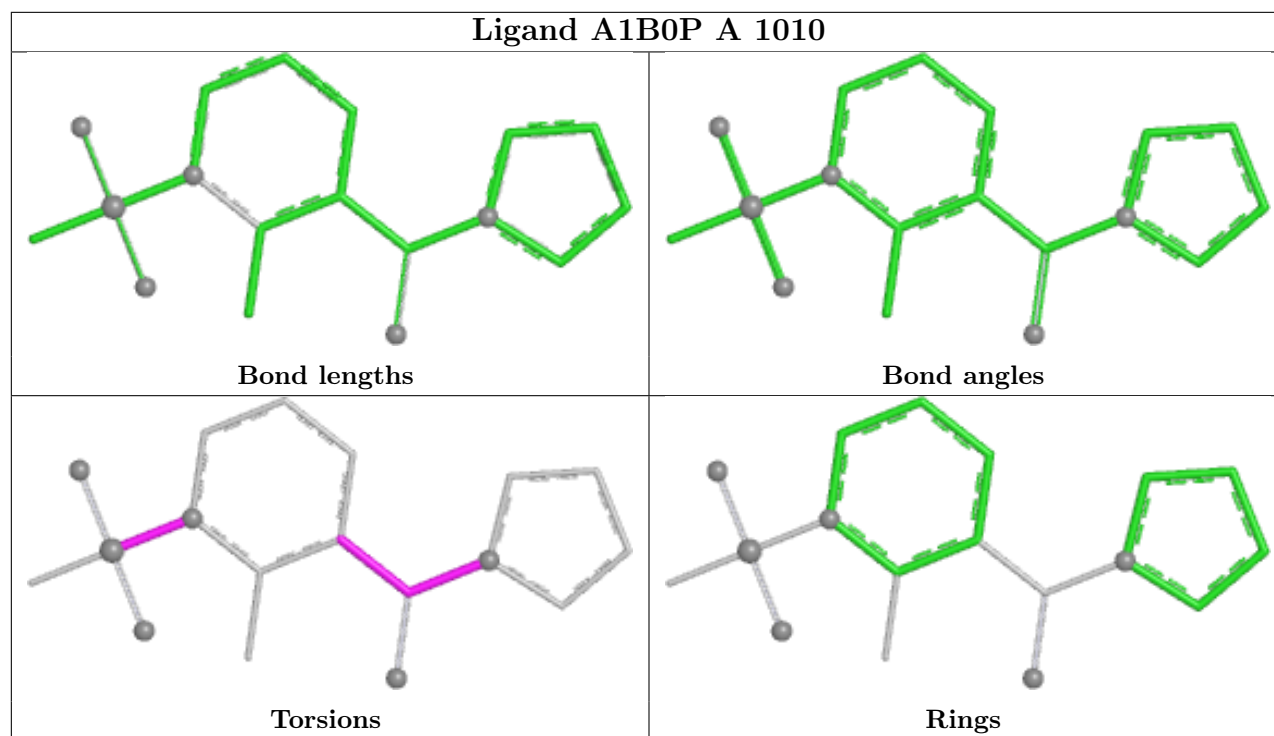
Mol	Chain	Res	Type	Atoms
3	A	1003[A]	MES	C7-C8-S-O1S
3	A	1003[A]	MES	C7-C8-S-O3S
3	A	1003[B]	MES	C8-C7-N4-C3
8	A	1010	A1B0P	C6-C7-N1-C8
8	A	1010	A1B0P	O2-C7-N1-C8
8	A	1010	A1B0P	C6-C7-N1-C11
8	A	1010	A1B0P	O2-C7-N1-C11
8	A	1010	A1B0P	C1-N-S-C2
8	A	1010	A1B0P	C1-N-S-O1
8	A	1010	A1B0P	C3-N-S-C2
8	A	1010	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 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003[B]	MES	1	0
4	A	1004	DMS	4	0
5	A	1006	PO4	4	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%)	2.99	269 (47%) 0 1	6, 35, 72, 120	157 (27%)

All (269) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	411	ALA	15.2
1	A	589	VAL	13.8
1	A	475	TRP	12.2
1	A	292	TRP	11.9
1	A	412	ILE	11.6
1	A	431	PHE	10.8
1	A	435	VAL	10.6
1	A	512	LEU	10.5
1	A	409	LEU	10.4
1	A	293	HIS	10.3
1	A	637	VAL	10.3
1	A	294	TYR	10.3
1	A	359	VAL	10.2
1	A	399	PHE	10.1
1	A	274	LEU	10.1
1	A	474	ILE	10.0
1	A	694	TRP	10.0
1	A	363	THR	10.0
1	A	806	THR	10.0
1	A	504	LEU	9.9
1	A	284	ILE	9.8
1	A	744	ALA	9.7
1	A	425	ALA	9.5
1	A	434	LEU	9.4
1	A	788	VAL	9.4
1	A	426	VAL	9.3
1	A	600	GLY	9.2

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Mol	Chain	Res	Type	RSRZ
1	A	407	ALA	9.2
1	A	276	ILE	9.1
1	A	507	VAL	9.1
1	A	691	ILE	9.1
1	A	635	LEU	9.0
1	A	476	TYR	9.0
1	A	525	LYS	9.0
1	A	366	PRO	8.9
1	A	505	SER	8.9
1	A	281	ILE	8.8
1	A	422	ALA	8.8
1	A	643	VAL	8.8
1	A	410	GLY	8.7
1	A	403	VAL	8.7
1	A	369	GLY	8.6
1	A	408	ALA	8.6
1	A	719[A]	LYS	8.5
1	A	642	ALA	8.4
1	A	319	SER	8.2
1	A	584	THR	8.2
1	A	367	LYS	8.2
1	A	791	SER	8.2
1	A	277	ILE	8.1
1	A	641	ILE	8.1
1	A	741[A]	SER	8.1
1	A	288	HIS	8.0
1	A	636	THR	8.0
1	A	291	SER	7.9
1	A	800	THR	7.8
1	A	745	GLY	7.8
1	A	477	MET	7.7
1	A	317	ALA	7.7
1	A	763[A]	SER	7.6
1	A	361	THR	7.6
1	A	789	PRO	7.6
1	A	438	GLU	7.6
1	A	295	ASP	7.6
1	A	439	ARG	7.5
1	A	638	THR	7.5
1	A	785[A]	SER	7.5
1	A	885	SER	7.5
1	A	889	PHE	7.5

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Mol	Chain	Res	Type	RSRZ
1	A	790	THR	7.5
1	A	405	SER	7.4
1	A	298	HIS	7.4
1	A	311	THR	7.4
1	A	419	TRP	7.4
1	A	473	ALA	7.3
1	A	429	SER	7.3
1	A	499	SER	7.3
1	A	535	THR	7.2
1	A	509	GLY	7.1
1	A	430	GLY	7.0
1	A	596	ARG	7.0
1	A	649	ARG	6.9
1	A	300	TYR	6.8
1	A	280	ARG	6.8
1	A	421	SER	6.8
1	A	595	ARG	6.7
1	A	536	ALA	6.7
1	A	400	THR	6.7
1	A	358	LYS	6.6
1	A	599	ARG	6.6
1	A	743	GLY	6.6
1	A	801	HIS	6.6
1	A	598	GLN	6.5
1	A	597	ASP	6.5
1	A	705	GLN	6.5
1	A	320	MET	6.5
1	A	514	LYS	6.5
1	A	864[A]	GLN	6.5
1	A	511	GLY	6.4
1	A	481	ALA	6.4
1	A	631	SER	6.4
1	A	428	ASP	6.3
1	A	423	ARG	6.3
1	A	513	HIS	6.3
1	A	273	ASN	6.2
1	A	484	LEU	6.2
1	A	500	ARG	6.2
1	A	437	LYS	6.2
1	A	539	ASP	6.2
1	A	406	ASN	6.1
1	A	640	GLU	6.1

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Mol	Chain	Res	Type	RSRZ
1	A	534	ASP	6.0
1	A	886	MET	6.0
1	A	312	LYS	6.0
1	A	644	LYS	6.0
1	A	692	GLN	6.0
1	A	279	LYS	6.0
1	A	301	LYS	6.0
1	A	639	GLU	6.0
1	A	746	TRP	5.9
1	A	360	ASP	5.9
1	A	397	GLU	5.9
1	A	278	GLY	5.8
1	A	451	VAL	5.8
1	A	884	PRO	5.8
1	A	452	TYR	5.8
1	A	887	LYS	5.8
1	A	318	SER	5.7
1	A	283	LYS	5.7
1	A	302	THR	5.7
1	A	404	ARG	5.7
1	A	645	ASN	5.7
1	A	588	THR	5.7
1	A	441	LEU	5.6
1	A	634	HIS	5.6
1	A	502	ASN	5.6
1	A	290	THR	5.6
1	A	440	ASN	5.5
1	A	503	SER	5.5
1	A	285	LYS	5.5
1	A	398	GLU	5.5
1	A	802	GLU	5.5
1	A	580	VAL	5.5
1	A	436	ASP	5.4
1	A	508	GLU	5.4
1	A	693	GLN	5.4
1	A	689	LYS	5.3
1	A	418	LYS	5.3
1	A	445	GLY	5.3
1	A	296	GLN	5.3
1	A	368	GLU	5.2
1	A	286	GLN	5.2
1	A	424	GLU	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	309	TYR	5.2
1	A	401	ARG	5.2
1	A	356	LYS	5.2
1	A	402	LYS	5.1
1	A	742	GLN	5.1
1	A	583	PRO	5.1
1	A	299	PRO	5.1
1	A	630	LYS	5.0
1	A	275	ASP	4.9
1	A	289	GLU	4.9
1	A	698	ARG	4.9
1	A	365	GLU	4.8
1	A	442	HIS	4.8
1	A	764	LEU	4.8
1	A	287	GLU	4.8
1	A	581	GLN	4.8
1	A	310	GLU	4.8
1	A	591	ASP	4.8
1	A	479	LEU	4.7
1	A	582	ARG	4.7
1	A	544	LEU	4.6
1	A	695	GLU	4.6
1	A	357	GLU	4.5
1	A	888	ARG	4.5
1	A	510	GLU	4.4
1	A	453	ASN	4.4
1	A	364	GLN	4.4
1	A	303	TRP	4.4
1	A	593	ILE	4.4
1	A	454	MET	4.4
1	A	427	GLU	4.4
1	A	297	ASP	4.4
1	A	448	GLU	4.3
1	A	420	LYS	4.3
1	A	305	TYR	4.3
1	A	575	ASN	4.2
1	A	282	GLU	4.2
1	A	478	TRP	4.1
1	A	344	THR	4.1
1	A	690	ASP	4.1
1	A	501	GLU	4.1
1	A	455	MET	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	446	LYS	3.9
1	A	449	THR	3.9
1	A	396	ARG	3.7
1	A	592	ILE	3.7
1	A	433	GLU	3.6
1	A	648	VAL	3.6
1	A	891	ARG	3.6
1	A	882	TYR	3.5
1	A	590	MET	3.5
1	A	670	LEU	3.5
1	A	568	ILE	3.5
1	A	577	VAL	3.4
1	A	563	LYS	3.4
1	A	443	LEU	3.4
1	A	578	VAL	3.4
1	A	680	ALA	3.3
1	A	482	ARG	3.3
1	A	881	ASP	3.3
1	A	629	PHE	3.3
1	A	750	GLU	3.2
1	A	524	LYS	3.2
1	A	701	ASN	3.1
1	A	558	GLU	3.1
1	A	304	ALA	3.0
1	A	307	GLY	3.0
1	A	677	ALA	3.0
1	A	540	THR	3.0
1	A	652	ARG	2.9
1	A	542	ILE	2.9
1	A	830	VAL	2.9
1	A	308	SER	2.9
1	A	559	GLY	2.9
1	A	876	ASN	2.9
1	A	890	ARG	2.9
1	A	579	ARG	2.8
1	A	647	LEU	2.8
1	A	306	HIS	2.8
1	A	372	LYS	2.7
1	A	880	THR	2.6
1	A	818	ILE	2.6
1	A	601	SER	2.6
1	A	632	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	489	LEU	2.6
1	A	676	SER	2.6
1	A	604	VAL	2.6
1	A	603	GLN	2.6
1	A	571	LEU	2.5
1	A	432	TRP	2.5
1	A	824	MET	2.4
1	A	567	ALA	2.4
1	A	570	LYS	2.4
1	A	480	GLY	2.4
1	A	808	ASP	2.3
1	A	555	ASN	2.3
1	A	545	GLU	2.3
1	A	664	ASP	2.3
1	A	883	MET	2.3
1	A	383	LYS	2.3
1	A	362	ARG	2.3
1	A	854	THR	2.3
1	A	862	ASN	2.3
1	A	825	GLU	2.3
1	A	564	LEU	2.3
1	A	561	HIS	2.2
1	A	548	LYS	2.2
1	A	338	VAL	2.2
1	A	495	ASP	2.1
1	A	337	MET	2.1
1	A	483	PHE	2.1
1	A	569	PHE	2.1
1	A	494	GLU	2.1
1	A	627	GLY	2.1
1	A	834	GLU	2.0
1	A	646	TRP	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 monosaccharides in this entry.

6.4 Ligands

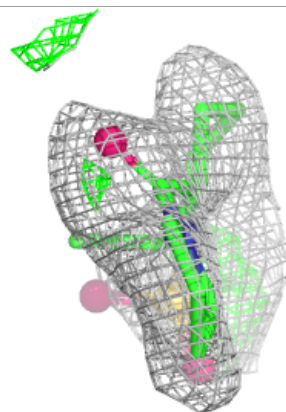
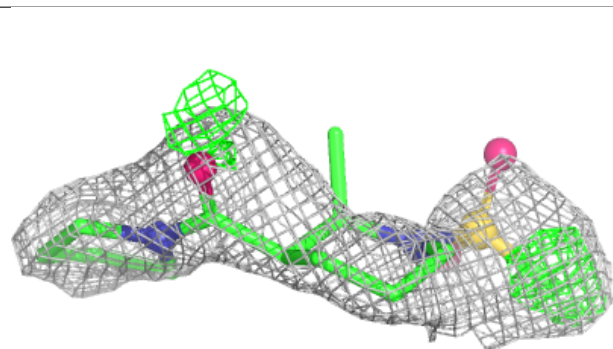
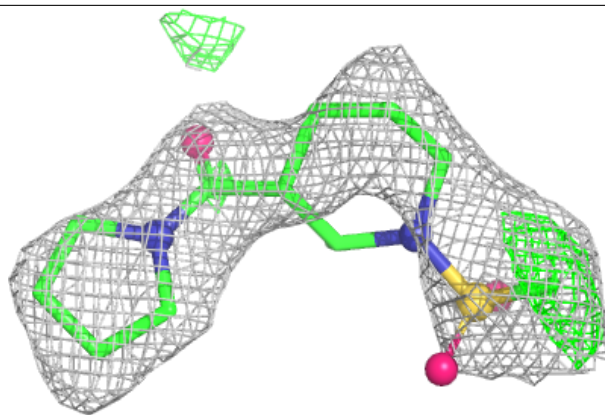
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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.