



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 25, 2024 – 07:41 PM EST

PDB ID : 7HKT
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 Z1983897532 (DNV2_NS5A-x0615)
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Deposited on : 2024-10-15
Resolution : 1.92 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	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)

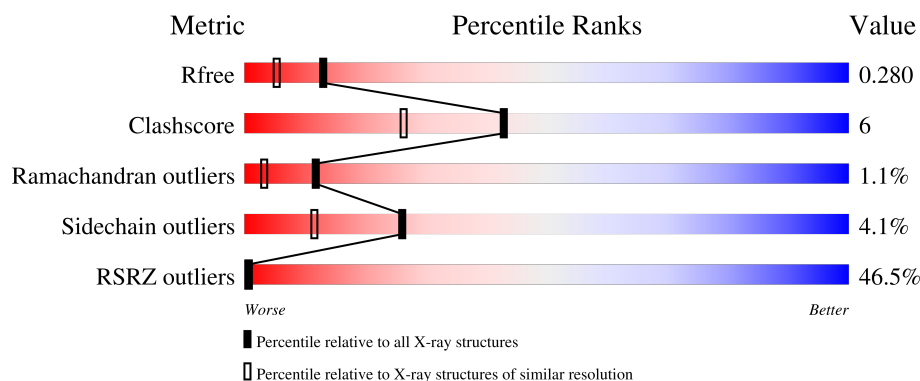
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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	1028 (1.92-1.92)
Clashscore	180529	1100 (1.92-1.92)
Ramachandran outliers	177936	1087 (1.92-1.92)
Sidechain outliers	177891	1087 (1.92-1.92)
RSRZ outliers	164620	1028 (1.92-1.92)

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 $\leq 5\%$.

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) : 2.40

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PO4	A	1008	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5339 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 Genome polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	583	4822	3036	865	887	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
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).



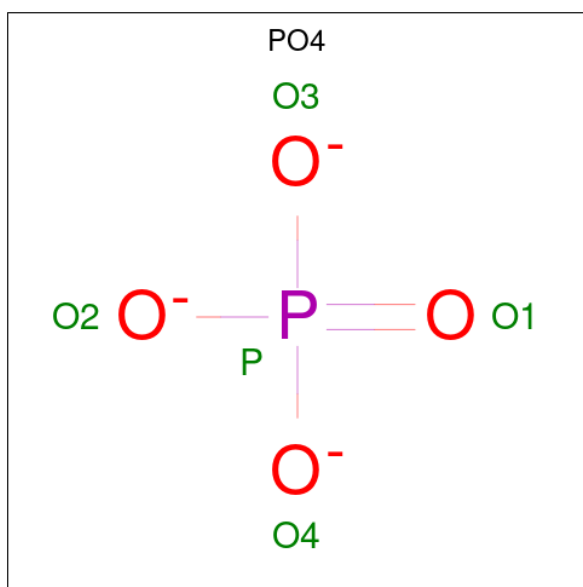
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is 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	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		

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



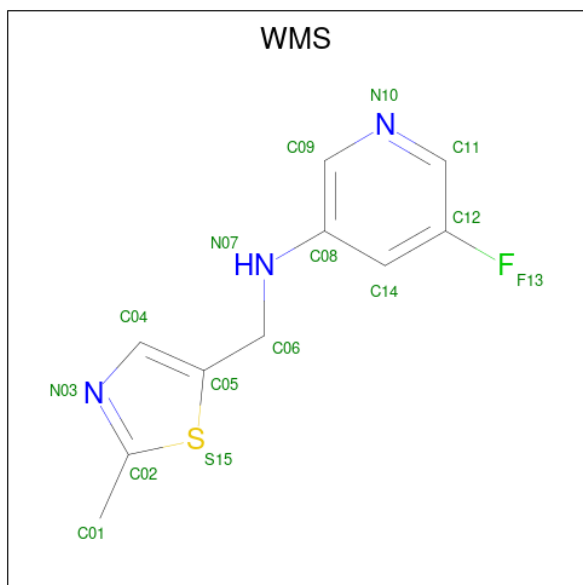
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		

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

- Molecule 7 is 5-fluoro-N-[(2-methyl-1,3-thiazol-5-yl)methyl]pyridin-3-amine (three-letter code: WMS) (formula: C₁₀H₁₀FN₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	F	N	S	0	1
			15	10	1	3	1		
7	A	1	Total	C	F	N	S	0	0
			15	10	1	3	1		

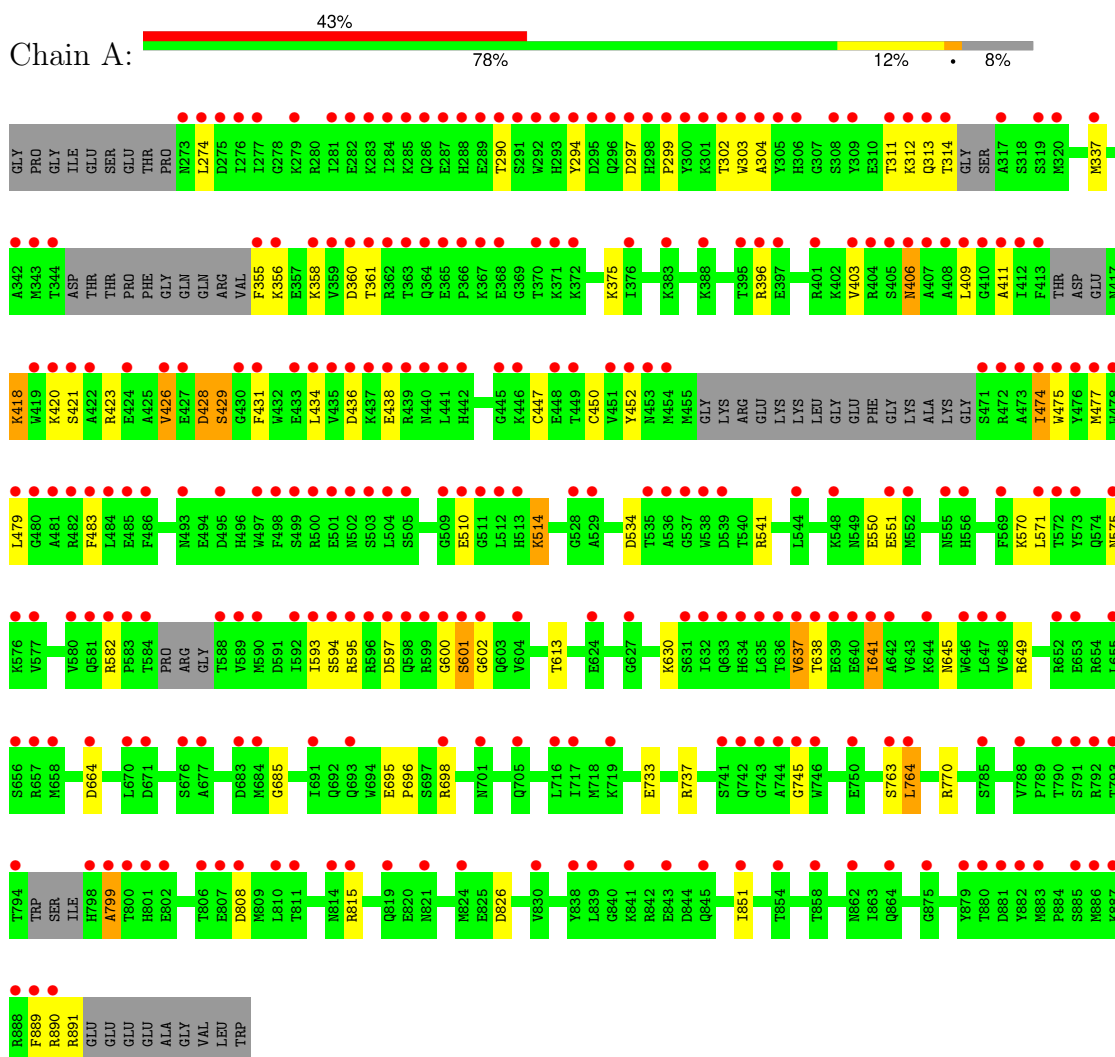
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	417	Total	O	0	1
			418	418		

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. 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. 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: Genome polyprotein



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 116.17Å 146.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.63 – 1.92 49.63 – 1.92	Depositor EDS
% Data completeness (in resolution range)	95.8 (49.63-1.92) 95.9 (49.63-1.92)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC5	Depositor
R, R_{free}	0.212 , 0.255 0.260 , 0.280	Depositor DCC
R_{free} test set	2779 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	37.9	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 100.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5339	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% 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: DMS, PEG, PO4, ZN, MES, WMS

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	0.68	0/4929	0.79	1/6645 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	815	ARG	NE-CZ-NH2	-5.00	117.80	120.30

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	4822	0	4721	56	0
2	A	2	0	0	0	0
3	A	24	0	26	0	0
4	A	12	0	18	2	0
5	A	21	0	30	1	1
6	A	10	0	0	4	0
7	A	30	0	0	1	0
8	A	418	0	0	11	2
All	All	5339	0	4795	59	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 6.

All (59) 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:638:THR:O	1:A:641:ILE:HG23	1.68	0.92
1:A:600:GLY:O	1:A:601:SER:OG	1.96	0.82
1:A:474:ILE:H	1:A:474:ILE:HD12	1.47	0.79
1:A:637:VAL:O	1:A:641:ILE:HG22	1.87	0.75
1:A:698:ARG:NH2	8:A:1101:HOH:O	2.26	0.69
1:A:474:ILE:HD12	1:A:474:ILE:N	2.07	0.68
1:A:303:TRP:CE2	1:A:595:ARG:HD2	2.30	0.67
4:A:1004:DMS:H11	8:A:1281:HOH:O	1.96	0.65
1:A:638:THR:HA	1:A:641:ILE:CG2	2.30	0.62
1:A:311:THR:O	1:A:312:LYS:HG3	2.00	0.62
1:A:733:GLU:O	1:A:737:ARG:HG3	2.01	0.61
1:A:302:THR:OG1	1:A:360:ASP:OD1	2.11	0.61
1:A:304:ALA:HB3	1:A:594:SER:OG	2.02	0.60
4:A:1004:DMS:C1	8:A:1329:HOH:O	2.50	0.59
1:A:534:ASP:OD1	6:A:1008:PO4:P	2.61	0.59
1:A:337:MET:HG2	8:A:1338:HOH:O	2.03	0.58
1:A:294:TYR:CD1	1:A:294:TYR:O	2.58	0.56
1:A:808:ASP:HB3	8:A:1385:HOH:O	2.05	0.56
1:A:510:GLU:O	1:A:514:LYS:HG3	2.07	0.55
1:A:314:THR:O	1:A:314:THR:HG22	2.05	0.55
1:A:534:ASP:OD1	6:A:1008:PO4:O4	2.26	0.54
1:A:431:PHE:O	1:A:434:LEU:HB2	2.09	0.53
1:A:571:LEU:O	1:A:575:ASN:O	2.28	0.52
1:A:745:GLY:N	8:A:1117:HOH:O	2.44	0.51
1:A:799:ALA:HB2	7:A:1013:WMS:C04	2.41	0.50
1:A:638:THR:C	1:A:641:ILE:HG23	2.32	0.50
1:A:396:ARG:NH2	1:A:436:ASP:OD1	2.41	0.50
1:A:550:GLU:OE2	1:A:613:THR:OG1	2.25	0.50
1:A:411:ALA:HB2	1:A:479:LEU:HD13	1.94	0.49
1:A:664:ASP:OD1	6:A:1008:PO4:P	2.71	0.49
1:A:409:LEU:HD22	8:A:1508:HOH:O	2.13	0.48
1:A:403:VAL:HG21	1:A:426:VAL:HG21	1.95	0.48
1:A:664:ASP:OD1	6:A:1008:PO4:O4	2.32	0.48
1:A:452:TYR:HB3	1:A:475:TRP:HB3	1.97	0.47
1:A:826:ASP:OD1	1:A:826:ASP:C	2.52	0.47
1:A:602:GLY:HA3	8:A:1196:HOH:O	2.15	0.46
1:A:770:ARG:HD2	1:A:851:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:ARG:NE	1:A:597:ASP:OD2	2.49	0.46
1:A:889:PHE:O	1:A:891:ARG:N	2.48	0.46
1:A:698:ARG:N	8:A:1106:HOH:O	2.35	0.45
1:A:313:GLN:HG2	1:A:314:THR:H	1.81	0.45
1:A:428:ASP:CG	1:A:429:SER:N	2.71	0.44
1:A:299:PRO:HD3	1:A:582:ARG:NH1	2.32	0.44
1:A:541:ARG:HD2	1:A:685:GLY:O	2.17	0.44
1:A:764:LEU:HD12	1:A:764:LEU:HA	1.85	0.44
5:A:1009:PEG:H32	8:A:1276:HOH:O	2.18	0.44
1:A:406:ASN:OD1	1:A:423:ARG:NH1	2.49	0.43
1:A:645:ASN:O	1:A:649:ARG:HB2	2.19	0.42
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.60	0.42
1:A:396:ARG:HG2	1:A:483:PHE:CZ	2.55	0.42
1:A:600:GLY:C	1:A:601:SER:OG	2.57	0.42
1:A:474:ILE:N	1:A:474:ILE:CD1	2.76	0.42
1:A:570:LYS:HG3	8:A:1202:HOH:O	2.20	0.41
1:A:551[A]:GLU:HG2	1:A:551[A]:GLU:O	2.20	0.41
1:A:304:ALA:O	1:A:593:ILE:HA	2.21	0.41
1:A:303:TRP:CZ2	1:A:595:ARG:HD2	2.55	0.41
1:A:695:GLU:HA	1:A:696:PRO:HD3	1.98	0.40
1:A:303:TRP:CE3	1:A:593:ILE:HD12	2.56	0.40
1:A:361:THR:O	1:A:595:ARG:NH2	2.54	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)
8:A:1282:HOH:O	8:A:1416:HOH:O[2_545]	1.87	0.33
8:A:1180:HOH:O	8:A:1180:HOH:O[2_445]	2.13	0.07
5:A:1009:PEG:O2	5:A:1009:PEG:O2[2_545]	2.15	0.05

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	576/637 (90%)	543 (94%)	27 (5%)	6 (1%)	13 4

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	418	LYS
1	A	420	LYS
1	A	601	SER
1	A	799	ALA
1	A	890	ARG
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	518/554 (94%)	496 (96%)	22 (4%)	25 11

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	274	LEU
1	A	290	THR
1	A	297	ASP
1	A	355	PHE
1	A	356	LYS
1	A	358	LYS
1	A	375	LYS
1	A	418	LYS
1	A	421	SER
1	A	426	VAL
1	A	428	ASP
1	A	429	SER
1	A	438	GLU
1	A	474	ILE

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Mol	Chain	Res	Type
1	A	477	MET
1	A	514	LYS
1	A	630	LYS
1	A	637	VAL
1	A	641	ILE
1	A	763[A]	SER
1	A	763[B]	SER
1	A	764	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	273	ASN
1	A	417	ASN
1	A	760	GLN
1	A	786	HIS

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 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DMS	A	1004	-	3,3,3	0.19	0	3,3,3	0.23	0
4	DMS	A	1005	-	3,3,3	0.28	0	3,3,3	0.07	0
5	PEG	A	1009	-	6,6,6	0.21	0	5,5,5	0.20	0
5	PEG	A	1011	-	6,6,6	0.17	0	5,5,5	0.10	0
7	WMS	A	1012[A]	-	14,16,16	0.50	0	14,21,21	0.98	1 (7%)
6	PO4	A	1010	-	4,4,4	0.78	0	6,6,6	0.42	0
4	DMS	A	1006	-	3,3,3	0.22	0	3,3,3	0.31	0
5	PEG	A	1007	-	6,6,6	0.20	0	5,5,5	0.10	0
6	PO4	A	1008	-	4,4,4	1.90	1 (25%)	6,6,6	0.73	0
3	MES	A	1003[A]	-	12,12,12	0.70	0	15,16,16	0.32	0
3	MES	A	1003[B]	-	12,12,12	0.69	0	15,16,16	0.49	0
7	WMS	A	1013	-	14,16,16	0.65	0	14,21,21	0.97	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	WMS	A	1012[A]	-	-	3/3/5/5	0/2/2/2
5	PEG	A	1011	-	-	2/4/4/4	-
5	PEG	A	1009	-	-	2/4/4/4	-
5	PEG	A	1007	-	-	1/4/4/4	-
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
7	WMS	A	1013	-	-	0/3/5/5	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1008	PO4	P-O1	3.66	1.59	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1013	WMS	C04-C05-S15	-3.14	108.88	112.00
7	A	1012[A]	WMS	C04-C05-S15	-3.13	108.89	112.00

There are no chirality outliers.

All (16) torsion outliers are listed below:

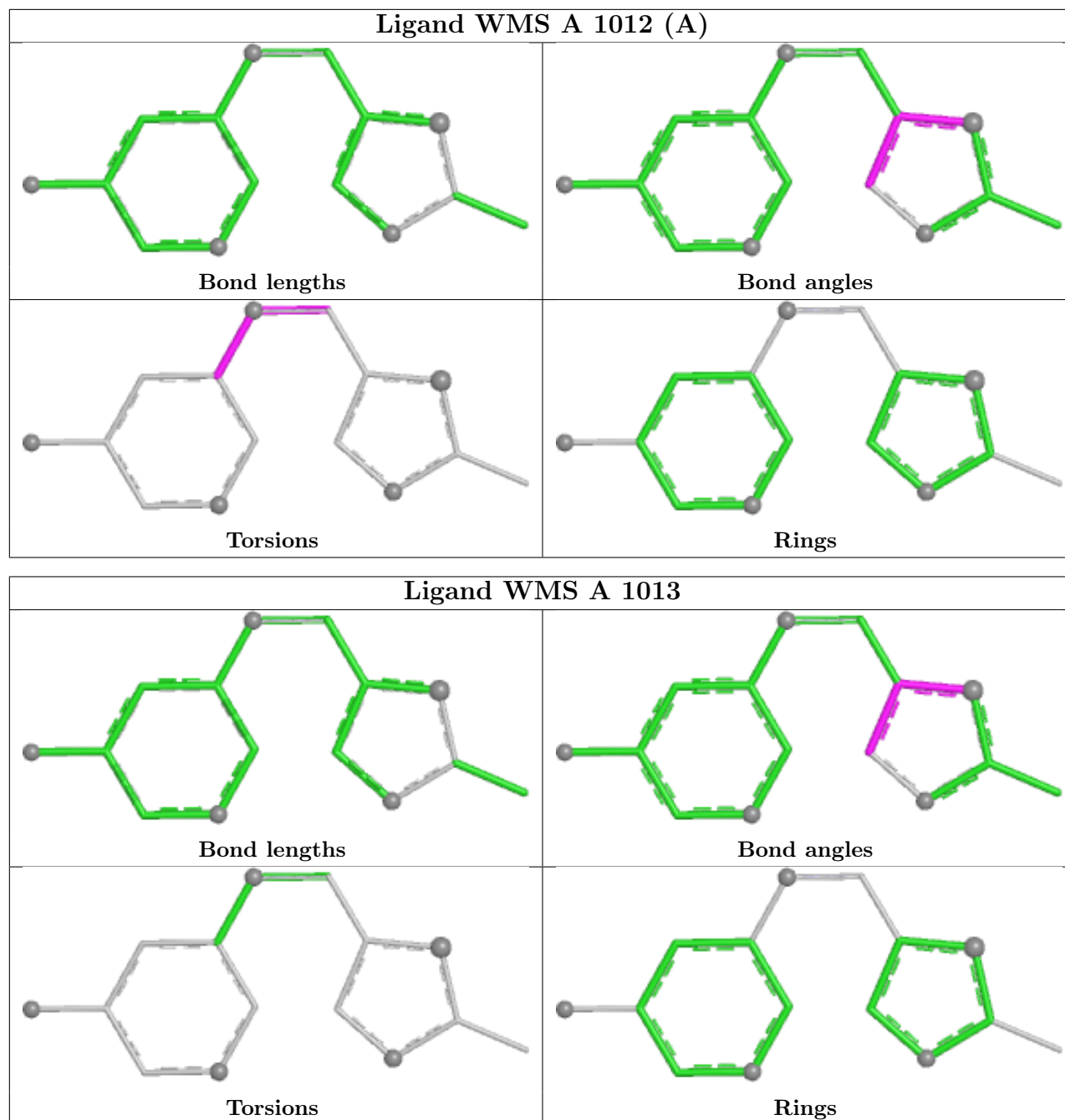
Mol	Chain	Res	Type	Atoms
3	A	1003[A]	MES	C7-C8-S-O1S
3	A	1003[A]	MES	C7-C8-S-O3S
3	A	1003[B]	MES	C8-C7-N4-C3
7	A	1012[A]	WMS	C09-C08-N07-C06
7	A	1012[A]	WMS	C14-C08-N07-C06
3	A	1003[B]	MES	C7-C8-S-O3S
5	A	1009	PEG	O2-C3-C4-O4
5	A	1011	PEG	O2-C3-C4-O4
3	A	1003[B]	MES	C8-C7-N4-C5
3	A	1003[A]	MES	C7-C8-S-O2S
3	A	1003[B]	MES	C7-C8-S-O1S
3	A	1003[B]	MES	C7-C8-S-O2S
7	A	1012[A]	WMS	C05-C06-N07-C08
5	A	1007	PEG	O1-C1-C2-O2
5	A	1009	PEG	C1-C2-O2-C3
5	A	1011	PEG	C4-C3-O2-C2

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1004	DMS	2	0
5	A	1009	PEG	1	1
6	A	1008	PO4	4	0
7	A	1013	WMS	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.



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 ⓘ

Warning: The R factor obtained from EDS is 0.2882, which does not match the depositor's R factor of 0.21248. Please interpret the results in this section carefully.

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	583/637 (91%)	2.76	271 (46%) 0 1	9, 44, 118, 162	144 (24%)

All (271) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	475	TRP	11.6
1	A	435	VAL	11.1
1	A	593	ILE	10.8
1	A	839	LEU	10.4
1	A	635	LEU	10.2
1	A	580	VAL	10.1
1	A	716	LEU	9.9
1	A	632	ILE	9.9
1	A	691	ILE	9.8
1	A	717	ILE	9.8
1	A	483	PHE	9.7
1	A	571	LEU	9.7
1	A	637	VAL	9.7
1	A	434	LEU	9.7
1	A	810	LEU	9.7
1	A	479	LEU	9.4
1	A	431	PHE	9.2
1	A	636	THR	9.1
1	A	641	ILE	9.1
1	A	785[A]	SER	9.1
1	A	573	TYR	9.1
1	A	763[A]	SER	9.0
1	A	484	LEU	9.0
1	A	292	TRP	9.0

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Mol	Chain	Res	Type	RSRZ
1	A	481	ALA	8.9
1	A	395	THR	8.9
1	A	480	GLY	8.9
1	A	838	TYR	8.8
1	A	359	VAL	8.7
1	A	851	ILE	8.7
1	A	366	PRO	8.6
1	A	276	ILE	8.3
1	A	512[A]	LEU	8.3
1	A	589	VAL	8.2
1	A	511	GLY	8.2
1	A	858	THR	8.2
1	A	370	THR	8.1
1	A	594	SER	8.1
1	A	294	TYR	8.0
1	A	601	SER	7.9
1	A	572	THR	7.9
1	A	474	ILE	7.9
1	A	799	ALA	7.9
1	A	293	HIS	7.9
1	A	277	ILE	7.9
1	A	788	VAL	7.8
1	A	304	ALA	7.8
1	A	363	THR	7.8
1	A	303	TRP	7.8
1	A	639	GLU	7.7
1	A	476	TYR	7.7
1	A	485	GLU	7.7
1	A	361	THR	7.6
1	A	814	ASN	7.6
1	A	551[A]	GLU	7.6
1	A	741[A]	SER	7.4
1	A	684	MET	7.4
1	A	411	ALA	7.3
1	A	705	GLN	7.3
1	A	439	ARG	7.2
1	A	305	TYR	7.2
1	A	698	ARG	7.2
1	A	638	THR	7.1
1	A	274	LEU	7.1
1	A	800	THR	7.1
1	A	745	GLY	7.0

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Mol	Chain	Res	Type	RSRZ
1	A	798	HIS	7.0
1	A	419	TRP	7.0
1	A	299	PRO	7.0
1	A	633	GLN	6.9
1	A	452	TYR	6.9
1	A	600	GLY	6.8
1	A	314	THR	6.8
1	A	864[A]	GLN	6.7
1	A	482	ARG	6.7
1	A	790	THR	6.7
1	A	438	GLU	6.7
1	A	284	ILE	6.7
1	A	808	ASP	6.6
1	A	510	GLU	6.6
1	A	504	LEU	6.5
1	A	575	ASN	6.5
1	A	634	HIS	6.4
1	A	372	LYS	6.3
1	A	576	LYS	6.3
1	A	599	ARG	6.3
1	A	640	GLU	6.3
1	A	719[A]	LYS	6.2
1	A	311	THR	6.2
1	A	367	LYS	6.1
1	A	581	GLN	6.0
1	A	801	HIS	6.0
1	A	582	ARG	6.0
1	A	655	LEU	5.9
1	A	397	GLU	5.9
1	A	451	VAL	5.9
1	A	295	ASP	5.9
1	A	598	GLN	5.9
1	A	656	SER	5.8
1	A	539	ASP	5.8
1	A	453	ASN	5.8
1	A	371	LYS	5.8
1	A	841	LYS	5.8
1	A	590	MET	5.7
1	A	360	ASP	5.7
1	A	807	GLU	5.7
1	A	396	ARG	5.6
1	A	862	ASN	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	595	ARG	5.5
1	A	437	LYS	5.5
1	A	436	ASP	5.5
1	A	498	PHE	5.5
1	A	882	TYR	5.4
1	A	317	ALA	5.3
1	A	505	SER	5.3
1	A	412	ILE	5.3
1	A	596	ARG	5.2
1	A	358	LYS	5.2
1	A	657	ARG	5.2
1	A	433	GLU	5.2
1	A	300	TYR	5.1
1	A	312	LYS	5.1
1	A	302	THR	5.1
1	A	422	ALA	5.1
1	A	449	THR	5.1
1	A	388	LYS	5.0
1	A	427	GLU	5.0
1	A	597	ASP	4.9
1	A	440	ASN	4.9
1	A	298	HIS	4.8
1	A	794	THR	4.8
1	A	881	ASP	4.8
1	A	683	ASP	4.7
1	A	407	ALA	4.7
1	A	355	PHE	4.7
1	A	880	THR	4.6
1	A	843	GLU	4.6
1	A	509	GLY	4.6
1	A	368	GLU	4.6
1	A	442	HIS	4.5
1	A	744	ALA	4.5
1	A	275	ASP	4.5
1	A	499	SER	4.5
1	A	403	VAL	4.5
1	A	592	ILE	4.5
1	A	513	HIS	4.4
1	A	301	LYS	4.4
1	A	544	LEU	4.4
1	A	793	THR	4.3
1	A	658	MET	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	448	GLU	4.2
1	A	746	TRP	4.2
1	A	309	TYR	4.2
1	A	627	GLY	4.2
1	A	273	ASN	4.1
1	A	290	THR	4.1
1	A	500	ARG	4.1
1	A	413	PHE	4.1
1	A	306	HIS	4.1
1	A	536	ALA	4.0
1	A	653	GLU	4.0
1	A	845	GLN	4.0
1	A	408	ALA	3.9
1	A	802	GLU	3.9
1	A	286	GLN	3.9
1	A	313	GLN	3.9
1	A	308	SER	3.8
1	A	365	GLU	3.8
1	A	569	PHE	3.8
1	A	424	GLU	3.7
1	A	441	LEU	3.7
1	A	288	HIS	3.7
1	A	405	SER	3.7
1	A	287	GLU	3.7
1	A	297	ASP	3.6
1	A	583	PRO	3.6
1	A	362	ARG	3.6
1	A	889	PHE	3.5
1	A	426	VAL	3.5
1	A	502	ASN	3.4
1	A	445	GLY	3.4
1	A	584	THR	3.4
1	A	478	TRP	3.3
1	A	528	GLY	3.3
1	A	404	ARG	3.3
1	A	291	SER	3.3
1	A	750	GLU	3.3
1	A	535	THR	3.2
1	A	743	GLY	3.2
1	A	875	GLY	3.2
1	A	503	SER	3.2
1	A	454	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	473	ALA	3.1
1	A	344	THR	3.1
1	A	364	GLN	3.1
1	A	501	GLU	3.0
1	A	791	SER	3.0
1	A	289	GLU	3.0
1	A	652	ARG	3.0
1	A	409	LEU	3.0
1	A	806	THR	2.9
1	A	493	ASN	2.9
1	A	296	GLN	2.8
1	A	337	MET	2.8
1	A	883	MET	2.8
1	A	764	LEU	2.8
1	A	279	LYS	2.8
1	A	664	ASP	2.7
1	A	282	GLU	2.7
1	A	830	VAL	2.7
1	A	588	THR	2.7
1	A	410	GLY	2.6
1	A	430	GLY	2.6
1	A	538	TRP	2.6
1	A	320	MET	2.6
1	A	420	LYS	2.6
1	A	356	LYS	2.5
1	A	548	LYS	2.5
1	A	886	MET	2.5
1	A	888	ARG	2.5
1	A	676	SER	2.5
1	A	647	LEU	2.5
1	A	811	THR	2.5
1	A	555	ASN	2.5
1	A	446	LYS	2.5
1	A	890	ARG	2.5
1	A	537	GLY	2.4
1	A	854	THR	2.4
1	A	406	ASN	2.4
1	A	285	LYS	2.4
1	A	556	HIS	2.4
1	A	815	ARG	2.4
1	A	677	ALA	2.4
1	A	631	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	495	ASP	2.4
1	A	577	VAL	2.4
1	A	529	ALA	2.3
1	A	885	SER	2.3
1	A	821	ASN	2.3
1	A	879	TYR	2.3
1	A	477	MET	2.3
1	A	281	ILE	2.3
1	A	602	GLY	2.3
1	A	693	GLN	2.3
1	A	671	ASP	2.2
1	A	819	GLN	2.2
1	A	792	ARG	2.2
1	A	642	ALA	2.2
1	A	319	SER	2.2
1	A	887	LYS	2.2
1	A	824	MET	2.2
1	A	742	GLN	2.2
1	A	624	GLU	2.2
1	A	376	ILE	2.2
1	A	283	LYS	2.1
1	A	383	LYS	2.1
1	A	604	VAL	2.1
1	A	701	ASN	2.1
1	A	342	ALA	2.1
1	A	646	TRP	2.1
1	A	486	PHE	2.1
1	A	644	LYS	2.1
1	A	401	ARG	2.1
1	A	472	ARG	2.1
1	A	648	VAL	2.0
1	A	471	SER	2.0
1	A	497	TRP	2.0
1	A	343	MET	2.0
1	A	552	MET	2.0
1	A	421	SER	2.0
1	A	670	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

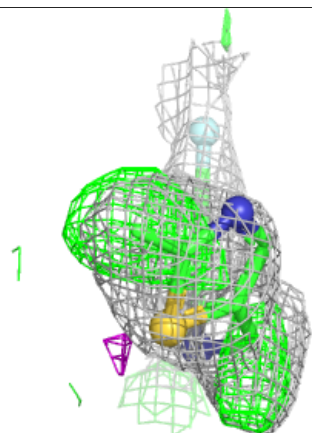
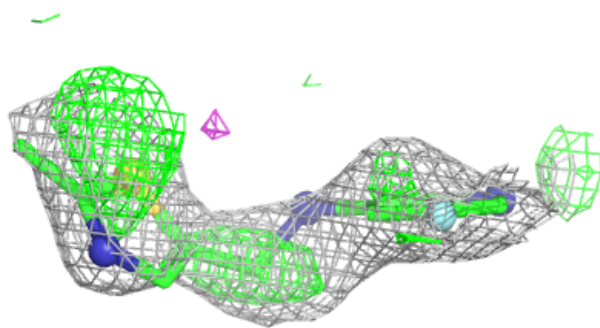
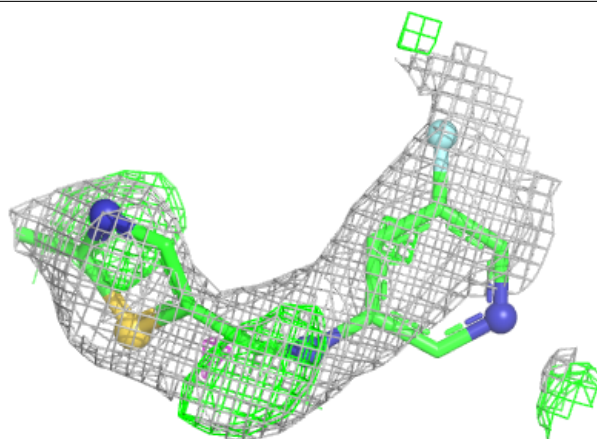
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	PEG	A	1007	7/7	0.56	0.22	98,101,110,118	0
7	WMS	A	1012[A]	15/15	0.73	0.36	42,47,54,55	15
6	PO4	A	1010	5/5	0.76	0.13	94,109,113,118	0
7	WMS	A	1013	15/15	0.77	0.18	41,44,47,50	15
6	PO4	A	1008	5/5	0.78	0.15	48,54,61,79	0
5	PEG	A	1009	7/7	0.78	0.18	106,116,124,131	0
5	PEG	A	1011	7/7	0.86	0.13	82,84,88,89	0
4	DMS	A	1005	4/4	0.88	0.18	76,93,93,94	0
4	DMS	A	1004	4/4	0.94	0.14	68,68,68,78	0
3	MES	A	1003[A]	12/12	0.94	0.27	873,892,918,919	12
3	MES	A	1003[B]	12/12	0.94	0.27	32,41,46,46	12
4	DMS	A	1006	4/4	0.95	0.12	65,67,69,75	0
2	ZN	A	1001	1/1	0.99	0.05	33,33,33,33	0
2	ZN	A	1002	1/1	0.99	0.04	66,66,66,66	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.

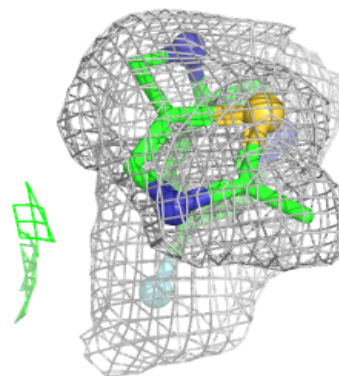
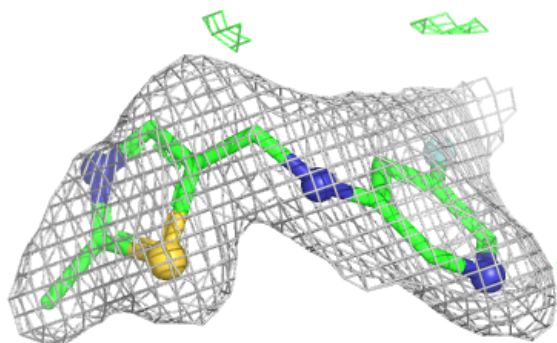
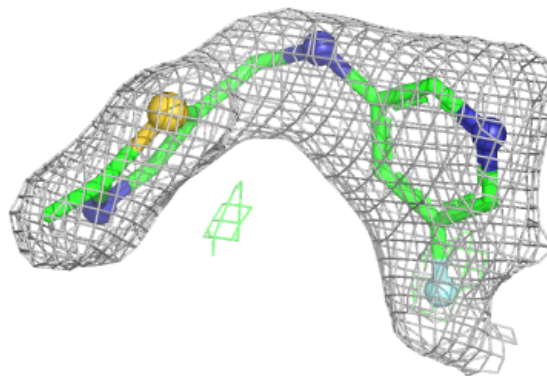
Electron density around WMS A 1012 (A):

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



Electron density around WMS A 1013:

$2mF_o-DF_c$ (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.