



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2025 – 11:06 AM EDT

PDB ID : 7I2H
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 Z1198177230 (DNV2_NS5A-x0411)
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Deposited on : 2025-03-06
Resolution : 1.84 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)

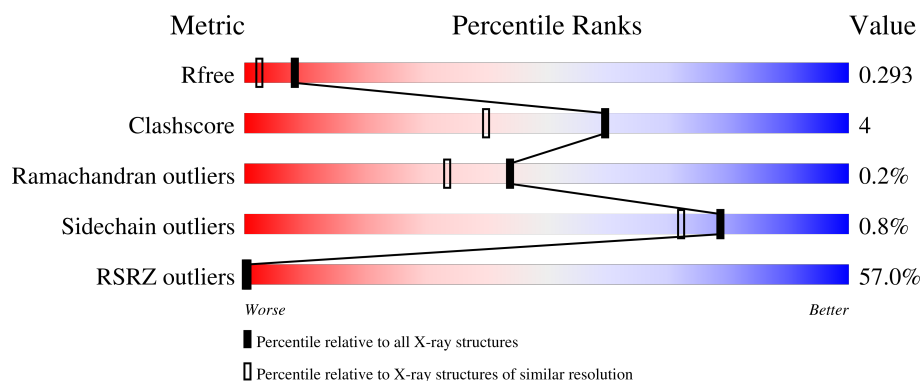
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	1150 (1.84-1.84)
Clashscore	180529	1248 (1.84-1.84)
Ramachandran outliers	177936	1240 (1.84-1.84)
Sidechain outliers	177891	1240 (1.84-1.84)
RSRZ outliers	164620	1149 (1.84-1.84)

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) : 2.41.4

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PO4	A	1007	-	-	X	-
7	K6U	A	1010	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5078 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NS5 RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	567	Total	C	N	O	S	0	7	0
			4690	2953	841	862	34			

There are 2 discrepancies between the modelled and reference sequences:

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

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

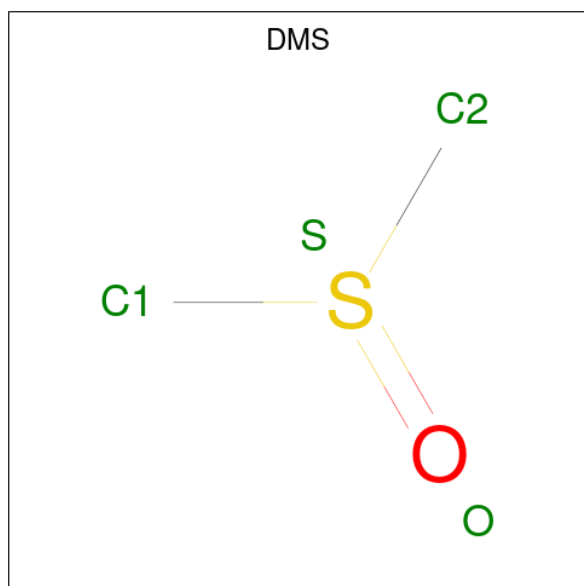
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: 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 (three-letter code: DMS) (formula: C_2H_6OS).



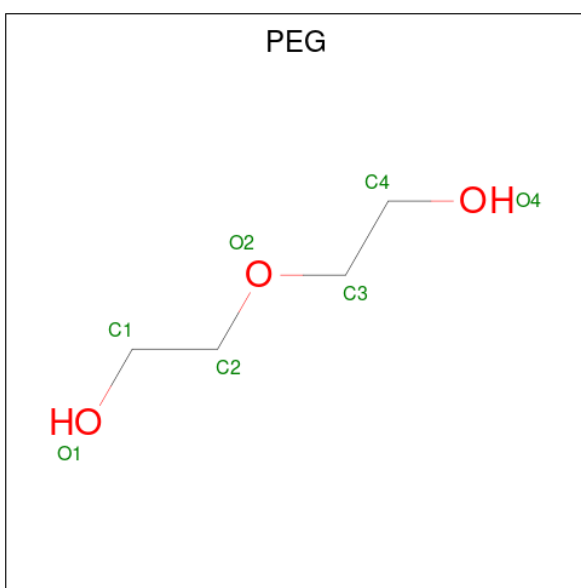
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

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



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

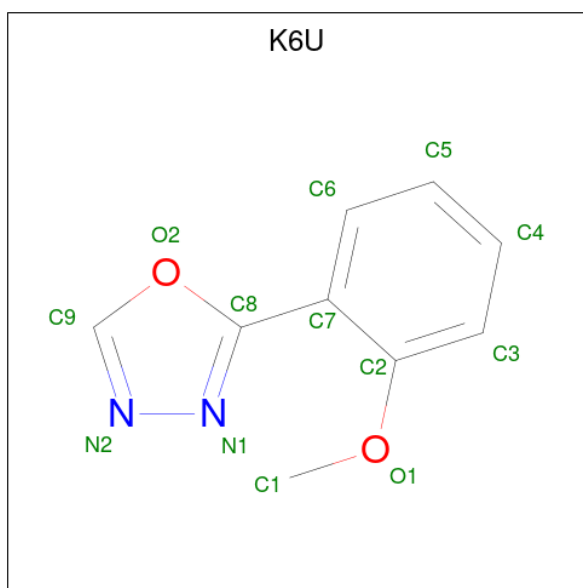
- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 7 is (2M)-2-(2-methoxyphenyl)-1,3,4-oxadiazole (three-letter code: K6U) (formula:

C₉H₈N₂O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			13	9	2	2		
7	A	1	Total	C	N	O	0	0
			13	9	2	2		

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

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

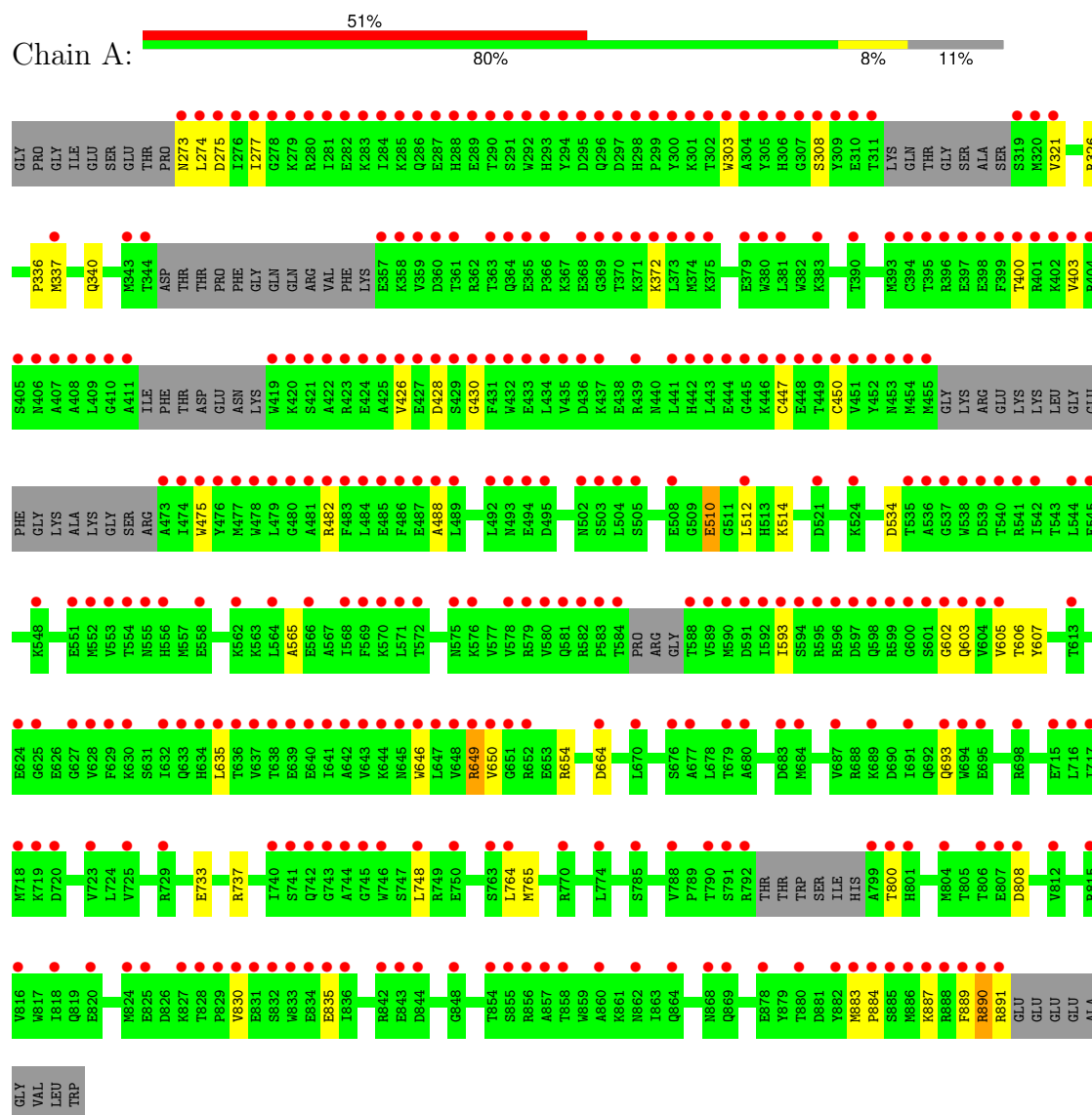
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	306	Total	O	0	0
			306	306		

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	82.38Å 115.50Å 146.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.50 – 1.84 37.50 – 1.84	Depositor EDS
% Data completeness (in resolution range)	95.7 (37.50-1.84) 95.7 (37.50-1.84)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.203 , 0.244 0.274 , 0.293	Depositor DCC
R_{free} test set	3159 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å ²)	35.2	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 149.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	5078	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.07% 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: PEG, PO4, CL, K6U, MES, ZN, DMS

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	1/4795 (0.0%)	0.84	0/6467

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	510	GLU	CD-OE2	6.71	1.33	1.25

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	4690	0	4584	38	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	26	0	0	1	0
8	A	1	0	0	0	0
9	A	306	0	0	6	3
All	All	5078	0	4638	40	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (40) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:ASP:OD1	5:A:1007:PO4:O4	2.06	0.73
1:A:607:TYR:H	7:A:1010:K6U:C9	2.04	0.71
1:A:510:GLU:O	1:A:514:LYS:HG3	1.92	0.69
1:A:649:ARG:HG2	1:A:650:VAL:HG13	1.74	0.68
1:A:336:PRO:O	1:A:340:GLN:HG2	1.96	0.66
1:A:534:ASP:OD1	5:A:1007:PO4:O4	2.18	0.61
4:A:1004:DMS:C1	9:A:1192:HOH:O	2.51	0.58
1:A:830:VAL:HG13	1:A:835:GLU:HB3	1.84	0.58
1:A:800:THR:HG21	9:A:1102:HOH:O	2.04	0.57
1:A:605:VAL:HA	9:A:1108:HOH:O	2.06	0.54
1:A:372:LYS:HG3	1:A:635:LEU:HD23	1.88	0.53
1:A:337:MET:HG2	9:A:1295:HOH:O	2.10	0.52
1:A:372:LYS:CG	1:A:635:LEU:HD23	2.41	0.51
4:A:1004:DMS:H11	9:A:1192:HOH:O	2.08	0.51
1:A:603:GLN:HB2	1:A:606:THR:OG1	2.11	0.51
1:A:475:TRP:O	1:A:482:ARG:NH2	2.46	0.48
1:A:664:ASP:OD1	5:A:1007:PO4:P	2.71	0.48
1:A:890:ARG:O	1:A:891:ARG:HB2	2.12	0.48
1:A:482:ARG:NH1	1:A:602:GLY:O	2.46	0.47
1:A:764:LEU:HG	1:A:765:MET:HE2	1.97	0.46
1:A:733:GLU:O	1:A:737:ARG:HG3	2.15	0.46
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.55	0.46
1:A:748:LEU:HD13	3:A:1003[B]:MES:H61	1.98	0.46
1:A:887:LYS:HG3	1:A:890:ARG:NH2	2.30	0.46
1:A:400:THR:HG23	1:A:426:VAL:HG11	1.97	0.45
1:A:887:LYS:HG3	1:A:890:ARG:HH21	1.82	0.44
1:A:428:ASP:OD1	1:A:430:GLY:N	2.49	0.44
1:A:488:ALA:HB1	1:A:565:ALA:HA	2.00	0.44
1:A:274:LEU:HA	1:A:277:ILE:HG12	2.00	0.43
1:A:275:ASP:OD1	1:A:275:ASP:N	2.52	0.42
1:A:889:PHE:C	1:A:891:ARG:H	2.21	0.42
1:A:321:VAL:HG11	1:A:326:ARG:CZ	2.50	0.41
1:A:273:ASN:N	1:A:275:ASP:OD1	2.52	0.41
1:A:883:MET:N	1:A:884:PRO:CD	2.84	0.41
1:A:737:ARG:HB3	9:A:1343:HOH:O	2.20	0.41
1:A:303:TRP:CD2	1:A:593:ILE:HD12	2.55	0.41
1:A:512[B]:LEU:HD23	1:A:512[B]:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:PRO:O	1:A:340:GLN:CG	2.67	0.41
1:A:403:VAL:HG11	1:A:426:VAL:HG21	2.03	0.40
1:A:646:TRP:CZ2	1:A:654:ARG:HG3	2.56	0.40

All (3) 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:1105:HOH:O	9:A:1105:HOH:O[2_445]	1.75	0.45
9:A:1251:HOH:O	9:A:1368:HOH:O[2_445]	2.09	0.11
9:A:1247:HOH:O	9:A:1344:HOH:O[2_545]	2.18	0.02

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	560/637 (88%)	535 (96%)	24 (4%)	1 (0%)	44 33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	890	ARG

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	503/554 (91%)	499 (99%)	4 (1%)	79 72

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

Mol	Chain	Res	Type
1	A	308	SER
1	A	649	ARG
1	A	693	GLN
1	A	808	ASP

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	493	ASN
1	A	645	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 ⓘ

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	PO4	A	1008	-	4,4,4	1.04	0	6,6,6	0.42	0
4	DMS	A	1004	-	3,3,3	0.47	0	3,3,3	0.39	0
3	MES	A	1003[B]	-	12,12,12	0.87	0	15,16,16	0.62	0
5	PO4	A	1007	-	4,4,4	3.49	3 (75%)	6,6,6	0.71	0
4	DMS	A	1006	-	3,3,3	0.12	0	3,3,3	0.40	0
7	K6U	A	1011	-	10,14,14	0.37	0	10,18,18	0.81	1 (10%)
3	MES	A	1003[A]	-	12,12,12	0.82	0	15,16,16	0.52	0
6	PEG	A	1009	-	6,6,6	0.14	0	5,5,5	0.10	0
7	K6U	A	1010	-	10,14,14	0.31	0	10,18,18	0.89	1 (10%)
4	DMS	A	1005	-	3,3,3	0.24	0	3,3,3	0.02	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
3	MES	A	1003[B]	-	-	4/6/14/14	0/1/1/1
7	K6U	A	1011	-	-	2/3/6/6	0/2/2/2
3	MES	A	1003[A]	-	-	3/6/14/14	0/1/1/1
6	PEG	A	1009	-	-	2/4/4/4	-
7	K6U	A	1010	-	-	2/3/6/6	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1007	PO4	P-O1	6.04	1.64	1.50
5	A	1007	PO4	P-O2	2.40	1.61	1.54
5	A	1007	PO4	P-O3	2.14	1.60	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1010	K6U	C7-C8-N1	2.61	128.24	123.86
7	A	1011	K6U	C7-C8-N1	2.35	127.81	123.86

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	1009	PEG	O2-C3-C4-O4
7	A	1011	K6U	C3-C2-O1-C1
7	A	1011	K6U	C7-C2-O1-C1
3	A	1003[A]	MES	C7-C8-S-O2S
7	A	1010	K6U	C3-C2-O1-C1
3	A	1003[B]	MES	C8-C7-N4-C5
7	A	1010	K6U	C7-C2-O1-C1
3	A	1003[B]	MES	C7-C8-S-O3S
3	A	1003[B]	MES	C7-C8-S-O2S
6	A	1009	PEG	C4-C3-O2-C2

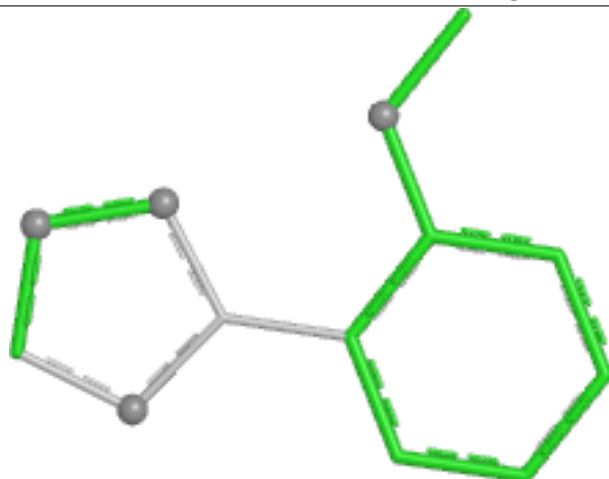
There are no ring outliers.

4 monomers are involved in 7 short contacts:

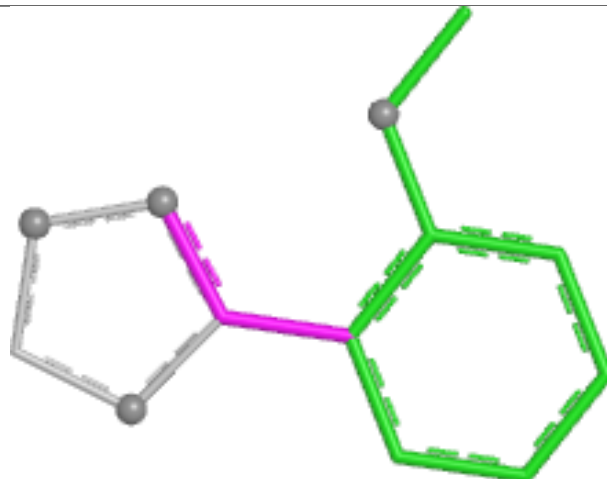
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1004	DMS	2	0
3	A	1003[B]	MES	1	0
5	A	1007	PO4	3	0
7	A	1010	K6U	1	0

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.

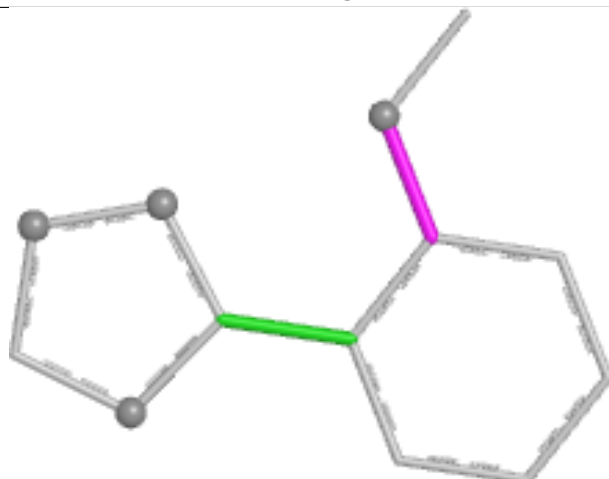
Ligand K6U A 1011



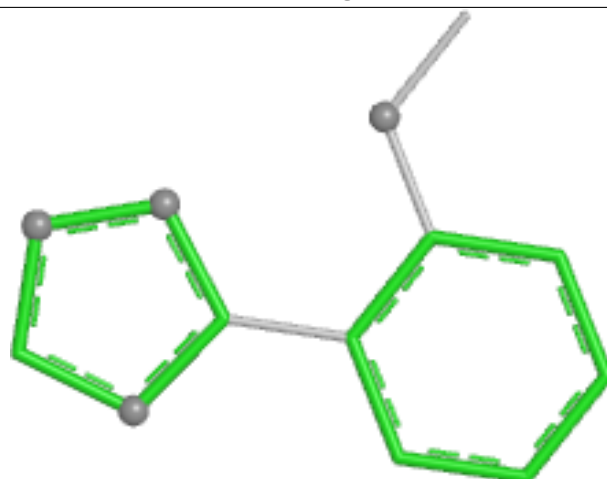
Bond lengths



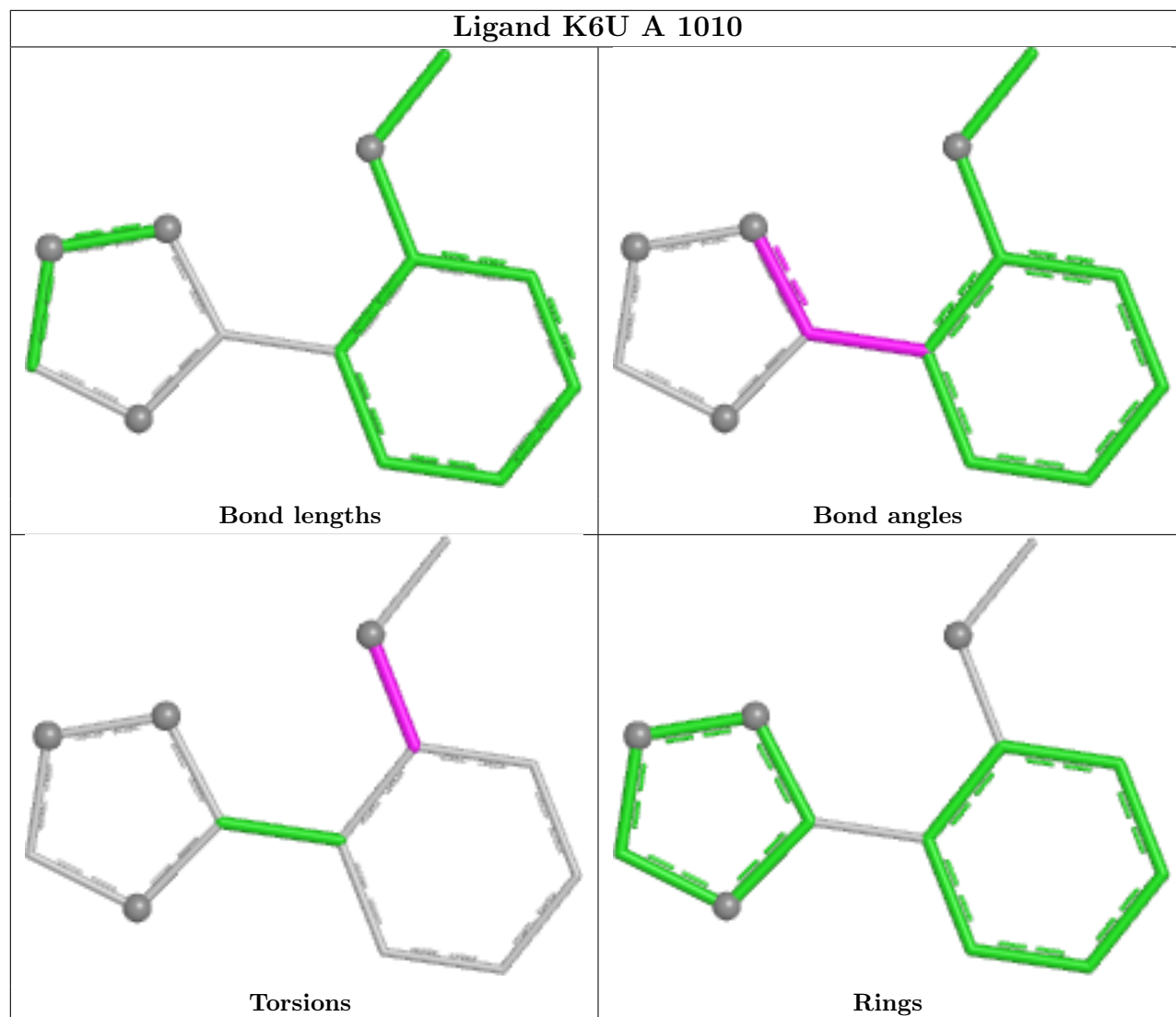
Bond angles



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, 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	567/637 (89%)	4.36	323 (56%) 0 0	8, 38, 93, 147	169 (29%)

All (323) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	505	SER	18.1
1	A	492	LEU	17.8
1	A	292	TRP	17.4
1	A	443	LEU	16.8
1	A	542	ILE	16.7
1	A	502	ASN	16.6
1	A	538	TRP	16.4
1	A	300	TYR	15.9
1	A	277	ILE	15.8
1	A	536	ALA	15.3
1	A	291	SER	15.3
1	A	535	THR	15.2
1	A	450	CYS	15.1
1	A	435	VAL	15.0
1	A	432	TRP	14.9
1	A	889	PHE	14.8
1	A	304	ALA	14.6
1	A	589	VAL	14.5
1	A	294	TYR	14.5
1	A	635	LEU	14.5
1	A	495	ASP	14.4
1	A	503	SER	14.4
1	A	299	PRO	14.4
1	A	801[A]	HIS	14.3
1	A	431	PHE	14.0
1	A	790	THR	14.0
1	A	452	TYR	13.9

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Mol	Chain	Res	Type	RSRZ
1	A	309	TYR	13.8
1	A	359	VAL	13.7
1	A	430	GLY	13.7
1	A	293	HIS	13.7
1	A	605	VAL	13.5
1	A	480	GLY	13.5
1	A	483	PHE	13.5
1	A	451	VAL	13.5
1	A	434	LEU	13.5
1	A	590	MET	13.5
1	A	594	SER	13.4
1	A	445	GLY	13.2
1	A	478	TRP	12.9
1	A	283	LYS	12.9
1	A	750	GLU	12.8
1	A	484	LEU	12.5
1	A	481	ALA	12.4
1	A	400	THR	12.3
1	A	584	THR	12.2
1	A	508	GLU	12.2
1	A	282	GLU	12.0
1	A	442	HIS	11.9
1	A	476	TYR	11.8
1	A	595	ARG	11.8
1	A	399	PHE	11.8
1	A	422	ALA	11.7
1	A	541	ARG	11.7
1	A	540	THR	11.6
1	A	298	HIS	11.6
1	A	487	GLU	11.5
1	A	449	THR	11.4
1	A	537	GLY	11.4
1	A	886	MET	11.4
1	A	426	VAL	11.3
1	A	405	SER	11.3
1	A	453	ASN	11.2
1	A	398	GLU	11.1
1	A	290	THR	11.1
1	A	493	ASN	11.0
1	A	475	TRP	11.0
1	A	885	SER	11.0
1	A	830	VAL	10.9

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Mol	Chain	Res	Type	RSRZ
1	A	774	LEU	10.9
1	A	295	ASP	10.8
1	A	425	ALA	10.8
1	A	479	LEU	10.8
1	A	637	VAL	10.7
1	A	428	ASP	10.6
1	A	650	VAL	10.6
1	A	539	ASP	10.5
1	A	544	LEU	10.5
1	A	636	THR	10.5
1	A	273	ASN	10.4
1	A	580	VAL	10.2
1	A	512[A]	LEU	10.0
1	A	716	LEU	9.9
1	A	401	ARG	9.7
1	A	888	ARG	9.5
1	A	485	GLU	9.4
1	A	599	ARG	9.4
1	A	311	THR	9.4
1	A	474	ILE	9.3
1	A	741[A]	SER	9.3
1	A	360	ASP	9.3
1	A	454	MET	9.2
1	A	598	GLN	9.2
1	A	604	VAL	9.1
1	A	791	SER	9.0
1	A	446	LYS	9.0
1	A	380	TRP	8.9
1	A	494	GLU	8.8
1	A	763[A]	SER	8.7
1	A	403	VAL	8.7
1	A	358	LYS	8.7
1	A	887	LYS	8.7
1	A	448	GLU	8.7
1	A	792	ARG	8.7
1	A	482	ARG	8.6
1	A	641	ILE	8.6
1	A	419	TRP	8.6
1	A	444	GLU	8.6
1	A	433	GLU	8.5
1	A	477	MET	8.5
1	A	407	ALA	8.4

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Mol	Chain	Res	Type	RSRZ
1	A	429	SER	8.4
1	A	638	THR	8.3
1	A	287	GLU	8.3
1	A	719[A]	LYS	8.2
1	A	421	SER	8.2
1	A	373	LEU	8.2
1	A	551	GLU	8.2
1	A	404	ARG	8.2
1	A	288	HIS	8.1
1	A	278	GLY	8.1
1	A	603	GLN	8.1
1	A	836	ILE	8.1
1	A	890	ARG	8.0
1	A	409	LEU	8.0
1	A	406	ASN	7.8
1	A	593	ILE	7.8
1	A	651	GLY	7.8
1	A	402	LYS	7.8
1	A	583	PRO	7.7
1	A	370	THR	7.7
1	A	860	ALA	7.6
1	A	296	GLN	7.4
1	A	639	GLU	7.4
1	A	649	ARG	7.4
1	A	842	ARG	7.4
1	A	634	HIS	7.4
1	A	455	MET	7.3
1	A	717	ILE	7.3
1	A	357	GLU	7.3
1	A	596	ARG	7.2
1	A	856	ARG	7.2
1	A	644	LYS	7.2
1	A	410	GLY	7.1
1	A	375	LYS	7.1
1	A	423	ARG	7.0
1	A	642	ALA	6.9
1	A	473	ALA	6.9
1	A	281	ILE	6.8
1	A	884	PRO	6.8
1	A	582	ARG	6.7
1	A	592	ILE	6.7
1	A	633	GLN	6.6

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Mol	Chain	Res	Type	RSRZ
1	A	569	PHE	6.5
1	A	891	ARG	6.5
1	A	297	ASP	6.5
1	A	640	GLU	6.4
1	A	729	ARG	6.4
1	A	441	LEU	6.4
1	A	770	ARG	6.3
1	A	408	ALA	6.3
1	A	411	ALA	6.3
1	A	843	GLU	6.3
1	A	424	GLU	6.2
1	A	864[A]	GLN	6.2
1	A	715	GLU	6.2
1	A	745	GLY	6.2
1	A	344	THR	6.2
1	A	374	MET	6.1
1	A	844	ASP	6.1
1	A	302	THR	6.0
1	A	882	TYR	5.9
1	A	648	VAL	5.9
1	A	286	GLN	5.8
1	A	785[A]	SER	5.8
1	A	600	GLY	5.7
1	A	420	LYS	5.7
1	A	597	ASP	5.6
1	A	562	LYS	5.6
1	A	698	ARG	5.6
1	A	883	MET	5.5
1	A	364	GLN	5.5
1	A	395	THR	5.5
1	A	371	LYS	5.4
1	A	834	GLU	5.2
1	A	832	SER	5.2
1	A	743	GLY	5.2
1	A	647	LEU	5.2
1	A	303	TRP	5.1
1	A	588	THR	5.1
1	A	835	GLU	5.1
1	A	799	ALA	5.0
1	A	564	LEU	4.9
1	A	652	ARG	4.8
1	A	396	ARG	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	670	LEU	4.7
1	A	308	SER	4.7
1	A	744	ALA	4.7
1	A	305	TYR	4.6
1	A	831	GLU	4.6
1	A	571	LEU	4.6
1	A	372	LYS	4.5
1	A	284	ILE	4.4
1	A	437	LYS	4.4
1	A	680	ALA	4.4
1	A	645	ASN	4.4
1	A	274	LEU	4.4
1	A	289	GLU	4.3
1	A	764	LEU	4.3
1	A	691	ILE	4.3
1	A	742	GLN	4.2
1	A	815	ARG	4.2
1	A	397	GLU	4.2
1	A	629	PHE	4.2
1	A	746	TRP	4.1
1	A	570	LYS	4.1
1	A	578	VAL	4.1
1	A	390	THR	4.1
1	A	800	THR	4.1
1	A	556	HIS	4.0
1	A	280	ARG	4.0
1	A	343	MET	4.0
1	A	552	MET	4.0
1	A	285	LYS	3.9
1	A	276	ILE	3.9
1	A	548	LYS	3.9
1	A	488	ALA	3.9
1	A	379	GLU	3.8
1	A	558	GLU	3.8
1	A	566	GLU	3.8
1	A	427	GLU	3.8
1	A	625	GLY	3.8
1	A	572	THR	3.8
1	A	687	VAL	3.8
1	A	880	THR	3.7
1	A	806	THR	3.7
1	A	581	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	306	HIS	3.6
1	A	279	LYS	3.6
1	A	319	SER	3.5
1	A	591	ASP	3.5
1	A	693	GLN	3.5
1	A	275	ASP	3.4
1	A	545	GLU	3.4
1	A	829	PRO	3.4
1	A	820	GLU	3.3
1	A	447	CYS	3.3
1	A	361	THR	3.3
1	A	575	ASN	3.3
1	A	363	THR	3.2
1	A	827	LYS	3.2
1	A	858	THR	3.2
1	A	307	GLY	3.1
1	A	646	TRP	3.1
1	A	365	GLU	3.1
1	A	576	LYS	3.1
1	A	740	ILE	3.0
1	A	601	SER	3.0
1	A	613	THR	3.0
1	A	855	SER	2.9
1	A	568	ILE	2.9
1	A	628	VAL	2.9
1	A	679	THR	2.9
1	A	627	GLY	2.8
1	A	393	MET	2.8
1	A	524	LYS	2.8
1	A	632	ILE	2.8
1	A	818	ILE	2.8
1	A	337	MET	2.8
1	A	301	LYS	2.8
1	A	555	ASN	2.8
1	A	808	ASP	2.8
1	A	825	GLU	2.8
1	A	579	ARG	2.7
1	A	725	VAL	2.7
1	A	383	LYS	2.7
1	A	694	TRP	2.7
1	A	664	ASP	2.7
1	A	439	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	630	LYS	2.7
1	A	848	GLY	2.6
1	A	643	VAL	2.6
1	A	854	THR	2.6
1	A	553	VAL	2.6
1	A	320	MET	2.5
1	A	812	VAL	2.5
1	A	748	LEU	2.5
1	A	436	ASP	2.5
1	A	816	VAL	2.5
1	A	366	PRO	2.5
1	A	602	GLY	2.5
1	A	683	ASP	2.5
1	A	868	ASN	2.5
1	A	321	VAL	2.5
1	A	689	LYS	2.4
1	A	486	PHE	2.4
1	A	684	MET	2.4
1	A	676	SER	2.4
1	A	878	GLU	2.4
1	A	857	ALA	2.3
1	A	828	THR	2.3
1	A	381	LEU	2.3
1	A	862	ASN	2.3
1	A	788	VAL	2.3
1	A	554	THR	2.3
1	A	718	MET	2.3
1	A	310	GLU	2.3
1	A	695	GLU	2.3
1	A	723	VAL	2.2
1	A	489	LEU	2.2
1	A	824	MET	2.2
1	A	807	GLU	2.2
1	A	720	ASP	2.1
1	A	369	GLY	2.1
1	A	624	GLU	2.1
1	A	833	TRP	2.1
1	A	368	GLU	2.1
1	A	521	ASP	2.1
1	A	677	ALA	2.1
1	A	804	MET	2.1
1	A	504	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	394	CYS	2.0
1	A	869	GLN	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](#)

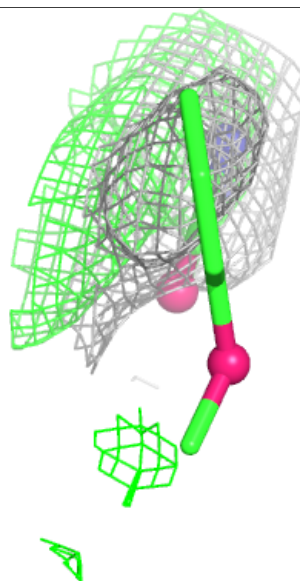
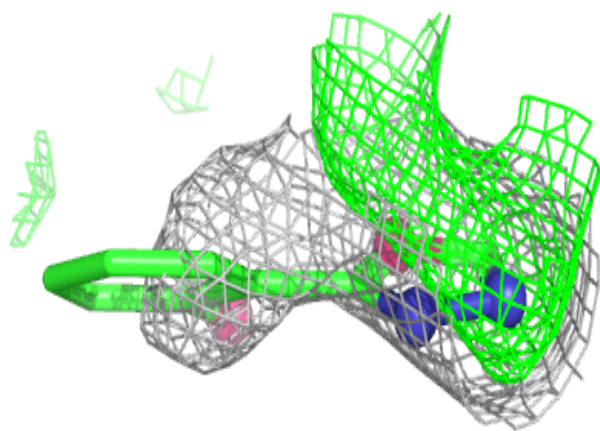
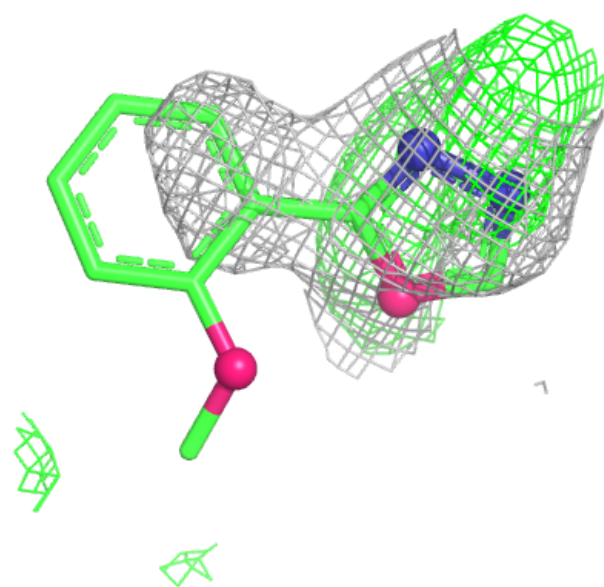
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	K6U	A	1010	13/13	0.55	0.57	52,54,57,58	13
7	K6U	A	1011	13/13	0.58	0.28	39,41,46,46	13
6	PEG	A	1009	7/7	0.73	0.20	70,77,86,87	0
5	PO4	A	1008	5/5	0.74	0.16	83,92,101,115	0
5	PO4	A	1007	5/5	0.80	0.13	42,46,55,81	0
4	DMS	A	1005	4/4	0.86	0.17	85,96,101,102	0
3	MES	A	1003[A]	12/12	0.93	0.25	767,781,797,797	12
3	MES	A	1003[B]	12/12	0.93	0.25	27,35,41,43	12
4	DMS	A	1004	4/4	0.94	0.14	49,57,58,64	0
4	DMS	A	1006	4/4	0.95	0.12	58,61,65,67	0
8	CL	A	1012	1/1	0.97	0.14	50,50,50,50	0
2	ZN	A	1002	1/1	0.98	0.04	60,60,60,60	0
2	ZN	A	1001	1/1	1.00	0.01	30,30,30,30	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.

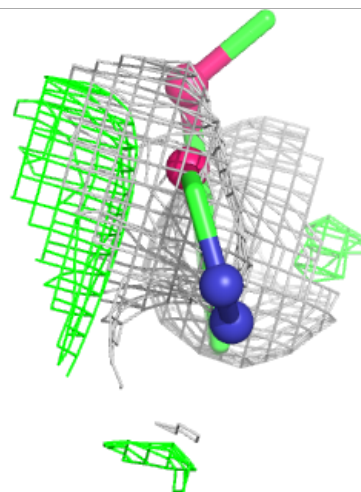
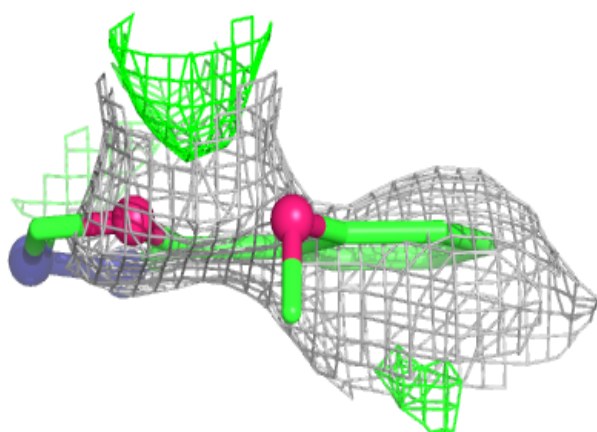
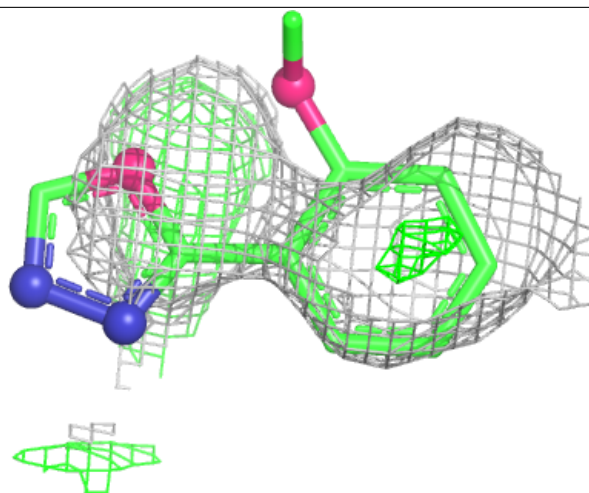
Electron density around K6U A 1010:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around K6U 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 [i](#)

There are no such residues in this entry.