



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:58 PM UTC

PDB ID : 7I2Q / pdb_00007i2q
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 Z26333434 (DNV2_NS5A-x0693)
Authors : Aschenbrenner, J.C.; Saini, M.; Chopra, A.; Marples, P.G.; Balcomb, B.H.; Lithgo, R.M.; Fearon, D.; von Delft, F.; Ruiz, F.X.; Arnold, E.
Deposited on : 2025-03-06
Resolution : 2.26 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)

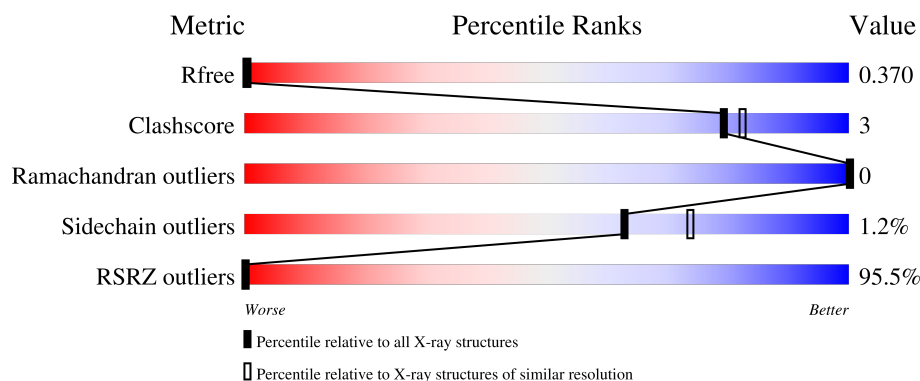
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	637	

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PO4	A	1006	-	-	-	X
6	RYM	A	1009	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 4981 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	574	4742	2985	849	874	34	0	7	0

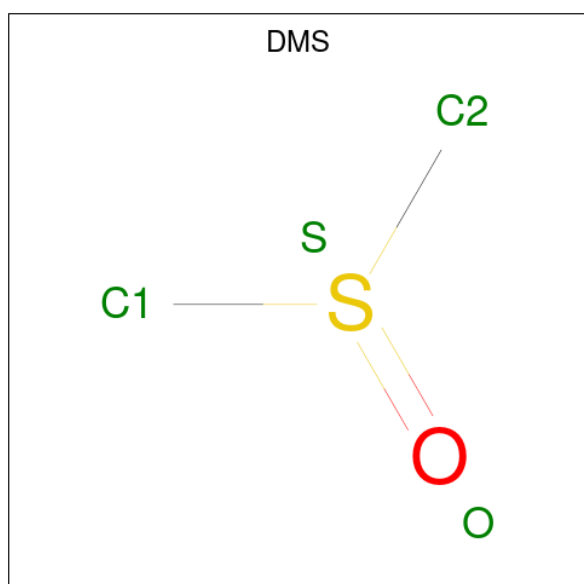
There are 2 discrepancies between the modelled and reference sequences:

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 (CCD ID: ZN) (formula: Zn).

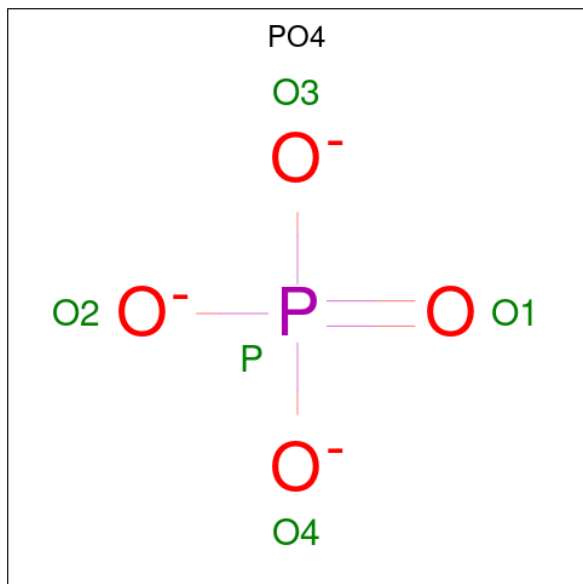
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



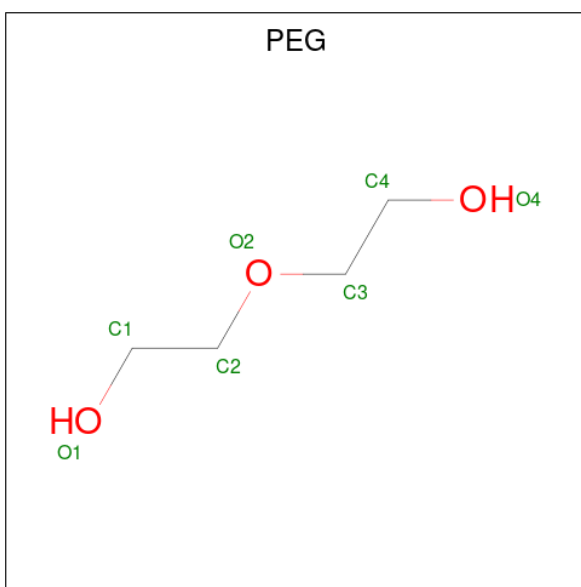
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



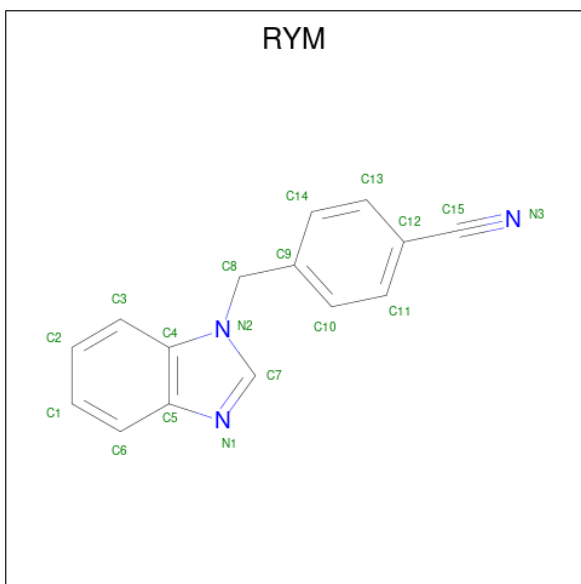
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 6 is 4-(benzimidazol-1-ylmethyl)benzenecarbonitrile (CCD ID: RYM) (formula: $C_{15}H_{11}N_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	N	0	0
			18	15	3		

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 8 is CHLORIDE ION (CCD ID: 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	177	Total	O	0	0
			177	177		

A866	A867	M868	Q869	V870	R871	S872	L873	I874	G875	M876	E877	E878	Y879	T880	D881	Y882	M883	P884	S885	P886	K887	R888	F889	R890	ARG	GLU	GLU	GLU	GLU	GLU	ALA	GLY	VAL	LEU	TRP
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	82.61Å 116.01Å 146.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.60 – 2.26 49.60 – 2.26	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.60-2.26) 98.3 (49.60-2.26)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.243 , 0.312 0.354 , 0.370	Depositor DCC
R_{free} test set	1706 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	43.9	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 773.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.70	EDS
Total number of atoms	4981	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.93% 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: RYM, ZN, MES, PO4, DMS, PEG, CL

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	1.01	0/4847	1.41	5/6536 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	837	PRO	N-CA-C	6.40	121.30	111.57
1	A	815	ARG	CA-C-N	6.27	128.53	120.70
1	A	815	ARG	C-N-CA	6.27	128.53	120.70
1	A	713	PHE	CB-CA-C	5.80	119.43	110.14
1	A	743	GLY	CA-C-O	-5.16	118.60	122.37

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	4742	0	4644	26	0
2	A	2	0	0	0	0
3	A	12	0	18	1	0
4	A	10	0	0	0	0
5	A	7	0	10	0	0
6	A	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	12	0	13	1	0
8	A	1	0	0	0	0
9	A	177	0	0	0	1
All	All	4981	0	4685	26	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (26) 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:513:HIS:HB3	1:A:765:MET:HE1	1.59	0.84
1:A:505:SER:HB2	1:A:615:MET:HE3	1.86	0.57
1:A:328:LEU:HD12	1:A:779:ILE:HG12	1.86	0.57
1:A:505:SER:HB3	1:A:660:ILE:HD12	1.87	0.55
1:A:760:GLN:CD	1:A:809:MET:HE3	2.32	0.55
1:A:730:ASN:OD1	1:A:732:ASP:HB2	2.09	0.52
1:A:765:MET:HA	1:A:765:MET:HE2	1.92	0.51
1:A:336:PRO:O	1:A:340:GLN:HG2	2.12	0.49
1:A:842:ARG:HG2	1:A:846:TRP:CE2	2.48	0.49
1:A:431:PHE:O	1:A:434:LEU:N	2.46	0.48
1:A:538:TRP:C	1:A:538:TRP:CD1	2.91	0.48
1:A:758:TYR:CE1	3:A:1005:DMS:H11	2.48	0.48
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.55	0.46
1:A:760:GLN:NE2	1:A:803:TRP:O	2.50	0.44
1:A:730:ASN:O	1:A:733:GLU:HB2	2.18	0.43
1:A:323:GLY:CA	7:A:1010:MES:H81	2.48	0.43
1:A:510:GLU:O	1:A:514:LYS:HG3	2.18	0.42
1:A:512[A]:LEU:HD12	1:A:512[A]:LEU:HA	1.79	0.42
1:A:619:LEU:HD11	1:A:655:LEU:HD21	2.02	0.42
1:A:863:ILE:HG21	1:A:883:MET:HE2	2.01	0.42
1:A:764:LEU:HG	1:A:765:MET:HE3	2.02	0.42
1:A:712:HIS:C	1:A:713:PHE:CD1	2.98	0.41
1:A:713:PHE:CD1	1:A:713:PHE:N	2.88	0.41
1:A:330:LYS:N	1:A:331:PRO:CD	2.84	0.41
1:A:726:VAL:HG21	1:A:768:HIS:CD2	2.56	0.41
1:A:842:ARG:HG2	1:A:846:TRP:CZ2	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1179:HOH:O	9:A:1211:HOH:O[2_545]	2.15	0.05

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	567/637 (89%)	529 (93%)	38 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	510/554 (92%)	504 (99%)	6 (1%)	63	74

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	396	ARG
1	A	438	GLU
1	A	641	ILE
1	A	664	ASP
1	A	687	VAL
1	A	887	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	513	HIS
1	A	555	ASN
1	A	603	GLN
1	A	845	GLN
1	A	868	ASN

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 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 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	$\# Z > 2$
3	DMS	A	1004	-	3,3,3	0.27	0	3,3,3	0.03	0
4	PO4	A	1007	-	4,4,4	0.73	0	6,6,6	0.46	0
6	RYM	A	1009	-	20,20,20	0.22	0	27,27,27	0.35	0
7	MES	A	1010	-	12,12,12	0.69	0	15,16,16	0.29	0
3	DMS	A	1003	-	3,3,3	0.23	0	3,3,3	0.05	0
4	PO4	A	1006	-	4,4,4	0.69	0	6,6,6	0.50	0
5	PEG	A	1008	-	6,6,6	0.18	0	5,5,5	0.09	0
3	DMS	A	1005	-	3,3,3	0.16	0	3,3,3	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	RYM	A	1009	-	-	0/6/6/6	0/3/3/3
7	MES	A	1010	-	-	1/6/14/14	0/1/1/1
5	PEG	A	1008	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

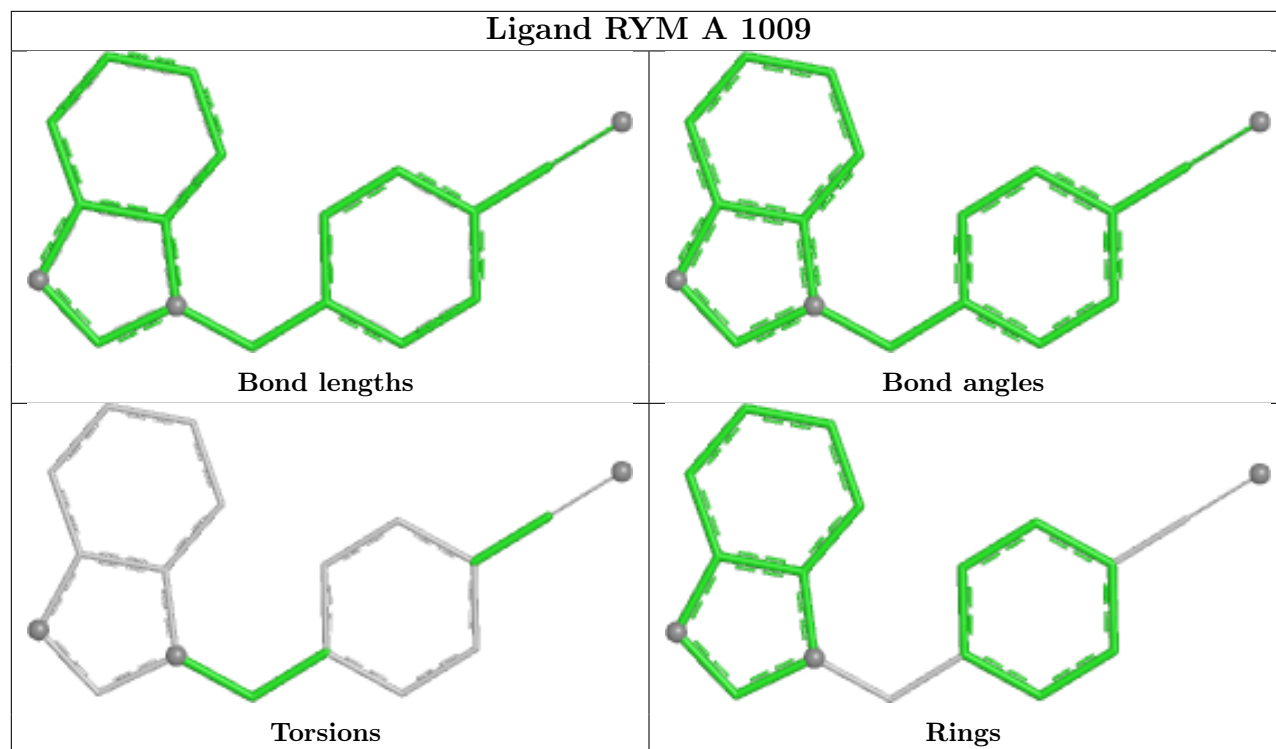
Mol	Chain	Res	Type	Atoms
7	A	1010	MES	C8-C7-N4-C3
5	A	1008	PEG	O1-C1-C2-O2
5	A	1008	PEG	O2-C3-C4-O4
5	A	1008	PEG	C4-C3-O2-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1010	MES	1	0
3	A	1005	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.



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	574/637 (90%)	10.45	548 (95%) 0 0	6, 41, 93, 169	265 (46%)

All (548) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	745	GLY	36.1
1	A	411	ALA	32.5
1	A	290	THR	32.5
1	A	744	ALA	32.1
1	A	743	GLY	30.8
1	A	429	SER	29.9
1	A	425	ALA	28.9
1	A	287	GLU	28.8
1	A	313	GLN	28.5
1	A	364	GLN	27.9
1	A	408	ALA	26.8
1	A	304	ALA	25.8
1	A	275	ASP	24.7
1	A	317	ALA	24.7
1	A	641	ILE	24.5
1	A	584	THR	24.3
1	A	889	PHE	23.9
1	A	282	GLU	22.7
1	A	420	LYS	22.6
1	A	423	ARG	22.4
1	A	292	TRP	22.4
1	A	406	ASN	22.3
1	A	806	THR	22.3
1	A	405	SER	22.2
1	A	887	LYS	22.2
1	A	309	TYR	22.2
1	A	274	LEU	22.2

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Mol	Chain	Res	Type	RSRZ
1	A	284	ILE	22.1
1	A	676	SER	21.7
1	A	426	VAL	21.6
1	A	453	ASN	21.5
1	A	570	LYS	21.4
1	A	648	VAL	21.3
1	A	451	VAL	21.3
1	A	589	VAL	21.3
1	A	636	THR	21.0
1	A	428	ASP	20.8
1	A	481	ALA	20.8
1	A	296	GLN	20.6
1	A	801[A]	HIS	20.5
1	A	444	GLU	20.5
1	A	369	GLY	20.4
1	A	410	GLY	20.3
1	A	291	SER	20.2
1	A	277	ILE	20.0
1	A	403	VAL	20.0
1	A	860	ALA	19.9
1	A	742	GLN	19.9
1	A	740	ILE	19.8
1	A	452	TYR	19.7
1	A	303	TRP	19.6
1	A	564	LEU	19.5
1	A	635	LEU	19.4
1	A	424	GLU	19.4
1	A	278	GLY	19.4
1	A	289	GLU	19.4
1	A	419	TRP	19.4
1	A	478	TRP	19.4
1	A	400	THR	19.2
1	A	882	TYR	18.8
1	A	305	TYR	18.8
1	A	294	TYR	18.8
1	A	794	THR	18.6
1	A	741[A]	SER	18.6
1	A	849	SER	18.6
1	A	285	LYS	18.6
1	A	399	PHE	18.6
1	A	286	GLN	18.5
1	A	311	THR	18.5

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Mol	Chain	Res	Type	RSRZ
1	A	583	PRO	18.5
1	A	754	LEU	18.4
1	A	579	ARG	18.4
1	A	298	HIS	18.3
1	A	312	LYS	18.2
1	A	314	THR	18.1
1	A	544	LEU	18.0
1	A	788	VAL	18.0
1	A	281	ILE	17.8
1	A	716	LEU	17.8
1	A	632	ILE	17.6
1	A	857	ALA	17.6
1	A	672	ASP	17.6
1	A	368	GLU	17.5
1	A	858	THR	17.5
1	A	302	THR	17.3
1	A	708	PHE	17.3
1	A	276	ILE	17.3
1	A	631	SER	17.3
1	A	763[A]	SER	17.3
1	A	308	SER	17.2
1	A	872	SER	17.2
1	A	682	ASN	17.1
1	A	559	GLY	17.1
1	A	787	TRP	17.1
1	A	572	THR	17.0
1	A	645	ASN	17.0
1	A	592	ILE	17.0
1	A	475	TRP	16.9
1	A	664	ASP	16.9
1	A	404	ARG	16.8
1	A	629	PHE	16.8
1	A	307	GLY	16.8
1	A	833	TRP	16.7
1	A	421	SER	16.7
1	A	367	LYS	16.7
1	A	593	ILE	16.7
1	A	633	GLN	16.6
1	A	880	THR	16.6
1	A	535	THR	16.5
1	A	293	HIS	16.5
1	A	441	LEU	16.5

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Mol	Chain	Res	Type	RSRZ
1	A	273	ASN	16.5
1	A	628	VAL	16.4
1	A	627	GLY	16.3
1	A	530	MET	16.3
1	A	295	ASP	16.3
1	A	665	CYS	16.2
1	A	373	LEU	16.1
1	A	890	ARG	16.1
1	A	588	THR	16.1
1	A	531	TYR	16.1
1	A	356	LYS	16.1
1	A	486	PHE	16.1
1	A	571	LEU	16.0
1	A	634	HIS	16.0
1	A	418	LYS	15.9
1	A	398	GLU	15.9
1	A	446	LYS	15.9
1	A	746	TRP	15.9
1	A	480	GLY	15.8
1	A	357	GLU	15.8
1	A	706	VAL	15.8
1	A	875	GLY	15.7
1	A	280	ARG	15.7
1	A	790	THR	15.7
1	A	620	ILE	15.6
1	A	476	TYR	15.6
1	A	681	LEU	15.6
1	A	558	GLU	15.6
1	A	871	ARG	15.5
1	A	366	PRO	15.5
1	A	850	LEU	15.5
1	A	477	MET	15.5
1	A	888	ARG	15.5
1	A	455	MET	15.5
1	A	591	ASP	15.5
1	A	835	GLU	15.3
1	A	569	PHE	15.2
1	A	383	LYS	15.2
1	A	360	ASP	15.2
1	A	582	ARG	15.1
1	A	605	VAL	15.1
1	A	362	ARG	15.0

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Mol	Chain	Res	Type	RSRZ
1	A	396	ARG	15.0
1	A	474	ILE	15.0
1	A	484	LEU	15.0
1	A	649	ARG	14.9
1	A	855	SER	14.9
1	A	864[A]	GLN	14.9
1	A	886	MET	14.9
1	A	407	ALA	14.9
1	A	677	ALA	14.9
1	A	374	MET	14.8
1	A	365	GLU	14.8
1	A	575	ASN	14.8
1	A	361	THR	14.7
1	A	610	ASN	14.7
1	A	799	ALA	14.7
1	A	774	LEU	14.7
1	A	297	ASP	14.7
1	A	854	THR	14.6
1	A	789	PRO	14.6
1	A	747	SER	14.6
1	A	603	GLN	14.5
1	A	680	ALA	14.4
1	A	748	LEU	14.3
1	A	834	GLU	14.3
1	A	881	ASP	14.3
1	A	394	CYS	14.3
1	A	561	HIS	14.2
1	A	786	HIS	14.2
1	A	679	THR	14.2
1	A	532	ALA	14.2
1	A	838	TYR	14.1
1	A	344	THR	14.0
1	A	853	LEU	14.0
1	A	580	VAL	13.9
1	A	397	GLU	13.9
1	A	613	THR	13.9
1	A	707	PRO	13.9
1	A	283	LYS	13.9
1	A	581	GLN	13.8
1	A	873	LEU	13.8
1	A	574	GLN	13.7
1	A	640	GLU	13.7

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Mol	Chain	Res	Type	RSRZ
1	A	785[A]	SER	13.7
1	A	384	GLU	13.7
1	A	876	ASN	13.7
1	A	482	ARG	13.6
1	A	427	GLU	13.6
1	A	705	GLN	13.6
1	A	566	GLU	13.4
1	A	594	SER	13.4
1	A	851	ILE	13.4
1	A	625	GLY	13.3
1	A	358	LYS	13.3
1	A	557	MET	13.2
1	A	624	GLU	13.2
1	A	719[A]	LYS	13.1
1	A	879	TYR	13.1
1	A	626	GLU	13.1
1	A	393	MET	13.1
1	A	363	THR	13.0
1	A	877	GLU	13.0
1	A	555	ASN	13.0
1	A	601	SER	13.0
1	A	440	ASN	12.8
1	A	856	ARG	12.8
1	A	619	LEU	12.8
1	A	622	GLN	12.8
1	A	573	TYR	12.8
1	A	487	GLU	12.8
1	A	422	ALA	12.7
1	A	436	ASP	12.6
1	A	739	ARG	12.6
1	A	402	LYS	12.6
1	A	753	CYS	12.6
1	A	549	ASN	12.6
1	A	692	GLN	12.5
1	A	306	HIS	12.5
1	A	791	SER	12.5
1	A	551	GLU	12.4
1	A	310	GLU	12.3
1	A	687	VAL	12.3
1	A	590	MET	12.2
1	A	621	ARG	12.2
1	A	279	LYS	12.2

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Mol	Chain	Res	Type	RSRZ
1	A	598	GLN	12.2
1	A	321	VAL	12.1
1	A	454	MET	12.1
1	A	606	THR	12.0
1	A	379	GLU	12.0
1	A	568	ILE	12.0
1	A	545	GLU	11.9
1	A	861	LYS	11.8
1	A	359	VAL	11.8
1	A	388	LYS	11.7
1	A	409	LEU	11.7
1	A	600	GLY	11.7
1	A	751	THR	11.7
1	A	750	GLU	11.7
1	A	548	LYS	11.6
1	A	737	ARG	11.4
1	A	448	GLU	11.4
1	A	387	LYS	11.4
1	A	534	ASP	11.4
1	A	401	ARG	11.3
1	A	840	GLY	11.3
1	A	576	LYS	11.2
1	A	496	HIS	11.2
1	A	792	ARG	11.2
1	A	556	HIS	11.1
1	A	371	LYS	11.1
1	A	599	ARG	11.1
1	A	623	MET	11.1
1	A	749	ARG	10.9
1	A	825	GLU	10.9
1	A	602	GLY	10.9
1	A	301	LYS	10.9
1	A	821	ASN	10.8
1	A	550	GLU	10.8
1	A	560	GLU	10.7
1	A	533	ASP	10.7
1	A	485	GLU	10.6
1	A	432	TRP	10.5
1	A	604	VAL	10.5
1	A	434	LEU	10.5
1	A	845	GLN	10.5
1	A	793	THR	10.4

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Mol	Chain	Res	Type	RSRZ
1	A	694	TRP	10.2
1	A	449	THR	10.1
1	A	563	LYS	10.1
1	A	512[A]	LEU	10.0
1	A	839	LEU	9.9
1	A	800	THR	9.9
1	A	372	LYS	9.8
1	A	865	THR	9.8
1	A	375	LYS	9.8
1	A	779	ILE	9.7
1	A	852	GLY	9.6
1	A	842	ARG	9.5
1	A	878	GLU	9.5
1	A	695	GLU	9.4
1	A	815	ARG	9.4
1	A	337	MET	9.3
1	A	644	LYS	9.2
1	A	638	THR	9.0
1	A	870	VAL	9.0
1	A	841	LYS	8.9
1	A	336	PRO	8.9
1	A	807	GLU	8.8
1	A	701	ASN	8.6
1	A	652	ARG	8.6
1	A	318	SER	8.5
1	A	691	ILE	8.5
1	A	508	GLU	8.5
1	A	288	HIS	8.4
1	A	536	ALA	8.2
1	A	597	ASP	8.2
1	A	501	GLU	8.2
1	A	437	LYS	8.1
1	A	885	SER	8.1
1	A	524	LYS	8.0
1	A	827	LYS	8.0
1	A	299	PRO	7.9
1	A	493	ASN	7.9
1	A	327	LEU	7.8
1	A	328	LEU	7.8
1	A	609	LEU	7.8
1	A	717	ILE	7.7
1	A	673	ARG	7.7

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Mol	Chain	Res	Type	RSRZ
1	A	831	GLU	7.7
1	A	542	ILE	7.6
1	A	430	GLY	7.6
1	A	637	VAL	7.6
1	A	541	ARG	7.4
1	A	319	SER	7.4
1	A	772	LEU	7.3
1	A	732	ASP	7.2
1	A	596	ARG	7.2
1	A	552	MET	7.2
1	A	525	LYS	7.2
1	A	693	GLN	7.1
1	A	300	TYR	7.1
1	A	433	GLU	7.0
1	A	660	ILE	7.0
1	A	803	TRP	6.9
1	A	874	ILE	6.9
1	A	431	PHE	6.9
1	A	702	ASP	6.9
1	A	808	ASP	6.8
1	A	341	MET	6.8
1	A	445	GLY	6.7
1	A	757	SER	6.7
1	A	690	ASP	6.7
1	A	820	GLU	6.6
1	A	340	GLN	6.6
1	A	539	ASP	6.6
1	A	503	SER	6.6
1	A	715	GLU	6.5
1	A	764	LEU	6.4
1	A	630	LYS	6.4
1	A	670	LEU	6.4
1	A	546	ASP	6.2
1	A	776	ALA	6.1
1	A	521	ASP	6.1
1	A	683	ASP	6.1
1	A	343	MET	6.1
1	A	685	GLY	6.1
1	A	723	VAL	6.1
1	A	720	ASP	6.0
1	A	497	TRP	6.0
1	A	650	VAL	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	567	ALA	5.9
1	A	439	ARG	5.9
1	A	538	TRP	5.9
1	A	642	ALA	5.8
1	A	663	ASP	5.8
1	A	509	GLY	5.8
1	A	816	VAL	5.8
1	A	483	PHE	5.8
1	A	704	THR	5.7
1	A	540	THR	5.7
1	A	730	ASN	5.7
1	A	646	TRP	5.7
1	A	830	VAL	5.7
1	A	611	THR	5.7
1	A	523	SER	5.6
1	A	828	THR	5.6
1	A	479	LEU	5.6
1	A	810	LEU	5.6
1	A	826	ASP	5.6
1	A	507	VAL	5.6
1	A	867	ILE	5.6
1	A	819	GLN	5.5
1	A	781	SER	5.5
1	A	866	ALA	5.5
1	A	780	CYS	5.5
1	A	802	GLU	5.5
1	A	647	LEU	5.4
1	A	386	GLY	5.4
1	A	578	VAL	5.4
1	A	498	PHE	5.4
1	A	674	PHE	5.4
1	A	554	THR	5.4
1	A	738	ALA	5.4
1	A	495	ASP	5.3
1	A	450	CYS	5.2
1	A	537	GLY	5.2
1	A	381	LEU	5.2
1	A	836	ILE	5.2
1	A	829	PRO	5.1
1	A	832	SER	5.1
1	A	447	CYS	5.1
1	A	671	ASP	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	758	TYR	5.0
1	A	783	VAL	5.0
1	A	805	THR	5.0
1	A	814	ASN	4.9
1	A	320	MET	4.9
1	A	615	MET	4.9
1	A	811	THR	4.9
1	A	726	VAL	4.9
1	A	334	ILE	4.9
1	A	443	LEU	4.8
1	A	595	ARG	4.8
1	A	710	SER	4.7
1	A	491	PHE	4.7
1	A	639	GLU	4.7
1	A	729	ARG	4.6
1	A	435	VAL	4.6
1	A	370	THR	4.6
1	A	562	LYS	4.6
1	A	338	VAL	4.6
1	A	612	PHE	4.6
1	A	438	GLU	4.6
1	A	725	VAL	4.6
1	A	818	ILE	4.6
1	A	769	ARG	4.6
1	A	494	GLU	4.5
1	A	698	ARG	4.5
1	A	728	CYS	4.5
1	A	378	ALA	4.5
1	A	616	GLU	4.5
1	A	329	THR	4.5
1	A	733	GLU	4.4
1	A	804	MET	4.4
1	A	678	LEU	4.4
1	A	868	ASN	4.4
1	A	824	MET	4.3
1	A	520	ARG	4.3
1	A	656	SER	4.3
1	A	529	ALA	4.3
1	A	339	THR	4.3
1	A	492	LEU	4.3
1	A	848	GLY	4.3
1	A	884	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	377	THR	4.2
1	A	711	HIS	4.2
1	A	325	VAL	4.2
1	A	499	SER	4.2
1	A	862	ASN	4.2
1	A	392	ARG	4.2
1	A	863	ILE	4.1
1	A	514	LYS	4.1
1	A	518	ILE	4.1
1	A	823	TRP	4.0
1	A	390	THR	4.0
1	A	658	MET	4.0
1	A	837	PRO	4.0
1	A	342	ALA	4.0
1	A	510	GLU	3.9
1	A	380	TRP	3.9
1	A	442	HIS	3.9
1	A	724	LEU	3.9
1	A	755	GLY	3.9
1	A	721	GLY	3.8
1	A	395	THR	3.8
1	A	504	LEU	3.8
1	A	607	TYR	3.8
1	A	502	ASN	3.6
1	A	777	ASN	3.6
1	A	736	GLY	3.6
1	A	759	ALA	3.6
1	A	768	HIS	3.6
1	A	762	TRP	3.6
1	A	784	PRO	3.5
1	A	846	TRP	3.5
1	A	766	TYR	3.5
1	A	713	PHE	3.5
1	A	577	VAL	3.5
1	A	376	ILE	3.5
1	A	651	GLY	3.5
1	A	513	HIS	3.5
1	A	547	LEU	3.4
1	A	684	MET	3.4
1	A	382	TRP	3.4
1	A	519	LEU	3.3
1	A	697	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	812	VAL	3.3
1	A	883	MET	3.3
1	A	765	MET	3.3
1	A	515	LEU	3.3
1	A	655	LEU	3.3
1	A	735	ILE	3.3
1	A	565	ALA	3.2
1	A	330	LYS	3.2
1	A	734	LEU	3.2
1	A	699	GLY	3.2
1	A	669	PRO	3.2
1	A	522	VAL	3.2
1	A	718	MET	3.2
1	A	689	LYS	3.1
1	A	324	VAL	3.1
1	A	662	GLY	3.1
1	A	869	GLN	3.1
1	A	675	ALA	3.0
1	A	332	TRP	3.0
1	A	659	ALA	3.0
1	A	809	MET	3.0
1	A	847	CYS	3.0
1	A	335	ILE	3.0
1	A	517	TYR	3.0
1	A	618	GLN	2.9
1	A	760	GLN	2.9
1	A	526	GLU	2.9
1	A	527	GLY	2.9
1	A	657	ARG	2.9
1	A	553	VAL	2.9
1	A	643	VAL	2.9
1	A	767	PHE	2.8
1	A	686	LYS	2.8
1	A	654	ARG	2.8
1	A	516	GLY	2.7
1	A	703	TRP	2.7
1	A	389	LYS	2.7
1	A	489	LEU	2.7
1	A	722	ARG	2.7
1	A	775	ALA	2.7
1	A	490	GLY	2.6
1	A	500	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	331	PRO	2.6
1	A	714	HIS	2.5
1	A	326	ARG	2.5
1	A	488	ALA	2.5
1	A	756	LYS	2.4
1	A	653	GLU	2.4
1	A	859	TRP	2.4
1	A	782	ALA	2.4
1	A	709	CYS	2.3
1	A	322	ASN	2.3
1	A	817	TRP	2.2
1	A	333	ASP	2.2
1	A	844	ASP	2.2
1	A	696	PRO	2.2
1	A	385	LEU	2.1
1	A	391	PRO	2.1
1	A	666	VAL	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 oligosaccharides 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.

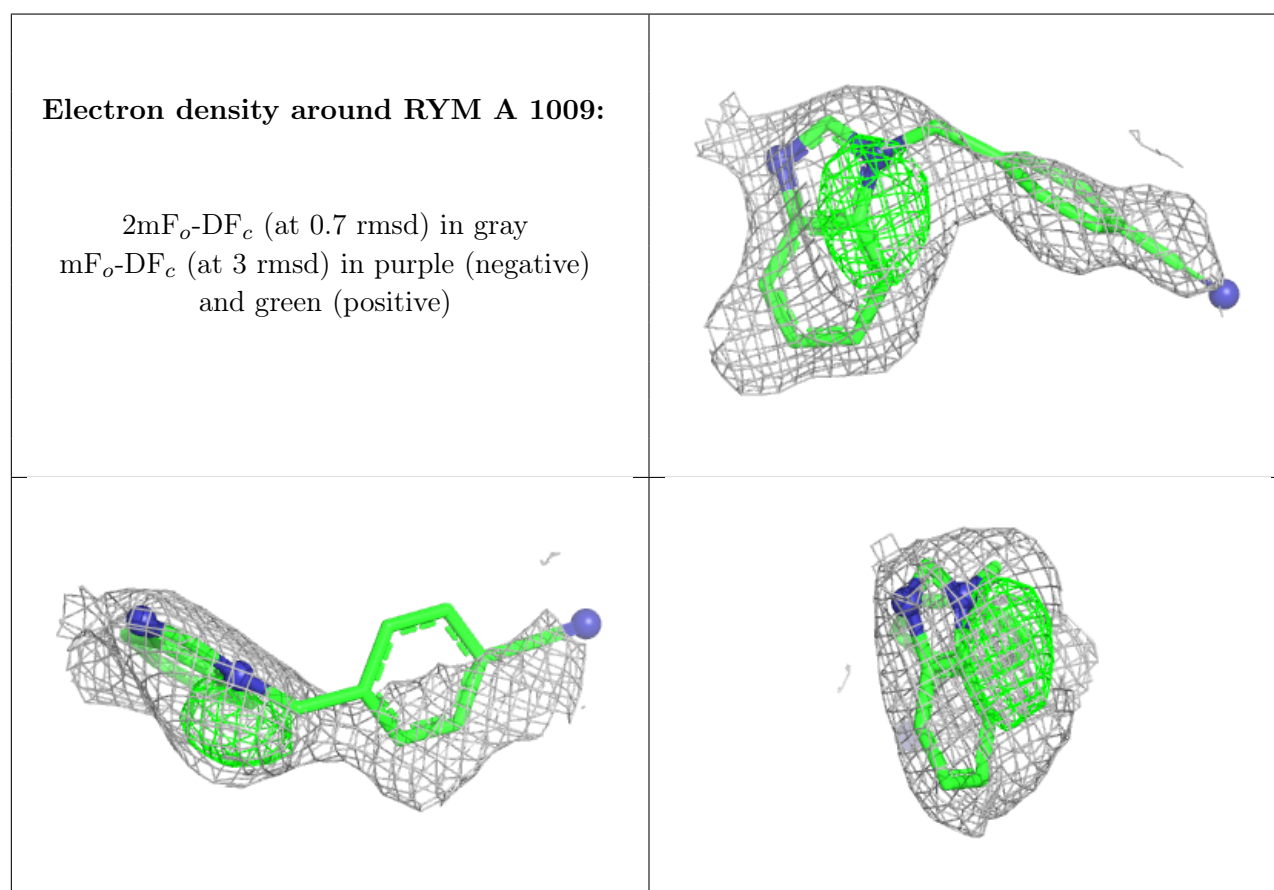
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	RYM	A	1009	18/18	0.55	0.41	20,21,21,21	18
4	PO4	A	1006	5/5	0.57	0.52	48,50,50,52	5
4	PO4	A	1007	5/5	0.61	0.20	114,118,125,125	0
3	DMS	A	1003	4/4	0.70	0.33	96,99,101,101	0
5	PEG	A	1008	7/7	0.72	0.29	102,106,111,114	0
3	DMS	A	1005	4/4	0.72	0.33	82,90,92,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	DMS	A	1004	4/4	0.80	0.22	98,105,106,110	0
7	MES	A	1010	12/12	0.87	0.30	11,23,40,281	12
8	CL	A	1011	1/1	0.90	0.16	2,2,2,2	1
2	ZN	A	1001	1/1	0.97	0.04	39,39,39,39	0
2	ZN	A	1002	1/1	0.99	0.07	77,77,77,77	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.