Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2025 – 11:39 AM EDT

PDB ID	:	7I2V
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:

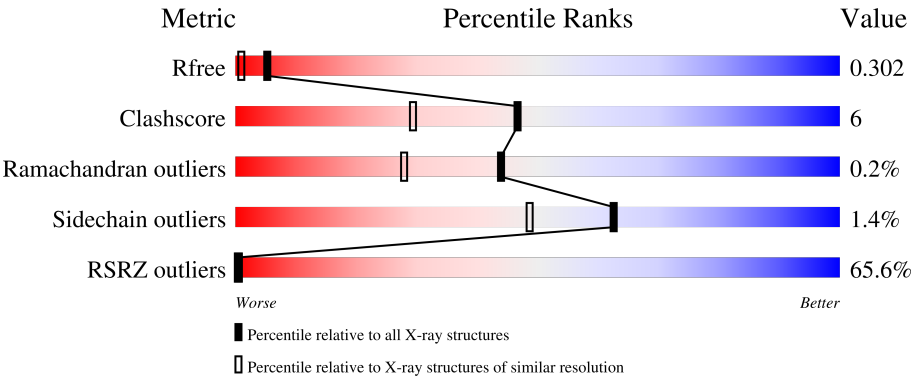
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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}	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 <=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	59% 79% 10% • 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) : 2.41.4

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PO4	A	1007	-	-	X	-
7	NY4	A	1010	-	-	-	X

2 Entry composition

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
			Total	C	N	O	S			
1	A	572	4725	2977	844	870	34	0	7	0

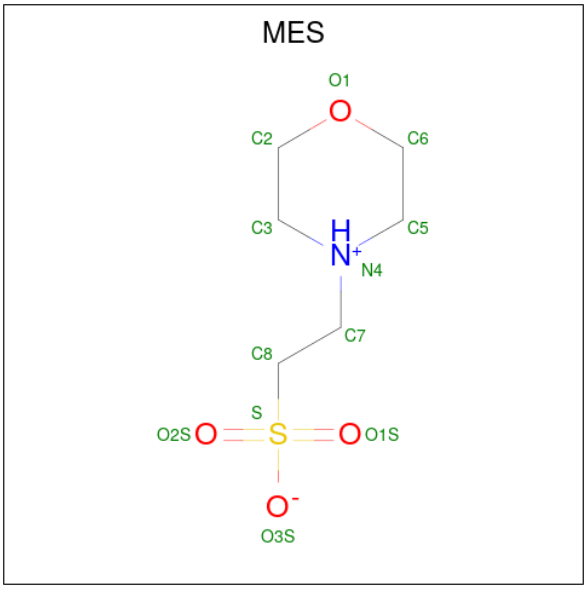
There are 2 discrepancies between the modelled and reference sequences:

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

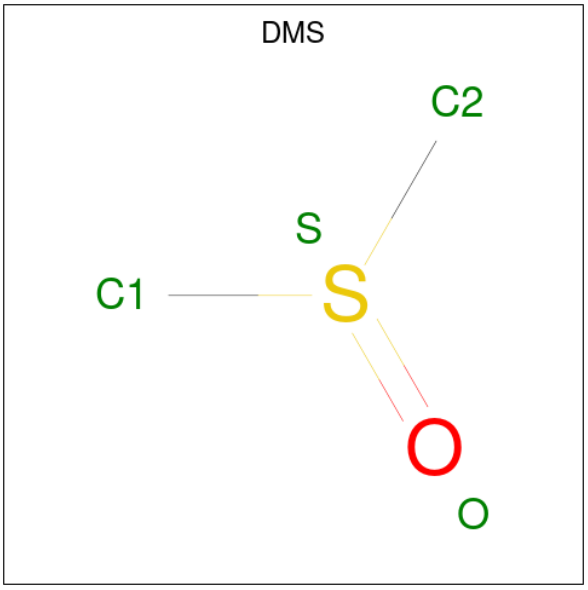
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	2	2	2	0	0

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



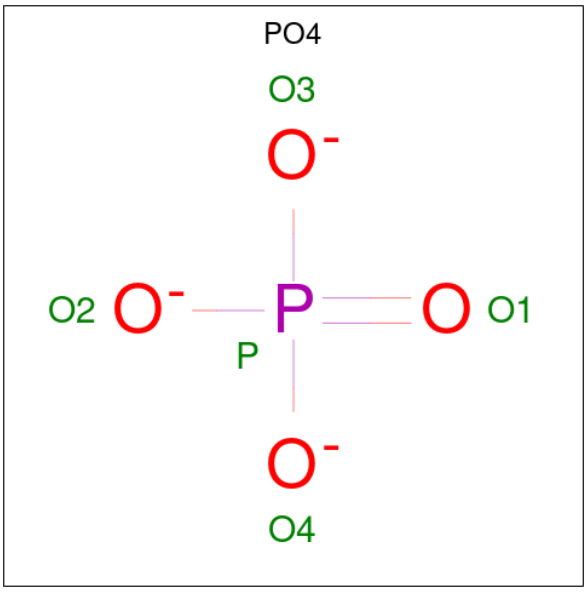
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	1
			24	12	2	8	2		

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



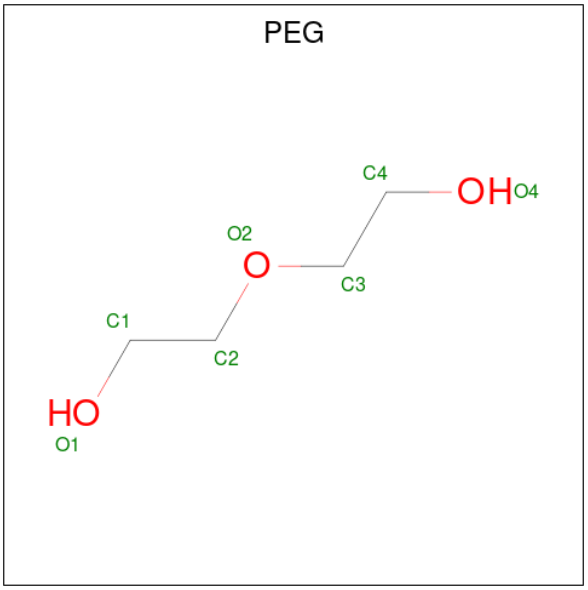
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	O	S		0	0
			4	2	1	1			
4	A	1	Total	C	O	S		0	0
			4	2	1	1			
4	A	1	Total	C	O	S		0	0
			4	2	1	1			

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

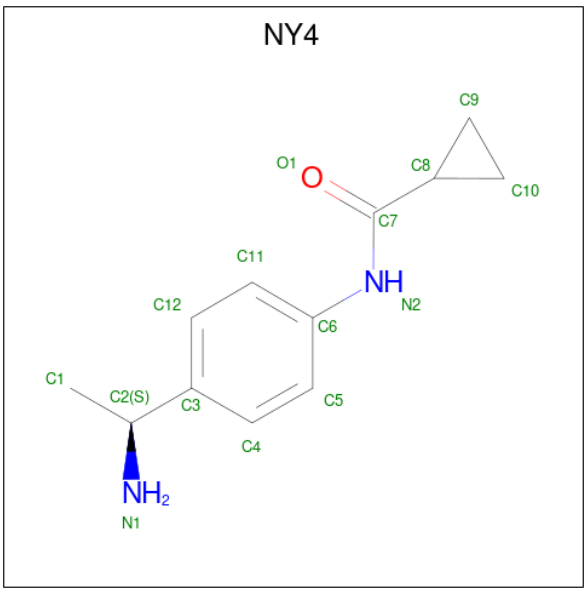
- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 7 is N-{4-[(1S)-1-aminoethyl]phenyl}cyclopropanecarboxamide (three-letter code:

NY4) (formula: $C_{12}H_{16}N_2O$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 9 is water.

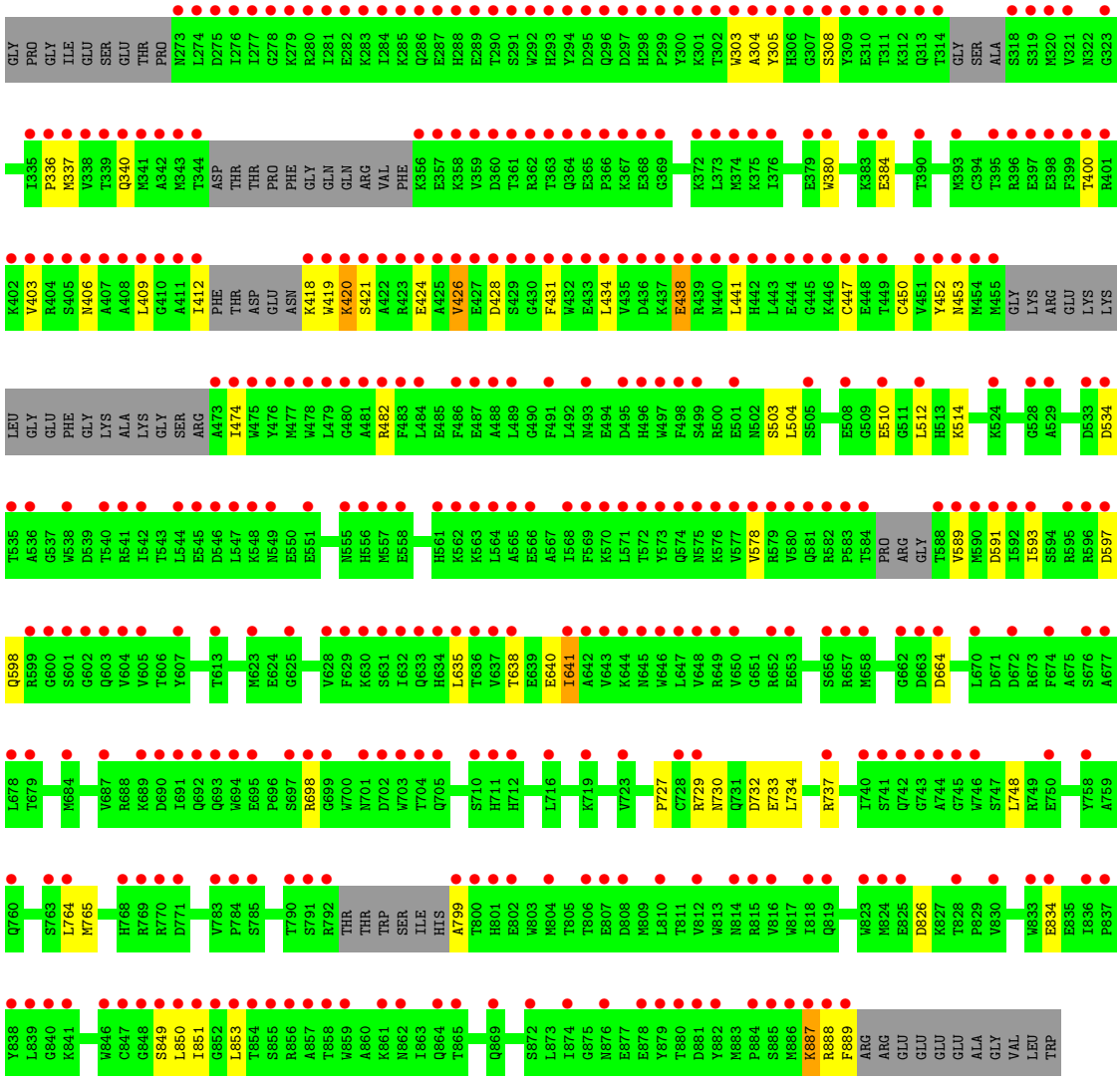
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	303	Total O 303 303	0	0

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: NS5 RNA-dependent RNA polymerase

Chain A:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 (5.16%)	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]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, PO4, NY4, PEG, DMS, MES, ZN

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	0.73	0/4830	0.82	0/6513

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	4725	0	4628	51	0
2	A	2	0	0	0	0
3	A	24	0	26	1	0
4	A	12	0	18	2	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	5	1
All	All	5099	0	4682	53	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 6.

All (53) 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
1:A:308:SER:HB3	1:A:589:VAL:HG22	1.73	0.70
1:A:380:TRP:O	1:A:384:GLU:HG2	1.93	0.68
1:A:418:LYS:HD2	1:A:419:TRP:CE2	2.34	0.62
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:308:SER:HB3	1:A:589:VAL:CG2	2.32	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
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:888:ARG:HG3	1:A:889:PHE:N	2.22	0.55
1:A:764:LEU:HG	1:A:765:MET:HE2	1.88	0.54
1:A:400:THR:HG23	1:A:426:VAL:CG1	2.37	0.54
1:A:418:LYS:O	1:A:418:LYS:HD3	2.08	0.54
1:A:664:ASP:OD1	5:A:1007:PO4:P	2.67	0.53
1:A:452:TYR:O	1:A:578:VAL:HA	2.08	0.53
1:A:400:THR:HG23	1:A:426:VAL:HG11	1.91	0.53
4:A:1004:DMS:C1	9:A:1188:HOH:O	2.57	0.52
1:A:438:GLU:O	1:A:441:LEU:HB2	2.10	0.52
1:A:419:TRP:HE1	1:A:428:ASP:CG	2.14	0.51
1:A:431:PHE:O	1:A:434:LEU:HB2	2.11	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:730:ASN:OD1	1:A:732:ASP:HB2	2.13	0.49
1:A:850:LEU:HD22	1:A:853:LEU:HD12	1.94	0.49
1:A:834:GLU:CD	1:A:887:LYS:HB2	2.32	0.49
1:A:826:ASP:OD1	1:A:826:ASP:C	2.51	0.49
1:A:597:ASP:O	1:A:598:GLN:HB2	2.14	0.48
1:A:474:ILE:HD12	1:A:474:ILE:N	2.30	0.47
1:A:512[A]:LEU:HG	1:A:727:PRO:CB	2.45	0.46
1:A:421:SER:OG	1:A:424:GLU:HG3	2.16	0.45
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:850:LEU:HD22	1:A:853:LEU:CD1	2.48	0.44
1:A:503:SER:O	1:A:504:LEU:HB2	2.17	0.44
4:A:1004:DMS:H11	9:A:1188:HOH:O	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:849:SER:OG	1:A:851:ILE:HG12	2.19	0.43
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:420:LYS:HD2	1:A:421:SER:N	2.35	0.42
1:A:748:LEU:HD13	3:A:1003[B]:MES:H61	2.02	0.42
1:A:420:LYS:HE3	1:A:420:LYS:HB3	1.87	0.41
1:A:698:ARG:NH2	9:A:1122:HOH:O	2.53	0.41
1:A:403:VAL:HG21	1:A:426:VAL:HG21	2.03	0.41
1:A:403:VAL:HG12	1:A:409:LEU:HD12	2.04	0.40

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%)	44 28

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%)	501 (99%)	7 (1%)	62 49

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

Mol	Chain	Res	Type
1	A	420	LYS
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 (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	603	GLN
1	A	645	ASN
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

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

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.

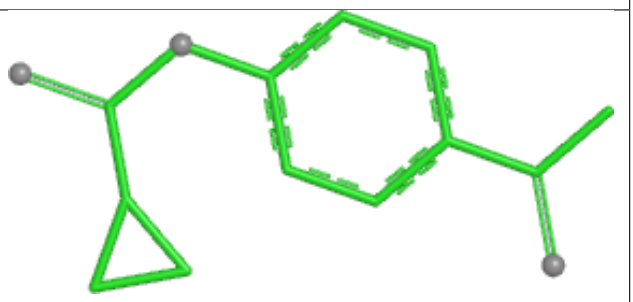
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1004	DMS	2	0
3	A	1003[B]	MES	1	0
5	A	1007	PO4	3	0

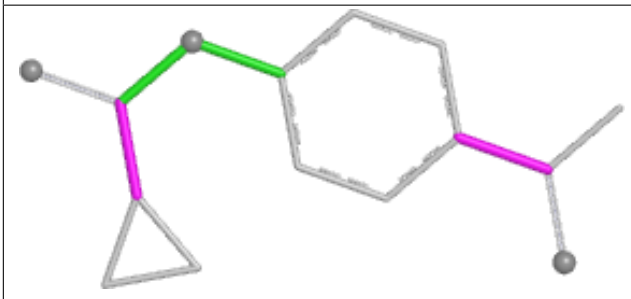
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand NY4 A 1010

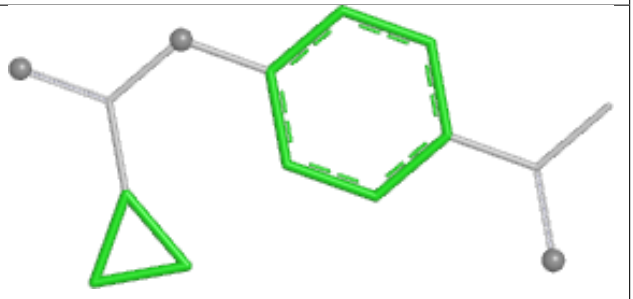
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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%)	4.49	375 (65%)	0	0	6, 39, 96, 142	140 (24%)

All (375) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	580	VAL	18.0
1	A	474	ILE	17.6
1	A	426	VAL	17.2
1	A	592	ILE	17.2
1	A	303	TRP	17.1
1	A	475	TRP	16.9
1	A	403	VAL	16.9
1	A	637	VAL	16.7
1	A	889	PHE	15.1
1	A	632	ILE	15.0
1	A	573	TYR	15.0
1	A	419	TRP	14.6
1	A	359	VAL	14.5
1	A	409	LEU	14.5
1	A	309	TYR	14.5
1	A	589	VAL	14.3
1	A	636	THR	14.3
1	A	577	VAL	13.5
1	A	422	ALA	13.5
1	A	512[A]	LEU	13.4
1	A	571	LEU	13.4
1	A	400	THR	13.3
1	A	479	LEU	13.3
1	A	588	THR	13.2
1	A	838	TYR	13.0
1	A	311	THR	12.9
1	A	857	ALA	12.5

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Mol	Chain	Res	Type	RSRZ
1	A	840	GLY	12.4
1	A	635	LEU	12.1
1	A	631	SER	11.9
1	A	363	THR	11.8
1	A	850	LEU	11.8
1	A	540	THR	11.7
1	A	572	THR	11.7
1	A	839	LEU	11.7
1	A	600	GLY	11.6
1	A	380	TRP	11.6
1	A	858	THR	11.5
1	A	445	GLY	11.5
1	A	602	GLY	11.5
1	A	853	LEU	11.5
1	A	768	HIS	11.2
1	A	421	SER	11.2
1	A	367	LYS	11.1
1	A	728	CYS	11.1
1	A	576	LYS	11.1
1	A	293	HIS	11.0
1	A	801[A]	HIS	11.0
1	A	851	ILE	11.0
1	A	575	ASN	11.0
1	A	314	THR	10.9
1	A	473	ALA	10.9
1	A	405	SER	10.8
1	A	591	ASP	10.8
1	A	854	THR	10.8
1	A	396	ARG	10.7
1	A	710	SER	10.7
1	A	366	PRO	10.7
1	A	308	SER	10.5
1	A	358	LYS	10.5
1	A	711	HIS	10.4
1	A	582	ARG	10.4
1	A	601	SER	10.4
1	A	284	ILE	10.3
1	A	852	GLY	10.3
1	A	888	ARG	10.3
1	A	597	ASP	10.3
1	A	837	PRO	10.2
1	A	885	SER	10.1

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Mol	Chain	Res	Type	RSRZ
1	A	541	ARG	10.1
1	A	301	LYS	10.1
1	A	449	THR	10.1
1	A	402	LYS	10.1
1	A	763[A]	SER	10.1
1	A	849	SER	10.0
1	A	855	SER	10.0
1	A	481	ALA	9.9
1	A	856	ARG	9.8
1	A	505	SER	9.7
1	A	603	GLN	9.7
1	A	590	MET	9.6
1	A	361	THR	9.5
1	A	546	ASP	9.5
1	A	356	LYS	9.4
1	A	581	GLN	9.4
1	A	886	MET	9.4
1	A	771	ASP	9.4
1	A	705	GLN	9.4
1	A	294	TYR	9.3
1	A	404	ARG	9.3
1	A	633	GLN	9.3
1	A	478	TRP	9.2
1	A	281	ILE	9.2
1	A	599	ARG	9.2
1	A	712	HIS	9.1
1	A	634	HIS	9.1
1	A	887	LYS	9.0
1	A	423	ARG	9.0
1	A	411	ALA	9.0
1	A	302	THR	8.9
1	A	312	LYS	8.9
1	A	424	GLU	8.9
1	A	428	ASP	8.9
1	A	770	ARG	8.8
1	A	401	ARG	8.7
1	A	551	GLU	8.7
1	A	383	LYS	8.7
1	A	410	GLY	8.6
1	A	799	ALA	8.5
1	A	435	VAL	8.5
1	A	864[A]	GLN	8.4

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Mol	Chain	Res	Type	RSRZ
1	A	746	TRP	8.4
1	A	596	ARG	8.3
1	A	431	PHE	8.3
1	A	420	LYS	8.3
1	A	630	LYS	8.3
1	A	745	GLY	8.3
1	A	729	ARG	8.3
1	A	412	ILE	8.2
1	A	548	LYS	8.2
1	A	384	GLU	8.1
1	A	697	SER	8.1
1	A	841	LYS	8.1
1	A	657	ARG	8.1
1	A	664	ASP	7.9
1	A	398	GLU	7.8
1	A	360	ASP	7.8
1	A	418	LYS	7.8
1	A	397	GLU	7.8
1	A	292	TRP	7.7
1	A	656	SER	7.7
1	A	313	GLN	7.7
1	A	446	LYS	7.7
1	A	769	ARG	7.7
1	A	694	TRP	7.6
1	A	357	GLU	7.6
1	A	663	ASP	7.6
1	A	791	SER	7.6
1	A	719[A]	LYS	7.6
1	A	741[A]	SER	7.5
1	A	434	LEU	7.4
1	A	289	GLU	7.4
1	A	368	GLU	7.3
1	A	290	THR	7.2
1	A	427	GLU	7.2
1	A	310	GLU	7.1
1	A	448	GLU	7.1
1	A	286	GLN	6.9
1	A	698	ARG	6.9
1	A	362	ARG	6.9
1	A	764	LEU	6.7
1	A	277	ILE	6.6
1	A	425	ALA	6.5

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Mol	Chain	Res	Type	RSRZ
1	A	658	MET	6.5
1	A	744	ALA	6.5
1	A	847	CYS	6.3
1	A	364	GLN	6.3
1	A	785[A]	SER	6.1
1	A	484	LEU	6.1
1	A	296	GLN	6.1
1	A	652	ARG	6.1
1	A	641	ILE	6.0
1	A	365	GLU	6.0
1	A	593	ILE	5.9
1	A	645	ASN	5.9
1	A	318	SER	5.9
1	A	496	HIS	5.8
1	A	583	PRO	5.8
1	A	638	THR	5.7
1	A	443	LEU	5.7
1	A	299	PRO	5.7
1	A	344	THR	5.6
1	A	476	TYR	5.6
1	A	305	TYR	5.6
1	A	441	LEU	5.4
1	A	584	THR	5.4
1	A	784	PRO	5.3
1	A	429	SER	5.3
1	A	562	LYS	5.3
1	A	444	GLU	5.3
1	A	653	GLU	5.2
1	A	298	HIS	5.2
1	A	501	GLU	5.1
1	A	274	LEU	5.1
1	A	678	LEU	5.1
1	A	439	ARG	5.1
1	A	488	ALA	5.1
1	A	287	GLU	5.0
1	A	275	ASP	5.0
1	A	295	ASP	4.9
1	A	432	TRP	4.9
1	A	455	MET	4.9
1	A	407	ALA	4.9
1	A	643	VAL	4.9
1	A	750	GLU	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	846	TRP	4.8
1	A	480	GLY	4.8
1	A	278	GLY	4.7
1	A	285	LYS	4.6
1	A	544	LEU	4.6
1	A	483	PHE	4.5
1	A	800	THR	4.5
1	A	742	GLN	4.5
1	A	564	LEU	4.5
1	A	874	ILE	4.5
1	A	442	HIS	4.4
1	A	649	ARG	4.4
1	A	406	ASN	4.4
1	A	792	ARG	4.4
1	A	288	HIS	4.4
1	A	440	ASN	4.4
1	A	297	ASP	4.4
1	A	743	GLY	4.4
1	A	687	VAL	4.3
1	A	699	GLY	4.3
1	A	568	ILE	4.3
1	A	818	ILE	4.3
1	A	393	MET	4.3
1	A	454	MET	4.3
1	A	451	VAL	4.3
1	A	790	THR	4.3
1	A	806	THR	4.2
1	A	570	LYS	4.2
1	A	408	ALA	4.1
1	A	563	LYS	4.1
1	A	495	ASP	4.1
1	A	452	TYR	4.1
1	A	436	ASP	4.1
1	A	642	ALA	4.0
1	A	379	GLU	4.0
1	A	453	ASN	4.0
1	A	300	TYR	4.0
1	A	882	TYR	4.0
1	A	670	LEU	4.0
1	A	701	ASN	4.0
1	A	861	LYS	3.9
1	A	830	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	282	GLU	3.9
1	A	487	GLU	3.9
1	A	880	THR	3.9
1	A	672	ASP	3.9
1	A	304	ALA	3.9
1	A	816	VAL	3.9
1	A	604	VAL	3.8
1	A	399	PHE	3.8
1	A	629	PHE	3.8
1	A	508	GLU	3.7
1	A	437	LYS	3.7
1	A	807	GLU	3.7
1	A	529	ALA	3.7
1	A	319	SER	3.6
1	A	390	THR	3.6
1	A	804	MET	3.6
1	A	644	LYS	3.6
1	A	783	VAL	3.5
1	A	703	TRP	3.5
1	A	648	VAL	3.5
1	A	306	HIS	3.5
1	A	558	GLU	3.5
1	A	555	ASN	3.5
1	A	628	VAL	3.4
1	A	307	GLY	3.4
1	A	430	GLY	3.4
1	A	677	ALA	3.4
1	A	497	TRP	3.4
1	A	848	GLY	3.4
1	A	545	GLU	3.4
1	A	486	PHE	3.4
1	A	716	LEU	3.3
1	A	279	LYS	3.3
1	A	646	TRP	3.3
1	A	865	THR	3.3
1	A	549	ASN	3.3
1	A	872	SER	3.3
1	A	702	ASP	3.2
1	A	834	GLU	3.2
1	A	337	MET	3.2
1	A	477	MET	3.2
1	A	528	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	491	PHE	3.1
1	A	276	ILE	3.1
1	A	690	ASP	3.1
1	A	320	MET	3.1
1	A	283	LYS	3.0
1	A	374	MET	3.0
1	A	498	PHE	3.0
1	A	723	VAL	3.0
1	A	524	LYS	3.0
1	A	510	GLU	3.0
1	A	740	ILE	2.9
1	A	343	MET	2.9
1	A	578	VAL	2.9
1	A	693	GLN	2.8
1	A	336	PRO	2.8
1	A	280	ARG	2.8
1	A	737	ARG	2.8
1	A	579	ARG	2.8
1	A	876	ASN	2.8
1	A	819	GLN	2.8
1	A	623	MET	2.8
1	A	273	ASN	2.7
1	A	607	TYR	2.7
1	A	879	TYR	2.7
1	A	625	GLY	2.7
1	A	547	LEU	2.7
1	A	375	LYS	2.7
1	A	823	TRP	2.7
1	A	647	LEU	2.6
1	A	395	THR	2.6
1	A	704	THR	2.6
1	A	321	VAL	2.6
1	A	534	ASP	2.6
1	A	676	SER	2.6
1	A	679	THR	2.6
1	A	338	VAL	2.6
1	A	760	GLN	2.6
1	A	574	GLN	2.5
1	A	291	SER	2.5
1	A	373	LEU	2.5
1	A	489	LEU	2.5
1	A	808	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	810	LEU	2.5
1	A	812	VAL	2.5
1	A	691	ILE	2.4
1	A	340	GLN	2.4
1	A	493	ASN	2.4
1	A	341	MET	2.4
1	A	828	THR	2.4
1	A	859	TRP	2.4
1	A	542	ILE	2.4
1	A	650	VAL	2.4
1	A	342	ALA	2.3
1	A	881	ASP	2.3
1	A	815	ARG	2.3
1	A	689	LYS	2.3
1	A	561	HIS	2.3
1	A	433	GLU	2.3
1	A	438	GLU	2.3
1	A	825	GLU	2.3
1	A	674	PHE	2.3
1	A	536	ALA	2.3
1	A	533	ASP	2.2
1	A	376	ILE	2.2
1	A	556	HIS	2.2
1	A	824	MET	2.2
1	A	878	GLU	2.2
1	A	662	GLY	2.2
1	A	684	MET	2.2
1	A	814	ASN	2.2
1	A	884	PRO	2.2
1	A	538	TRP	2.2
1	A	836	ILE	2.2
1	A	535	THR	2.2
1	A	613	THR	2.2
1	A	692	GLN	2.2
1	A	802	GLU	2.2
1	A	869	GLN	2.2
1	A	758	TYR	2.2
1	A	369	GLY	2.2
1	A	833	TRP	2.1
1	A	605	VAL	2.1
1	A	482	ARG	2.1
1	A	499	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	566	GLU	2.1
1	A	862	ASN	2.1
1	A	339	THR	2.1
1	A	372	LYS	2.1
1	A	447	CYS	2.1
1	A	565	ALA	2.1
1	A	569	PHE	2.1
1	A	323	GLY	2.1
1	A	595	ARG	2.0
1	A	695	GLU	2.0
1	A	557	MET	2.0
1	A	335	ILE	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 monosaccharides 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, 95^{th} 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
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

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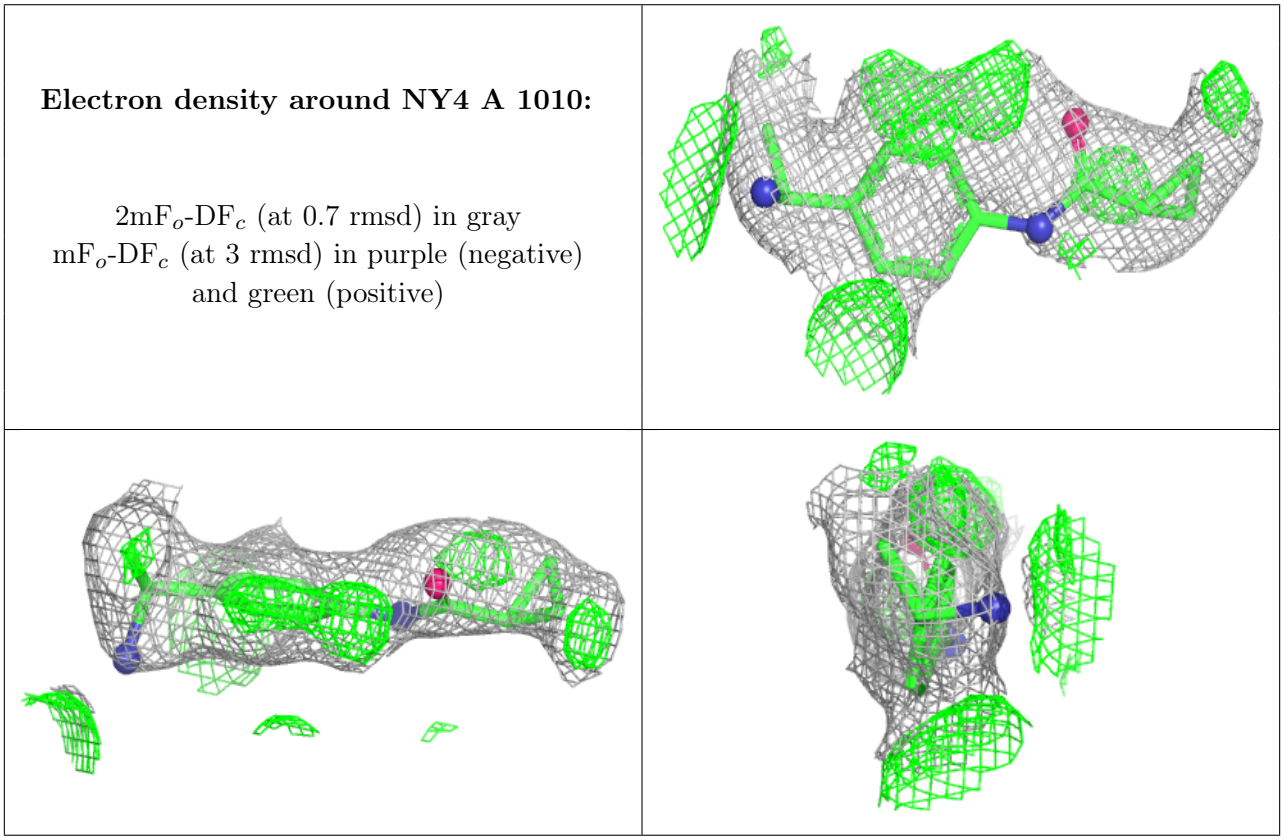
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	A	1002	1/1	0.99	0.04	61,61,61,61	0

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.

Electron density around NY4 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.