Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2025 – 10:37 AM EDT

PDB ID	:	7I2O
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 Z1787627869 (DNV2_NS5A-x0587)
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Deposited on	:	2025-03-06
Resolution	:	1.86 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:

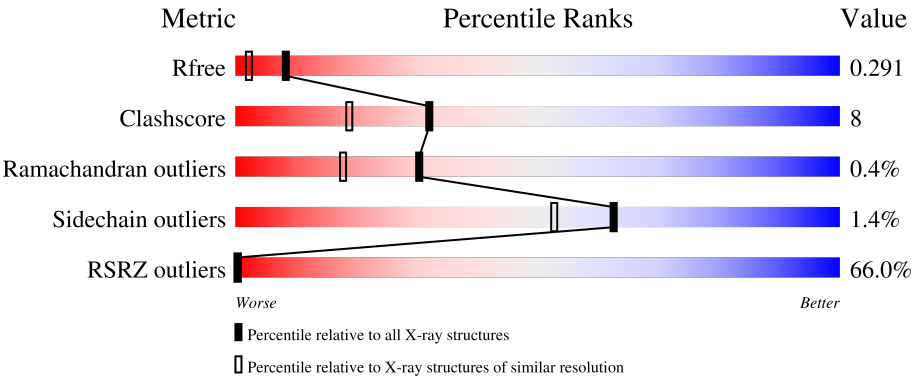
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3097 (1.86-1.86)
Clashscore	180529	3359 (1.86-1.86)
Ramachandran outliers	177936	3335 (1.86-1.86)
Sidechain outliers	177891	3335 (1.86-1.86)
RSRZ outliers	164620	3097 (1.86-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	637	59% 78% 11% • 10%

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	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5112 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	571	4719	2972	847	866	34	0	6	0

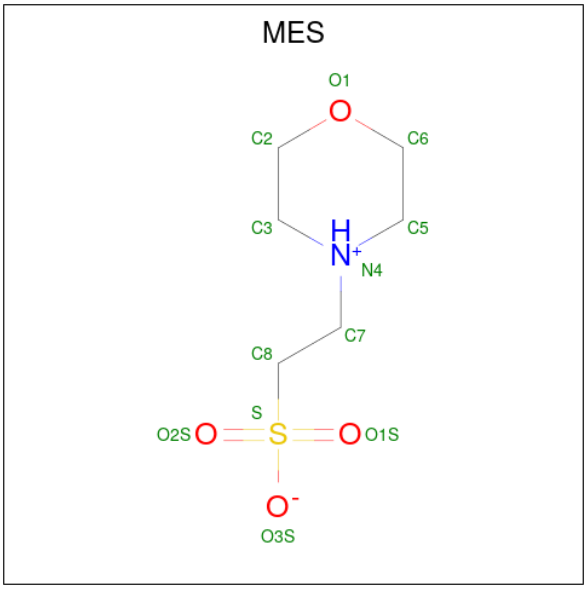
There are 2 discrepancies between the modelled and reference sequences:

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

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

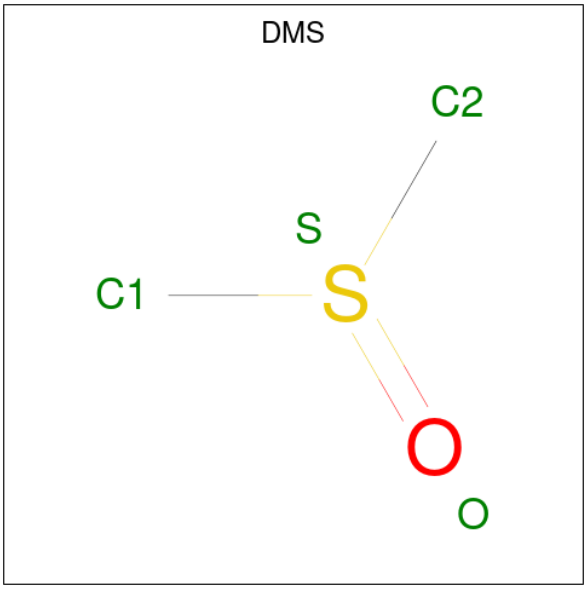
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	2	2	2	0	0

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



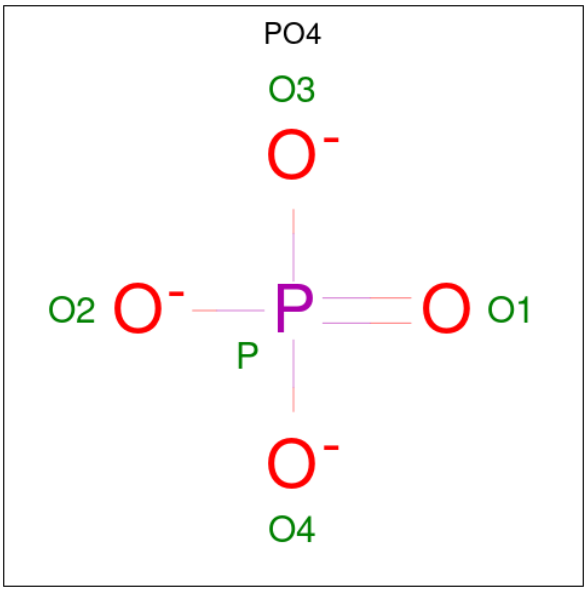
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	1
			24	12	2	8	2		

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



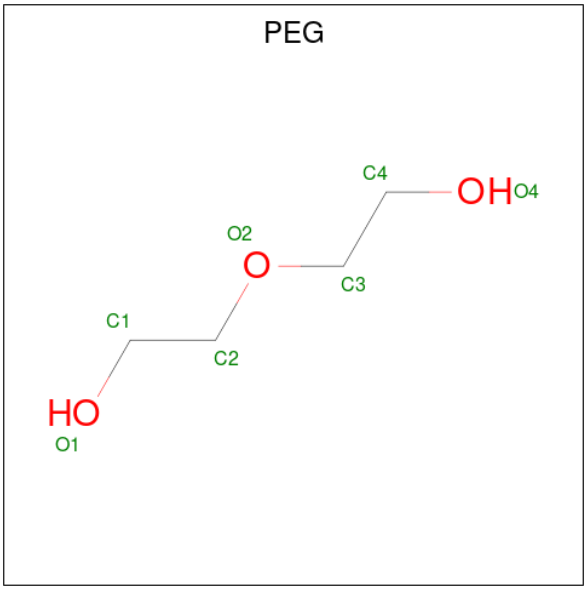
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	O	S		0	0
			4	2	1	1			
4	A	1	Total	C	O	S		0	0
			4	2	1	1			
4	A	1	Total	C	O	S		0	0
			4	2	1	1			

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



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

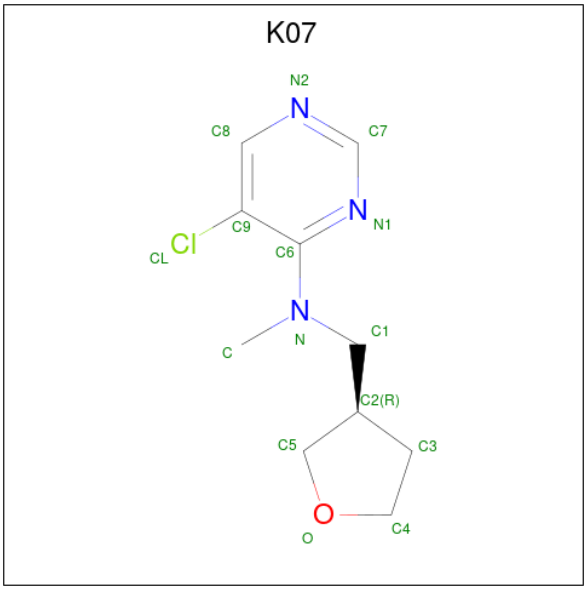
- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 7 is 5-chloro-N-methyl-N-{[(3R)-oxolan-3-yl]methyl}pyrimidin-4-amine (three-

letter code: K07) (formula: $C_{10}H_{14}ClN_3O$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 8 is water.

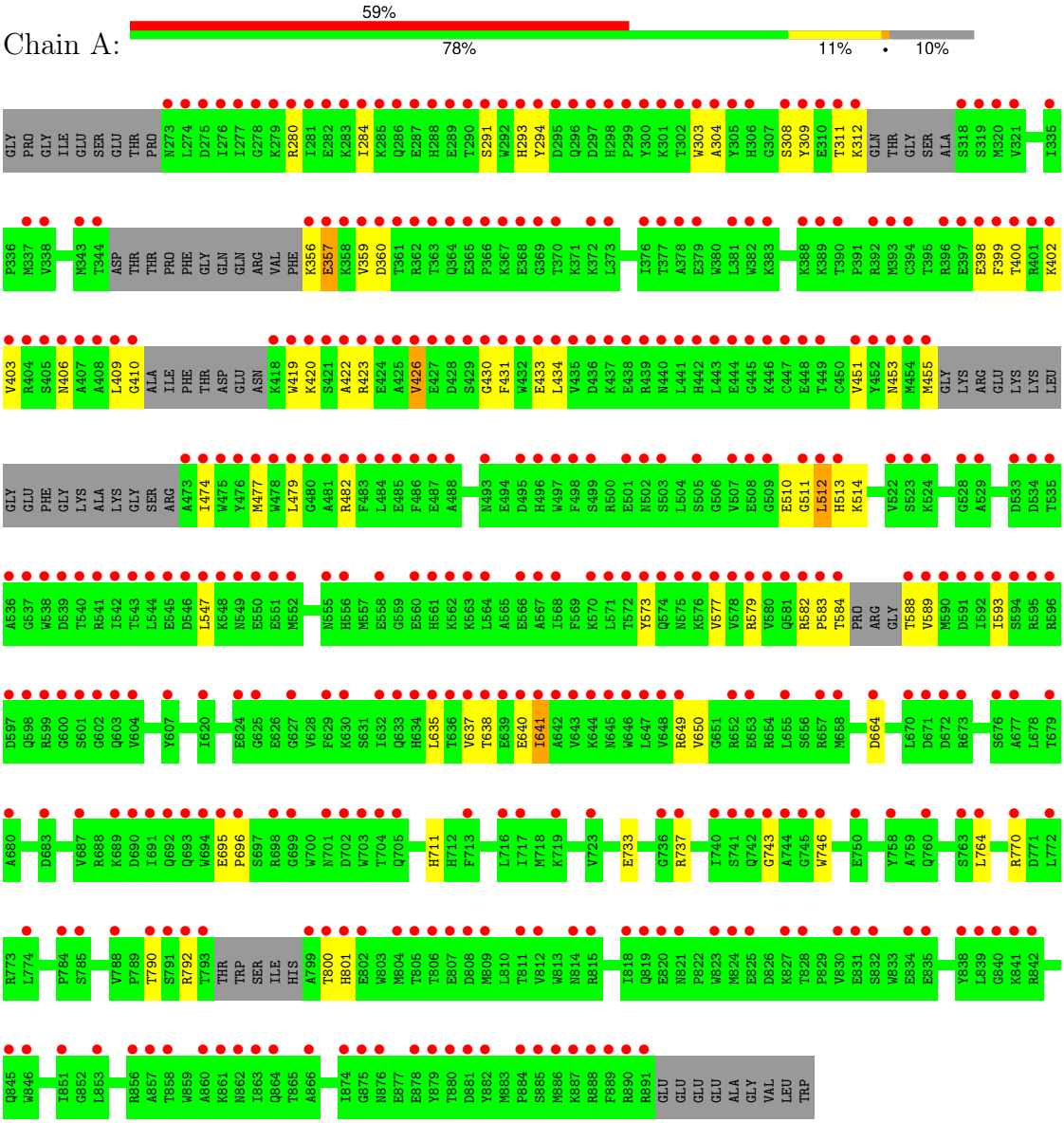
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	323	Total	O	0	0
			323	323		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: NS5 RNA-dependent RNA polymerase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	82.45Å 116.26Å 146.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.47 – 1.86 73.47 – 1.86	Depositor EDS
% Data completeness (in resolution range)	97.2 (73.47-1.86) 97.2 (73.47-1.86)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.98 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.197 , 0.244 0.265 , 0.291	Depositor DCC
R_{free} test set	3086 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å^2)	37.1	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 168.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	5112	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PO4, K07, DMS, MES, PEG

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	0/4824	0.80	0/6503

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	511	GLY	Mainchain
1	A	512[B]	LEU	Mainchain
1	A	800	THR	Mainchain
1	A	801[A]	HIS	Mainchain
1	A	801[B]	HIS	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4719	0	4626	71	0
2	A	2	0	0	0	0
3	A	24	0	26	0	0
4	A	12	0	18	2	0
5	A	10	0	0	2	0
6	A	7	0	10	0	0
7	A	15	0	0	3	0
8	A	323	0	0	4	2
All	All	5112	0	4680	75	2

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 8.

All (75) 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:746:TRP:NE1	1:A:792:ARG:CZ	1.99	1.25
1:A:430:GLY:HA2	1:A:433:GLU:OE1	1.51	1.10
1:A:746:TRP:CD1	1:A:792:ARG:NH2	2.21	1.08
1:A:746:TRP:HE1	1:A:792:ARG:CZ	1.82	0.92
1:A:746:TRP:NE1	1:A:792:ARG:NH2	2.20	0.89
7:A:1010:K07:C	7:A:1010:K07:CL	2.63	0.84
1:A:746:TRP:CE2	1:A:792:ARG:CZ	2.63	0.81
1:A:746:TRP:CE2	1:A:792:ARG:NE	2.48	0.81
1:A:746:TRP:CZ2	1:A:792:ARG:NE	2.49	0.81
1:A:664:ASP:OD1	5:A:1007:PO4:O4	2.00	0.80
1:A:312:LYS:HA	1:A:588:THR:HG21	1.64	0.79
1:A:430:GLY:HA2	1:A:433:GLU:CD	2.02	0.79
1:A:311:THR:O	1:A:312:LYS:HG3	1.83	0.78
1:A:746:TRP:HE1	1:A:792:ARG:NH1	1.84	0.75
1:A:733:GLU:O	1:A:737:ARG:HG3	1.87	0.75
1:A:474:ILE:HD12	1:A:474:ILE:N	2.04	0.72
1:A:638:THR:O	1:A:641:ILE:HG23	1.88	0.72
1:A:294:TYR:CD1	1:A:294:TYR:O	2.44	0.70
1:A:649:ARG:HG2	1:A:650:VAL:HG13	1.77	0.67
1:A:474:ILE:HD12	1:A:474:ILE:H	1.59	0.66
1:A:400:THR:O	1:A:403:VAL:HG22	1.97	0.65
1:A:291:SER:O	1:A:309:TYR:HA	1.97	0.65
1:A:746:TRP:CZ2	1:A:792:ARG:CD	2.80	0.65
1:A:638:THR:HA	1:A:641:ILE:CG2	2.28	0.64
1:A:294:TYR:O	1:A:294:TYR:HD1	1.82	0.61
1:A:357:GLU:CD	1:A:357:GLU:C	2.58	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1004:DMS:C1	8:A:1259:HOH:O	2.48	0.61
1:A:746:TRP:CZ2	1:A:792:ARG:HG3	2.37	0.60
1:A:400:THR:HA	1:A:426:VAL:HG21	1.85	0.59
1:A:664:ASP:OD1	5:A:1007:PO4:P	2.61	0.58
1:A:637:VAL:O	1:A:641:ILE:HG22	2.04	0.57
1:A:746:TRP:NE1	1:A:792:ARG:NH1	2.45	0.57
1:A:356:LYS:HG2	1:A:357:GLU:H	1.70	0.56
1:A:356:LYS:HB3	1:A:359:VAL:CG1	2.36	0.56
1:A:399:PHE:O	1:A:403:VAL:HG13	2.08	0.54
4:A:1004:DMS:H11	8:A:1259:HOH:O	2.05	0.54
1:A:582:ARG:HG2	1:A:584:THR:OG1	2.07	0.54
1:A:746:TRP:HZ2	1:A:792:ARG:CD	2.18	0.54
1:A:312:LYS:HA	1:A:588:THR:CG2	2.37	0.53
1:A:356:LYS:HB3	1:A:359:VAL:HG12	1.92	0.52
1:A:451:VAL:HG13	1:A:577:VAL:HG12	1.92	0.51
1:A:547:LEU:HD13	1:A:573:TYR:O	2.11	0.51
1:A:422:ALA:HB1	1:A:479:LEU:HD22	1.92	0.51
1:A:510:GLU:O	1:A:514:LYS:HG3	2.11	0.50
1:A:280:ARG:O	1:A:284:ILE:HG13	2.13	0.48
1:A:409:LEU:O	1:A:410:GLY:C	2.51	0.48
1:A:398:GLU:O	1:A:402:LYS:HG3	2.14	0.48
1:A:304:ALA:O	1:A:593:ILE:HA	2.13	0.47
1:A:635:LEU:HD23	1:A:640:GLU:HG2	1.95	0.47
1:A:431:PHE:O	1:A:434:LEU:HB2	2.15	0.47
1:A:356:LYS:HG2	1:A:357:GLU:N	2.30	0.46
1:A:583:PRO:O	1:A:584:THR:C	2.55	0.45
1:A:746:TRP:CE2	1:A:792:ARG:NH2	2.80	0.45
1:A:743:GLY:HA3	1:A:746:TRP:HE1	1.81	0.45
1:A:790:THR:HG21	8:A:1389:HOH:O	2.16	0.45
1:A:512[A]:LEU:HD21	1:A:711:HIS:NE2	2.32	0.45
7:A:1010:K07:N2	8:A:1108:HOH:O	2.36	0.45
1:A:477:MET:HB2	1:A:482:ARG:NE	2.32	0.45
1:A:746:TRP:CD1	1:A:792:ARG:CZ	2.72	0.44
1:A:746:TRP:CG	1:A:792:ARG:NH2	2.81	0.44
1:A:293:HIS:CD2	1:A:308:SER:HB2	2.53	0.44
1:A:746:TRP:CZ2	1:A:792:ARG:CG	3.00	0.44
1:A:770:ARG:HD3	7:A:1010:K07:N2	2.32	0.44
1:A:746:TRP:HZ2	1:A:792:ARG:HD2	1.84	0.43
1:A:400:THR:HG23	1:A:426:VAL:CG1	2.49	0.43
1:A:764:LEU:HD12	1:A:764:LEU:HA	1.83	0.42
1:A:512[B]:LEU:HD11	1:A:711:HIS:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:ASN:ND2	1:A:579:ARG:HD2	2.36	0.41
1:A:583:PRO:HA	1:A:588:THR:HA	2.02	0.41
1:A:423:ARG:O	1:A:426:VAL:HG12	2.21	0.41
1:A:695:GLU:HA	1:A:696:PRO:HD3	1.95	0.41
1:A:400:THR:HG23	1:A:426:VAL:HG11	2.02	0.40
1:A:303:TRP:CE3	1:A:593:ILE:HD12	2.56	0.40

All (2) 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:1122:HOH:O	8:A:1122:HOH:O[2_445]	1.79	0.41
8:A:1262:HOH:O	8:A:1344:HOH:O[2_545]	1.89	0.31

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	563/637 (88%)	540 (96%)	21 (4%)	2 (0%)	30 18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	406	ASN
1	A	420	LYS

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	507/554 (92%)	500 (99%)	7 (1%)	62 53

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	357	GLU
1	A	360	ASP
1	A	419	TRP
1	A	426	VAL
1	A	455	MET
1	A	589	VAL
1	A	641	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	819	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 11 ligands modelled in this entry, 2 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	$\#\|Z\| > 2$
4	DMS	A	1004	-	3,3,3	0.43	0	3,3,3	0.26	0
7	K07	A	1010	-	15,16,16	0.35	0	17,21,21	0.82	1 (5%)
3	MES	A	1003[A]	-	12,12,12	0.67	0	15,16,16	0.47	0
3	MES	A	1003[B]	-	12,12,12	0.69	0	15,16,16	0.29	0
4	DMS	A	1006	-	3,3,3	0.23	0	3,3,3	0.12	0
5	PO4	A	1007	-	4,4,4	3.69	4 (100%)	6,6,6	0.91	0
5	PO4	A	1008	-	4,4,4	1.21	1 (25%)	6,6,6	0.35	0
4	DMS	A	1005	-	3,3,3	0.23	0	3,3,3	0.07	0
6	PEG	A	1009	-	6,6,6	0.15	0	5,5,5	0.21	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
6	PEG	A	1009	-	-	2/4/4/4	-
7	K07	A	1010	-	-	2/8/15/15	0/2/2/2
3	MES	A	1003[A]	-	-	1/6/14/14	0/1/1/1
3	MES	A	1003[B]	-	-	5/6/14/14	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1007	PO4	P-O1	6.11	1.64	1.50
5	A	1007	PO4	P-O4	-2.59	1.47	1.54
5	A	1008	PO4	P-O1	2.40	1.56	1.50
5	A	1007	PO4	P-O3	2.36	1.61	1.54
5	A	1007	PO4	P-O2	2.19	1.61	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1010	K07	C8-C9-C6	-2.42	115.65	119.49

There are no chirality outliers.

All (10) torsion outliers are listed below:

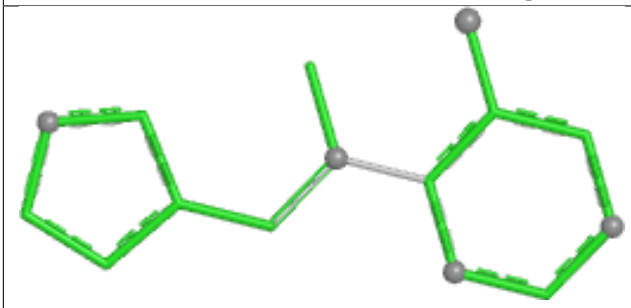
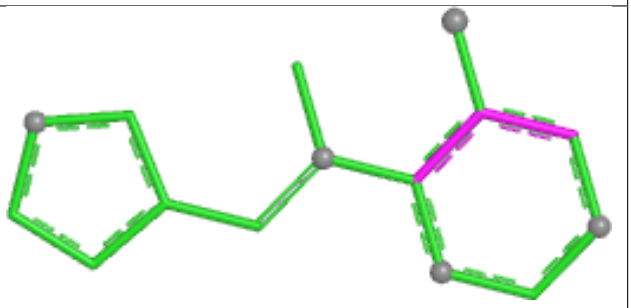
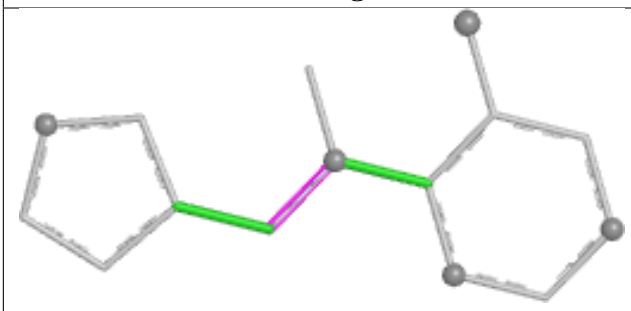
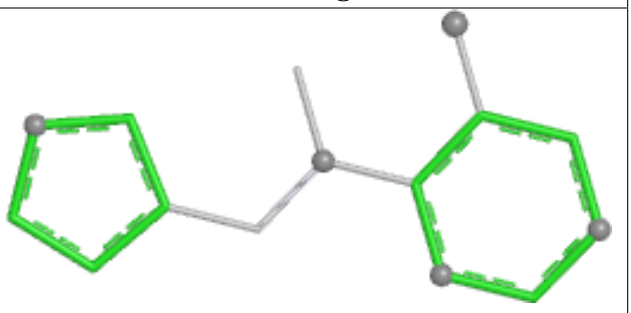
Mol	Chain	Res	Type	Atoms
3	A	1003[B]	MES	C8-C7-N4-C3
3	A	1003[B]	MES	C7-C8-S-O2S
3	A	1003[B]	MES	C7-C8-S-O3S
7	A	1010	K07	C2-C1-N-C
3	A	1003[B]	MES	C8-C7-N4-C5
6	A	1009	PEG	O2-C3-C4-O4
3	A	1003[B]	MES	C7-C8-S-O1S
7	A	1010	K07	C2-C1-N-C6
3	A	1003[A]	MES	C8-C7-N4-C3
6	A	1009	PEG	C4-C3-O2-C2

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1004	DMS	2	0
7	A	1010	K07	3	0
5	A	1007	PO4	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand K07 A 1010	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	571/637 (89%)	4.36	377 (66%)	0	0	6, 39, 78, 140	207 (36%)

All (377) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	889	PHE	17.6
1	A	830	VAL	15.1
1	A	478	TRP	14.3
1	A	589	VAL	14.3
1	A	886	MET	13.2
1	A	717	ILE	12.6
1	A	885	SER	12.5
1	A	839	LEU	12.5
1	A	294	TYR	12.4
1	A	409	LEU	12.3
1	A	863	ILE	12.2
1	A	774	LEU	12.1
1	A	716	LEU	11.9
1	A	475	TRP	11.8
1	A	426	VAL	11.7
1	A	284	ILE	11.5
1	A	851	ILE	11.5
1	A	838	TYR	11.5
1	A	637	VAL	11.4
1	A	407	ALA	11.4
1	A	840	GLY	11.3
1	A	641	ILE	11.2
1	A	435	VAL	11.2
1	A	888	ARG	11.2
1	A	646	TRP	11.2
1	A	592	ILE	11.1
1	A	431	PHE	11.1

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Mol	Chain	Res	Type	RSRZ
1	A	884	PRO	11.1
1	A	512[A]	LEU	11.0
1	A	434	LEU	11.0
1	A	425	ALA	10.9
1	A	474	ILE	10.9
1	A	856	ARG	10.9
1	A	882	TYR	10.9
1	A	814	ASN	10.9
1	A	303	TRP	10.8
1	A	281	ILE	10.8
1	A	860	ALA	10.7
1	A	719[A]	LYS	10.6
1	A	542	ILE	10.5
1	A	479	LEU	10.4
1	A	298	HIS	10.3
1	A	746	TRP	10.3
1	A	763[A]	SER	10.2
1	A	655	LEU	10.2
1	A	648	VAL	10.0
1	A	578	VAL	10.0
1	A	580	VAL	10.0
1	A	801[A]	HIS	9.9
1	A	593	ILE	9.9
1	A	363	THR	9.8
1	A	476	TYR	9.8
1	A	359	VAL	9.7
1	A	636	THR	9.7
1	A	800	THR	9.6
1	A	571	LEU	9.6
1	A	511	GLY	9.6
1	A	422	ALA	9.6
1	A	887	LYS	9.5
1	A	429	SER	9.4
1	A	293	HIS	9.3
1	A	588	THR	9.3
1	A	274	LEU	9.3
1	A	864[A]	GLN	9.2
1	A	408	ALA	9.2
1	A	477	MET	9.1
1	A	785[A]	SER	9.1
1	A	311	THR	9.1
1	A	428	ASP	9.0

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Mol	Chain	Res	Type	RSRZ
1	A	577	VAL	9.0
1	A	647	LEU	8.9
1	A	573	TYR	8.8
1	A	601	SER	8.8
1	A	635	LEU	8.7
1	A	890	ARG	8.7
1	A	543	THR	8.7
1	A	299	PRO	8.6
1	A	563	LYS	8.6
1	A	441	LEU	8.6
1	A	276	ILE	8.6
1	A	309	TYR	8.6
1	A	358	LYS	8.5
1	A	791	SER	8.4
1	A	713	PHE	8.3
1	A	564	LEU	8.1
1	A	834	GLU	8.1
1	A	567	ALA	8.1
1	A	594	SER	8.1
1	A	591	ASP	8.1
1	A	638	THR	8.1
1	A	600	GLY	8.0
1	A	770	ARG	8.0
1	A	400	THR	8.0
1	A	498	PHE	8.0
1	A	582	ARG	8.0
1	A	279	LYS	7.9
1	A	308	SER	7.9
1	A	439	ARG	7.9
1	A	344	THR	7.9
1	A	590	MET	7.9
1	A	430	GLY	7.8
1	A	584	THR	7.8
1	A	366	PRO	7.8
1	A	448	GLU	7.7
1	A	575	ASN	7.7
1	A	792	ARG	7.7
1	A	583	PRO	7.7
1	A	743	GLY	7.7
1	A	744	ALA	7.7
1	A	562	LYS	7.7
1	A	290	THR	7.7

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Mol	Chain	Res	Type	RSRZ
1	A	547	LEU	7.7
1	A	480	GLY	7.7
1	A	793	THR	7.6
1	A	835	GLU	7.6
1	A	295	ASP	7.6
1	A	841	LYS	7.6
1	A	291	SER	7.6
1	A	568	ILE	7.5
1	A	657	ARG	7.5
1	A	423	ARG	7.4
1	A	513	HIS	7.4
1	A	645	ASN	7.4
1	A	534	ASP	7.4
1	A	891	ARG	7.4
1	A	555	ASN	7.4
1	A	544	LEU	7.3
1	A	845	GLN	7.3
1	A	576	LYS	7.3
1	A	301	LYS	7.3
1	A	505	SER	7.3
1	A	304	ALA	7.2
1	A	561	HIS	7.2
1	A	482	ARG	7.2
1	A	312	LYS	7.2
1	A	388	LYS	7.2
1	A	741	SER	7.1
1	A	499	SER	7.1
1	A	280	ARG	7.0
1	A	862	ASN	7.0
1	A	649	ARG	7.0
1	A	790	THR	7.0
1	A	424	GLU	6.9
1	A	283	LYS	6.9
1	A	438	GLU	6.9
1	A	302	THR	6.9
1	A	745	GLY	6.9
1	A	436	ASP	6.9
1	A	421	SER	6.9
1	A	574	GLN	6.8
1	A	634	HIS	6.8
1	A	639	GLU	6.8
1	A	680	ALA	6.8

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Mol	Chain	Res	Type	RSRZ
1	A	640	GLU	6.8
1	A	451	VAL	6.8
1	A	296	GLN	6.6
1	A	502	ASN	6.6
1	A	595	ARG	6.6
1	A	558	GLU	6.5
1	A	369	GLY	6.5
1	A	285	LYS	6.4
1	A	742	GLN	6.4
1	A	861	LYS	6.4
1	A	273	ASN	6.4
1	A	539	ASP	6.4
1	A	552	MET	6.4
1	A	356	LYS	6.3
1	A	509	GLY	6.3
1	A	452	TYR	6.2
1	A	410	GLY	6.2
1	A	541	ARG	6.2
1	A	658	MET	6.2
1	A	603	GLN	6.1
1	A	818	ILE	6.1
1	A	572	THR	6.1
1	A	536	ALA	6.1
1	A	288	HIS	6.0
1	A	433	GLU	6.0
1	A	485	GLU	6.0
1	A	566	GLU	6.0
1	A	579	ARG	6.0
1	A	419	TRP	5.9
1	A	427	GLU	5.9
1	A	881	ASP	5.9
1	A	362	ARG	5.8
1	A	676	SER	5.8
1	A	632	ILE	5.8
1	A	396	ARG	5.8
1	A	305	TYR	5.8
1	A	300	TYR	5.7
1	A	581	GLN	5.7
1	A	524	LYS	5.6
1	A	698	ARG	5.6
1	A	705	GLN	5.6
1	A	364	GLN	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	406	ASN	5.6
1	A	876	ASN	5.5
1	A	551	GLU	5.5
1	A	398	GLU	5.5
1	A	397	GLU	5.4
1	A	545	GLU	5.4
1	A	473	ALA	5.4
1	A	824	MET	5.4
1	A	437	LYS	5.4
1	A	537	GLY	5.4
1	A	383	LYS	5.3
1	A	570	LYS	5.3
1	A	701	ASN	5.3
1	A	548	LYS	5.3
1	A	599	ARG	5.3
1	A	875	GLY	5.2
1	A	550	GLU	5.2
1	A	784	PRO	5.2
1	A	277	ILE	5.2
1	A	629	PHE	5.2
1	A	799	ALA	5.2
1	A	402	LYS	5.1
1	A	393	MET	5.1
1	A	286	GLN	5.1
1	A	442	HIS	5.1
1	A	289	GLU	5.0
1	A	546	ASP	5.0
1	A	404	ARG	5.0
1	A	481	ALA	5.0
1	A	604	VAL	5.0
1	A	361	THR	5.0
1	A	653	GLU	5.0
1	A	503	SER	5.0
1	A	420	LYS	4.9
1	A	360	ASP	4.9
1	A	365	GLU	4.8
1	A	764	LEU	4.8
1	A	560	GLU	4.8
1	A	440	ASN	4.7
1	A	310	GLU	4.7
1	A	275	ASP	4.6
1	A	418	LYS	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	292	TRP	4.6
1	A	690	ASP	4.6
1	A	357	GLU	4.5
1	A	405	SER	4.5
1	A	455	MET	4.5
1	A	528	GLY	4.5
1	A	874	ILE	4.5
1	A	880	THR	4.4
1	A	443	LEU	4.4
1	A	832	SER	4.4
1	A	453	ASN	4.4
1	A	449	THR	4.4
1	A	297	ASP	4.4
1	A	444	GLU	4.4
1	A	750	GLU	4.4
1	A	484	LEU	4.4
1	A	446	LYS	4.3
1	A	368	GLU	4.3
1	A	278	GLY	4.2
1	A	495	ASP	4.2
1	A	501	GLU	4.2
1	A	825	GLU	4.2
1	A	693	GLN	4.2
1	A	808	ASP	4.2
1	A	486	PHE	4.2
1	A	633	GLN	4.1
1	A	487	GLU	4.1
1	A	318	SER	4.1
1	A	827	LYS	4.1
1	A	788	VAL	4.0
1	A	376	ILE	4.0
1	A	394	CYS	3.9
1	A	673	ARG	3.9
1	A	483	PHE	3.9
1	A	287	GLU	3.9
1	A	337	MET	3.8
1	A	403	VAL	3.8
1	A	540	THR	3.8
1	A	556	HIS	3.7
1	A	702	ASP	3.7
1	A	630	LYS	3.7
1	A	597	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	625	GLY	3.6
1	A	598	GLN	3.6
1	A	694	TRP	3.6
1	A	804	MET	3.6
1	A	821	ASN	3.5
1	A	670	LEU	3.5
1	A	878	GLU	3.5
1	A	390	THR	3.5
1	A	642	ALA	3.5
1	A	692	GLN	3.4
1	A	846	TRP	3.4
1	A	677	ALA	3.4
1	A	373	LEU	3.4
1	A	496	HIS	3.3
1	A	319	SER	3.3
1	A	691	ILE	3.3
1	A	807	GLU	3.3
1	A	377	THR	3.3
1	A	687	VAL	3.3
1	A	432	TRP	3.3
1	A	493	ASN	3.3
1	A	819	GLN	3.2
1	A	811	THR	3.2
1	A	282	GLU	3.1
1	A	627	GLY	3.1
1	A	664	ASP	3.1
1	A	758	TYR	3.1
1	A	370	THR	3.1
1	A	704	THR	3.1
1	A	672	ASP	3.1
1	A	338	VAL	3.0
1	A	379	GLU	3.0
1	A	695	GLU	3.0
1	A	454	MET	3.0
1	A	736	GLY	3.0
1	A	624	GLU	2.9
1	A	679	THR	2.9
1	A	828	THR	2.9
1	A	343	MET	2.9
1	A	372	LYS	2.9
1	A	535	THR	2.9
1	A	596	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	607	TYR	2.8
1	A	497	TRP	2.8
1	A	671	ASP	2.8
1	A	858	THR	2.8
1	A	378	ALA	2.8
1	A	740	ILE	2.8
1	A	445	GLY	2.8
1	A	820	GLU	2.8
1	A	806	THR	2.7
1	A	802	GLU	2.7
1	A	401	ARG	2.7
1	A	529	ALA	2.7
1	A	538	TRP	2.7
1	A	533	ASP	2.7
1	A	367	LYS	2.7
1	A	809	MET	2.7
1	A	392	ARG	2.6
1	A	879	TYR	2.6
1	A	523	SER	2.6
1	A	815	ARG	2.6
1	A	643	VAL	2.6
1	A	652	ARG	2.6
1	A	689	LYS	2.6
1	A	321	VAL	2.5
1	A	760	GLN	2.5
1	A	823	TRP	2.5
1	A	602	GLY	2.5
1	A	508	GLU	2.4
1	A	320	MET	2.4
1	A	696	PRO	2.4
1	A	507	VAL	2.4
1	A	737	ARG	2.4
1	A	306	HIS	2.4
1	A	723	VAL	2.4
1	A	805	THR	2.4
1	A	812	VAL	2.3
1	A	853	LEU	2.3
1	A	857	ALA	2.3
1	A	447	CYS	2.3
1	A	699	GLY	2.3
1	A	683	ASP	2.3
1	A	831	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	389	LYS	2.2
1	A	842	ARG	2.2
1	A	399	PHE	2.1
1	A	382	TRP	2.1
1	A	620	ILE	2.1
1	A	488	ALA	2.1
1	A	866	ALA	2.1
1	A	381	LEU	2.1
1	A	772	LEU	2.1
1	A	703	TRP	2.1
1	A	522	VAL	2.0
1	A	644	LYS	2.0
1	A	335	ILE	2.0
1	A	549	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PO4	A	1007	5/5	0.72	0.16	41,45,54,74	0
7	K07	A	1010	15/15	0.75	0.37	47,50,55,68	15
5	PO4	A	1008	5/5	0.79	0.14	91,101,116,130	0
6	PEG	A	1009	7/7	0.81	0.17	69,80,83,84	0
4	DMS	A	1005	4/4	0.82	0.56	98,102,102,104	4
4	DMS	A	1006	4/4	0.82	0.54	78,80,80,81	4
4	DMS	A	1004	4/4	0.88	0.19	54,59,61,62	0
3	MES	A	1003[B]	12/12	0.97	0.35	734,758,811,814	12
3	MES	A	1003[A]	12/12	0.97	0.35	25,31,33,34	12

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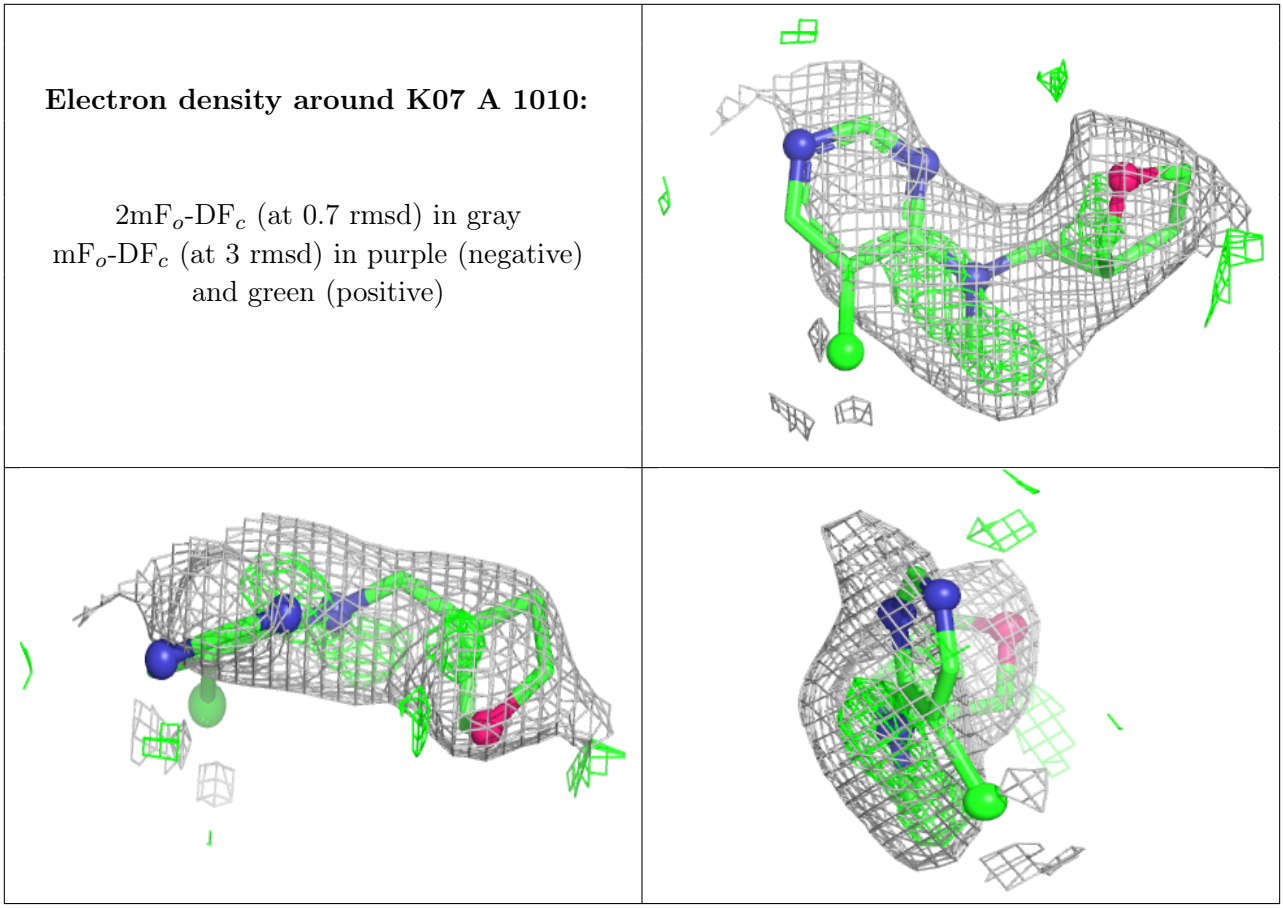
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	A	1002	1/1	0.99	0.04	60,60,60,60	0
2	ZN	A	1001	1/1	1.00	0.03	29,29,29,29	0

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 K07 A 1010:

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



6.5 Other polymers

There are no such residues in this entry.