Full wwPDB X-ray Structure Validation Report (i)

Mar 27, 2025 – 10:19 AM EDT

PDB ID	:	7I2G
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 Z1079512010 (DNV2_NS5A-x0379)
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	:	1.85 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 (i) 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 (i)) were used in the production of this report:

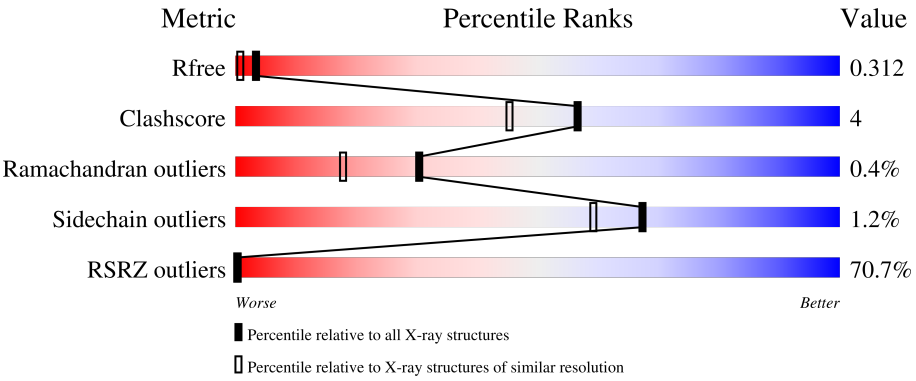
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (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 1.85 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	3097 (1.86-1.86)
Clashscore	180529	3359 (1.86-1.86)
Ramachandran outliers	177936	3335 (1.86-1.86)
Sidechain outliers	177891	3335 (1.86-1.86)
RSRZ outliers	164620	3097 (1.86-1.86)

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	63% 81% 8% 11%

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	1006	-	-	X	-
8	UWS	A	1010	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5088 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	570	4698	2962	840	862	34	0	5	0

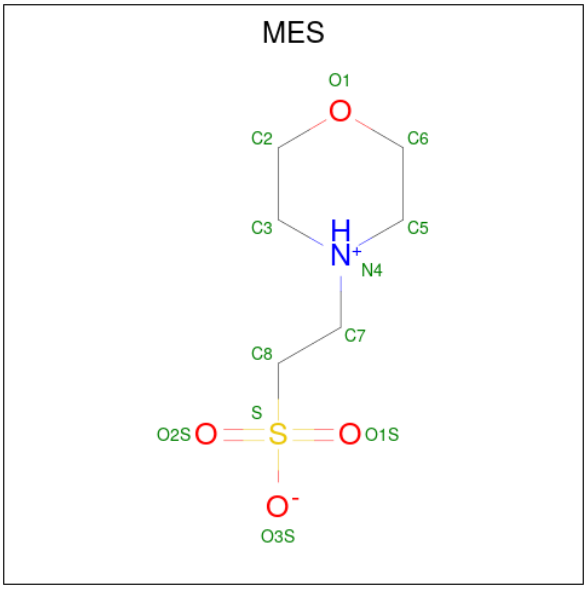
There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

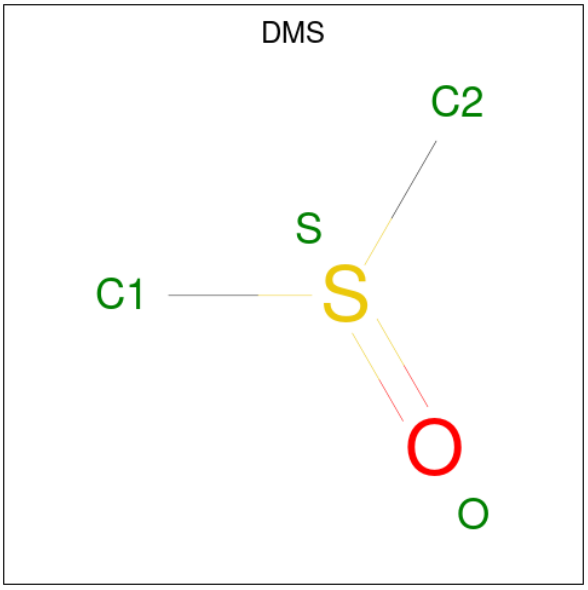
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	2	2	2	0	0

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



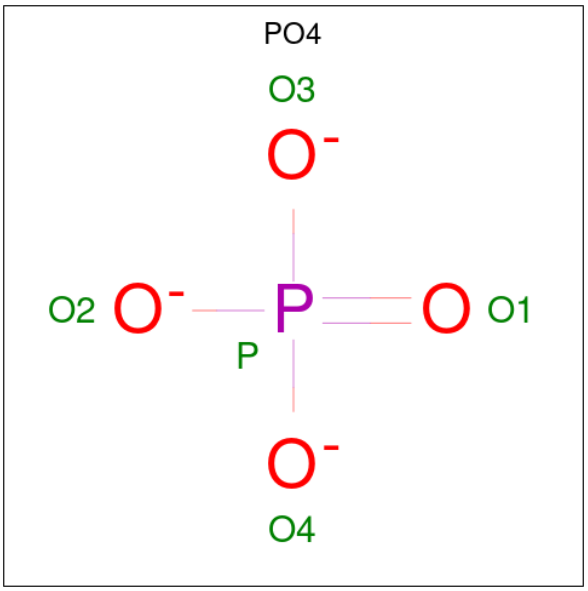
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	1
			24	12	2	8	2		

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



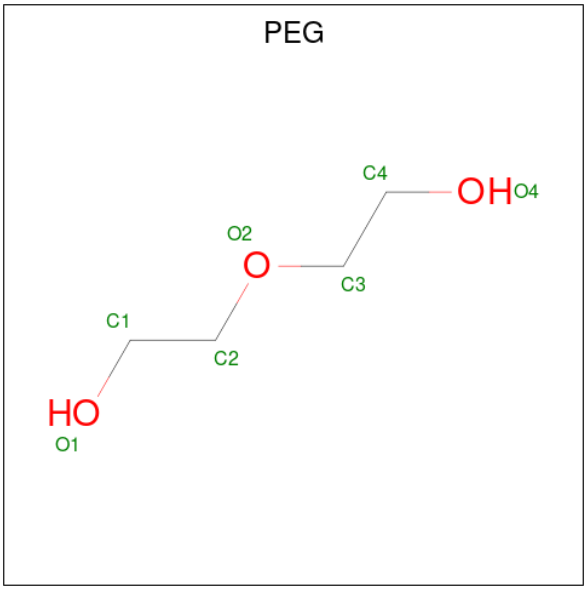
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

- 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: $C_4H_{10}O_3$).

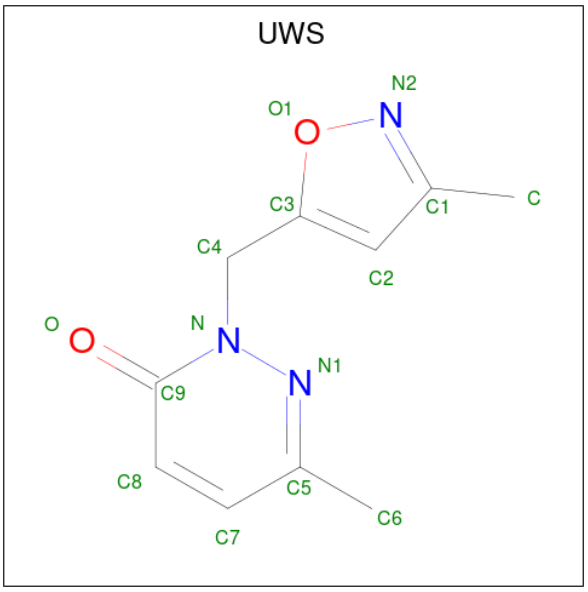


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 4 3	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total Cl 2 2	0	0

- Molecule 8 is 6-methyl-2-[(3-methyl-1,2-oxazol-5-yl)methyl]pyridazin-3(2H)-one (three-letter code: UWS) (formula: $C_{10}H_{11}N_3O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O 15 10 3 2	0	0
8	A	1	Total C N O 15 10 3 2	0	0

- Molecule 9 is water.

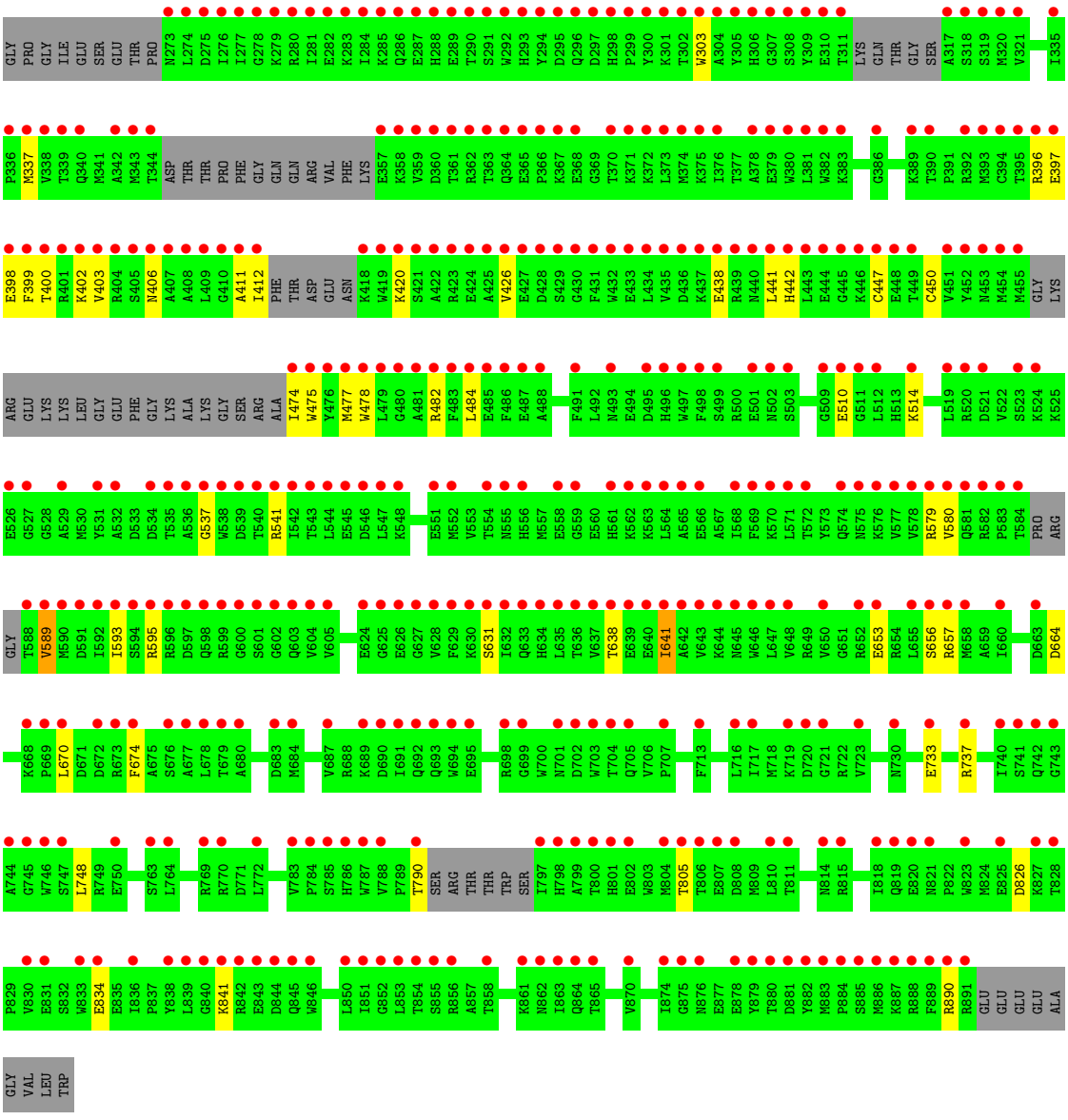
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	307	Total O 307 307	0	0

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	82.42Å 116.04Å 147.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.69 – 1.85 73.69 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.0 (73.69-1.85) 98.0 (73.69-1.85)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.98 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.207 , 0.247 0.291 , 0.312	Depositor DCC
R_{free} test set	3139 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å^2)	35.3	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 281.7	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	0.82	EDS
Total number of atoms	5088	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% 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: UWS, PEG, DMS, ZN, PO4, CL, MES

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	0/4803	0.78	0/6478

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	4698	0	4603	40	0
2	A	2	0	0	0	0
3	A	24	0	26	1	0
4	A	8	0	12	2	0
5	A	10	0	0	2	0
6	A	7	0	10	0	0
7	A	2	0	0	0	0
8	A	30	0	0	0	0
9	A	307	0	0	8	1
All	All	5088	0	4651	42	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 (42) 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:670:LEU:HA	9:A:1177:HOH:O	1.31	1.24
1:A:397:GLU:OE1	1:A:397:GLU:N	2.09	0.85
1:A:664:ASP:OD1	5:A:1006:PO4:O4	2.00	0.79
1:A:670:LEU:HD12	9:A:1177:HOH:O	1.85	0.77
1:A:510:GLU:OE1	1:A:514:LYS:HE3	1.88	0.73
1:A:400:THR:O	1:A:403:VAL:HG22	1.89	0.73
1:A:537:GLY:O	1:A:541:ARG:HG2	1.91	0.71
1:A:438:GLU:O	1:A:441:LEU:HB2	2.00	0.62
1:A:400:THR:HG23	1:A:426:VAL:HG11	1.82	0.62
1:A:653:GLU:O	1:A:656:SER:OG	2.14	0.61
1:A:579:ARG:O	1:A:579:ARG:HG3	1.99	0.61
1:A:580:VAL:HG21	1:A:593:ILE:HD11	1.83	0.60
1:A:664:ASP:OD1	5:A:1006:PO4:P	2.60	0.59
1:A:638:THR:O	1:A:641:ILE:HG22	2.03	0.58
4:A:1004:DMS:C1	9:A:1245:HOH:O	2.51	0.58
1:A:396:ARG:HB2	1:A:397:GLU:OE1	2.04	0.57
1:A:653:GLU:OE2	1:A:657:ARG:NE	2.37	0.57
1:A:403:VAL:HG21	1:A:426:VAL:HG21	1.86	0.57
1:A:733:GLU:O	1:A:737:ARG:HG3	2.05	0.57
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.46	0.55
1:A:337:MET:HG2	9:A:1302:HOH:O	2.11	0.51
1:A:580:VAL:CG2	1:A:593:ILE:HD11	2.41	0.51
1:A:399:PHE:O	1:A:403:VAL:HG13	2.10	0.51
1:A:442:HIS:CE1	1:A:484:LEU:HD13	2.48	0.48
1:A:398:GLU:O	1:A:402:LYS:HG3	2.13	0.48
4:A:1004:DMS:H13	9:A:1245:HOH:O	2.11	0.48
1:A:589:VAL:CG2	1:A:589:VAL:O	2.64	0.46
1:A:412:ILE:HG12	1:A:478:TRP:HA	1.97	0.46
1:A:411:ALA:HA	1:A:477:MET:O	2.15	0.45
1:A:653:GLU:OE2	1:A:657:ARG:CZ	2.65	0.45
1:A:510:GLU:OE1	1:A:514:LYS:CE	2.64	0.44
1:A:826:ASP:OD1	1:A:826:ASP:C	2.57	0.43
1:A:475:TRP:CD1	1:A:475:TRP:N	2.86	0.43
1:A:510:GLU:OE1	1:A:510:GLU:HA	2.19	0.42
1:A:790:THR:HG22	9:A:1324:HOH:O	2.17	0.42
1:A:579:ARG:O	1:A:579:ARG:CG	2.67	0.42
1:A:834:GLU:OE2	1:A:890:ARG:NE	2.49	0.42
1:A:303:TRP:CE2	1:A:595:ARG:HD2	2.54	0.42
1:A:653:GLU:OE2	1:A:657:ARG:NH2	2.53	0.41
1:A:674:PHE:N	9:A:1124:HOH:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:748:LEU:HD13	3:A:1003[B]:MES:H61	2.03	0.41
1:A:841:LYS:NZ	9:A:1126:HOH:O	2.55	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:1313:HOH:O	9:A:1313:HOH:O[4_545]	2.19	0.01

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	561/637 (88%)	536 (96%)	23 (4%)	2 (0%)	30 18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	420	LYS
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	504/554 (91%)	498 (99%)	6 (1%)	67 59

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	474	ILE
1	A	482	ARG
1	A	589	VAL
1	A	631	SER
1	A	641	ILE
1	A	805	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	742	GLN
1	A	845	GLN

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 13 ligands modelled in this entry, 4 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	$\#\|Z\| > 2$
8	UWS	A	1011	-	14,16,16	1.30	3 (21%)	13,22,22	0.94	1 (7%)
5	PO4	A	1007	-	4,4,4	0.85	0	6,6,6	0.44	0
8	UWS	A	1010	-	14,16,16	1.27	2 (14%)	13,22,22	0.96	1 (7%)
5	PO4	A	1006	-	4,4,4	3.06	1 (25%)	6,6,6	0.98	0
3	MES	A	1003[B]	-	12,12,12	0.79	0	15,16,16	0.64	0
4	DMS	A	1004	-	3,3,3	0.38	0	3,3,3	0.16	0
3	MES	A	1003[A]	-	12,12,12	0.92	0	15,16,16	0.67	0
4	DMS	A	1005	-	3,3,3	0.26	0	3,3,3	0.06	0
6	PEG	A	1008	-	6,6,6	0.16	0	5,5,5	0.15	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
8	UWS	A	1011	-	-	0/3/4/4	0/2/2/2
8	UWS	A	1010	-	-	2/3/4/4	0/2/2/2
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
6	PEG	A	1008	-	-	2/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1006	PO4	P-O1	5.16	1.62	1.50
8	A	1010	UWS	C2-C3	-3.79	1.34	1.39
8	A	1011	UWS	C2-C3	-3.67	1.34	1.39
8	A	1010	UWS	C4-C3	-2.27	1.48	1.51
8	A	1011	UWS	C4-C3	-2.05	1.49	1.51
8	A	1011	UWS	C7-C5	2.05	1.44	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1010	UWS	C4-C3-C2	3.09	133.90	129.50
8	A	1011	UWS	C4-C3-C2	3.04	133.82	129.50

There are no chirality outliers.

All (12) 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	UWS	C2-C3-C4-N
6	A	1008	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[A]	MES	C7-C8-S-O2S
3	A	1003[B]	MES	C7-C8-S-O1S
3	A	1003[B]	MES	C7-C8-S-O2S
6	A	1008	PEG	C4-C3-O2-C2
8	A	1010	UWS	C3-C4-N-N1

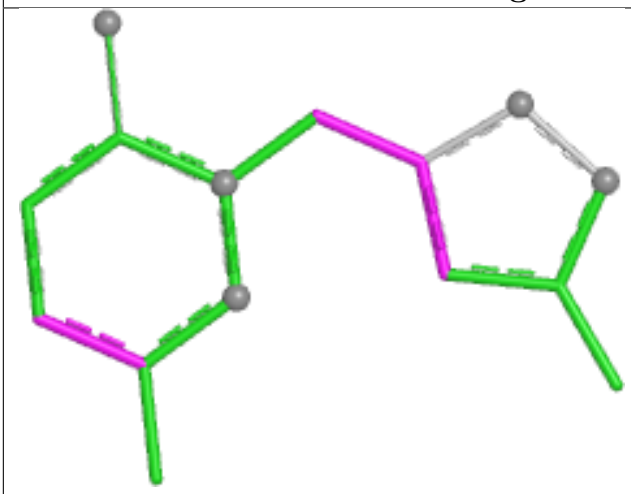
There are no ring outliers.

3 monomers are involved in 5 short contacts:

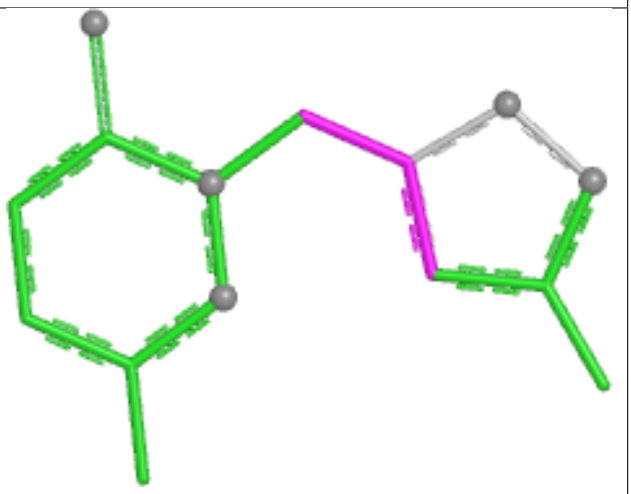
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1006	PO4	2	0
3	A	1003[B]	MES	1	0
4	A	1004	DMS	2	0

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.

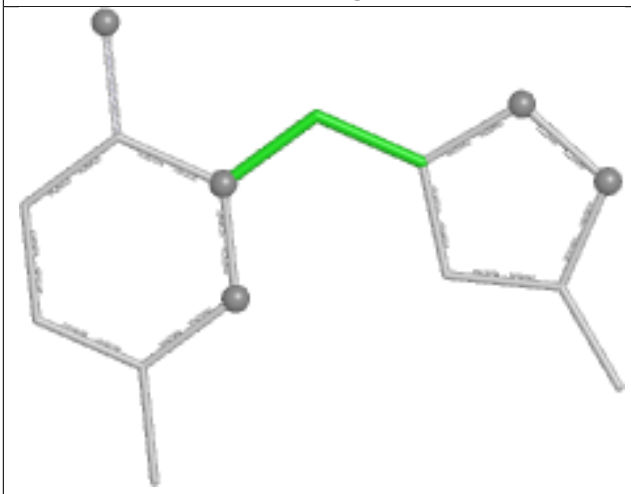
Ligand UWS A 1011



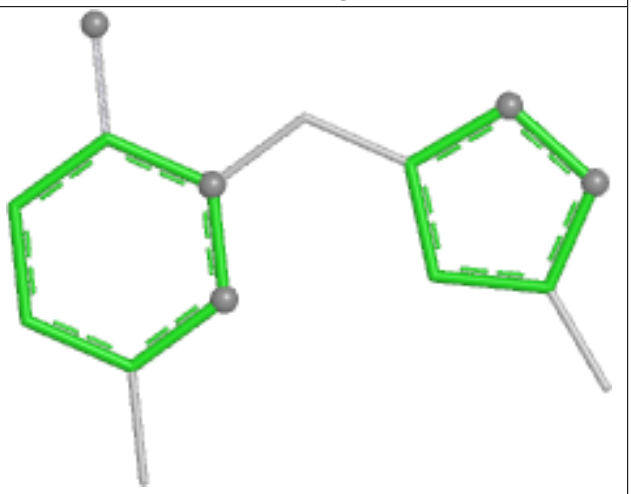
Bond lengths



Bond angles

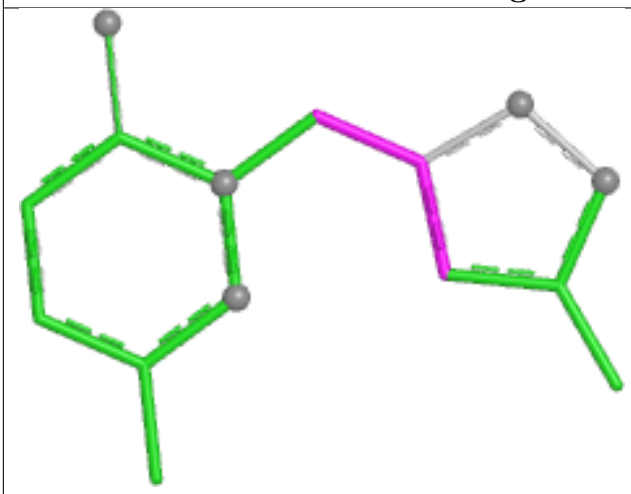


Torsions

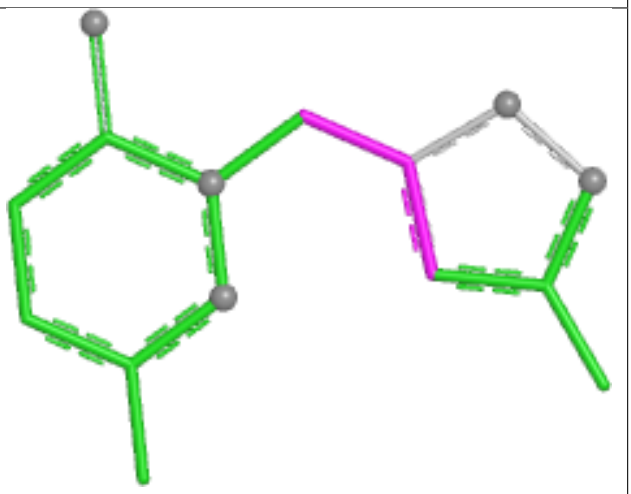


Rings

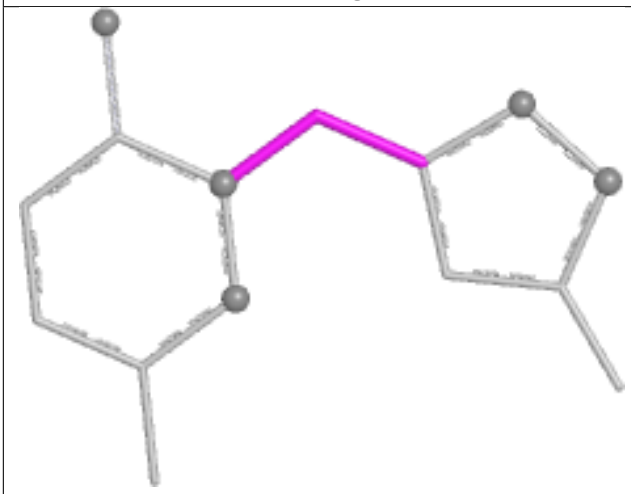
Ligand UWS A 1010



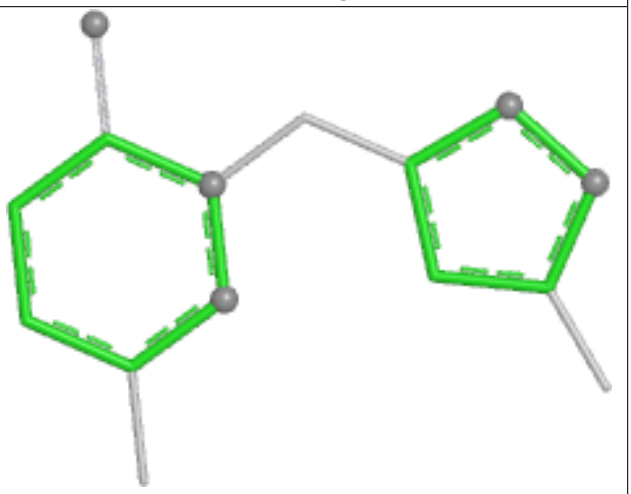
Bond lengths



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	570/637 (89%)	5.89	403 (70%)	0	0	6, 34, 89, 138	198 (34%)

All (403) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	292	TRP	17.8
1	A	411	ALA	17.8
1	A	432	TRP	17.4
1	A	399	PHE	16.6
1	A	592	ILE	16.5
1	A	646	TRP	16.5
1	A	478	TRP	16.1
1	A	431	PHE	16.1
1	A	303	TRP	15.9
1	A	593	ILE	15.8
1	A	637	VAL	15.7
1	A	483	PHE	15.7
1	A	426	VAL	15.6
1	A	512[A]	LEU	15.6
1	A	443	LEU	15.4
1	A	632	ILE	15.4
1	A	409	LEU	15.4
1	A	294	TYR	15.3
1	A	519	LEU	15.3
1	A	628	VAL	15.2
1	A	441	LEU	15.2
1	A	600	GLY	15.1
1	A	601	SER	15.0
1	A	309	TYR	14.9
1	A	641	ILE	14.9
1	A	376	ILE	14.7
1	A	799	ALA	14.7

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Mol	Chain	Res	Type	RSRZ
1	A	580	VAL	14.6
1	A	412	ILE	14.5
1	A	282	GLU	14.5
1	A	373	LEU	14.4
1	A	863	ILE	14.4
1	A	655	LEU	14.4
1	A	499	SER	14.4
1	A	636	THR	14.3
1	A	289	GLU	14.2
1	A	589	VAL	14.2
1	A	421	SER	14.2
1	A	582	ARG	14.1
1	A	648	VAL	14.0
1	A	304	ALA	14.0
1	A	422	ALA	13.9
1	A	538	TRP	13.9
1	A	403	VAL	13.8
1	A	410	GLY	13.8
1	A	430	GLY	13.8
1	A	407	ALA	13.8
1	A	400	THR	13.8
1	A	428	ASP	13.7
1	A	542	ILE	13.7
1	A	577	VAL	13.7
1	A	670	LEU	13.6
1	A	669	PRO	13.6
1	A	635	LEU	13.6
1	A	691	ILE	13.6
1	A	839	LEU	13.5
1	A	853	LEU	13.5
1	A	293	HIS	13.4
1	A	716	LEU	13.3
1	A	395	THR	13.1
1	A	408	ALA	13.1
1	A	629	PHE	13.1
1	A	305	TYR	13.0
1	A	719[A]	LYS	12.9
1	A	846	TRP	12.9
1	A	274	LEU	12.8
1	A	575	ASN	12.8
1	A	511	GLY	12.8
1	A	855	SER	12.7

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Mol	Chain	Res	Type	RSRZ
1	A	291	SER	12.6
1	A	288	HIS	12.6
1	A	359	VAL	12.6
1	A	668	LYS	12.6
1	A	713	PHE	12.6
1	A	479	LEU	12.6
1	A	851	ILE	12.5
1	A	438	GLU	12.5
1	A	797	ILE	12.4
1	A	419	TRP	12.4
1	A	484	LEU	12.3
1	A	850	LEU	12.3
1	A	588	THR	12.3
1	A	283	LYS	12.2
1	A	576	LYS	12.0
1	A	474	ILE	12.0
1	A	429	SER	12.0
1	A	290	THR	11.8
1	A	804	MET	11.7
1	A	660	ILE	11.7
1	A	638	THR	11.7
1	A	437	LYS	11.7
1	A	631	SER	11.6
1	A	360	ASP	11.5
1	A	717	ILE	11.5
1	A	645	ASN	11.5
1	A	656	SER	11.5
1	A	311	THR	11.4
1	A	405	SER	11.4
1	A	798	HIS	11.2
1	A	838	TYR	11.2
1	A	402	LYS	11.2
1	A	591	ASP	11.2
1	A	840	GLY	11.1
1	A	599	ARG	11.0
1	A	361	THR	11.0
1	A	306	HIS	11.0
1	A	298	HIS	11.0
1	A	644	LYS	11.0
1	A	537	GLY	11.0
1	A	864[A]	GLN	10.9
1	A	371	LYS	10.9

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Mol	Chain	Res	Type	RSRZ
1	A	509	GLY	10.9
1	A	546	ASP	10.9
1	A	639	GLU	10.9
1	A	536	ALA	10.8
1	A	657	ARG	10.8
1	A	856	ARG	10.7
1	A	398	GLU	10.7
1	A	452	TYR	10.7
1	A	852	GLY	10.7
1	A	740	ILE	10.6
1	A	541	ARG	10.6
1	A	744	ALA	10.6
1	A	514	LYS	10.6
1	A	830	VAL	10.6
1	A	302	THR	10.5
1	A	423	ARG	10.5
1	A	741	SER	10.5
1	A	482	ARG	10.5
1	A	854	THR	10.5
1	A	357	GLU	10.4
1	A	693	GLN	10.4
1	A	844	ASP	10.4
1	A	317	ALA	10.4
1	A	595	ARG	10.4
1	A	297	ASP	10.3
1	A	372	LYS	10.3
1	A	401	ARG	10.2
1	A	594	SER	10.2
1	A	745	GLY	10.1
1	A	439	ARG	10.1
1	A	888	ARG	10.1
1	A	743	GLY	10.1
1	A	598	GLN	10.0
1	A	640	GLU	10.0
1	A	548	LYS	9.9
1	A	296	GLN	9.9
1	A	487	GLU	9.9
1	A	526	GLU	9.8
1	A	540	THR	9.8
1	A	275	ASP	9.7
1	A	442	HIS	9.7
1	A	510	GLU	9.7

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Mol	Chain	Res	Type	RSRZ
1	A	475	TRP	9.6
1	A	375	LYS	9.6
1	A	634	HIS	9.6
1	A	800	THR	9.5
1	A	689	LYS	9.5
1	A	581	GLN	9.4
1	A	433	GLU	9.4
1	A	534	ASP	9.3
1	A	436	ASP	9.3
1	A	406	ASN	9.3
1	A	420	LYS	9.2
1	A	485	GLU	9.2
1	A	633	GLN	9.2
1	A	396	ARG	9.2
1	A	626	GLU	9.2
1	A	653	GLU	9.1
1	A	358	LYS	9.1
1	A	658	MET	9.0
1	A	861	LYS	9.0
1	A	763[A]	SER	9.0
1	A	455	MET	9.0
1	A	810	LEU	9.0
1	A	287	GLU	9.0
1	A	397	GLU	9.0
1	A	630	LYS	8.9
1	A	770	ARG	8.9
1	A	746	TRP	8.9
1	A	579	ARG	8.8
1	A	862	ASN	8.8
1	A	344	THR	8.7
1	A	440	ASN	8.7
1	A	286	GLN	8.7
1	A	841	LYS	8.4
1	A	539	ASP	8.4
1	A	690	ASP	8.3
1	A	584	THR	8.3
1	A	747	SER	8.2
1	A	842	ARG	8.1
1	A	501	GLU	8.1
1	A	476	TYR	8.0
1	A	278	GLY	7.9
1	A	785[A]	SER	7.9

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Mol	Chain	Res	Type	RSRZ
1	A	562	LYS	7.9
1	A	843	GLU	7.8
1	A	790	THR	7.8
1	A	364	GLN	7.7
1	A	875	GLY	7.6
1	A	692	GLN	7.6
1	A	814	ASN	7.6
1	A	284	ILE	7.5
1	A	698	ARG	7.5
1	A	544	LEU	7.5
1	A	572	THR	7.2
1	A	590	MET	7.2
1	A	365	GLU	7.1
1	A	277	ILE	7.0
1	A	602	GLY	7.0
1	A	880	THR	7.0
1	A	279	LYS	6.9
1	A	281	ILE	6.8
1	A	451	VAL	6.8
1	A	603	GLN	6.7
1	A	418	LYS	6.7
1	A	881	ASP	6.7
1	A	571	LEU	6.7
1	A	280	ARG	6.6
1	A	695	GLU	6.6
1	A	481	ALA	6.6
1	A	742	GLN	6.5
1	A	363	THR	6.5
1	A	368	GLU	6.5
1	A	337	MET	6.4
1	A	845	GLN	6.4
1	A	379	GLU	6.4
1	A	362	ARG	6.2
1	A	448	GLU	6.2
1	A	604	VAL	6.2
1	A	705	GLN	6.1
1	A	310	GLU	6.1
1	A	818	ILE	6.1
1	A	564	LEU	6.0
1	A	694	TRP	5.9
1	A	737	ARG	5.9
1	A	566	GLU	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	884	PRO	5.8
1	A	299	PRO	5.8
1	A	680	ALA	5.8
1	A	393	MET	5.8
1	A	529	ALA	5.7
1	A	551	GLU	5.7
1	A	890	ARG	5.7
1	A	444	GLU	5.7
1	A	318	SER	5.6
1	A	876	ASN	5.5
1	A	301	LYS	5.5
1	A	784	PRO	5.5
1	A	383	LYS	5.4
1	A	524	LYS	5.4
1	A	825	GLU	5.4
1	A	889	PHE	5.4
1	A	699	GLY	5.4
1	A	750	GLU	5.3
1	A	404	ARG	5.3
1	A	488	ALA	5.2
1	A	295	ASP	5.2
1	A	449	THR	5.1
1	A	496	HIS	5.0
1	A	495	ASP	5.0
1	A	583	PRO	5.0
1	A	300	TYR	5.0
1	A	772	LEU	5.0
1	A	454	MET	4.9
1	A	801	HIS	4.9
1	A	733	GLU	4.8
1	A	627	GLY	4.8
1	A	477	MET	4.8
1	A	596	ARG	4.8
1	A	343	MET	4.8
1	A	891	ARG	4.8
1	A	828	THR	4.7
1	A	276	ILE	4.7
1	A	434	LEU	4.7
1	A	425	ALA	4.7
1	A	453	ASN	4.6
1	A	424	GLU	4.6
1	A	882	TYR	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	807	GLU	4.5
1	A	831	GLU	4.5
1	A	389	LYS	4.3
1	A	435	VAL	4.3
1	A	374	MET	4.3
1	A	273	ASN	4.3
1	A	307	GLY	4.3
1	A	597	ASP	4.2
1	A	808	ASP	4.2
1	A	427	GLU	4.2
1	A	447	CYS	4.2
1	A	806	THR	4.2
1	A	677	ALA	4.1
1	A	568	ILE	4.1
1	A	823	TRP	4.1
1	A	561	HIS	4.1
1	A	887	LYS	4.1
1	A	563	LYS	4.1
1	A	370	THR	4.0
1	A	819	GLN	4.0
1	A	578	VAL	4.0
1	A	565	ALA	3.9
1	A	445	GLY	3.9
1	A	392	ARG	3.9
1	A	702	ASP	3.8
1	A	815	ARG	3.8
1	A	486	PHE	3.8
1	A	308	SER	3.8
1	A	552	MET	3.7
1	A	886	MET	3.7
1	A	764	LEU	3.7
1	A	394	CYS	3.7
1	A	446	LYS	3.7
1	A	570	LYS	3.6
1	A	703	TRP	3.6
1	A	885	SER	3.6
1	A	285	LYS	3.6
1	A	625	GLY	3.6
1	A	687	VAL	3.5
1	A	676	SER	3.5
1	A	833	TRP	3.5
1	A	545	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	335	ILE	3.5
1	A	721	GLY	3.5
1	A	555	ASN	3.5
1	A	827	LYS	3.5
1	A	720	ASP	3.5
1	A	679	THR	3.4
1	A	647	LEU	3.4
1	A	556	HIS	3.4
1	A	338	VAL	3.4
1	A	642	ALA	3.4
1	A	821	ASN	3.4
1	A	493	ASN	3.3
1	A	390	THR	3.3
1	A	701	ASN	3.3
1	A	319	SER	3.3
1	A	834	GLU	3.3
1	A	491	PHE	3.3
1	A	321	VAL	3.2
1	A	788	VAL	3.2
1	A	673	ARG	3.2
1	A	502	ASN	3.1
1	A	878	GLU	3.1
1	A	652	ARG	3.1
1	A	480	GLY	3.1
1	A	342	ALA	3.0
1	A	497	TRP	3.0
1	A	574	GLN	3.0
1	A	684	MET	3.0
1	A	569	PHE	2.9
1	A	339	THR	2.9
1	A	531	TYR	2.9
1	A	836	ILE	2.8
1	A	678	LEU	2.8
1	A	527	GLY	2.8
1	A	672	ASP	2.8
1	A	547	LEU	2.8
1	A	366	PRO	2.8
1	A	674	PHE	2.7
1	A	554	THR	2.7
1	A	874	ILE	2.7
1	A	643	VAL	2.7
1	A	723	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	650	VAL	2.6
1	A	683	ASP	2.6
1	A	802	GLU	2.6
1	A	532	ALA	2.6
1	A	783	VAL	2.5
1	A	382	TRP	2.5
1	A	336	PRO	2.5
1	A	320	MET	2.5
1	A	378	ALA	2.5
1	A	624	GLU	2.5
1	A	367	LYS	2.5
1	A	498	PHE	2.4
1	A	858	THR	2.4
1	A	870	VAL	2.4
1	A	558	GLU	2.4
1	A	340	GLN	2.3
1	A	787	TRP	2.3
1	A	883	MET	2.3
1	A	786	HIS	2.3
1	A	769	ARG	2.2
1	A	820	GLU	2.2
1	A	521	ASP	2.2
1	A	543	THR	2.2
1	A	805	THR	2.1
1	A	523	SER	2.1
1	A	811	THR	2.1
1	A	520	ARG	2.1
1	A	380	TRP	2.1
1	A	704	THR	2.1
1	A	865	THR	2.1
1	A	663	ASP	2.1
1	A	707	PRO	2.1
1	A	503	SER	2.1
1	A	879	TYR	2.1
1	A	730	ASN	2.1
1	A	559	GLY	2.1
1	A	605	VAL	2.0
1	A	381	LEU	2.0
1	A	535	THR	2.0
1	A	386	GLY	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)

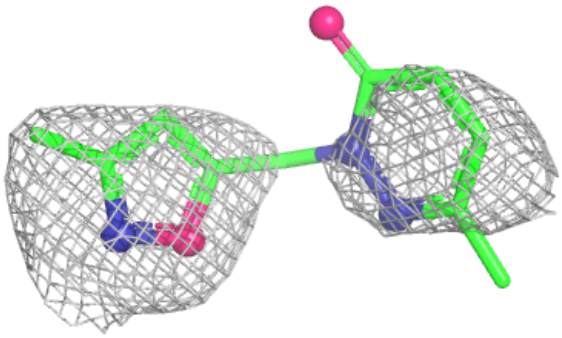
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

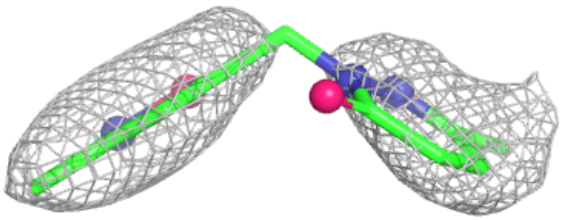
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	UWS	A	1011	15/15	0.70	0.31	43,46,50,53	15
6	PEG	A	1008	7/7	0.74	0.20	65,72,82,84	0
4	DMS	A	1005	4/4	0.75	0.28	90,104,105,111	0
8	UWS	A	1010	15/15	0.76	0.52	70,75,76,76	15
5	PO4	A	1007	5/5	0.76	0.17	73,87,97,110	0
5	PO4	A	1006	5/5	0.80	0.15	38,42,58,70	0
4	DMS	A	1004	4/4	0.89	0.18	53,55,57,57	0
3	MES	A	1003[B]	12/12	0.93	0.24	27,30,32,33	12
3	MES	A	1003[A]	12/12	0.93	0.24	848,857,888,888	12
7	CL	A	1012	1/1	0.96	0.08	60,60,60,60	0
7	CL	A	1009	1/1	0.98	0.12	45,45,45,45	0
2	ZN	A	1002	1/1	0.98	0.05	62,62,62,62	0
2	ZN	A	1001	1/1	0.99	0.02	28,28,28,28	0

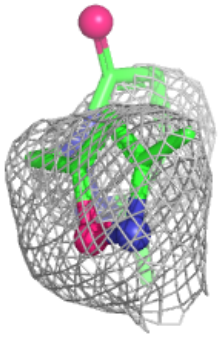
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around UWS 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)

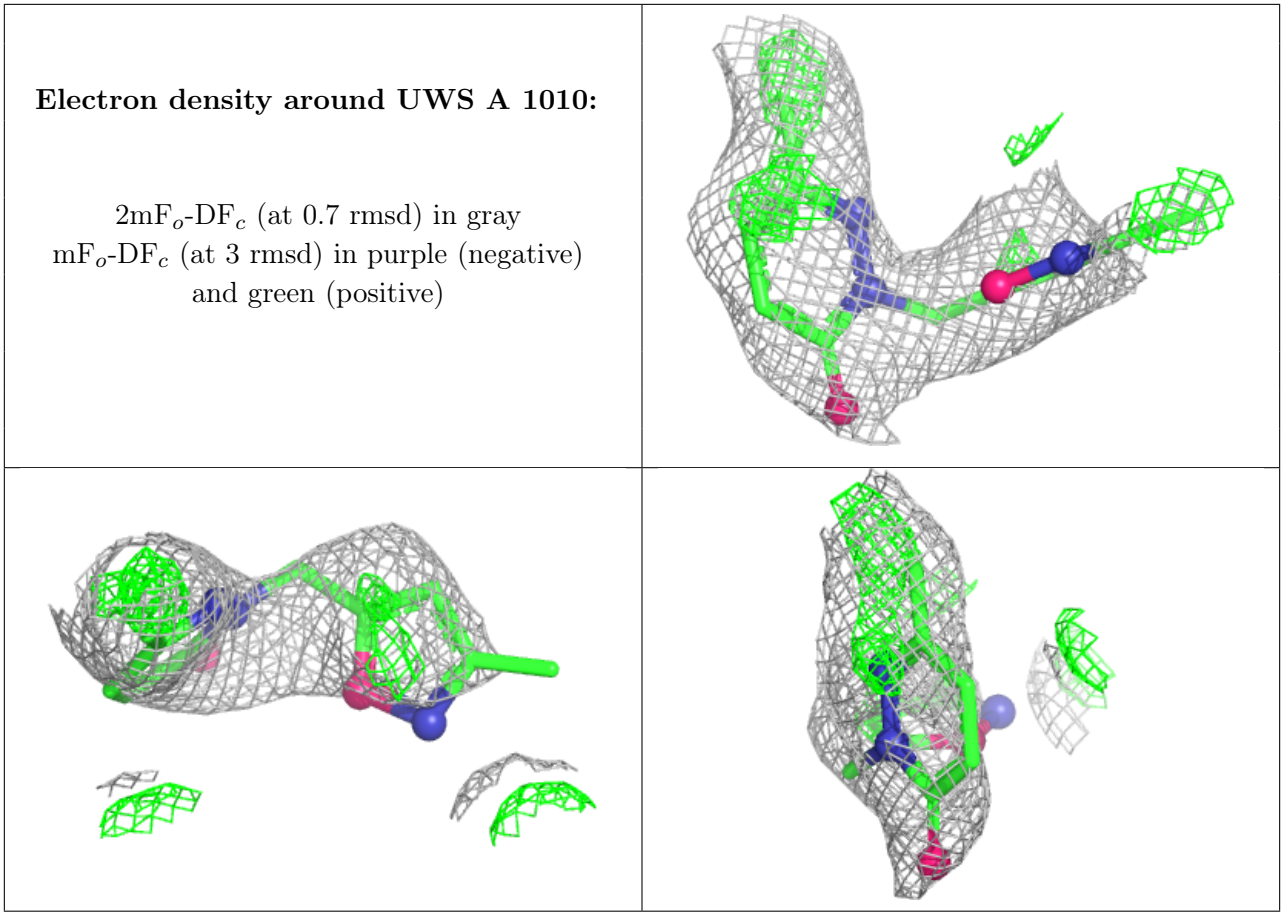






Electron density around UWS A 1010:

$2mF_o$-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

There are no such residues in this entry.