Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2025 – 10:20 AM EDT

PDB ID	:	7I2S
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 Z31721798 (DNV2_NS5A-x0771)
Authors	:	Aschenbrenner, J.C.; Saini, M.; Chopra, A.; Marples, P.G.; Balcomb, B.H.; Lithgo, R.M.; Fearon, D.; von Delft, F.; Ruiz, F.X.; Arnold, E.
Deposited on	:	2025-03-06
Resolution	:	1.56 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:

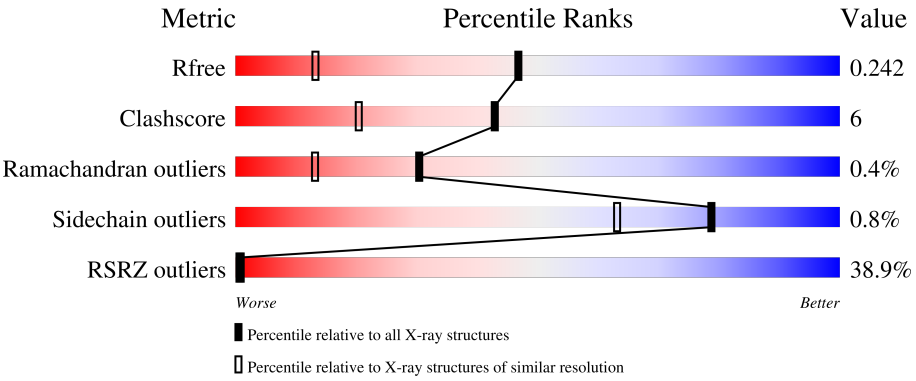
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (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 1.56 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	1935 (1.56-1.56)
Clashscore	180529	2073 (1.56-1.56)
Ramachandran outliers	177936	2037 (1.56-1.56)
Sidechain outliers	177891	2034 (1.56-1.56)
RSRZ outliers	164620	1935 (1.56-1.56)

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	35% 79% 11% • 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
4	DMS	A	1004	-	-	X	-
6	PO4	A	1008	-	-	X	-
7	NW4	A	1011	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5255 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	576	4757	2994	853	876	34	0	7	0

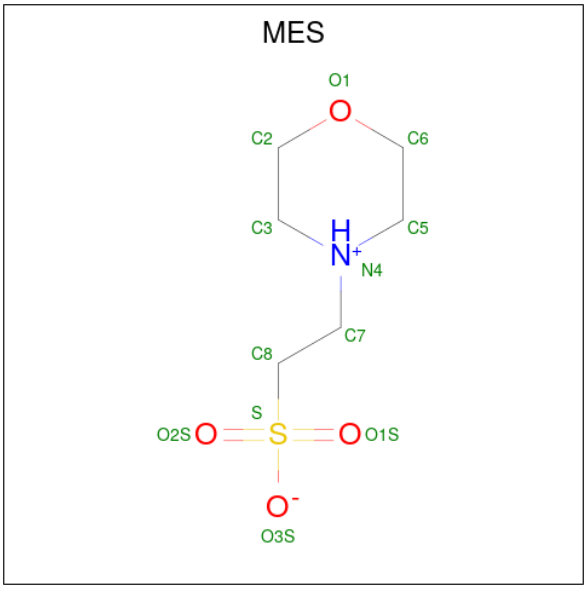
There are 2 discrepancies between the modelled and reference sequences:

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).

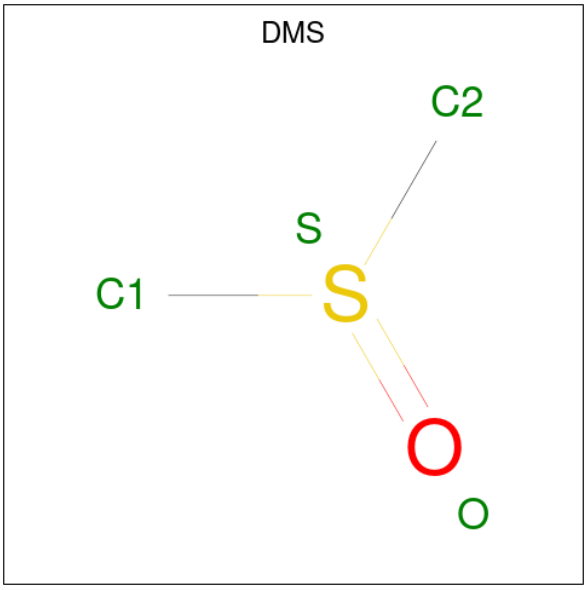
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	2	2	2	0	0

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



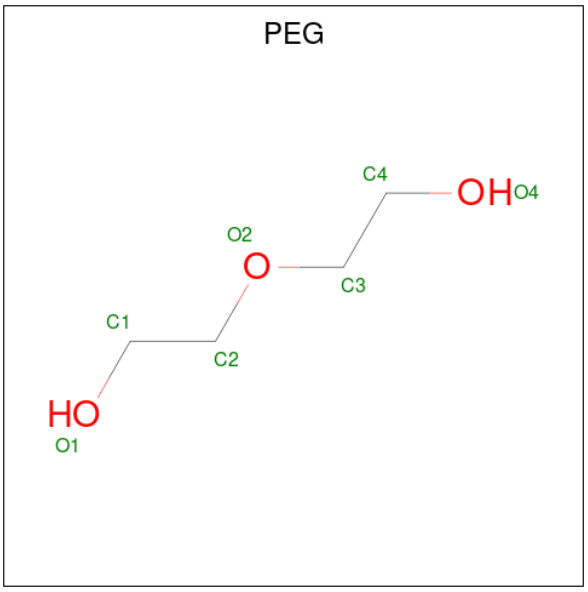
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	1
			24	12	2	8	2		

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



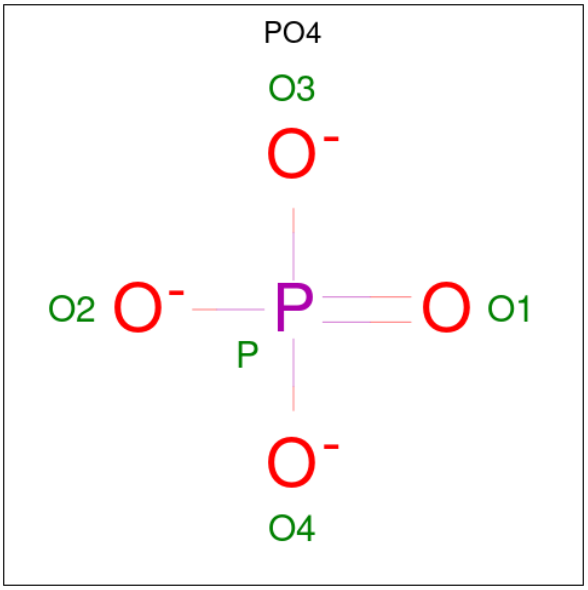
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	O	S		0	0
			4	2	1	1			
4	A	1	Total	C	O	S		0	0
			4	2	1	1			
4	A	1	Total	C	O	S		0	0
			4	2	1	1			

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



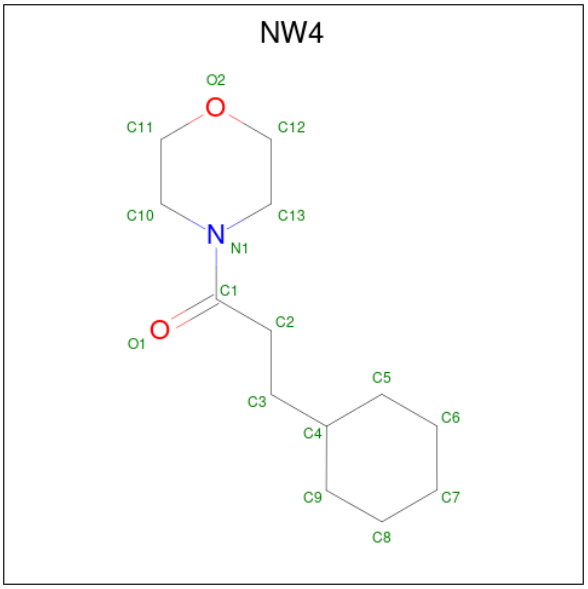
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 7 is 3-cyclohexyl-1-(morpholin-4-yl)propan-1-one (three-letter code: NW4) (formula: $C_{13}H_{23}NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O 16 13 1 2	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.

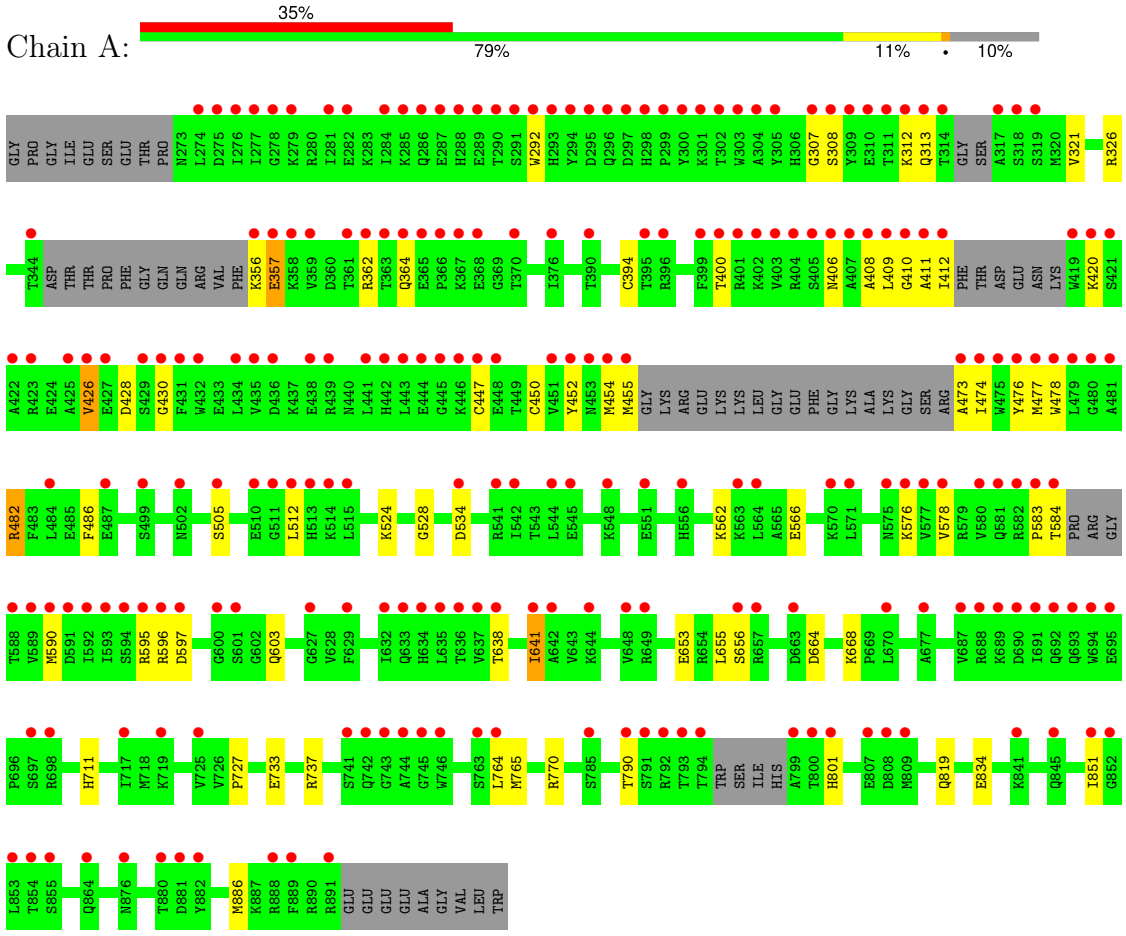
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	419	Total O 419 419	0	0

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	82.44Å 116.67Å 148.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.97 – 1.56 49.97 – 1.56	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.97-1.56) 99.5 (49.97-1.56)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.01 (at 1.56Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.188 , 0.211 0.222 , 0.242	Depositor DCC
R_{free} test set	5192 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	25.5	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 62.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5255	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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: PO4, DMS, NW4, PEG, MES, ZN, CL

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	0.74	0/4862	0.79	0/6557

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	4757	0	4660	54	0
2	A	2	0	0	0	0
3	A	24	0	26	0	0
4	A	12	0	18	4	0
5	A	14	0	20	0	0
6	A	10	0	0	4	0
7	A	16	0	0	0	0
8	A	1	0	0	0	0
9	A	419	0	0	13	2
All	All	5255	0	4724	58	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 (58) 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:454:MET:O	1:A:455:MET:HG3	1.54	1.07
1:A:664:ASP:OD1	6:A:1008:PO4:O4	1.90	0.88
1:A:595:ARG:NE	1:A:597:ASP:OD1	2.15	0.80
1:A:664:ASP:OD1	6:A:1008:PO4:P	2.43	0.77
1:A:411:ALA:HA	1:A:477:MET:O	1.89	0.71
1:A:474:ILE:HD12	1:A:474:ILE:N	2.06	0.70
1:A:512[B]:LEU:O	9:A:1101:HOH:O	2.07	0.70
1:A:356:LYS:O	1:A:356:LYS:HD2	1.92	0.69
1:A:576:LYS:NZ	1:A:596:ARG:O	2.27	0.68
1:A:454:MET:O	1:A:455:MET:CG	2.39	0.65
1:A:428:ASP:OD1	1:A:430:GLY:N	2.30	0.65
1:A:512[A]:LEU:HD21	1:A:711:HIS:NE2	2.12	0.64
1:A:534:ASP:OD1	6:A:1008:PO4:O4	2.17	0.63
1:A:733:GLU:O	1:A:737:ARG:HG3	1.99	0.62
1:A:409:LEU:O	1:A:482:ARG:HG2	2.00	0.61
1:A:638:THR:HA	1:A:641:ILE:CG2	2.30	0.61
4:A:1004:DMS:C1	9:A:1272:HOH:O	2.48	0.60
1:A:534:ASP:OD1	6:A:1008:PO4:P	2.60	0.59
4:A:1004:DMS:H11	9:A:1272:HOH:O	2.03	0.58
1:A:834:GLU:HG3	9:A:1152:HOH:O	2.04	0.57
1:A:512[A]:LEU:O	9:A:1101:HOH:O	2.17	0.57
1:A:790:THR:HG22	9:A:1367:HOH:O	2.07	0.55
1:A:801[B]:HIS:H	1:A:801[B]:HIS:CD2	2.24	0.54
1:A:400:THR:HA	1:A:426:VAL:HG21	1.89	0.54
1:A:362:ARG:HH21	1:A:364:GLN:HA	1.72	0.54
1:A:886:MET:HE1	9:A:1155:HOH:O	2.10	0.52
1:A:473:ALA:C	1:A:474:ILE:HD12	2.30	0.52
1:A:412:ILE:HG12	1:A:478:TRP:HA	1.92	0.52
1:A:764:LEU:HG	1:A:765:MET:HE3	1.91	0.50
1:A:819:GLN:NE2	9:A:1107:HOH:O	2.34	0.50
1:A:653:GLU:O	1:A:656:SER:OG	2.23	0.50
1:A:528:GLY:O	1:A:668:LYS:HE3	2.14	0.48
1:A:524:LYS:NZ	9:A:1118:HOH:O	2.47	0.48
1:A:562:LYS:NZ	9:A:1108:HOH:O	2.35	0.48
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.55	0.47
1:A:583:PRO:O	1:A:584:THR:C	2.52	0.47
1:A:562:LYS:HE3	1:A:566:GLU:OE2	2.16	0.46
1:A:764:LEU:HG	1:A:765:MET:CE	2.45	0.46
1:A:505:SER:OG	1:A:655:LEU:O	2.24	0.46
1:A:770:ARG:HD2	1:A:851:ILE:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:CYS:HB3	1:A:486:PHE:CE2	2.51	0.45
1:A:638:THR:O	1:A:641:ILE:HG23	2.16	0.45
1:A:357:GLU:N	1:A:357:GLU:OE2	2.50	0.45
1:A:512[A]:LEU:HG	1:A:727:PRO:HB3	1.99	0.44
1:A:410:GLY:O	1:A:476:TYR:HA	2.18	0.43
1:A:452:TYR:HB2	1:A:578:VAL:HG22	2.00	0.43
1:A:321:VAL:HG11	1:A:326:ARG:CZ	2.49	0.42
1:A:292:TRP:CZ2	1:A:307:GLY:HA3	2.55	0.42
1:A:308:SER:HA	1:A:590:MET:O	2.20	0.42
1:A:408:ALA:HB3	1:A:603:GLN:HE22	1.84	0.42
1:A:409:LEU:HD22	9:A:1515:HOH:O	2.20	0.42
4:A:1004:DMS:H13	9:A:1272:HOH:O	2.15	0.42
1:A:408:ALA:HB3	1:A:603:GLN:NE2	2.35	0.42
1:A:512[A]:LEU:HG	1:A:727:PRO:CB	2.51	0.41
1:A:312:LYS:O	1:A:313:GLN:HG3	2.21	0.41
1:A:638:THR:HA	1:A:641:ILE:HG22	2.03	0.41
4:A:1004:DMS:H12	9:A:1328:HOH:O	2.21	0.40
1:A:409:LEU:O	1:A:410:GLY:C	2.60	0.40

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:1162:HOH:O	9:A:1162:HOH:O[2_445]	1.56	0.64
9:A:1292:HOH:O	9:A:1415:HOH:O[2_545]	2.10	0.10

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	569/637 (89%)	551 (97%)	16 (3%)	2 (0%)	30 13

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	406	ASN
1	A	420	LYS

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	511/554 (92%)	507 (99%)	4 (1%)	79 63

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	357	GLU
1	A	426	VAL
1	A	482	ARG
1	A	641	ILE

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	603	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 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	PEG	A	1010	-	6,6,6	0.14	0	5,5,5	0.12	0
3	MES	A	1003[B]	-	12,12,12	0.70	0	15,16,16	0.32	0
3	MES	A	1003[A]	-	12,12,12	0.73	0	15,16,16	0.94	1 (6%)
6	PO4	A	1008	-	4,4,4	6.15	3 (75%)	6,6,6	0.95	0
6	PO4	A	1009	-	4,4,4	1.33	1 (25%)	6,6,6	0.49	0
4	DMS	A	1005	-	3,3,3	0.33	0	3,3,3	0.05	0
4	DMS	A	1006	-	3,3,3	0.25	0	3,3,3	0.42	0
5	PEG	A	1007	-	6,6,6	0.21	0	5,5,5	0.18	0
4	DMS	A	1004	-	3,3,3	0.95	0	3,3,3	0.65	0
7	NW4	A	1011	-	17,17,17	0.18	0	21,21,21	0.59	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
5	PEG	A	1010	-	-	3/4/4/4	-
3	MES	A	1003[B]	-	-	5/6/14/14	0/1/1/1
3	MES	A	1003[A]	-	-	3/6/14/14	0/1/1/1
5	PEG	A	1007	-	-	1/4/4/4	-
7	NW4	A	1011	-	-	4/9/25/25	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1008	PO4	P-O1	9.00	1.71	1.50
6	A	1008	PO4	P-O2	6.70	1.74	1.54
6	A	1008	PO4	P-O3	4.90	1.68	1.54
6	A	1009	PO4	P-O1	2.30	1.56	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1003[A]	MES	O2S-S-C8	-2.04	103.64	106.73

There are no chirality outliers.

All (16) 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-O2S
3	A	1003[A]	MES	C7-C8-S-O3S
3	A	1003[B]	MES	C8-C7-N4-C3
7	A	1011	NW4	O1-C1-N1-C10
7	A	1011	NW4	C2-C1-N1-C10
7	A	1011	NW4	C2-C1-N1-C13
7	A	1011	NW4	O1-C1-N1-C13
5	A	1010	PEG	O2-C3-C4-O4
5	A	1007	PEG	O2-C3-C4-O4
3	A	1003[B]	MES	C8-C7-N4-C5
3	A	1003[B]	MES	C7-C8-S-O3S
3	A	1003[B]	MES	C7-C8-S-O1S
3	A	1003[B]	MES	C7-C8-S-O2S
5	A	1010	PEG	O1-C1-C2-O2
5	A	1010	PEG	C4-C3-O2-C2

There are no ring outliers.

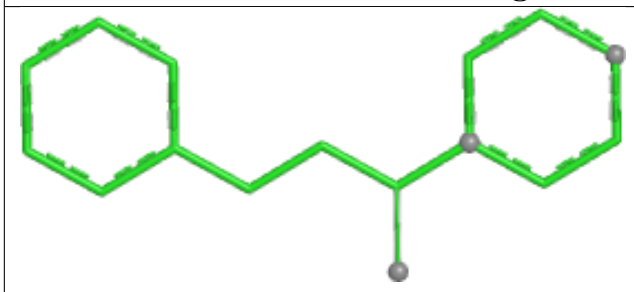
2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1008	PO4	4	0
4	A	1004	DMS	4	0

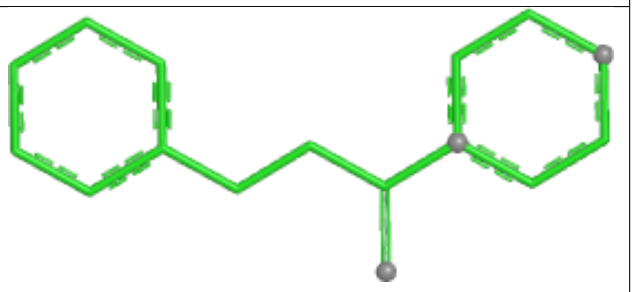
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

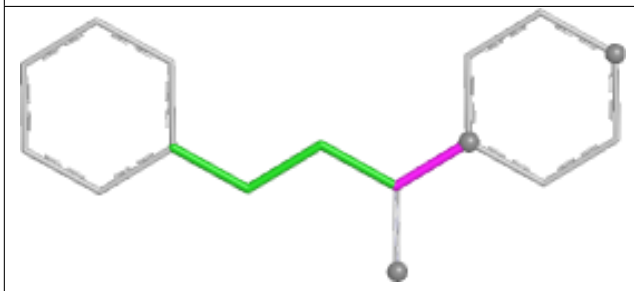
Ligand NW4 A 1011



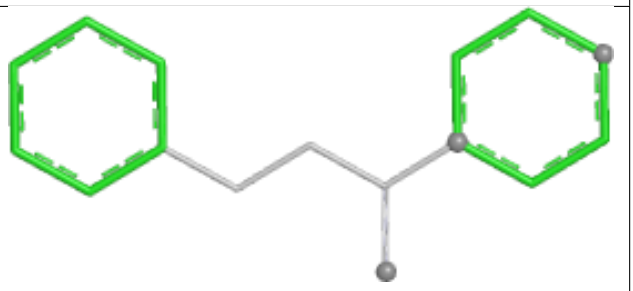
Bond lengths



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	576/637 (90%)	2.57	224 (38%) 1 1	5, 32, 85, 127	99 (17%)

All (224) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	851	ILE	15.6
1	A	853	LEU	14.2
1	A	303	TRP	13.6
1	A	512[A]	LEU	13.4
1	A	451	VAL	13.1
1	A	478	TRP	13.0
1	A	593	ILE	13.0
1	A	592	ILE	12.9
1	A	636	THR	12.5
1	A	725	VAL	12.4
1	A	515	LEU	12.3
1	A	635	LEU	12.3
1	A	426	VAL	12.3
1	A	475	TRP	12.2
1	A	801[A]	HIS	12.1
1	A	304	ALA	12.1
1	A	852	GLY	12.0
1	A	419	TRP	11.8
1	A	855	SER	11.1
1	A	589	VAL	11.0
1	A	854	THR	10.8
1	A	719[A]	LYS	10.6
1	A	409	LEU	10.5
1	A	412	ILE	10.3
1	A	400	THR	10.3
1	A	476	TYR	9.6
1	A	431	PHE	9.5

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Mol	Chain	Res	Type	RSRZ
1	A	411	ALA	9.5
1	A	292	TRP	9.3
1	A	511	GLY	9.2
1	A	513	HIS	9.1
1	A	841	LYS	9.1
1	A	317	ALA	9.0
1	A	888	ARG	9.0
1	A	594	SER	8.9
1	A	363	THR	8.8
1	A	576	LYS	8.7
1	A	697	SER	8.7
1	A	473	ALA	8.6
1	A	575	ASN	8.5
1	A	356	LYS	8.5
1	A	743	GLY	8.4
1	A	453	ASN	8.4
1	A	845	GLN	8.4
1	A	402	LYS	8.4
1	A	477	MET	8.4
1	A	499	SER	8.2
1	A	410	GLY	8.1
1	A	763[A]	SER	8.1
1	A	454	MET	8.1
1	A	584	THR	8.1
1	A	505	SER	8.1
1	A	601	SER	8.1
1	A	656	SER	8.0
1	A	590	MET	7.9
1	A	588	THR	7.9
1	A	785[A]	SER	7.9
1	A	302	THR	7.9
1	A	474	ILE	7.9
1	A	591	ASP	7.7
1	A	514	LYS	7.6
1	A	401	ARG	7.6
1	A	808	ASP	7.5
1	A	864[A]	GLN	7.5
1	A	657	ARG	7.5
1	A	649	ARG	7.5
1	A	408	ALA	7.4
1	A	298	HIS	7.4
1	A	421	SER	7.4

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Mol	Chain	Res	Type	RSRZ
1	A	396	ARG	7.3
1	A	595	ARG	7.3
1	A	405	SER	7.2
1	A	359	VAL	7.1
1	A	309	TYR	7.1
1	A	319	SER	7.1
1	A	809	MET	7.0
1	A	318	SER	6.9
1	A	284	ILE	6.8
1	A	689	LYS	6.8
1	A	299	PRO	6.7
1	A	741[A]	SER	6.7
1	A	698	ARG	6.6
1	A	600	GLY	6.6
1	A	541	ARG	6.6
1	A	403	VAL	6.6
1	A	548	LYS	6.6
1	A	502	ASN	6.5
1	A	583	PRO	6.5
1	A	404	ARG	6.4
1	A	510	GLU	6.4
1	A	688	ARG	6.4
1	A	551	GLU	6.2
1	A	290	THR	6.2
1	A	807	GLU	6.2
1	A	406	ASN	6.0
1	A	294	TYR	6.0
1	A	487	GLU	6.0
1	A	693	GLN	5.8
1	A	358	LYS	5.8
1	A	455	MET	5.7
1	A	597	ASP	5.7
1	A	420	LYS	5.7
1	A	596	ARG	5.5
1	A	365	GLU	5.3
1	A	407	ALA	5.3
1	A	441	LEU	5.3
1	A	742	GLN	5.2
1	A	314	THR	5.2
1	A	690	ASP	5.1
1	A	357	GLU	5.1
1	A	692	GLN	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	277	ILE	5.0
1	A	297	ASP	4.9
1	A	281	ILE	4.9
1	A	637	VAL	4.9
1	A	305	TYR	4.8
1	A	435	VAL	4.7
1	A	364	GLN	4.6
1	A	308	SER	4.6
1	A	422	ALA	4.5
1	A	442	HIS	4.5
1	A	799	ALA	4.5
1	A	362	ARG	4.5
1	A	301	LYS	4.4
1	A	361	THR	4.4
1	A	434	LEU	4.3
1	A	794	THR	4.2
1	A	571	LEU	4.2
1	A	791	SER	4.1
1	A	436	ASP	4.1
1	A	427	GLU	4.1
1	A	432	TRP	4.0
1	A	793	THR	4.0
1	A	278	GLY	3.9
1	A	274	LEU	3.8
1	A	279	LYS	3.8
1	A	300	TYR	3.8
1	A	452	TYR	3.8
1	A	293	HIS	3.7
1	A	445	GLY	3.7
1	A	448	GLU	3.7
1	A	479	LEU	3.7
1	A	484	LEU	3.7
1	A	694	TRP	3.6
1	A	288	HIS	3.6
1	A	370	THR	3.6
1	A	880	THR	3.5
1	A	889	PHE	3.5
1	A	790	THR	3.5
1	A	295	ASP	3.5
1	A	443	LEU	3.4
1	A	564	LEU	3.4
1	A	641	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	344	THR	3.4
1	A	481	ALA	3.3
1	A	891	ARG	3.3
1	A	276	ILE	3.2
1	A	275	ASP	3.2
1	A	744	ALA	3.2
1	A	366	PRO	3.2
1	A	423	ARG	3.2
1	A	577	VAL	3.2
1	A	746	TRP	3.1
1	A	544	LEU	3.1
1	A	638	THR	3.1
1	A	311	THR	3.1
1	A	792	ARG	3.0
1	A	296	GLN	3.0
1	A	399	PHE	3.0
1	A	287	GLU	3.0
1	A	376	ILE	3.0
1	A	291	SER	3.0
1	A	881	ASP	3.0
1	A	313	GLN	2.9
1	A	745	GLY	2.9
1	A	425	ALA	2.8
1	A	677	ALA	2.8
1	A	629	PHE	2.8
1	A	670	LEU	2.7
1	A	634	HIS	2.7
1	A	289	GLU	2.7
1	A	800	THR	2.6
1	A	286	GLN	2.6
1	A	582	ARG	2.6
1	A	627	GLY	2.6
1	A	563	LYS	2.6
1	A	580	VAL	2.6
1	A	480	GLY	2.6
1	A	312	LYS	2.6
1	A	439	ARG	2.5
1	A	438	GLU	2.5
1	A	444	GLU	2.5
1	A	545	GLU	2.5
1	A	282	GLU	2.4
1	A	581	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	447	CYS	2.4
1	A	430	GLY	2.4
1	A	648	VAL	2.4
1	A	307	GLY	2.3
1	A	632	ILE	2.3
1	A	644	LYS	2.3
1	A	570	LYS	2.3
1	A	429	SER	2.3
1	A	368	GLU	2.3
1	A	285	LYS	2.3
1	A	882	TYR	2.3
1	A	534	ASP	2.3
1	A	310	GLU	2.2
1	A	764	LEU	2.2
1	A	691	ILE	2.2
1	A	633	GLN	2.2
1	A	542	ILE	2.2
1	A	876	ASN	2.2
1	A	390	THR	2.2
1	A	663	ASP	2.1
1	A	395	THR	2.1
1	A	556	HIS	2.1
1	A	717	ILE	2.1
1	A	446	LYS	2.0
1	A	578	VAL	2.0
1	A	642	ALA	2.0
1	A	695	GLU	2.0
1	A	367	LYS	2.0
1	A	687	VAL	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)

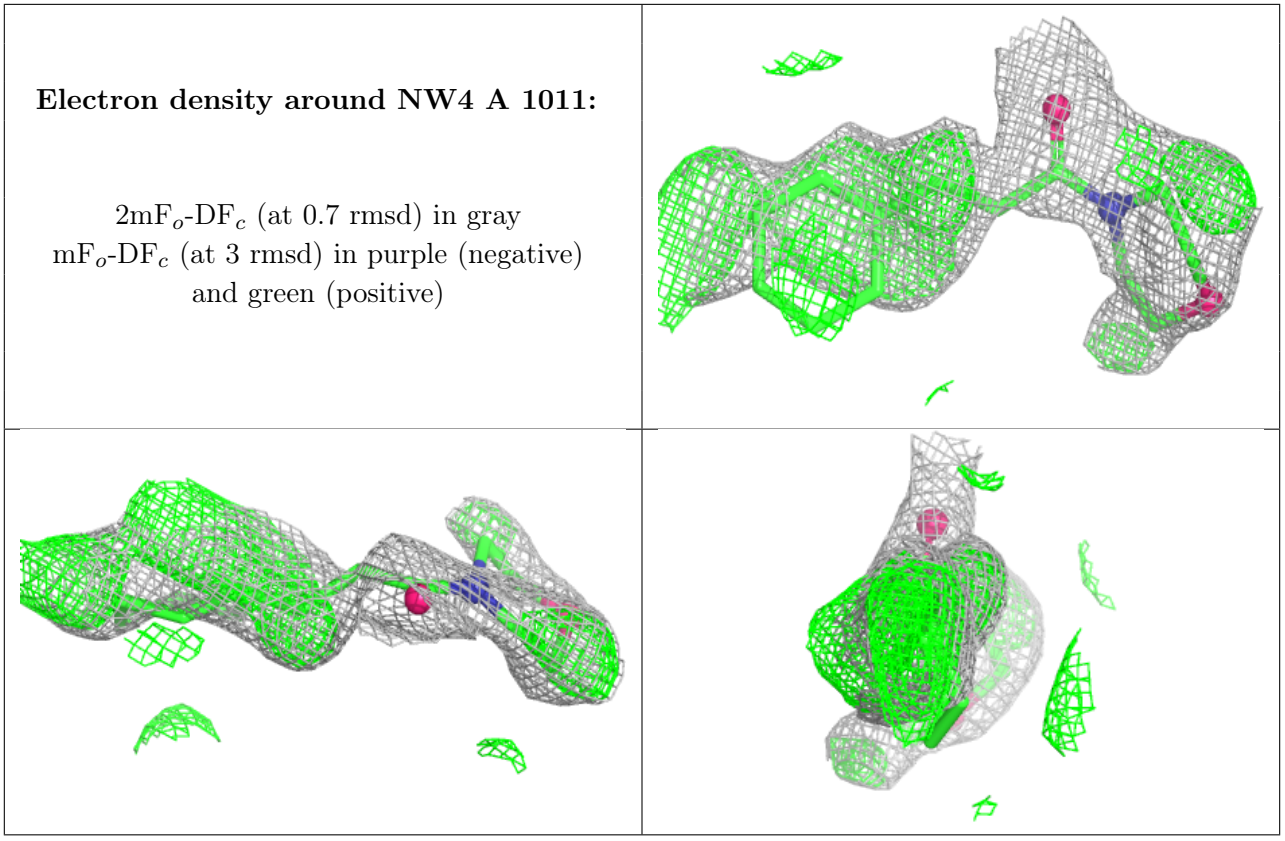
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	NW4	A	1011	16/16	0.59	0.45	44,46,47,48	16
6	PO4	A	1009	5/5	0.61	0.19	69,70,89,105	0
4	DMS	A	1005	4/4	0.68	0.27	63,78,86,96	0
5	PEG	A	1007	7/7	0.71	0.18	65,72,84,85	0
6	PO4	A	1008	5/5	0.75	0.17	30,32,42,60	0
5	PEG	A	1010	7/7	0.82	0.18	62,69,73,74	0
4	DMS	A	1004	4/4	0.90	0.16	36,38,40,41	0
4	DMS	A	1006	4/4	0.95	0.12	43,46,51,54	0
3	MES	A	1003[A]	12/12	0.97	0.33	18,22,24,24	12
3	MES	A	1003[B]	12/12	0.97	0.33	483,499,513,515	12
2	ZN	A	1002	1/1	0.98	0.07	47,47,47,47	0
8	CL	A	1012	1/1	0.99	0.06	36,36,36,36	0
2	ZN	A	1001	1/1	1.00	0.01	18,18,18,18	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 NW4 A 1011:

$2mF_o$-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

There are no such residues in this entry.