



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:42 PM UTC

PDB ID : 7HKX / pdb_00007hkk
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 Z3765495818 (DENV2_NS5A-x0825)
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Deposited on : 2024-10-15
Resolution : 1.82 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)

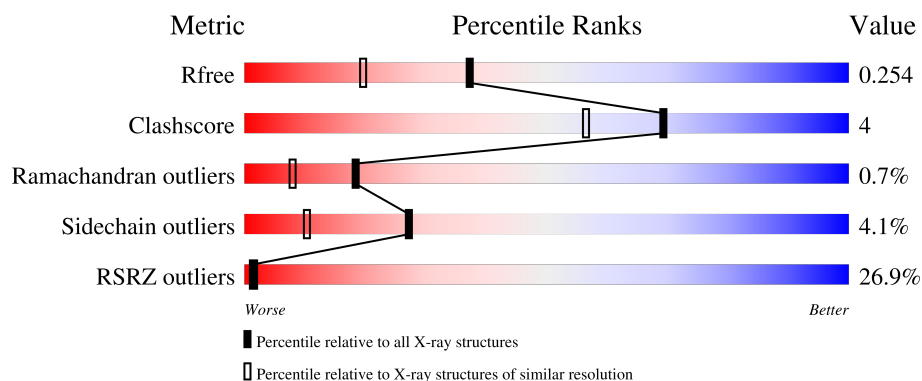
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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	24% 81% 9% 9%

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
6	PEG	A	1010	-	-	-	X
7	PO4	A	1009	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5371 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
1	A	581	Total	C	N	O	S	0	8	0
			4815	3032	864	885	34			

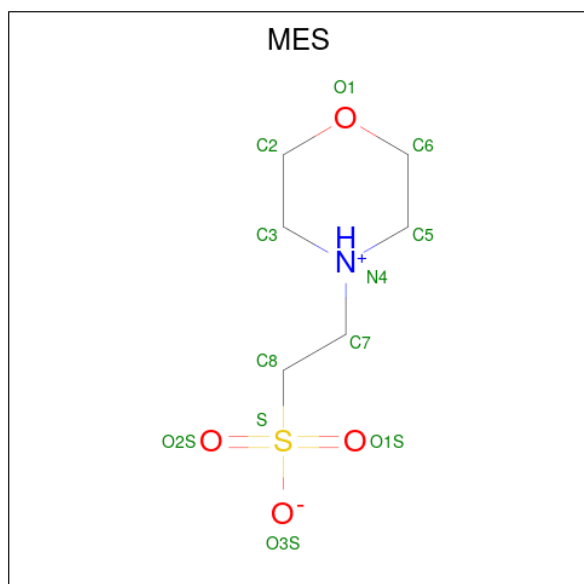
There are 2 discrepancies between the modelled and reference sequences:

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 (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).

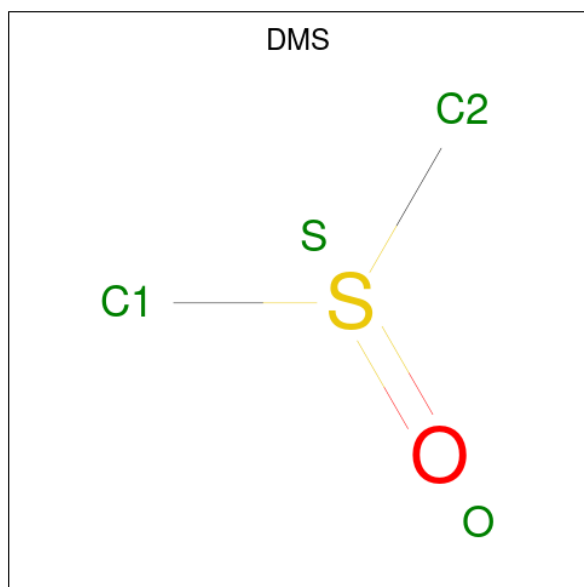


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	1
			24	12	2	8	2		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

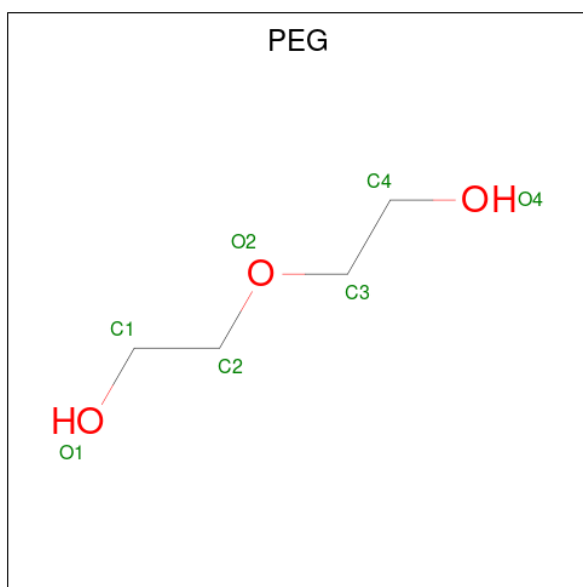
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



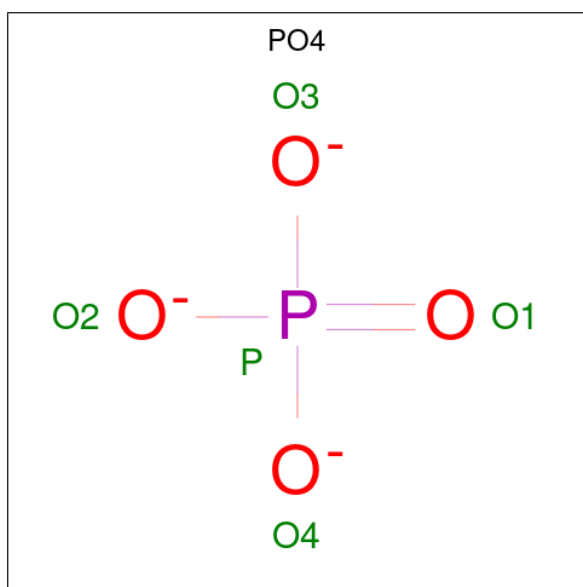
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



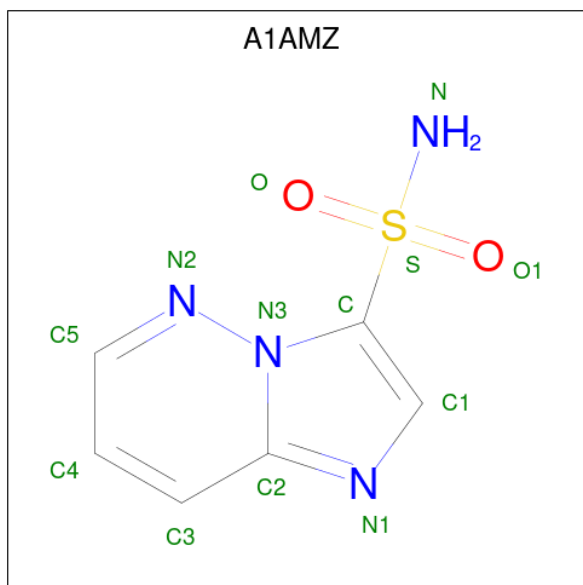
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	P	0	0
			5	4	1		

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

- Molecule 8 is (4R)-imidazo[1,2-b]pyridazine-3-sulfonamide (CCD ID: A1AMZ) (formula: $C_6H_6N_4O_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	S	0	0
			13	6	4	2	1		
8	A	1	Total	C	N	O	S	0	0
			13	6	4	2	1		
8	A	1	Total	C	N	O	S	0	0
			13	6	4	2	1		

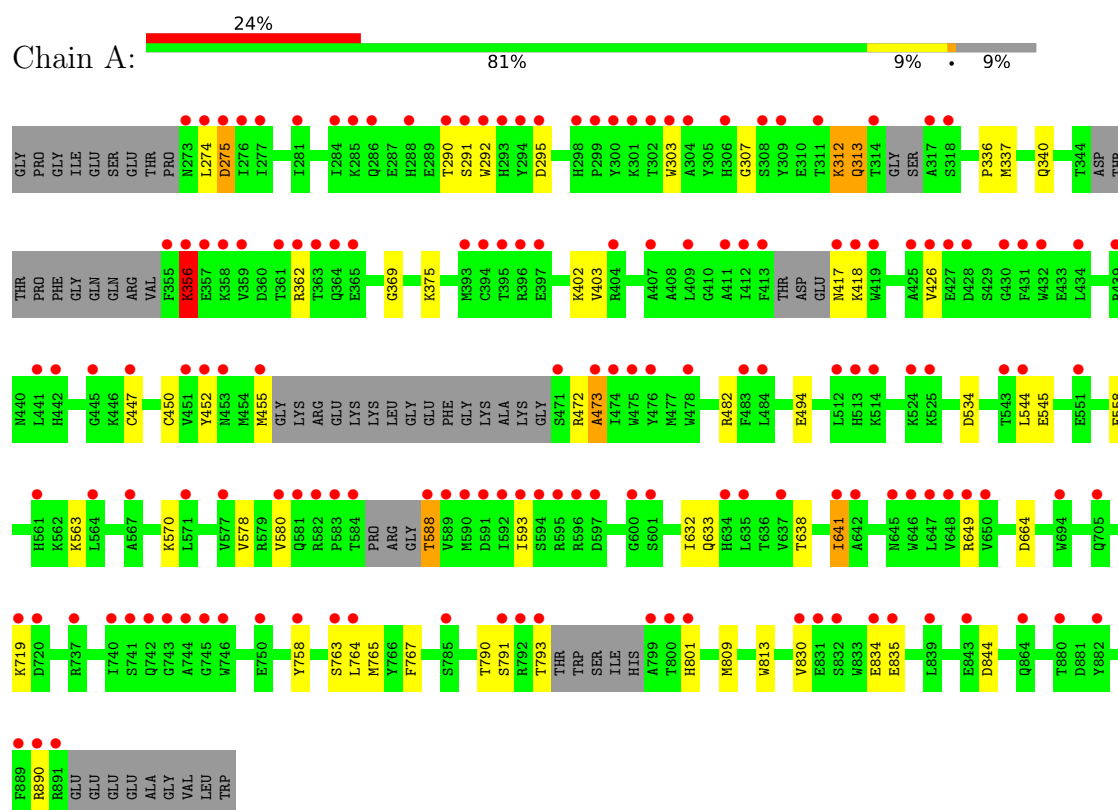
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	447	Total	O	0	1
			447	447		

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: Genome polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	82.01Å 116.51Å 148.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.58 – 1.82 91.58 – 1.82	Depositor EDS
% Data completeness (in resolution range)	99.2 (91.58-1.82) 99.5 (91.58-1.82)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 1.82Å)	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC5	Depositor
R, R_{free}	0.202 , 0.243 0.223 , 0.254	Depositor DCC
R_{free} test set	3311 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 59.4	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	0.94	EDS
Total number of atoms	5371	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% 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: CL, PO4, MES, DMS, A1AMZ, PEG, ZN

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	1.05	1/4922 (0.0%)	1.35	2/6635 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	813	TRP	C-O	5.12	1.29	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	844	ASP	CA-CB-CG	5.67	118.27	112.60
1	A	356	LYS	N-CA-C	-5.11	107.06	113.15

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	4815	0	4713	31	0
2	A	2	0	0	0	0
3	A	24	0	26	0	0
4	A	1	0	0	0	0
5	A	12	0	18	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	21	0	30	0	0
7	A	10	0	0	3	0
8	A	39	0	0	0	0
9	A	447	0	0	8	3
All	All	5371	0	4787	34	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 (34) 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	7:A:1009:PO4:O4	1.96	0.83
1:A:638:THR:O	1:A:641:ILE:HG22	1.91	0.69
5:A:1005:DMS:H11	9:A:1219:HOH:O	1.94	0.67
1:A:534:ASP:OD1	7:A:1009:PO4:O4	2.12	0.67
1:A:664:ASP:OD1	7:A:1009:PO4:P	2.56	0.64
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.41	0.60
5:A:1005:DMS:H12	9:A:1336:HOH:O	2.04	0.56
1:A:337:MET:HG2	9:A:1382:HOH:O	2.09	0.53
1:A:830:VAL:HG13	1:A:835:GLU:HB2	1.93	0.51
1:A:758:TYR:CD1	5:A:1007:DMS:H21	2.47	0.50
1:A:275:ASP:OD1	1:A:275:ASP:N	2.44	0.49
1:A:763[A]:SER:O	1:A:767:PHE:HB3	2.13	0.48
1:A:809:MET:HA	1:A:809:MET:HE2	1.96	0.48
1:A:356:LYS:O	1:A:356:LYS:HD2	2.14	0.47
1:A:336:PRO:O	1:A:340:GLN:HG3	2.17	0.45
1:A:580:VAL:HG21	1:A:593:ILE:HD11	1.99	0.45
1:A:303:TRP:CE3	1:A:593:ILE:HD12	2.52	0.45
1:A:545:GLU:HG3	9:A:1271:HOH:O	2.16	0.45
1:A:834:GLU:OE2	1:A:890:ARG:NE	2.51	0.44
1:A:764:LEU:C	1:A:765:MET:HE2	2.43	0.44
1:A:790:THR:HG22	9:A:1389:HOH:O	2.18	0.44
1:A:312:LYS:HA	1:A:588:THR:HG21	2.00	0.43
1:A:764:LEU:O	1:A:765:MET:HE2	2.18	0.43
1:A:452:TYR:O	1:A:578:VAL:HA	2.18	0.43
1:A:369:GLY:HA3	1:A:632:ILE:O	2.18	0.43
1:A:563:LYS:HE3	9:A:1124:HOH:O	2.19	0.43
1:A:801[B]:HIS:CD2	1:A:801[B]:HIS:H	2.37	0.43
1:A:719[A]:LYS:NZ	9:A:1108:HOH:O	2.39	0.43
1:A:295:ASP:OD1	1:A:295:ASP:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:LYS:O	1:A:313:GLN:HG3	2.19	0.42
1:A:402:LYS:NZ	1:A:494:GLU:OE2	2.52	0.42
1:A:292:TRP:CZ2	1:A:307:GLY:HA3	2.55	0.41
5:A:1005:DMS:C1	9:A:1219:HOH:O	2.61	0.41
1:A:472:ARG:O	1:A:473:ALA:HB2	2.22	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:1154:HOH:O	9:A:1154:HOH:O[2_445]	1.85	0.35
9:A:1408:HOH:O	9:A:1408:HOH:O[4_545]	2.05	0.15
9:A:1324:HOH:O	9:A:1324:HOH:O[4_545]	2.18	0.02

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	575/637 (90%)	542 (94%)	29 (5%)	4 (1%)	18 8

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	312	LYS
1	A	473	ALA
1	A	313	GLN
1	A	418	LYS

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	517/554 (93%)	496 (96%)	21 (4%)	27	10

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	274	LEU
1	A	275	ASP
1	A	290	THR
1	A	291	SER
1	A	356	LYS
1	A	362	ARG
1	A	375	LYS
1	A	403	VAL
1	A	417	ASN
1	A	426	VAL
1	A	455	MET
1	A	482	ARG
1	A	544	LEU
1	A	558	GLU
1	A	570	LYS
1	A	588	THR
1	A	633	GLN
1	A	641	ILE
1	A	649	ARG
1	A	791	SER
1	A	793	THR

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	298	HIS
1	A	313	GLN
1	A	417	ASN
1	A	581	GLN

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Mol	Chain	Res	Type
1	A	701	ASN
1	A	786	HIS

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 16 ligands modelled in this entry, 3 are monoatomic - leaving 13 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	A1AMZ	A	1013	-	12,14,14	1.40	1 (8%)	15,21,21	0.80	1 (6%)
7	PO4	A	1009	-	4,4,4	2.54	1 (25%)	6,6,6	0.51	0
7	PO4	A	1011	-	4,4,4	0.93	0	6,6,6	0.43	0
8	A1AMZ	A	1014	-	12,14,14	1.41	1 (8%)	15,21,21	0.83	1 (6%)
6	PEG	A	1010	-	6,6,6	0.11	0	5,5,5	0.07	0
5	DMS	A	1005	-	3,3,3	0.23	0	3,3,3	0.25	0
6	PEG	A	1008	-	6,6,6	0.15	0	5,5,5	0.06	0
3	MES	A	1003[B]	-	12,12,12	0.71	0	15,16,16	0.28	0
3	MES	A	1003[A]	-	12,12,12	0.69	0	15,16,16	0.29	0
5	DMS	A	1007	-	3,3,3	0.14	0	3,3,3	0.28	0
5	DMS	A	1006	-	3,3,3	0.27	0	3,3,3	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PEG	A	1012	-	6,6,6	0.11	0	5,5,5	0.07	0
8	A1AMZ	A	1015	-	12,14,14	1.26	1 (8%)	15,21,21	0.86	1 (6%)

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	A1AMZ	A	1013	-	-	2/4/6/6	0/2/2/2
8	A1AMZ	A	1014	-	-	1/4/6/6	0/2/2/2
6	PEG	A	1010	-	-	2/4/4/4	-
6	PEG	A	1008	-	-	3/4/4/4	-
3	MES	A	1003[B]	-	-	5/6/14/14	0/1/1/1
3	MES	A	1003[A]	-	-	1/6/14/14	0/1/1/1
6	PEG	A	1012	-	-	3/4/4/4	-
8	A1AMZ	A	1015	-	-	0/4/6/6	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1014	A1AMZ	C5-N2	4.76	1.37	1.31
8	A	1013	A1AMZ	C5-N2	4.72	1.37	1.31
7	A	1009	PO4	P-O1	4.49	1.61	1.50
8	A	1015	A1AMZ	C5-N2	4.22	1.36	1.31

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1015	A1AMZ	C-C1-N1	-2.79	110.90	114.45
8	A	1013	A1AMZ	C-C1-N1	-2.68	111.03	114.45
8	A	1014	A1AMZ	C-C1-N1	-2.30	111.52	114.45

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1003[B]	MES	C8-C7-N4-C3
3	A	1003[B]	MES	C8-C7-N4-C5
3	A	1003[B]	MES	C7-C8-S-O1S

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Mol	Chain	Res	Type	Atoms
8	A	1013	A1AMZ	C1-C-S-O
8	A	1013	A1AMZ	C1-C-S-O1
8	A	1014	A1AMZ	C1-C-S-O1
6	A	1008	PEG	C4-C3-O2-C2
6	A	1008	PEG	O1-C1-C2-O2
3	A	1003[B]	MES	C7-C8-S-O3S
6	A	1008	PEG	O2-C3-C4-O4
6	A	1012	PEG	O1-C1-C2-O2
6	A	1012	PEG	O2-C3-C4-O4
6	A	1010	PEG	O2-C3-C4-O4
3	A	1003[B]	MES	C7-C8-S-O2S
6	A	1010	PEG	C1-C2-O2-C3
6	A	1012	PEG	C4-C3-O2-C2
3	A	1003[A]	MES	C8-C7-N4-C3

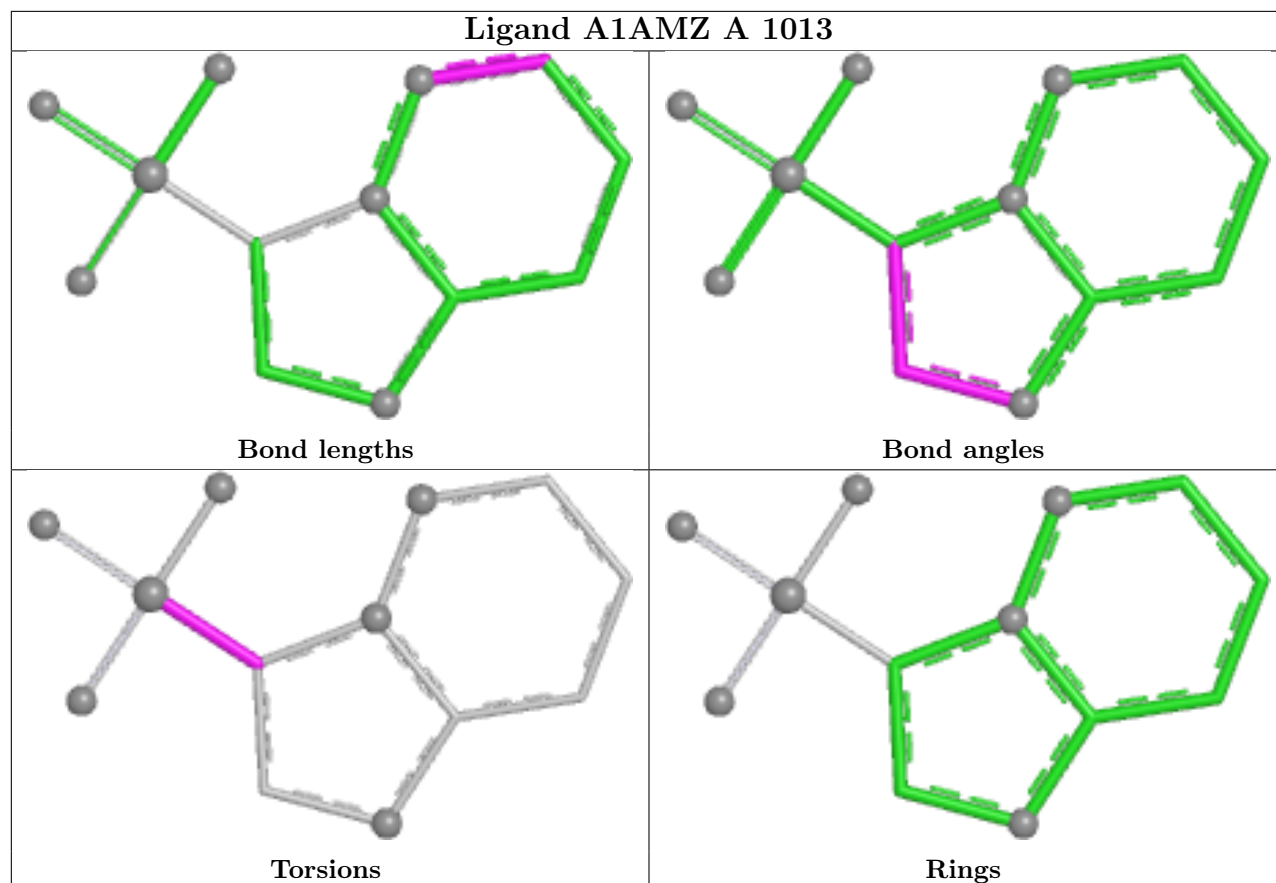
There are no ring outliers.

3 monomers are involved in 7 short contacts:

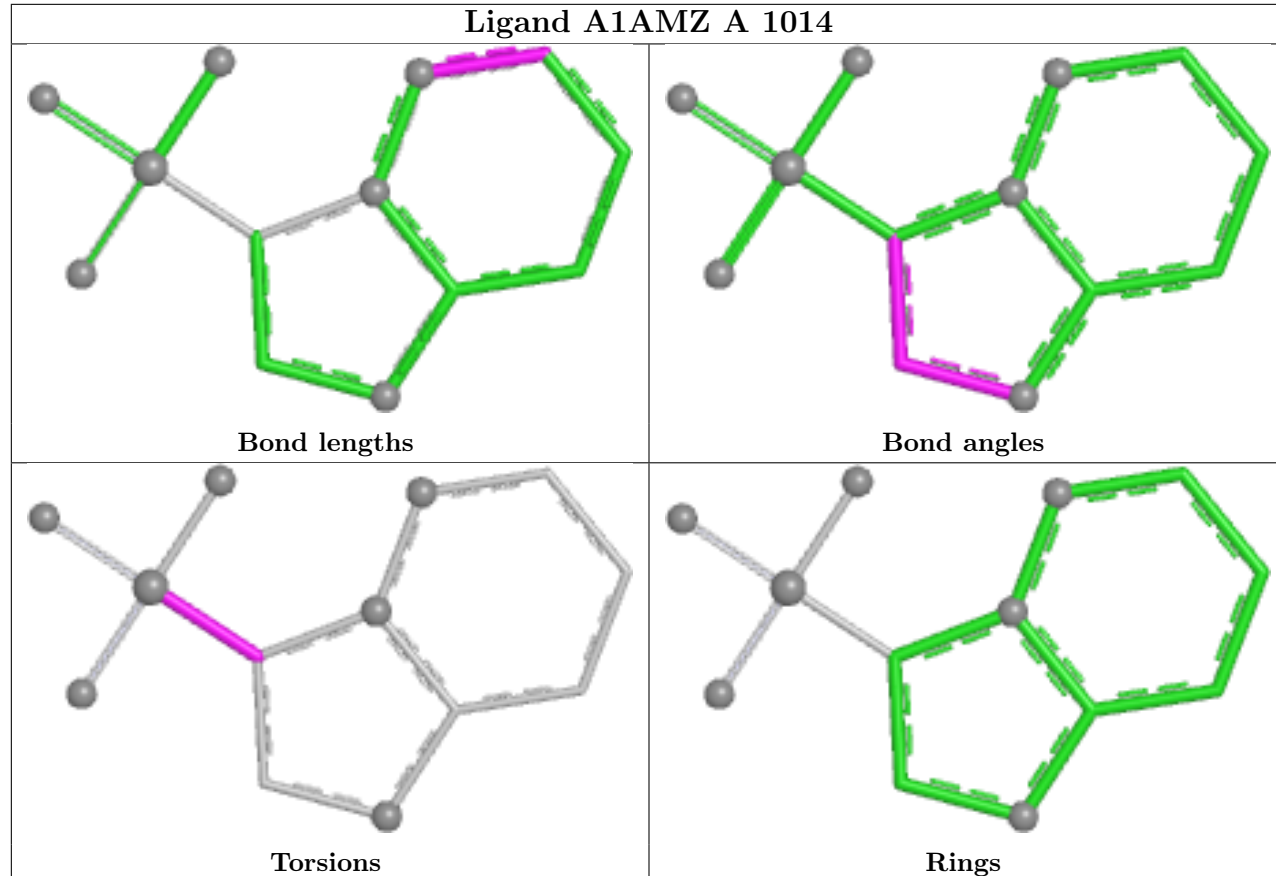
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1009	PO4	3	0
5	A	1005	DMS	3	0
5	A	1007	DMS	1	0

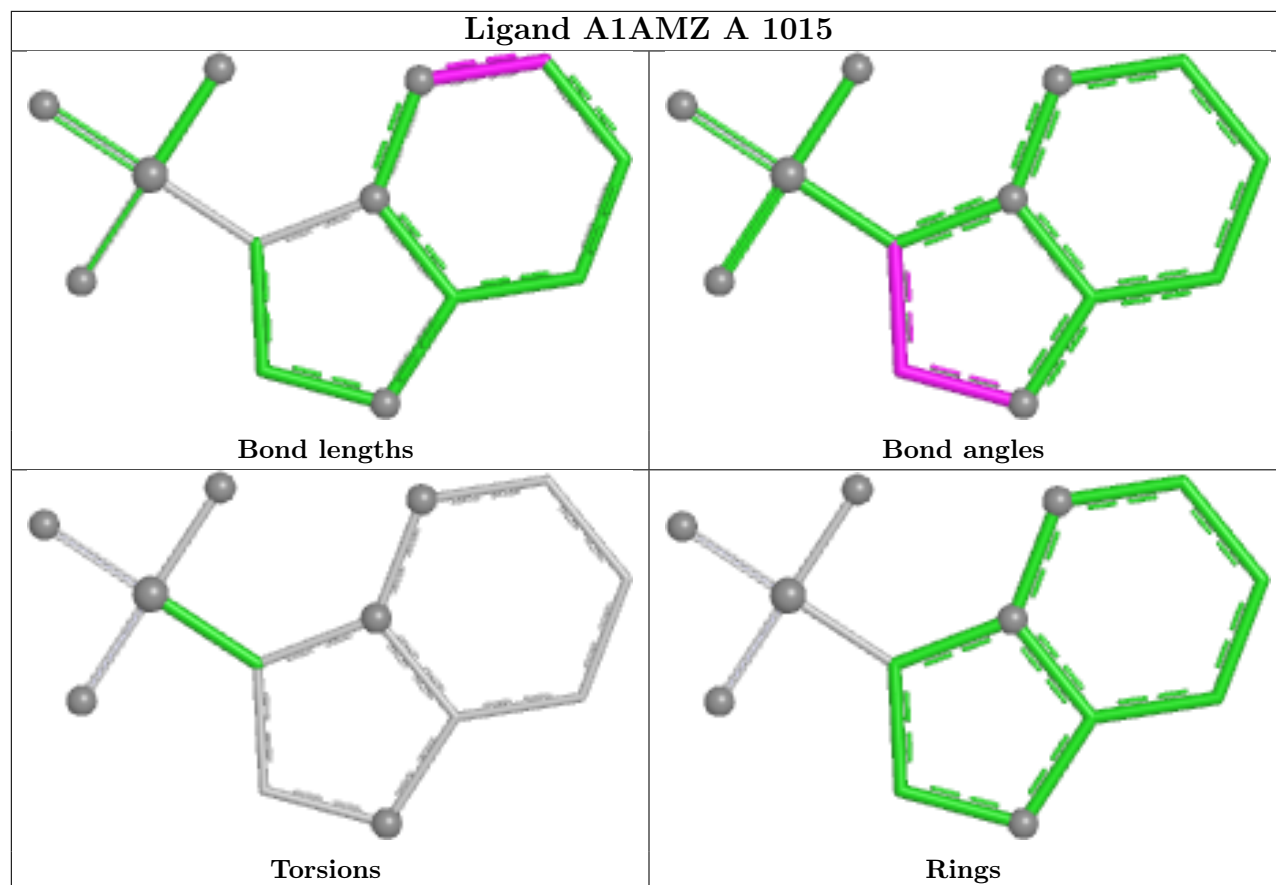
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 A1AMZ A 1013



Ligand A1AMZ A 1014





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	581/637 (91%)	1.53	156 (26%) 1 1	6, 37, 109, 152	50 (8%)

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	646	TRP	15.0
1	A	648	VAL	13.5
1	A	801[A]	HIS	13.5
1	A	741[A]	SER	12.9
1	A	740	ILE	12.9
1	A	512[A]	LEU	12.7
1	A	650	VAL	12.2
1	A	647	LEU	12.2
1	A	642	ALA	11.5
1	A	719[A]	LYS	11.0
1	A	758	TYR	10.2
1	A	832	SER	10.1
1	A	839	LEU	9.9
1	A	513	HIS	9.6
1	A	763[A]	SER	8.8
1	A	835	GLU	8.7
1	A	649	ARG	8.7
1	A	525	LYS	8.5
1	A	514	LYS	8.4
1	A	785[A]	SER	8.2
1	A	551[A]	GLU	8.1
1	A	524	LYS	8.1
1	A	864[A]	GLN	8.0
1	A	645	ASN	8.0
1	A	720	ASP	7.7
1	A	705	GLN	7.7
1	A	834	GLU	7.3

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Mol	Chain	Res	Type	RSRZ
1	A	742	GLN	7.2
1	A	737	ARG	6.9
1	A	363	THR	6.8
1	A	589	VAL	6.6
1	A	831	GLU	6.3
1	A	799	ALA	5.8
1	A	543	THR	5.7
1	A	600	GLY	5.7
1	A	595	ARG	5.6
1	A	292	TRP	5.6
1	A	594	SER	5.5
1	A	544	LEU	5.4
1	A	843	GLU	5.4
1	A	355	PHE	5.4
1	A	317	ALA	5.0
1	A	483	PHE	4.8
1	A	475	TRP	4.7
1	A	413	PHE	4.7
1	A	474	ILE	4.6
1	A	293	HIS	4.6
1	A	311	THR	4.4
1	A	411	ALA	4.3
1	A	431	PHE	4.2
1	A	294	TYR	4.2
1	A	395	THR	4.2
1	A	281	ILE	4.1
1	A	419	TRP	4.1
1	A	394	CYS	4.1
1	A	597	ASP	4.1
1	A	412	ILE	4.1
1	A	409	LEU	3.9
1	A	596	ARG	3.9
1	A	396	ARG	3.9
1	A	359	VAL	3.9
1	A	426	VAL	3.8
1	A	308	SER	3.8
1	A	393	MET	3.8
1	A	284	ILE	3.8
1	A	290	THR	3.7
1	A	356	LYS	3.7
1	A	792	ARG	3.7
1	A	473	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	793	THR	3.6
1	A	314	THR	3.6
1	A	299	PRO	3.6
1	A	365	GLU	3.5
1	A	583	PRO	3.5
1	A	584	THR	3.5
1	A	439	ARG	3.5
1	A	407	ALA	3.5
1	A	591	ASP	3.4
1	A	361	THR	3.4
1	A	588	THR	3.4
1	A	273	ASN	3.4
1	A	288	HIS	3.3
1	A	362	ARG	3.3
1	A	744	ALA	3.3
1	A	637	VAL	3.3
1	A	428	ASP	3.3
1	A	889	PHE	3.3
1	A	452	TYR	3.2
1	A	890	ARG	3.1
1	A	750	GLU	3.1
1	A	577	VAL	3.1
1	A	455	MET	3.1
1	A	634	HIS	3.1
1	A	304	ALA	3.1
1	A	298	HIS	3.0
1	A	274	LEU	3.0
1	A	590	MET	3.0
1	A	743	GLY	3.0
1	A	791	SER	3.0
1	A	277	ILE	2.9
1	A	484	LEU	2.9
1	A	447	CYS	2.9
1	A	303	TRP	2.8
1	A	582	ARG	2.8
1	A	309	TYR	2.8
1	A	564	LEU	2.8
1	A	561	HIS	2.7
1	A	593	ILE	2.7
1	A	276	ILE	2.7
1	A	430	GLY	2.7
1	A	800	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	295	ASP	2.6
1	A	434	LEU	2.6
1	A	635	LEU	2.6
1	A	882	TYR	2.6
1	A	581	GLN	2.6
1	A	641	ILE	2.6
1	A	592	ILE	2.5
1	A	364	GLN	2.5
1	A	318	SER	2.5
1	A	285	LYS	2.5
1	A	397	GLU	2.4
1	A	442	HIS	2.4
1	A	601	SER	2.4
1	A	404	ARG	2.3
1	A	427	GLU	2.3
1	A	880	THR	2.3
1	A	358	LYS	2.3
1	A	478	TRP	2.3
1	A	302	THR	2.3
1	A	425	ALA	2.3
1	A	746	TRP	2.3
1	A	471	SER	2.3
1	A	301	LYS	2.3
1	A	694	TRP	2.2
1	A	891	ARG	2.2
1	A	830	VAL	2.2
1	A	291	SER	2.2
1	A	745	GLY	2.2
1	A	476	TYR	2.2
1	A	306	HIS	2.2
1	A	451	VAL	2.2
1	A	275	ASP	2.2
1	A	571	LEU	2.2
1	A	418	LYS	2.1
1	A	286	GLN	2.1
1	A	445	GLY	2.1
1	A	417	ASN	2.1
1	A	300	TYR	2.1
1	A	432	TRP	2.1
1	A	453	ASN	2.1
1	A	764	LEU	2.1
1	A	580	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	441	LEU	2.0
1	A	567	ALA	2.0
1	A	357	GLU	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.

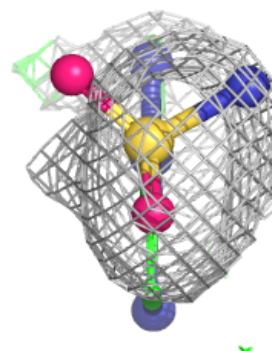
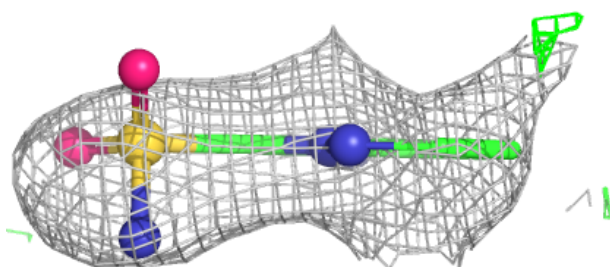
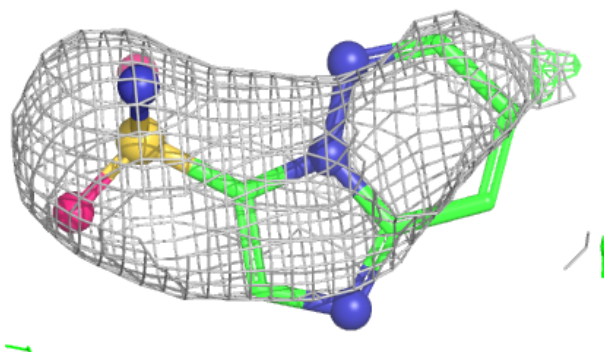
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	PEG	A	1010	7/7	0.40	0.42	258,260,263,264	7
6	PEG	A	1008	7/7	0.58	0.36	56,59,61,62	7
7	PO4	A	1011	5/5	0.68	0.16	72,82,95,102	0
8	A1AMZ	A	1015	13/13	0.70	0.24	97,99,104,104	13
7	PO4	A	1009	5/5	0.73	0.15	44,45,60,73	0
6	PEG	A	1012	7/7	0.79	0.17	58,64,67,68	0
8	A1AMZ	A	1014	13/13	0.80	0.18	61,63,66,69	13
5	DMS	A	1006	4/4	0.82	0.23	82,95,95,101	0
8	A1AMZ	A	1013	13/13	0.91	0.13	39,41,48,48	13
5	DMS	A	1005	4/4	0.96	0.12	45,46,47,48	0
5	DMS	A	1007	4/4	0.97	0.09	51,51,52,57	0
3	MES	A	1003[A]	12/12	0.97	0.33	23,25,27,27	12
3	MES	A	1003[B]	12/12	0.97	0.33	586,603,641,643	12
4	CL	A	1004	1/1	0.98	0.07	38,38,38,38	0
2	ZN	A	1002	1/1	0.99	0.06	53,53,53,53	0
2	ZN	A	1001	1/1	1.00	0.04	23,23,23,23	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.

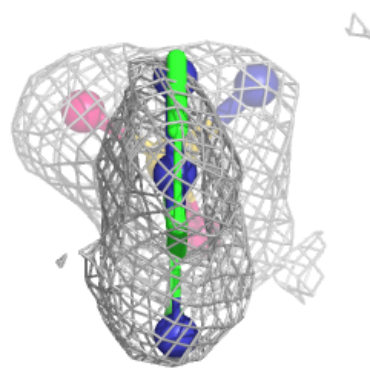
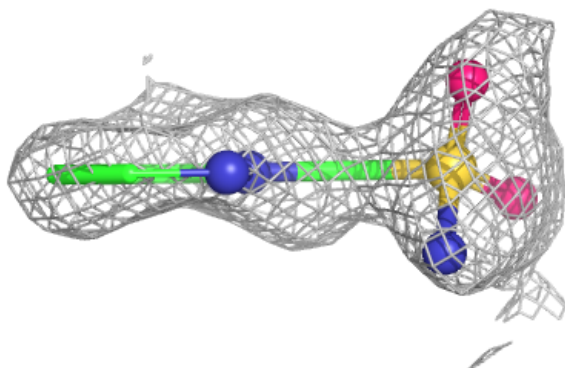
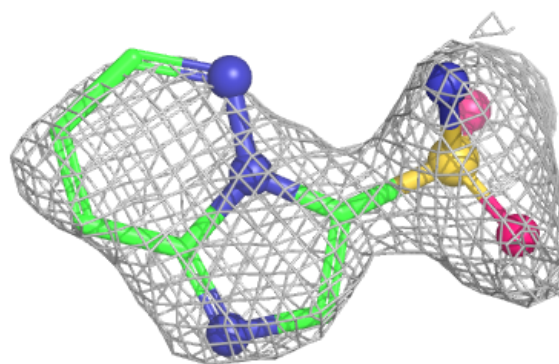
Electron density around A1AMZ A 1015:

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



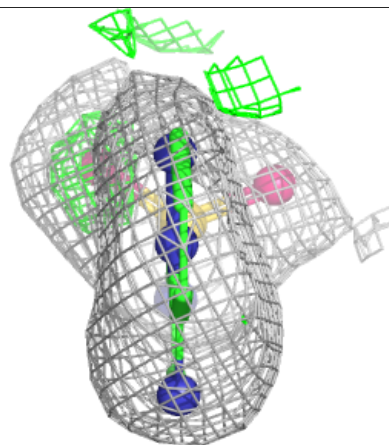
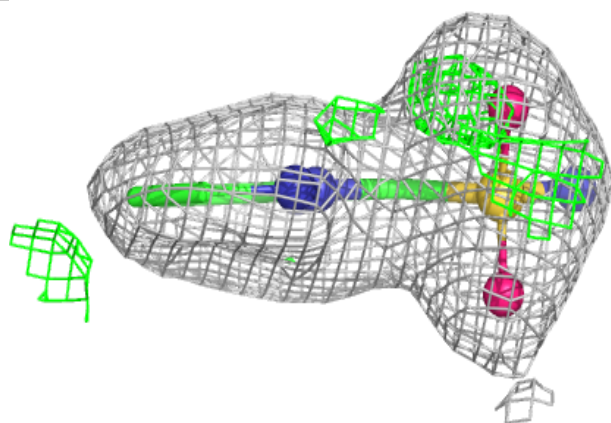
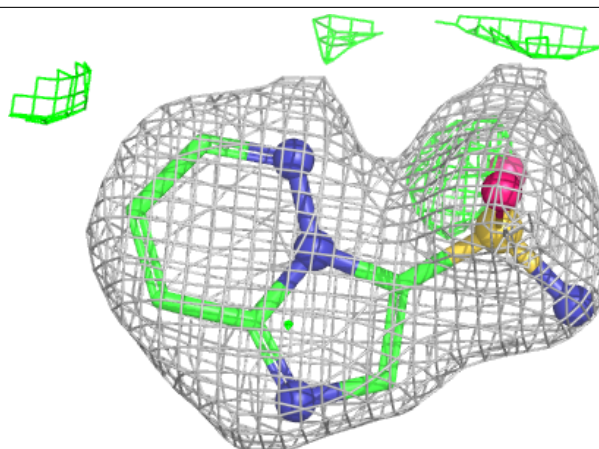
Electron density around A1AMZ A 1014:

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



Electron density around A1AMZ 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.