



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 04:40 AM UTC

PDB ID : 7I2V / pdb_00007i2v
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 Z415636694 (DNV2_NS5A-x0843)
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Deposited on : 2025-03-06
Resolution : 1.76 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)

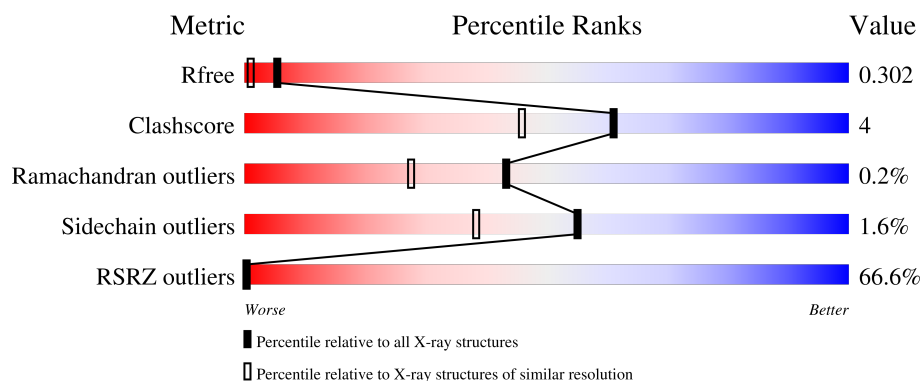
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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	60% 80% 9% 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	1007	-	-	X	-
7	NY4	A	1010	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5099 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	572	Total	C	N	O	S	0	7	0
			4725	2977	844	870	34			

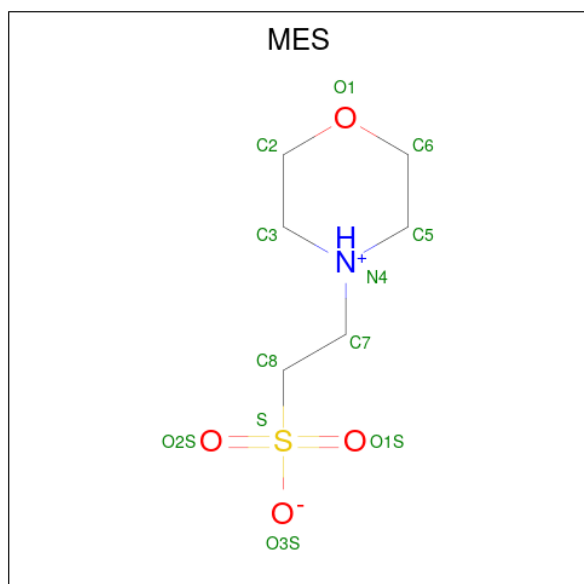
There are 2 discrepancies between the modelled and reference sequences:

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 (CCD ID: ZN) (formula: Zn).

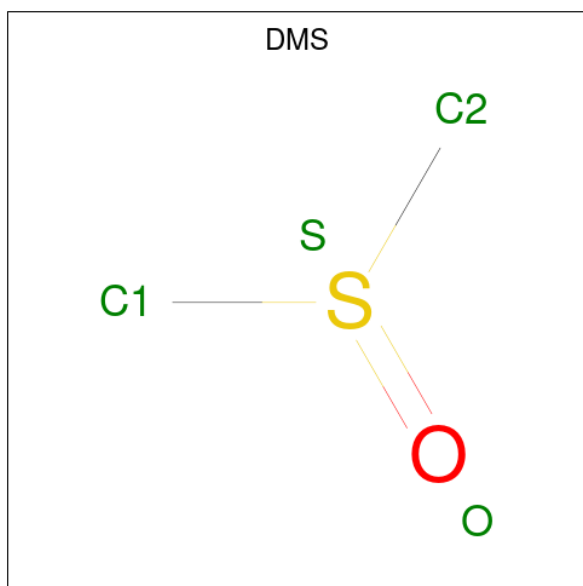
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

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



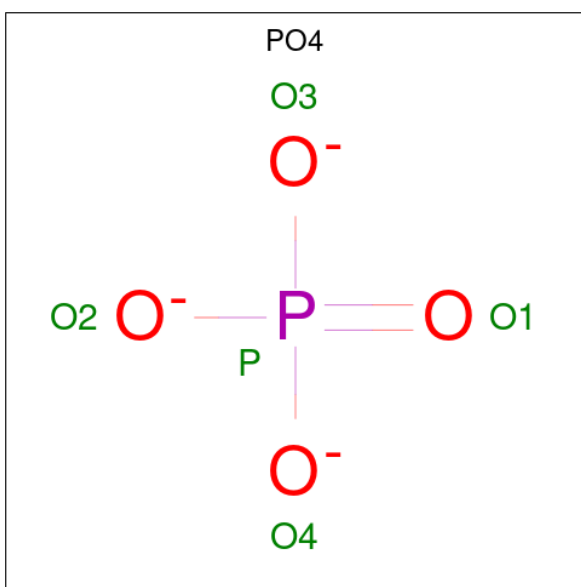
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	1
			24	12	2	8	2		

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



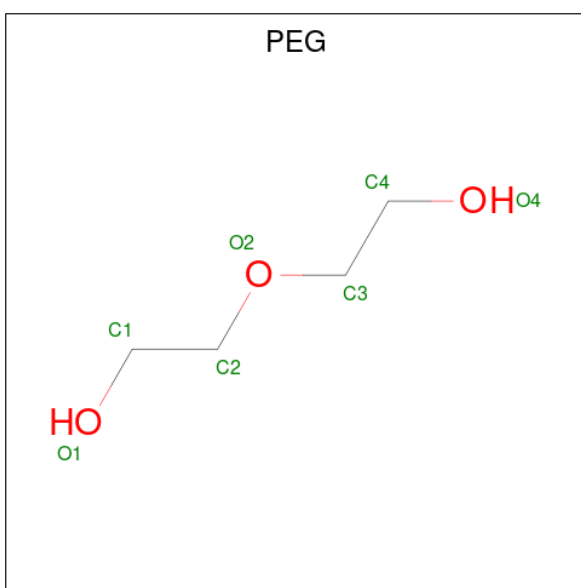
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

- 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		

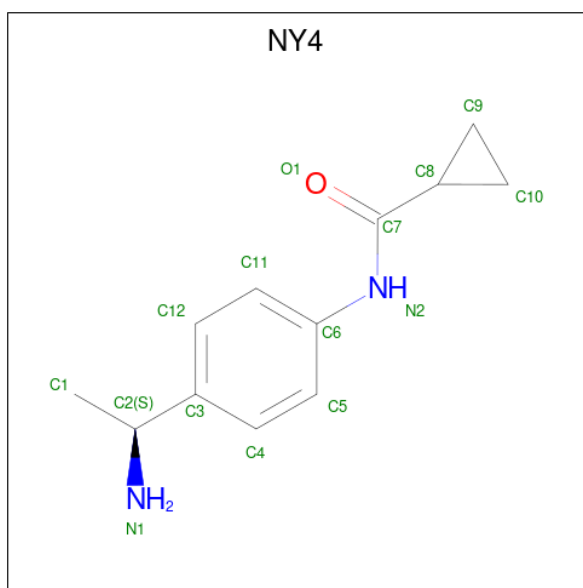
- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 7 is N-{4-[(1S)-1-aminoethyl]phenyl}cyclopropanecarboxamide (CCD ID: NY4)

(formula: C₁₂H₁₆N₂O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			15	12	2	1		

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

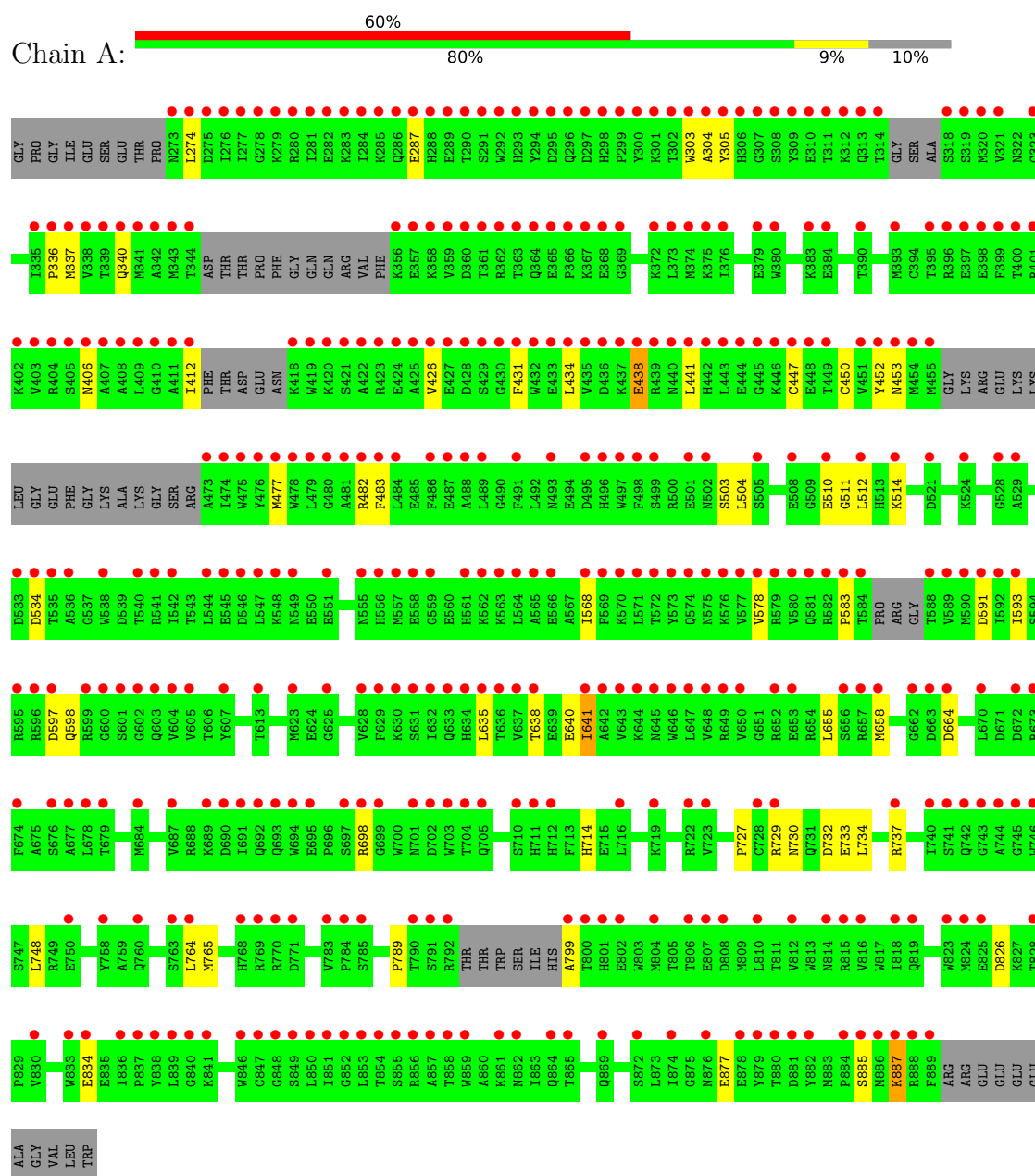
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	303	Total	O	0	0
			303	303		

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	82.31Å 115.78Å 146.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.41 – 1.76 73.41 – 1.76	Depositor EDS
% Data completeness (in resolution range)	92.8 (73.41-1.76) 92.8 (73.41-1.76)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.91 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.214 , 0.256 0.278 , 0.302	Depositor DCC
R_{free} test set	3568 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	33.0	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 106.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	5099	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% 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, DMS, MES, NY4, CL, 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	1.07	1/4830 (0.0%)	1.37	7/6513 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	714	HIS	CE1-NE2	5.50	1.38	1.32

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	877	GLU	CA-C-O	-6.21	114.56	121.51
1	A	511	GLY	CA-C-O	-6.12	117.11	121.88
1	A	789	PRO	CB-CA-C	-5.65	104.52	111.64
1	A	483	PHE	CA-CB-CG	-5.64	108.16	113.80
1	A	583	PRO	N-CA-C	5.26	121.44	113.81
1	A	568	ILE	N-CA-C	-5.11	105.51	110.42
1	A	885	SER	N-CA-C	-5.00	106.28	112.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4725	0	4628	37	0
2	A	2	0	0	0	0
3	A	24	0	26	1	0
4	A	12	0	18	3	0
5	A	10	0	0	3	0
6	A	7	0	10	0	0
7	A	15	0	0	0	0
8	A	1	0	0	0	0
9	A	303	0	0	6	1
All	All	5099	0	4682	40	1

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 (40) 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:534:ASP:OD1	5:A:1007:PO4:O4	1.91	0.89
1:A:510:GLU:O	1:A:514:LYS:HG3	1.91	0.70
4:A:1004:DMS:H11	9:A:1188:HOH:O	1.94	0.67
1:A:336:PRO:O	1:A:340:GLN:HG2	2.01	0.60
1:A:635:LEU:HD23	1:A:640:GLU:HG2	1.81	0.60
1:A:305:TYR:HA	1:A:593:ILE:HG22	1.84	0.59
1:A:337:MET:HG2	9:A:1305:HOH:O	2.03	0.58
4:A:1004:DMS:H12	9:A:1226:HOH:O	2.04	0.56
1:A:534:ASP:OD1	5:A:1007:PO4:P	2.63	0.56
1:A:303:TRP:CE3	1:A:593:ILE:HD12	2.41	0.55
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.46	0.55
1:A:834:GLU:CD	1:A:887:LYS:HB2	2.32	0.54
1:A:664:ASP:OD1	5:A:1007:PO4:P	2.67	0.53
1:A:826:ASP:OD1	1:A:826:ASP:C	2.51	0.53
1:A:452:TYR:O	1:A:578:VAL:HA	2.08	0.53
1:A:438:GLU:O	1:A:441:LEU:HB2	2.10	0.52
1:A:431:PHE:O	1:A:434:LEU:HB2	2.11	0.51
4:A:1004:DMS:C1	9:A:1188:HOH:O	2.57	0.51
1:A:412:ILE:O	1:A:412:ILE:HG13	2.10	0.51
1:A:764:LEU:HG	1:A:765:MET:CE	2.41	0.51
1:A:512[A]:LEU:HG	1:A:727:PRO:HB3	1.93	0.49
1:A:764:LEU:HG	1:A:765:MET:HE3	1.94	0.49
1:A:730:ASN:OD1	1:A:732:ASP:HB2	2.13	0.49
1:A:764:LEU:O	1:A:765:MET:HE2	2.12	0.49
1:A:597:ASP:O	1:A:598:GLN:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:764:LEU:C	1:A:765:MET:HE2	2.40	0.47
1:A:512[A]:LEU:HG	1:A:727:PRO:CB	2.45	0.46
1:A:655:LEU:HA	1:A:658:MET:HE2	1.98	0.46
1:A:799:ALA:HB1	9:A:1258:HOH:O	2.17	0.44
1:A:305:TYR:HE1	1:A:591:ASP:OD1	2.01	0.44
1:A:503:SER:O	1:A:504:LEU:HB2	2.17	0.44
1:A:304:ALA:O	1:A:593:ILE:HA	2.19	0.43
1:A:733:GLU:O	1:A:737:ARG:HG3	2.19	0.43
1:A:729:ARG:HD3	1:A:734:LEU:HD21	2.02	0.42
1:A:303:TRP:CD2	1:A:593:ILE:HD12	2.55	0.42
1:A:638:THR:O	1:A:641:ILE:HG22	2.20	0.42
1:A:336:PRO:O	1:A:340:GLN:CG	2.66	0.42
1:A:748:LEU:HD13	3:A:1003[B]:MES:H61	2.02	0.42
1:A:698:ARG:NH2	9:A:1122:HOH:O	2.53	0.41
1:A:452:TYR:CZ	1:A:477:MET:HE3	2.56	0.41

All (1) 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:1116:HOH:O	9:A:1116:HOH:O[2_445]	2.17	0.03

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	565/637 (89%)	543 (96%)	21 (4%)	1 (0%)	43 27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	406	ASN

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	508/554 (92%)	500 (98%)	8 (2%)	55 38

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

Mol	Chain	Res	Type
1	A	274	LEU
1	A	287	GLU
1	A	426	VAL
1	A	438	GLU
1	A	453	ASN
1	A	482	ARG
1	A	641	ILE
1	A	887	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	273	ASN
1	A	493	ASN
1	A	603	GLN
1	A	645	ASN
1	A	768	HIS
1	A	786	HIS
1	A	819	GLN
1	A	862	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 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	$\# Z > 2$
7	NY4	A	1010	-	16,16,16	0.39	0	22,22,22	0.56	0
3	MES	A	1003[A]	-	12,12,12	0.77	0	15,16,16	0.45	0
4	DMS	A	1006	-	3,3,3	0.25	0	3,3,3	0.22	0
5	PO4	A	1008	-	4,4,4	0.99	0	6,6,6	0.37	0
3	MES	A	1003[B]	-	12,12,12	0.73	0	15,16,16	0.73	0
4	DMS	A	1004	-	3,3,3	0.37	0	3,3,3	0.34	0
6	PEG	A	1009	-	6,6,6	0.20	0	5,5,5	0.24	0
4	DMS	A	1005	-	3,3,3	0.28	0	3,3,3	0.06	0
5	PO4	A	1007	-	4,4,4	3.57	2 (50%)	6,6,6	0.82	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	1009	-	-	1/4/4/4	-
3	MES	A	1003[B]	-	-	2/6/14/14	0/1/1/1
3	MES	A	1003[A]	-	-	3/6/14/14	0/1/1/1
7	NY4	A	1010	-	-	5/12/14/14	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1007	PO4	P-O1	6.06	1.64	1.50
5	A	1007	PO4	P-O2	2.91	1.63	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

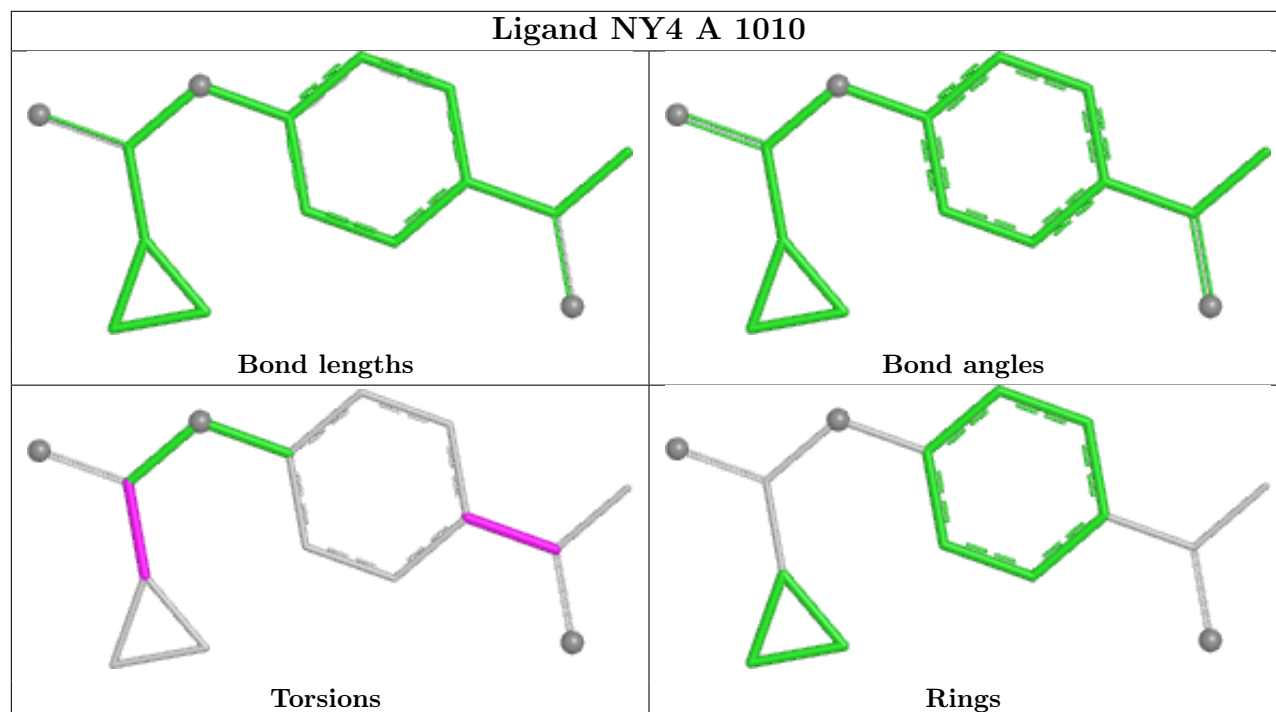
Mol	Chain	Res	Type	Atoms
3	A	1003[A]	MES	C7-C8-S-O1S
3	A	1003[A]	MES	C7-C8-S-O3S
3	A	1003[B]	MES	C8-C7-N4-C3
7	A	1010	NY4	N2-C7-C8-C10
7	A	1010	NY4	N2-C7-C8-C9
7	A	1010	NY4	O1-C7-C8-C10
7	A	1010	NY4	O1-C7-C8-C9
3	A	1003[A]	MES	C7-C8-S-O2S
6	A	1009	PEG	C4-C3-O2-C2
3	A	1003[B]	MES	C8-C7-N4-C5
7	A	1010	NY4	C1-C2-C3-C12

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003[B]	MES	1	0
4	A	1004	DMS	3	0
5	A	1007	PO4	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	572/637 (89%)	4.61	381 (66%) 0 0	6, 39, 96, 142	140 (24%)

All (381) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	580	VAL	18.5
1	A	474	ILE	18.0
1	A	426	VAL	17.7
1	A	592	ILE	17.5
1	A	303	TRP	17.5
1	A	403	VAL	17.4
1	A	475	TRP	17.2
1	A	637	VAL	17.1
1	A	632	ILE	15.4
1	A	889	PHE	15.3
1	A	573	TYR	15.2
1	A	359	VAL	15.0
1	A	419	TRP	14.9
1	A	409	LEU	14.8
1	A	589	VAL	14.7
1	A	309	TYR	14.7
1	A	636	THR	14.5
1	A	577	VAL	14.0
1	A	422	ALA	13.9
1	A	512[A]	LEU	13.7
1	A	571	LEU	13.7
1	A	400	THR	13.6
1	A	479	LEU	13.6
1	A	588	THR	13.5
1	A	838	TYR	13.2
1	A	311	THR	13.2
1	A	857	ALA	12.9

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Mol	Chain	Res	Type	RSRZ
1	A	840	GLY	12.7
1	A	635	LEU	12.4
1	A	363	THR	12.1
1	A	631	SER	12.1
1	A	850	LEU	12.1
1	A	540	THR	12.0
1	A	600	GLY	12.0
1	A	572	THR	12.0
1	A	839	LEU	12.0
1	A	445	GLY	11.9
1	A	602	GLY	11.9
1	A	380	TRP	11.8
1	A	858	THR	11.8
1	A	853	LEU	11.7
1	A	728	CYS	11.3
1	A	768	HIS	11.3
1	A	421	SER	11.3
1	A	851	ILE	11.3
1	A	473	ALA	11.2
1	A	575	ASN	11.2
1	A	293	HIS	11.2
1	A	801[A]	HIS	11.2
1	A	314	THR	11.2
1	A	367	LYS	11.1
1	A	576	LYS	11.1
1	A	405	SER	11.0
1	A	854	THR	11.0
1	A	591	ASP	10.9
1	A	366	PRO	10.9
1	A	710	SER	10.8
1	A	396	ARG	10.8
1	A	308	SER	10.7
1	A	852	GLY	10.6
1	A	711	HIS	10.6
1	A	284	ILE	10.6
1	A	601	SER	10.5
1	A	358	LYS	10.5
1	A	582	ARG	10.5
1	A	837	PRO	10.4
1	A	597	ASP	10.4
1	A	888	ARG	10.4
1	A	449	THR	10.3

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Mol	Chain	Res	Type	RSRZ
1	A	885	SER	10.3
1	A	481	ALA	10.2
1	A	763[A]	SER	10.2
1	A	541	ARG	10.2
1	A	849	SER	10.2
1	A	855	SER	10.2
1	A	301	LYS	10.1
1	A	402	LYS	10.1
1	A	856	ARG	9.9
1	A	505	SER	9.9
1	A	590	MET	9.8
1	A	603	GLN	9.8
1	A	361	THR	9.8
1	A	546	ASP	9.7
1	A	886	MET	9.6
1	A	581	GLN	9.5
1	A	771	ASP	9.5
1	A	294	TYR	9.5
1	A	705	GLN	9.5
1	A	478	TRP	9.5
1	A	356	LYS	9.4
1	A	281	ILE	9.4
1	A	633	GLN	9.4
1	A	404	ARG	9.4
1	A	411	ALA	9.3
1	A	712	HIS	9.2
1	A	599	ARG	9.2
1	A	634	HIS	9.2
1	A	302	THR	9.1
1	A	887	LYS	9.1
1	A	423	ARG	9.0
1	A	428	ASP	9.0
1	A	424	GLU	9.0
1	A	312	LYS	8.9
1	A	410	GLY	8.9
1	A	770	ARG	8.8
1	A	435	VAL	8.8
1	A	799	ALA	8.8
1	A	401	ARG	8.8
1	A	551	GLU	8.8
1	A	383	LYS	8.7
1	A	746	TRP	8.6

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Mol	Chain	Res	Type	RSRZ
1	A	745	GLY	8.5
1	A	864[A]	GLN	8.5
1	A	431	PHE	8.5
1	A	412	ILE	8.4
1	A	596	ARG	8.4
1	A	420	LYS	8.3
1	A	630	LYS	8.3
1	A	729	ARG	8.3
1	A	697	SER	8.3
1	A	384	GLU	8.2
1	A	548	LYS	8.2
1	A	657	ARG	8.2
1	A	841	LYS	8.2
1	A	664	ASP	8.1
1	A	360	ASP	8.0
1	A	292	TRP	7.9
1	A	398	GLU	7.9
1	A	656	SER	7.8
1	A	397	GLU	7.8
1	A	418	LYS	7.8
1	A	694	TRP	7.8
1	A	313	GLN	7.8
1	A	769	ARG	7.7
1	A	446	LYS	7.7
1	A	663	ASP	7.7
1	A	791	SER	7.7
1	A	357	GLU	7.7
1	A	741[A]	SER	7.6
1	A	434	LEU	7.6
1	A	719[A]	LYS	7.6
1	A	289	GLU	7.4
1	A	290	THR	7.4
1	A	368	GLU	7.4
1	A	427	GLU	7.3
1	A	310	GLU	7.2
1	A	448	GLU	7.2
1	A	286	GLN	7.0
1	A	698	ARG	7.0
1	A	362	ARG	7.0
1	A	764	LEU	6.9
1	A	277	ILE	6.8
1	A	425	ALA	6.7

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Mol	Chain	Res	Type	RSRZ
1	A	744	ALA	6.7
1	A	658	MET	6.6
1	A	847	CYS	6.5
1	A	364	GLN	6.4
1	A	484	LEU	6.3
1	A	785[A]	SER	6.2
1	A	641	ILE	6.2
1	A	296	GLN	6.2
1	A	652	ARG	6.2
1	A	593	ILE	6.1
1	A	365	GLU	6.1
1	A	645	ASN	6.0
1	A	318	SER	6.0
1	A	583	PRO	6.0
1	A	496	HIS	5.9
1	A	638	THR	5.9
1	A	299	PRO	5.9
1	A	443	LEU	5.9
1	A	344	THR	5.8
1	A	476	TYR	5.7
1	A	305	TYR	5.7
1	A	441	LEU	5.6
1	A	584	THR	5.5
1	A	784	PRO	5.5
1	A	429	SER	5.4
1	A	444	GLU	5.3
1	A	562	LYS	5.3
1	A	298	HIS	5.3
1	A	274	LEU	5.3
1	A	678	LEU	5.3
1	A	488	ALA	5.3
1	A	653	GLU	5.2
1	A	501	GLU	5.2
1	A	439	ARG	5.2
1	A	432	TRP	5.1
1	A	287	GLU	5.1
1	A	275	ASP	5.1
1	A	407	ALA	5.1
1	A	643	VAL	5.1
1	A	295	ASP	5.0
1	A	455	MET	5.0
1	A	846	TRP	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	480	GLY	5.0
1	A	750	GLU	4.9
1	A	278	GLY	4.9
1	A	544	LEU	4.7
1	A	564	LEU	4.7
1	A	800	THR	4.7
1	A	483	PHE	4.6
1	A	285	LYS	4.6
1	A	874	ILE	4.6
1	A	742	GLN	4.6
1	A	442	HIS	4.5
1	A	406	ASN	4.5
1	A	743	GLY	4.5
1	A	440	ASN	4.5
1	A	687	VAL	4.5
1	A	699	GLY	4.5
1	A	649	ARG	4.5
1	A	288	HIS	4.5
1	A	792	ARG	4.5
1	A	568	ILE	4.5
1	A	818	ILE	4.5
1	A	297	ASP	4.5
1	A	451	VAL	4.4
1	A	393	MET	4.4
1	A	454	MET	4.4
1	A	790	THR	4.4
1	A	806	THR	4.3
1	A	408	ALA	4.3
1	A	570	LYS	4.2
1	A	642	ALA	4.2
1	A	452	TYR	4.2
1	A	495	ASP	4.2
1	A	563	LYS	4.2
1	A	436	ASP	4.2
1	A	453	ASN	4.1
1	A	670	LEU	4.1
1	A	300	TYR	4.1
1	A	882	TYR	4.1
1	A	830	VAL	4.1
1	A	701	ASN	4.1
1	A	379	GLU	4.1
1	A	816	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	304	ALA	4.0
1	A	861	LYS	4.0
1	A	880	THR	4.0
1	A	282	GLU	4.0
1	A	604	VAL	4.0
1	A	487	GLU	4.0
1	A	672	ASP	4.0
1	A	399	PHE	3.9
1	A	629	PHE	3.9
1	A	529	ALA	3.9
1	A	508	GLU	3.8
1	A	437	LYS	3.8
1	A	807	GLU	3.8
1	A	319	SER	3.7
1	A	390	THR	3.7
1	A	804	MET	3.7
1	A	783	VAL	3.7
1	A	648	VAL	3.6
1	A	644	LYS	3.6
1	A	703	TRP	3.6
1	A	628	VAL	3.6
1	A	307	GLY	3.6
1	A	430	GLY	3.6
1	A	555	ASN	3.6
1	A	677	ALA	3.6
1	A	848	GLY	3.6
1	A	306	HIS	3.6
1	A	497	TRP	3.5
1	A	558	GLU	3.5
1	A	486	PHE	3.5
1	A	716	LEU	3.5
1	A	545	GLU	3.5
1	A	646	TRP	3.4
1	A	865	THR	3.4
1	A	549	ASN	3.4
1	A	872	SER	3.4
1	A	279	LYS	3.4
1	A	702	ASP	3.3
1	A	528	GLY	3.3
1	A	834	GLU	3.3
1	A	337	MET	3.3
1	A	477	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	276	ILE	3.2
1	A	491	PHE	3.2
1	A	690	ASP	3.2
1	A	320	MET	3.1
1	A	723	VAL	3.1
1	A	374	MET	3.1
1	A	283	LYS	3.1
1	A	498	PHE	3.1
1	A	740	ILE	3.1
1	A	578	VAL	3.0
1	A	510	GLU	3.0
1	A	524	LYS	3.0
1	A	343	MET	3.0
1	A	336	PRO	3.0
1	A	693	GLN	2.9
1	A	876	ASN	2.9
1	A	280	ARG	2.9
1	A	625	GLY	2.9
1	A	737	ARG	2.9
1	A	273	ASN	2.9
1	A	579	ARG	2.8
1	A	819	GLN	2.8
1	A	623	MET	2.8
1	A	607	TYR	2.8
1	A	879	TYR	2.8
1	A	547	LEU	2.8
1	A	823	TRP	2.8
1	A	321	VAL	2.8
1	A	647	LEU	2.8
1	A	395	THR	2.8
1	A	704	THR	2.8
1	A	375	LYS	2.7
1	A	534	ASP	2.7
1	A	338	VAL	2.7
1	A	676	SER	2.7
1	A	679	THR	2.7
1	A	760	GLN	2.6
1	A	574	GLN	2.6
1	A	291	SER	2.6
1	A	373	LEU	2.6
1	A	489	LEU	2.6
1	A	810	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	812	VAL	2.6
1	A	808	ASP	2.6
1	A	691	ILE	2.6
1	A	493	ASN	2.5
1	A	340	GLN	2.5
1	A	828	THR	2.5
1	A	859	TRP	2.5
1	A	341	MET	2.5
1	A	650	VAL	2.5
1	A	542	ILE	2.5
1	A	342	ALA	2.5
1	A	881	ASP	2.4
1	A	536	ALA	2.4
1	A	815	ARG	2.4
1	A	561	HIS	2.4
1	A	674	PHE	2.4
1	A	433	GLU	2.4
1	A	438	GLU	2.4
1	A	825	GLU	2.4
1	A	689	LYS	2.4
1	A	376	ILE	2.4
1	A	662	GLY	2.3
1	A	533	ASP	2.3
1	A	556	HIS	2.3
1	A	884	PRO	2.3
1	A	824	MET	2.3
1	A	814	ASN	2.3
1	A	836	ILE	2.3
1	A	878	GLU	2.3
1	A	538	TRP	2.3
1	A	369	GLY	2.3
1	A	684	MET	2.3
1	A	535	THR	2.3
1	A	613	THR	2.3
1	A	758	TYR	2.3
1	A	605	VAL	2.3
1	A	833	TRP	2.2
1	A	692	GLN	2.2
1	A	869	GLN	2.2
1	A	802	GLU	2.2
1	A	339	THR	2.2
1	A	862	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	565	ALA	2.2
1	A	499	SER	2.2
1	A	323	GLY	2.2
1	A	566	GLU	2.2
1	A	482	ARG	2.2
1	A	447	CYS	2.2
1	A	569	PHE	2.2
1	A	372	LYS	2.2
1	A	335	ILE	2.1
1	A	559	GLY	2.1
1	A	557	MET	2.1
1	A	695	GLU	2.1
1	A	595	ARG	2.1
1	A	502	ASN	2.1
1	A	514	LYS	2.0
1	A	673	ARG	2.0
1	A	722	ARG	2.0
1	A	521	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.

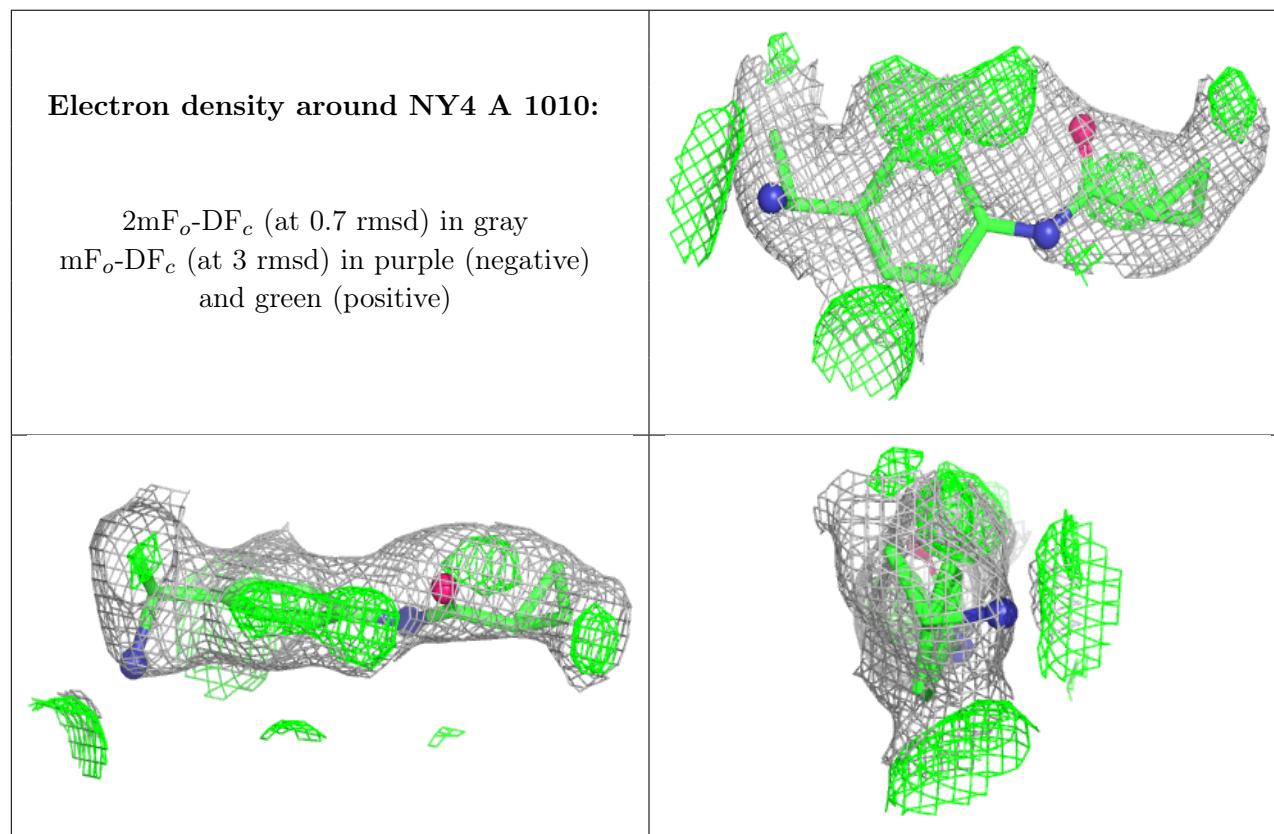
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NY4	A	1010	15/15	0.66	0.42	47,52,54,54	15
5	PO4	A	1008	5/5	0.69	0.21	100,110,124,133	0
5	PO4	A	1007	5/5	0.73	0.16	41,42,58,77	0
4	DMS	A	1005	4/4	0.81	0.23	69,92,95,100	0
6	PEG	A	1009	7/7	0.83	0.17	69,71,77,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	DMS	A	1006	4/4	0.90	0.16	57,59,61,68	0
3	MES	A	1003[A]	12/12	0.92	0.27	831,851,903,903	12
3	MES	A	1003[B]	12/12	0.92	0.27	24,30,33,34	12
4	DMS	A	1004	4/4	0.93	0.13	46,46,48,49	0
8	CL	A	1011	1/1	0.96	0.09	19,19,19,19	1
2	ZN	A	1001	1/1	0.99	0.04	28,28,28,28	0
2	ZN	A	1002	1/1	0.99	0.04	61,61,61,61	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.