



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 07:59 AM EDT

PDB ID : 7I2G / pdb_00007i2g
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 (DENV2_NS5A-x0379)
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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 ⓘ 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)

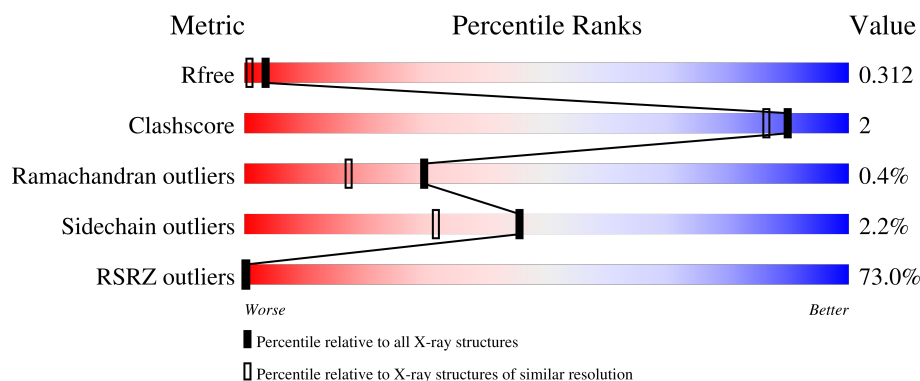
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	637	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PO4	A	1006	-	-	X	-
8	UWS	A	1010	-	-	-	X

2 Entry composition [i](#)

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

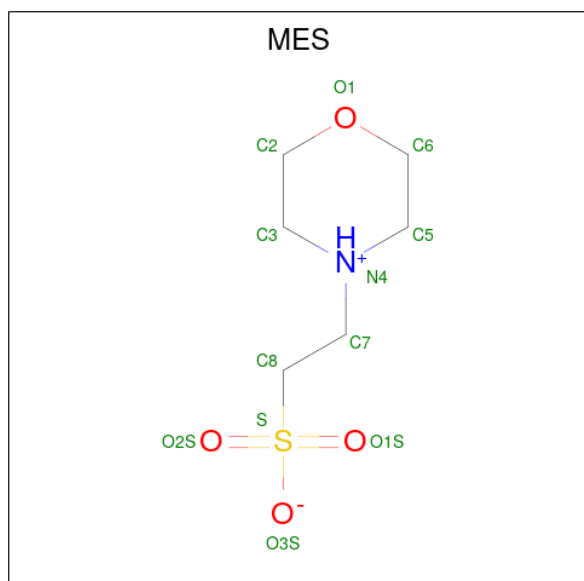
There are 2 discrepancies between the modelled and reference sequences:

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 (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).



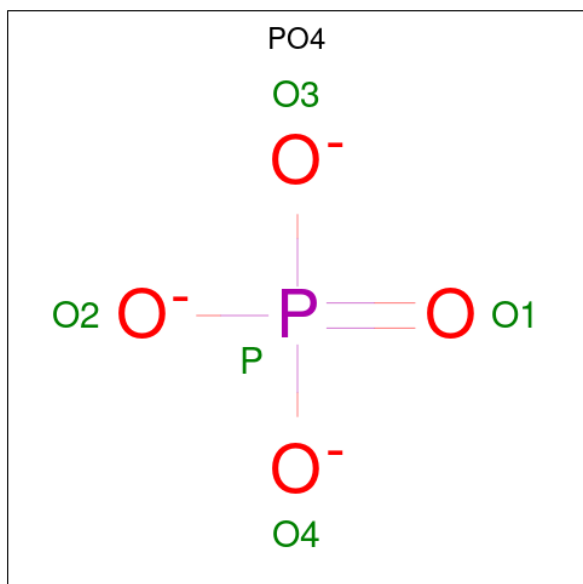
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	1
			24	12	2	8	2		

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



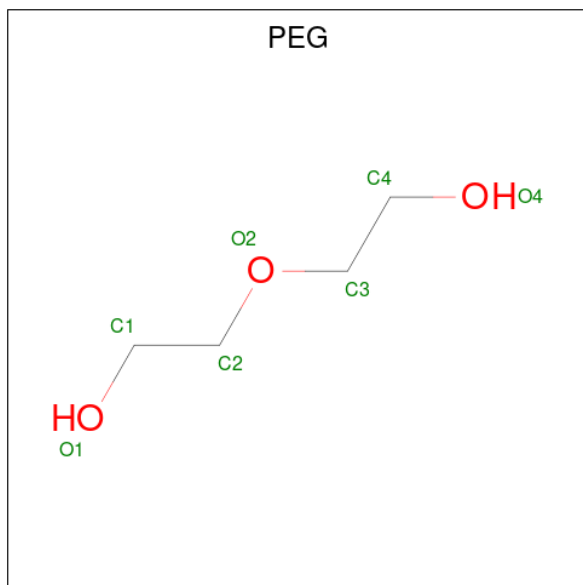
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

- 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: $C_4H_{10}O_3$).

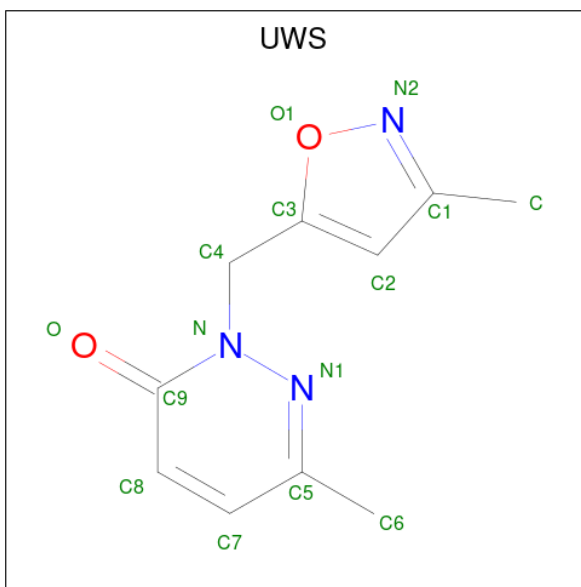


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 8 is 6-methyl-2-[(3-methyl-1,2-oxazol-5-yl)methyl]pyridazin-3(2H)-one (CCD ID: 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	0	0
			15	10	3	2		
8	A	1	Total	C	N	O	0	0
			15	10	3	2		

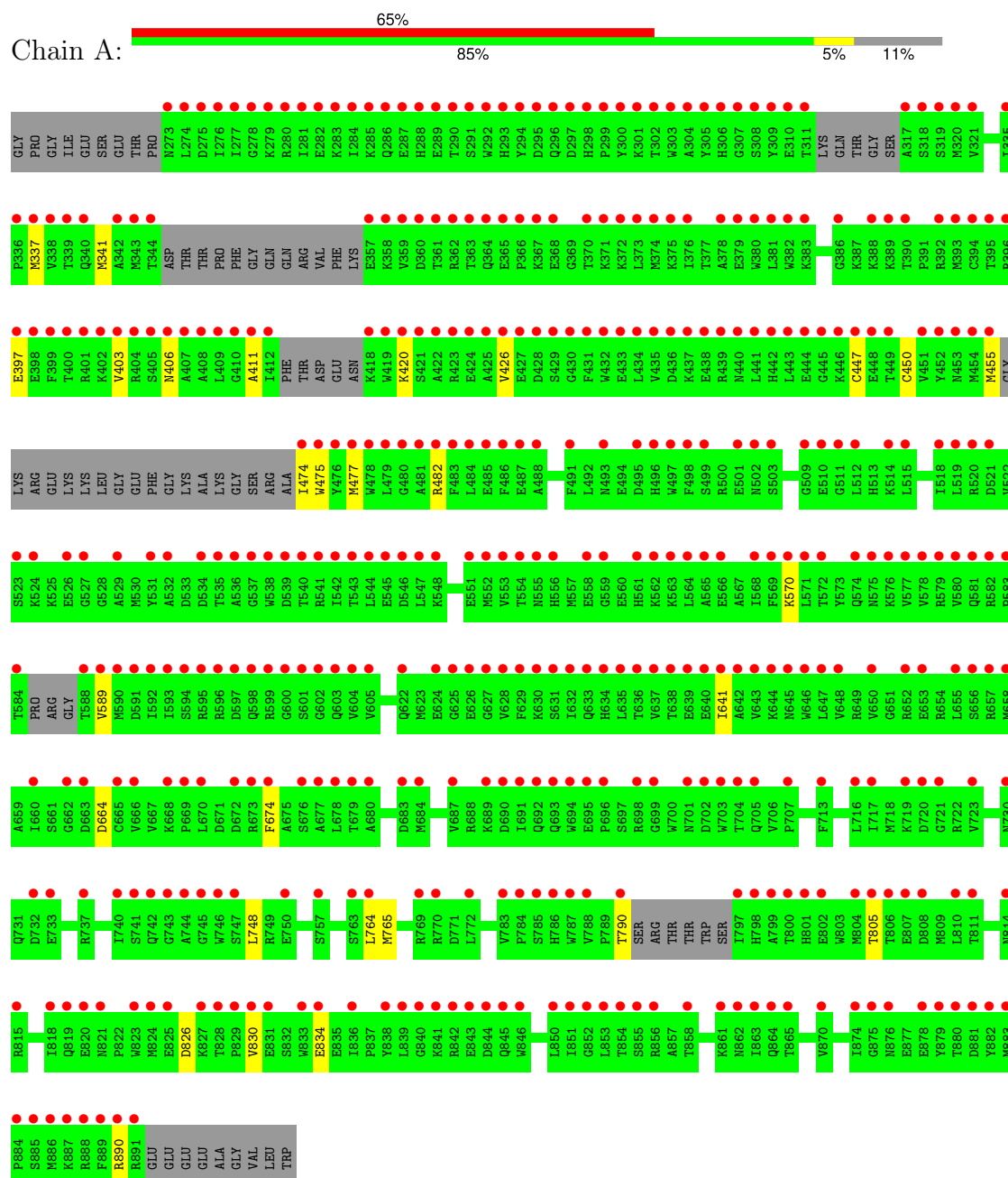
- Molecule 9 is water.

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

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	82.42Å 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
$\langle I/\sigma(I) \rangle$ 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	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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.*

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: PO4, UWS, PEG, ZN, CL, DMS, 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	1.04	0/4803	1.37	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 [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	4698	0	4603	14	0
2	A	2	0	0	0	0
3	A	24	0	26	1	0
4	A	8	0	12	3	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	6	1
All	All	5088	0	4651	17	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 2.

All (17) 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:664:ASP:OD1	5:A:1006:PO4:O4	2.00	0.79
4:A:1004:DMS:H11	9:A:1245:HOH:O	1.90	0.71
1:A:664:ASP:OD1	5:A:1006:PO4:P	2.60	0.59
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.46	0.55
4:A:1004:DMS:C1	9:A:1245:HOH:O	2.51	0.52
1:A:337:MET:HG2	9:A:1302:HOH:O	2.11	0.51
4:A:1004:DMS:H12	9:A:1208:HOH:O	2.10	0.51
1:A:764:LEU:O	1:A:765:MET:HE2	2.11	0.49
1:A:764:LEU:C	1:A:765:MET:HE2	2.38	0.48
1:A:826:ASP:OD1	1:A:826:ASP:C	2.57	0.47
1:A:411:ALA:HA	1:A:477:MET:O	2.15	0.45
1:A:475:TRP:CD1	1:A:475:TRP:N	2.86	0.43
1:A:790:THR:HG22	9:A:1324:HOH:O	2.17	0.42
1:A:834:GLU:OE2	1:A:890:ARG:NE	2.49	0.42
1:A:341:MET:HE2	1:A:341:MET:HB3	1.80	0.41
1:A:674:PHE:N	9:A:1124:HOH:O	2.54	0.41
1:A:748:LEU:HD13	3:A:1003[B]:MES:H61	2.03	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: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 17

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	420	LYS
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	504/554 (91%)	493 (98%)	11 (2%)	45	32

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	397	GLU
1	A	403	VAL
1	A	426	VAL
1	A	455	MET
1	A	474	ILE
1	A	482	ARG
1	A	570	LYS
1	A	589	VAL
1	A	641	ILE
1	A	805	THR
1	A	830	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	273	ASN
1	A	575	ASN
1	A	598	GLN
1	A	742	GLN
1	A	786	HIS
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	-	16,16,16	0.63	1 (6%)	17,22,22	0.39	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
8	UWS	A	1010	-	16,16,16	0.38	0	17,22,22	1.26	1 (5%)
5	PO4	A	1006	-	4,4,4	3.06	1 (25%)	6,6,6	0.98	0
3	MES	A	1003[A]	-	12,12,12	0.92	0	15,16,16	0.67	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
5	PO4	A	1007	-	4,4,4	0.85	0	6,6,6	0.44	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	-	-	0/4/4/4	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PEG	A	1008	-	-	2/4/4/4	-
8	UWS	A	1010	-	-	3/4/4/4	0/2/2/2
3	MES	A	1003[A]	-	-	3/6/14/14	0/1/1/1
3	MES	A	1003[B]	-	-	5/6/14/14	0/1/1/1

All (2) 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	1011	UWS	C7-C5	2.05	1.44	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1010	UWS	C3-C4-N	-4.94	106.42	112.36

There are no chirality outliers.

All (13) 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
6	A	1008	PEG	O2-C3-C4-O4
3	A	1003[B]	MES	C8-C7-N4-C5
8	A	1010	UWS	O1-C3-C4-N
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-C9
8	A	1010	UWS	C3-C4-N-N1

There are no ring outliers.

3 monomers are involved in 6 short contacts:

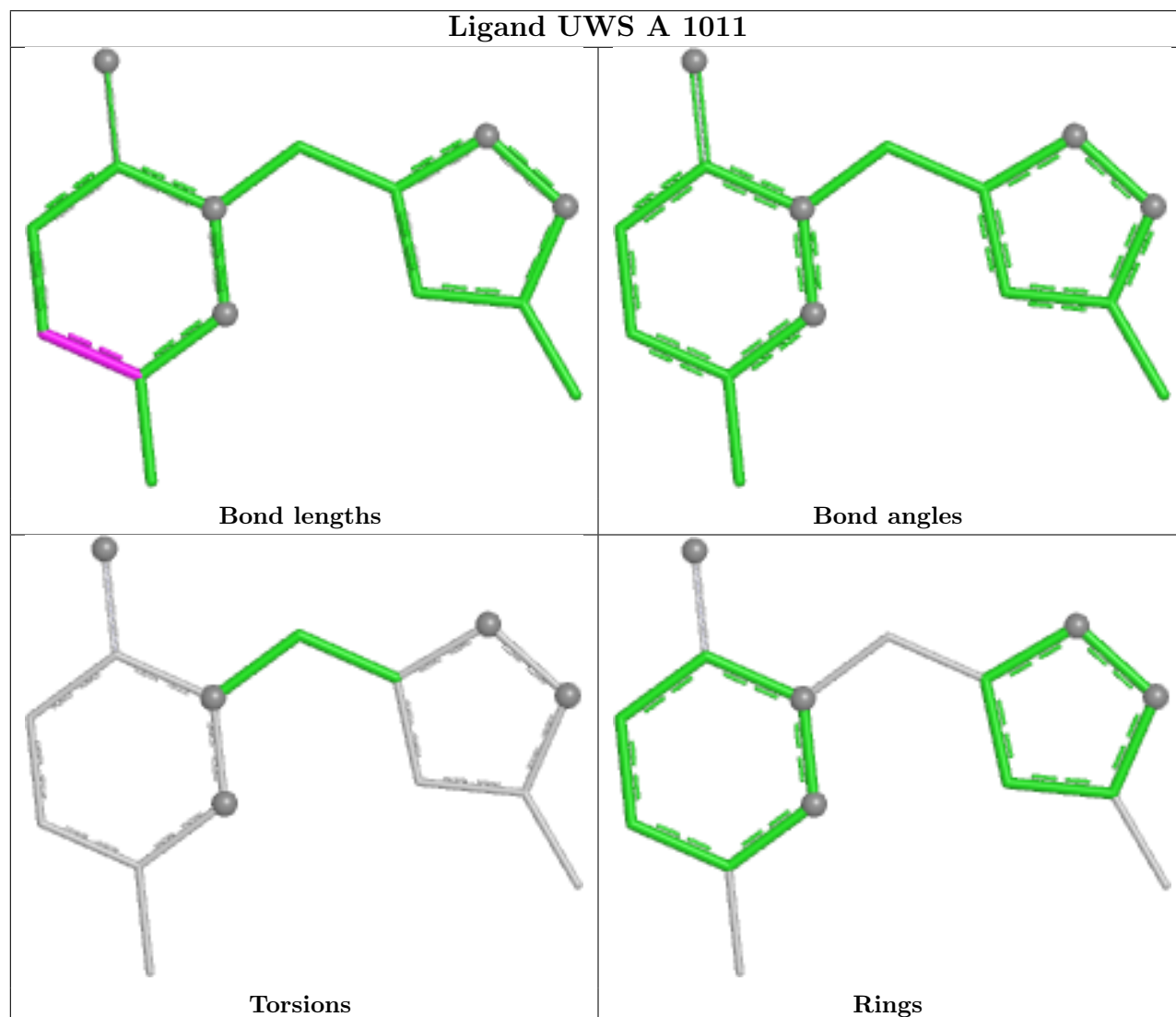
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1006	PO4	2	0
3	A	1003[B]	MES	1	0

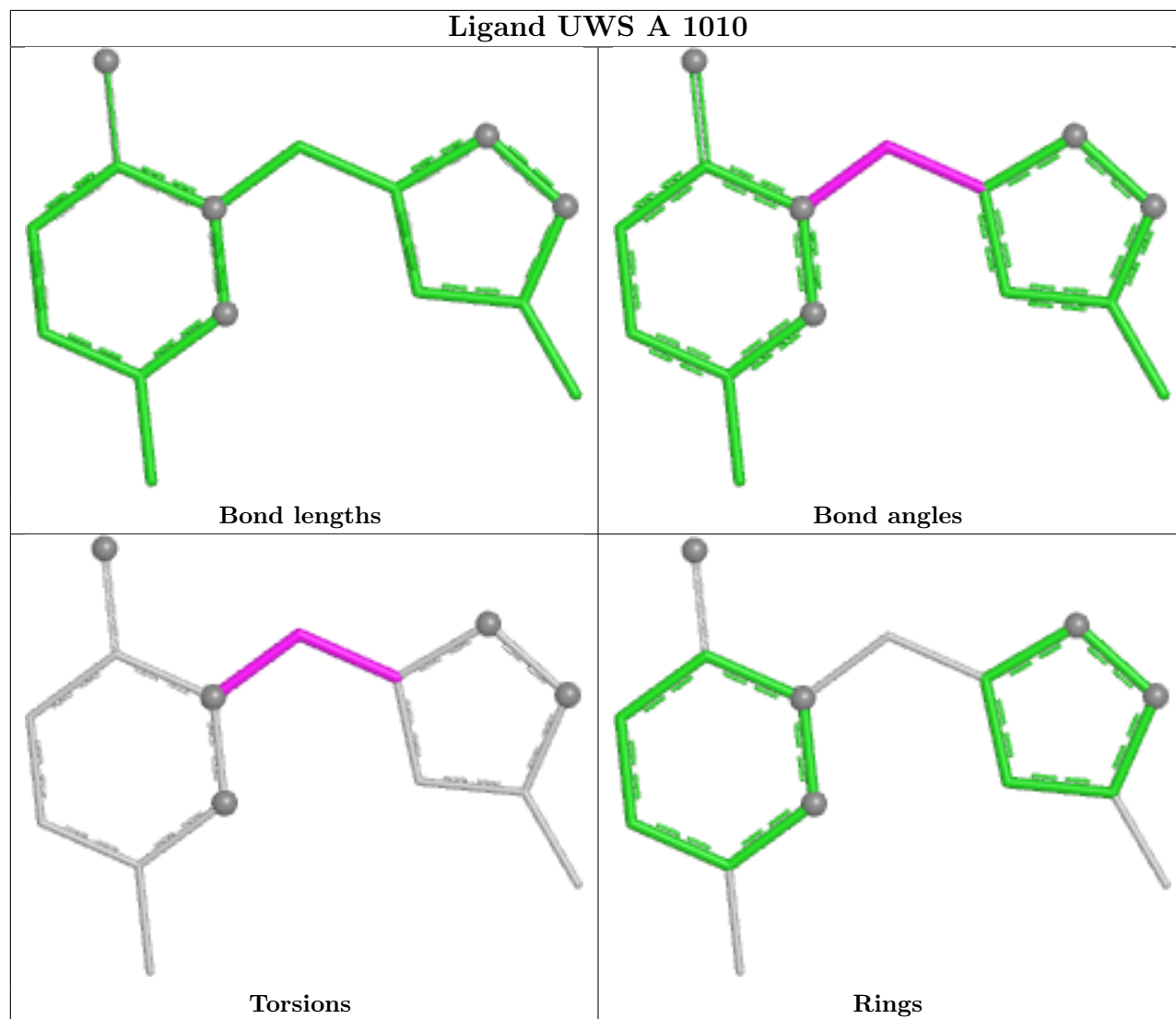
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1004	DMS	3	0

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	570/637 (89%)	6.08	416 (72%) 0 0	6, 34, 89, 138	198 (34%)

All (416) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	292	TRP	18.6
1	A	411	ALA	18.5
1	A	432	TRP	18.2
1	A	646	TRP	17.2
1	A	399	PHE	17.1
1	A	592	ILE	17.0
1	A	478	TRP	16.8
1	A	431	PHE	16.6
1	A	303	TRP	16.6
1	A	637	VAL	16.2
1	A	593	ILE	16.2
1	A	426	VAL	16.2
1	A	483	PHE	16.1
1	A	512[A]	LEU	16.1
1	A	443	LEU	15.9
1	A	409	LEU	15.9
1	A	632	ILE	15.9
1	A	294	TYR	15.8
1	A	519	LEU	15.8
1	A	628	VAL	15.7
1	A	600	GLY	15.6
1	A	441	LEU	15.6
1	A	309	TYR	15.4
1	A	641	ILE	15.3
1	A	601	SER	15.3
1	A	799	ALA	15.3
1	A	376	ILE	15.1

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Mol	Chain	Res	Type	RSRZ
1	A	580	VAL	15.1
1	A	412	ILE	15.0
1	A	373	LEU	14.9
1	A	655	LEU	14.9
1	A	863	ILE	14.9
1	A	499	SER	14.7
1	A	589	VAL	14.7
1	A	636	THR	14.7
1	A	304	ALA	14.5
1	A	648	VAL	14.5
1	A	282	GLU	14.5
1	A	421	SER	14.5
1	A	422	ALA	14.5
1	A	538	TRP	14.5
1	A	410	GLY	14.3
1	A	430	GLY	14.3
1	A	407	ALA	14.3
1	A	403	VAL	14.3
1	A	289	GLU	14.2
1	A	582	ARG	14.2
1	A	400	THR	14.1
1	A	577	VAL	14.1
1	A	670	LEU	14.1
1	A	542	ILE	14.1
1	A	635	LEU	14.0
1	A	839	LEU	14.0
1	A	853	LEU	14.0
1	A	691	ILE	14.0
1	A	669	PRO	14.0
1	A	428	ASP	13.9
1	A	293	HIS	13.7
1	A	716	LEU	13.7
1	A	408	ALA	13.6
1	A	629	PHE	13.5
1	A	395	THR	13.5
1	A	846	TRP	13.4
1	A	305	TYR	13.4
1	A	274	LEU	13.2
1	A	511	GLY	13.2
1	A	359	VAL	13.0
1	A	575	ASN	13.0
1	A	479	LEU	13.0

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Mol	Chain	Res	Type	RSRZ
1	A	713	PHE	13.0
1	A	855	SER	12.9
1	A	719[A]	LYS	12.9
1	A	419	TRP	12.9
1	A	291	SER	12.9
1	A	288	HIS	12.9
1	A	851	ILE	12.9
1	A	797	ILE	12.8
1	A	484	LEU	12.8
1	A	850	LEU	12.8
1	A	588	THR	12.6
1	A	668	LYS	12.6
1	A	438	GLU	12.5
1	A	474	ILE	12.4
1	A	283	LYS	12.2
1	A	429	SER	12.2
1	A	290	THR	12.1
1	A	576	LYS	12.1
1	A	660	ILE	12.0
1	A	804	MET	12.0
1	A	638	THR	12.0
1	A	631	SER	11.9
1	A	717	ILE	11.9
1	A	656	SER	11.7
1	A	311	THR	11.7
1	A	437	LYS	11.7
1	A	645	ASN	11.7
1	A	360	ASP	11.7
1	A	405	SER	11.6
1	A	838	TYR	11.5
1	A	840	GLY	11.5
1	A	798	HIS	11.5
1	A	537	GLY	11.4
1	A	361	THR	11.3
1	A	591	ASP	11.3
1	A	509	GLY	11.3
1	A	306	HIS	11.3
1	A	536	ALA	11.3
1	A	298	HIS	11.2
1	A	402	LYS	11.2
1	A	599	ARG	11.1
1	A	852	GLY	11.1

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Mol	Chain	Res	Type	RSRZ
1	A	744	ALA	11.1
1	A	864[A]	GLN	11.1
1	A	546	ASP	11.1
1	A	452	TYR	11.0
1	A	644	LYS	11.0
1	A	740	ILE	11.0
1	A	371	LYS	11.0
1	A	830	VAL	10.9
1	A	639	GLU	10.9
1	A	657	ARG	10.9
1	A	856	ARG	10.8
1	A	302	THR	10.8
1	A	317	ALA	10.8
1	A	854	THR	10.8
1	A	741	SER	10.8
1	A	398	GLU	10.7
1	A	541	ARG	10.7
1	A	423	ARG	10.6
1	A	514	LYS	10.6
1	A	482	ARG	10.6
1	A	693	GLN	10.6
1	A	844	ASP	10.5
1	A	745	GLY	10.5
1	A	595	ARG	10.5
1	A	297	ASP	10.5
1	A	743	GLY	10.5
1	A	357	GLU	10.5
1	A	594	SER	10.4
1	A	372	LYS	10.3
1	A	401	ARG	10.3
1	A	439	ARG	10.2
1	A	598	GLN	10.2
1	A	888	ARG	10.2
1	A	475	TRP	10.1
1	A	540	THR	10.1
1	A	296	GLN	10.0
1	A	640	GLU	10.0
1	A	442	HIS	10.0
1	A	548	LYS	10.0
1	A	275	ASP	9.9
1	A	487	GLU	9.9
1	A	526	GLU	9.8

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Mol	Chain	Res	Type	RSRZ
1	A	800	THR	9.8
1	A	634	HIS	9.8
1	A	510	GLU	9.7
1	A	375	LYS	9.7
1	A	581	GLN	9.6
1	A	689	LYS	9.5
1	A	406	ASN	9.5
1	A	534	ASP	9.4
1	A	436	ASP	9.4
1	A	433	GLU	9.4
1	A	633	GLN	9.3
1	A	810	LEU	9.3
1	A	746	TRP	9.3
1	A	658	MET	9.3
1	A	396	ARG	9.3
1	A	420	LYS	9.3
1	A	485	GLU	9.2
1	A	763[A]	SER	9.2
1	A	455	MET	9.2
1	A	626	GLU	9.2
1	A	653	GLU	9.2
1	A	358	LYS	9.1
1	A	861	LYS	9.1
1	A	862	ASN	9.0
1	A	287	GLU	9.0
1	A	397	GLU	9.0
1	A	770	ARG	9.0
1	A	630	LYS	9.0
1	A	344	THR	8.9
1	A	579	ARG	8.9
1	A	440	ASN	8.9
1	A	286	GLN	8.8
1	A	584	THR	8.6
1	A	539	ASP	8.6
1	A	690	ASP	8.5
1	A	841	LYS	8.5
1	A	747	SER	8.4
1	A	476	TYR	8.3
1	A	278	GLY	8.3
1	A	842	ARG	8.2
1	A	501	GLU	8.1
1	A	785[A]	SER	8.1

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Mol	Chain	Res	Type	RSRZ
1	A	790	THR	8.0
1	A	875	GLY	8.0
1	A	562	LYS	7.9
1	A	843	GLU	7.9
1	A	284	ILE	7.8
1	A	364	GLN	7.8
1	A	544	LEU	7.8
1	A	692	GLN	7.8
1	A	814	ASN	7.8
1	A	698	ARG	7.6
1	A	572	THR	7.5
1	A	590	MET	7.4
1	A	602	GLY	7.3
1	A	277	ILE	7.3
1	A	880	THR	7.2
1	A	365	GLU	7.1
1	A	281	ILE	7.0
1	A	451	VAL	7.0
1	A	279	LYS	7.0
1	A	571	LEU	6.9
1	A	481	ALA	6.9
1	A	603	GLN	6.9
1	A	881	ASP	6.8
1	A	418	LYS	6.8
1	A	280	ARG	6.7
1	A	363	THR	6.7
1	A	695	GLU	6.7
1	A	742	GLN	6.7
1	A	337	MET	6.6
1	A	368	GLU	6.5
1	A	845	GLN	6.5
1	A	604	VAL	6.4
1	A	379	GLU	6.4
1	A	818	ILE	6.3
1	A	362	ARG	6.3
1	A	705	GLN	6.3
1	A	694	TRP	6.2
1	A	448	GLU	6.2
1	A	564	LEU	6.2
1	A	310	GLU	6.2
1	A	680	ALA	6.1
1	A	884	PRO	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	529	ALA	6.0
1	A	737	ARG	6.0
1	A	299	PRO	6.0
1	A	393	MET	5.9
1	A	566	GLU	5.9
1	A	318	SER	5.8
1	A	890	ARG	5.8
1	A	551	GLU	5.8
1	A	444	GLU	5.8
1	A	876	ASN	5.7
1	A	784	PRO	5.7
1	A	889	PHE	5.6
1	A	699	GLY	5.6
1	A	301	LYS	5.6
1	A	383	LYS	5.5
1	A	524	LYS	5.5
1	A	825	GLU	5.5
1	A	488	ALA	5.5
1	A	750	GLU	5.4
1	A	404	ARG	5.4
1	A	295	ASP	5.3
1	A	449	THR	5.3
1	A	583	PRO	5.2
1	A	300	TYR	5.2
1	A	772	LEU	5.2
1	A	496	HIS	5.2
1	A	495	ASP	5.1
1	A	801	HIS	5.1
1	A	454	MET	5.1
1	A	627	GLY	5.1
1	A	477	MET	5.0
1	A	276	ILE	5.0
1	A	434	LEU	4.9
1	A	828	THR	4.9
1	A	343	MET	4.9
1	A	425	ALA	4.9
1	A	733	GLU	4.9
1	A	596	ARG	4.9
1	A	891	ARG	4.9
1	A	882	TYR	4.8
1	A	453	ASN	4.8
1	A	424	GLU	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	807	GLU	4.6
1	A	831	GLU	4.5
1	A	435	VAL	4.5
1	A	307	GLY	4.5
1	A	374	MET	4.4
1	A	389	LYS	4.4
1	A	273	ASN	4.4
1	A	677	ALA	4.4
1	A	823	TRP	4.4
1	A	597	ASP	4.4
1	A	808	ASP	4.4
1	A	447	CYS	4.3
1	A	568	ILE	4.3
1	A	806	THR	4.3
1	A	427	GLU	4.3
1	A	561	HIS	4.3
1	A	578	VAL	4.2
1	A	370	THR	4.2
1	A	887	LYS	4.2
1	A	563	LYS	4.1
1	A	565	ALA	4.1
1	A	819	GLN	4.1
1	A	445	GLY	4.1
1	A	486	PHE	4.0
1	A	392	ARG	4.0
1	A	702	ASP	4.0
1	A	308	SER	3.9
1	A	815	ARG	3.9
1	A	764	LEU	3.9
1	A	703	TRP	3.9
1	A	552	MET	3.9
1	A	886	MET	3.9
1	A	394	CYS	3.8
1	A	625	GLY	3.8
1	A	833	TRP	3.8
1	A	446	LYS	3.7
1	A	885	SER	3.7
1	A	687	VAL	3.7
1	A	721	GLY	3.7
1	A	570	LYS	3.7
1	A	335	ILE	3.7
1	A	676	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	285	LYS	3.7
1	A	555	ASN	3.6
1	A	647	LEU	3.6
1	A	545	GLU	3.6
1	A	679	THR	3.6
1	A	720	ASP	3.6
1	A	642	ALA	3.6
1	A	338	VAL	3.6
1	A	827	LYS	3.6
1	A	556	HIS	3.5
1	A	821	ASN	3.5
1	A	390	THR	3.5
1	A	493	ASN	3.5
1	A	319	SER	3.4
1	A	701	ASN	3.4
1	A	321	VAL	3.4
1	A	491	PHE	3.4
1	A	788	VAL	3.4
1	A	834	GLU	3.3
1	A	502	ASN	3.3
1	A	673	ARG	3.3
1	A	497	TRP	3.3
1	A	480	GLY	3.3
1	A	342	ALA	3.2
1	A	652	ARG	3.2
1	A	878	GLU	3.2
1	A	574	GLN	3.1
1	A	569	PHE	3.1
1	A	684	MET	3.1
1	A	531	TYR	3.0
1	A	339	THR	3.0
1	A	527	GLY	3.0
1	A	836	ILE	3.0
1	A	678	LEU	3.0
1	A	547	LEU	3.0
1	A	366	PRO	3.0
1	A	672	ASP	2.9
1	A	674	PHE	2.9
1	A	874	ILE	2.9
1	A	554	THR	2.9
1	A	643	VAL	2.8
1	A	723	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	382	TRP	2.8
1	A	650	VAL	2.8
1	A	532	ALA	2.7
1	A	783	VAL	2.7
1	A	683	ASP	2.7
1	A	336	PRO	2.7
1	A	378	ALA	2.7
1	A	802	GLU	2.7
1	A	320	MET	2.6
1	A	498	PHE	2.6
1	A	624	GLU	2.6
1	A	367	LYS	2.6
1	A	870	VAL	2.6
1	A	858	THR	2.6
1	A	787	TRP	2.5
1	A	558	GLU	2.5
1	A	340	GLN	2.4
1	A	786	HIS	2.4
1	A	883	MET	2.4
1	A	521	ASP	2.3
1	A	769	ARG	2.3
1	A	820	GLU	2.3
1	A	543	THR	2.3
1	A	380	TRP	2.3
1	A	805	THR	2.3
1	A	523	SER	2.3
1	A	811	THR	2.3
1	A	704	THR	2.2
1	A	865	THR	2.2
1	A	559	GLY	2.2
1	A	707	PRO	2.2
1	A	879	TYR	2.2
1	A	520	ARG	2.2
1	A	605	VAL	2.2
1	A	381	LEU	2.2
1	A	386	GLY	2.2
1	A	503	SER	2.2
1	A	663	ASP	2.2
1	A	730	ASN	2.2
1	A	535	THR	2.2
1	A	518	ILE	2.1
1	A	662	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	515	LEU	2.1
1	A	696	PRO	2.1
1	A	829	PRO	2.1
1	A	732	ASP	2.1
1	A	757	SER	2.1
1	A	622	GLN	2.1
1	A	824	MET	2.1
1	A	553	VAL	2.1
1	A	665	CYS	2.0
1	A	388	LYS	2.0
1	A	666	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 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
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

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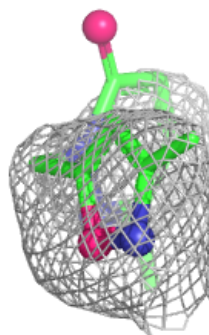
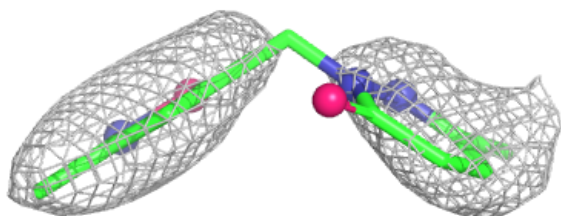
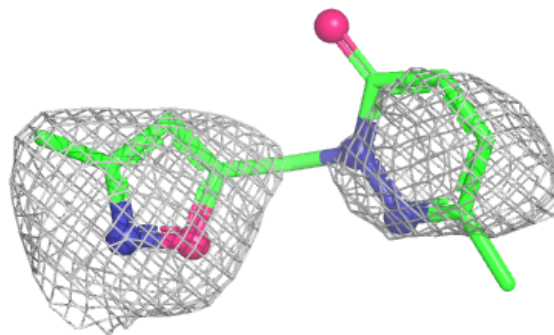
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	1001	1/1	0.99	0.02	28,28,28,28	0

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.

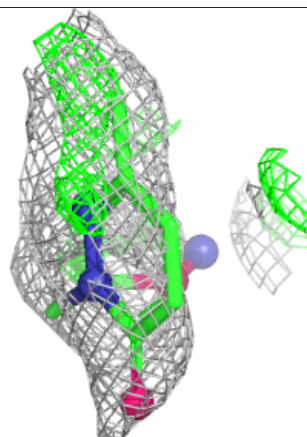
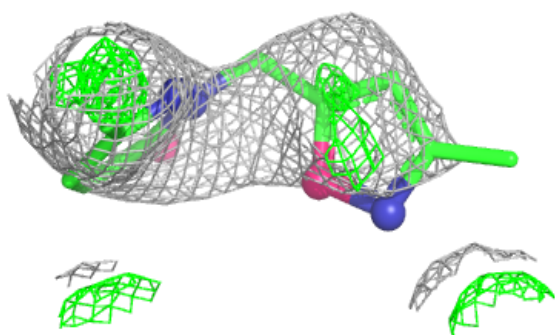
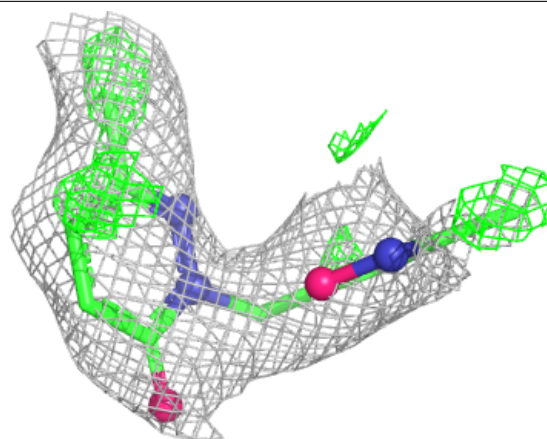
Electron density around UWS A 1011:

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 [i](#)

There are no such residues in this entry.