Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2025 – 11:53 AM EDT

PDB ID	:	7I2Q
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:

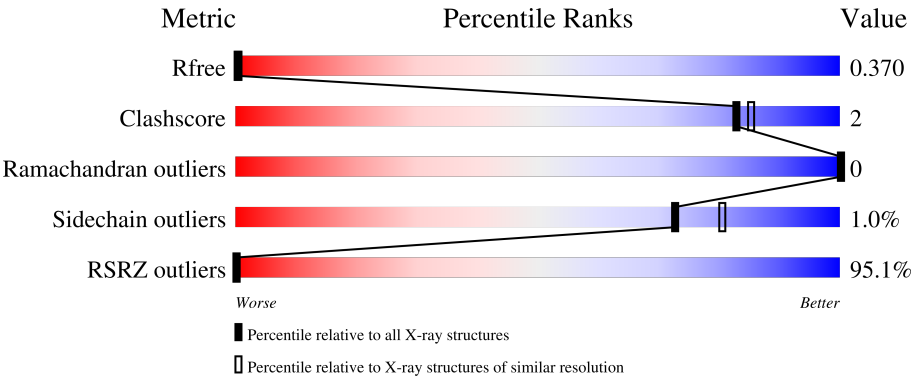
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (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 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}	164625	1763 (2.26-2.26)
Clashscore	180529	1919 (2.26-2.26)
Ramachandran outliers	177936	1884 (2.26-2.26)
Sidechain outliers	177891	1885 (2.26-2.26)
RSRZ outliers	164620	1763 (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 <=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	86% 84% 6% 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
4	PO4	A	1006	-	-	-	X
6	RYM	A	1009	-	-	-	X

2 Entry composition

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
1	A	574	Total	C	N	O	S	0	7	0
			4742	2985	849	874	34			

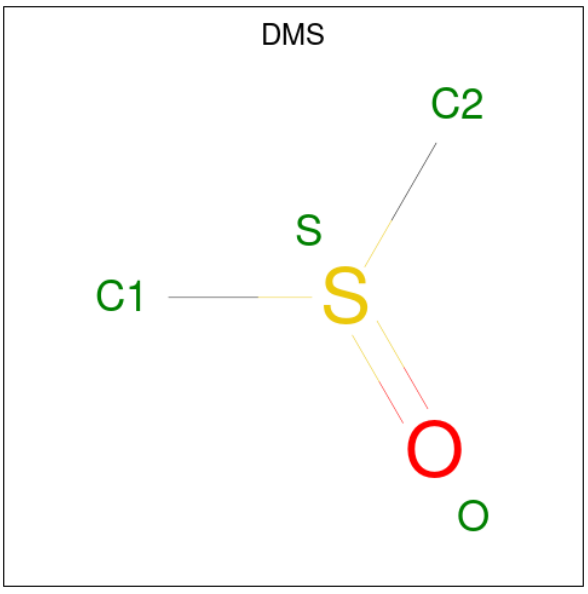
There are 2 discrepancies between the modelled and reference sequences:

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

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

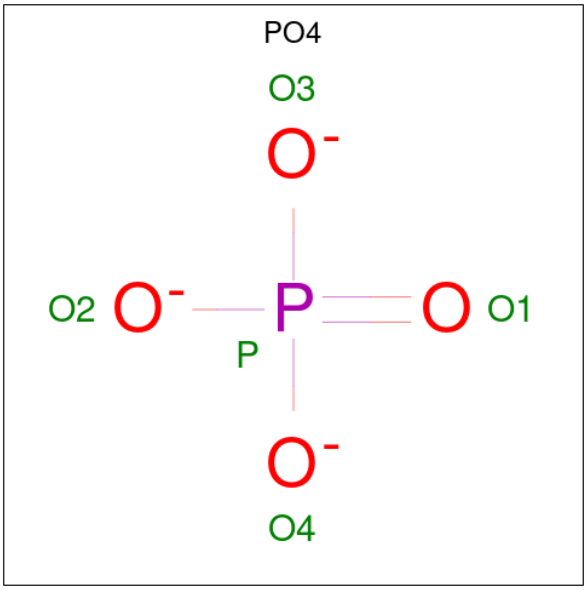
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



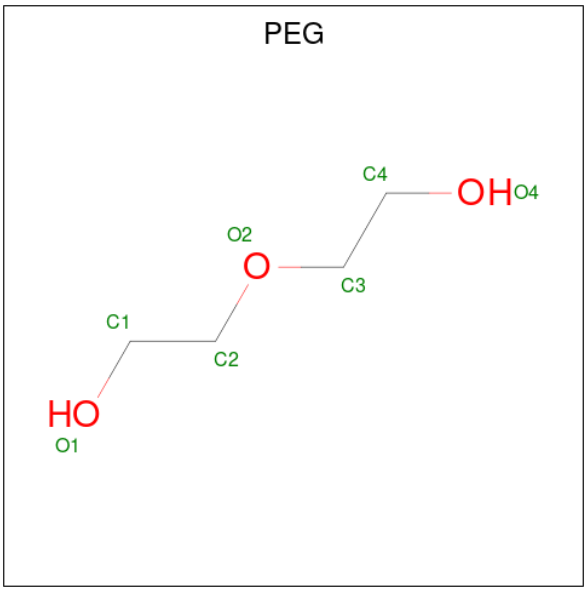
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O S 4 2 1 1	0	0
3	A	1	Total C O S 4 2 1 1	0	0
3	A	1	Total C O S 4 2 1 1	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



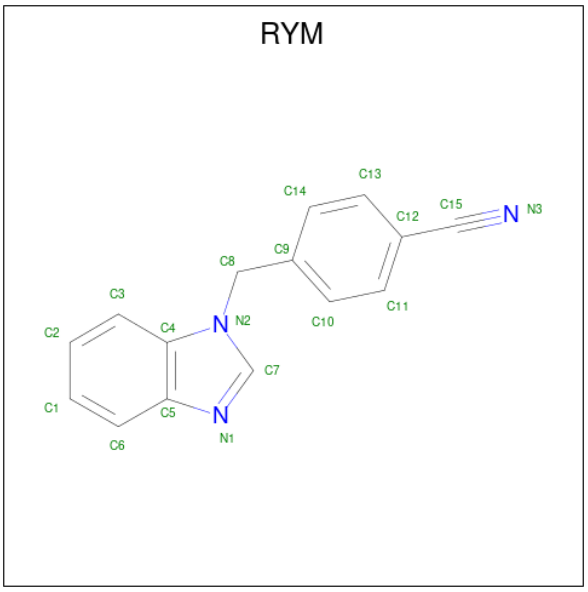
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	A	1	Total O P 5 4 1	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



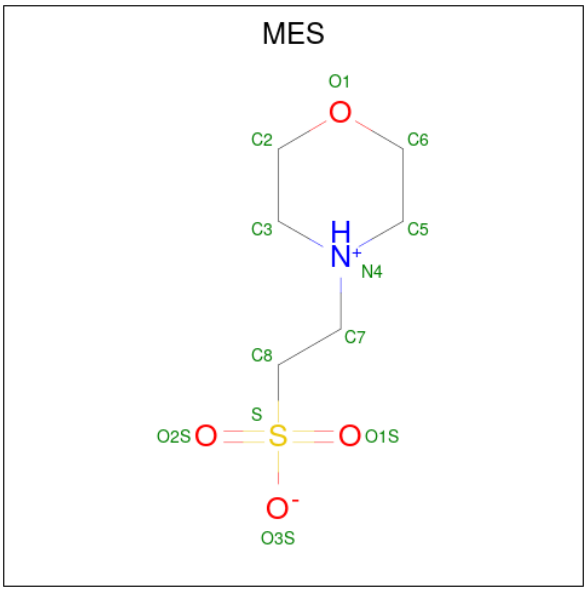
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is 4-(benzimidazol-1-ylmethyl)benzenecarbonitrile (three-letter code: 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 (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

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

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

- Molecule 9 is water.

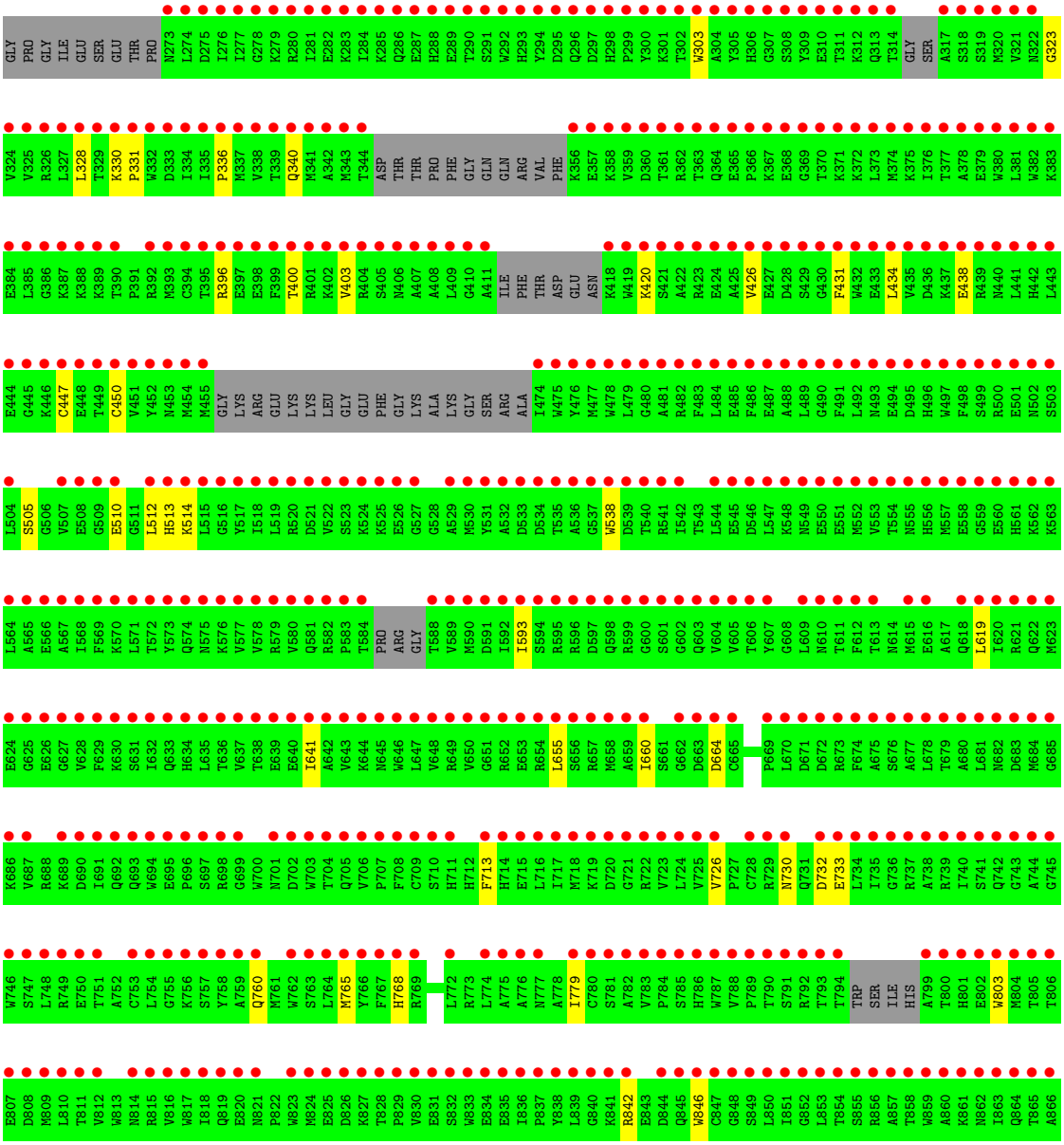
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	177	Total O 177 177	0	0

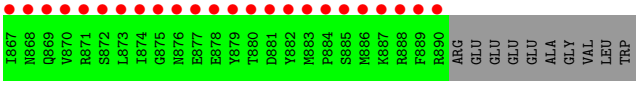
3 Residue-property plots (i)

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:




I867
N868
Q869
V870
R871
S872
L873
I874
G875
N876
E877
E878
Y879
T880
D881
Y882
M883
P884
S885
M886
K887
R888
P889
R890
ARG
GLU
GLU
GLU
GLU
ALA
GLY
VAL
LEU
TRP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	82.61Å 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
$< I/\sigma(I) >$ [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	1703 reflections (5.11%)	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]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[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: CL, RYM, ZN, PO4, MES, DMS, 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	0.66	0/4847	0.75	0/6536

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4742	0	4644	22	0
2	A	2	0	0	0	0
3	A	12	0	18	0	0
4	A	10	0	0	0	0
5	A	7	0	10	0	0
6	A	18	0	0	0	0
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	22	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 2.

All (22) 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: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:730:ASN:OD1	1:A:732:ASP:HB2	2.09	0.52
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:400:THR:O	1:A:403:VAL:HG22	2.14	0.47
1:A:513:HIS:HB3	1:A:765:MET:CE	2.46	0.46
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:538:TRP:C	1:A:538:TRP:CD1	2.91	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:303:TRP:CE3	1:A:593:ILE:HD12	2.55	0.42
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:403:VAL:HG21	1:A:426:VAL:HG21	2.02	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%)	505 (99%)	5 (1%)	73 80

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	396	ARG
1	A	420	LYS
1	A	438	GLU
1	A	641	ILE
1	A	664	ASP

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	760	GLN

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	1005	-	3,3,3	0.16	0	3,3,3	0.21	0
6	RYM	A	1009	-	19,20,20	0.77	0	22,27,27	0.61	0
3	DMS	A	1003	-	3,3,3	0.23	0	3,3,3	0.05	0
7	MES	A	1010	-	12,12,12	0.69	0	15,16,16	0.29	0
5	PEG	A	1008	-	6,6,6	0.18	0	5,5,5	0.09	0
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
4	PO4	A	1006	-	4,4,4	0.69	0	6,6,6	0.50	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
7	MES	A	1010	-	-	1/6/14/14	0/1/1/1
6	RYM	A	1009	-	-	2/6/6/6	0/3/3/3
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 (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1009	RYM	C9-C8-N2-C7
7	A	1010	MES	C8-C7-N4-C3
5	A	1008	PEG	O1-C1-C2-O2
5	A	1008	PEG	O2-C3-C4-O4
6	A	1009	RYM	C9-C8-N2-C4
5	A	1008	PEG	C4-C3-O2-C2

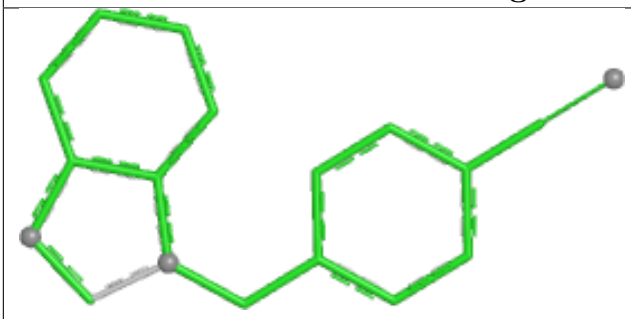
There are no ring outliers.

1 monomer is involved in 1 short contact:

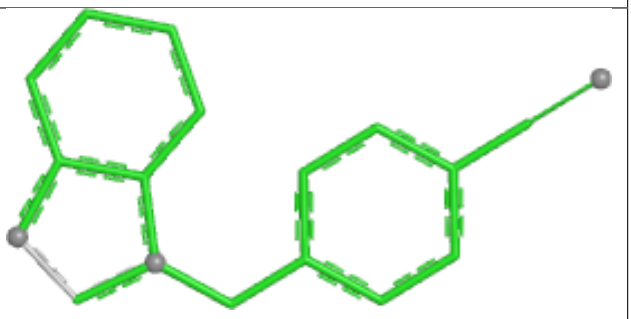
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1010	MES	1	0

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 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.

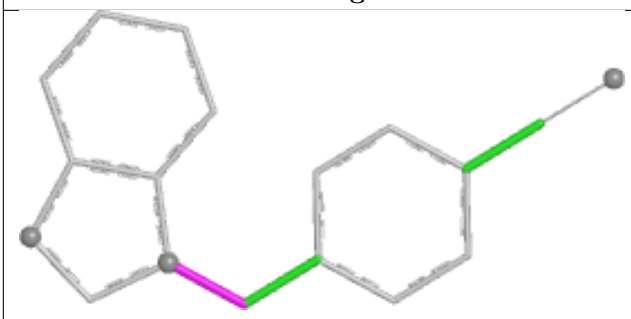
Ligand RYM A 1009



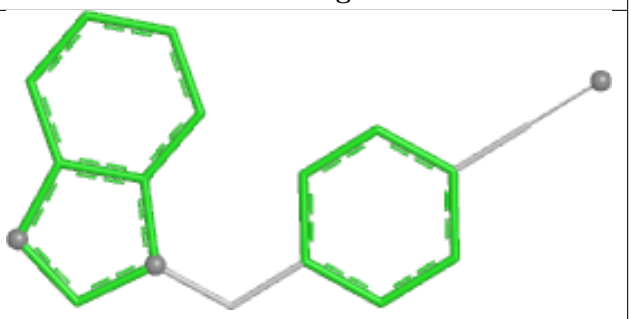
Bond lengths



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	574/637 (90%)	10.41	546 (95%)	0	6, 41, 93, 169	265 (46%)

All (546) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	745	GLY	35.8
1	A	290	THR	32.4
1	A	411	ALA	32.2
1	A	744	ALA	31.7
1	A	743	GLY	30.5
1	A	429	SER	30.1
1	A	287	GLU	29.6
1	A	313	GLN	28.8
1	A	425	ALA	28.5
1	A	364	GLN	28.2
1	A	408	ALA	26.5
1	A	304	ALA	25.4
1	A	275	ASP	25.0
1	A	641	ILE	24.4
1	A	317	ALA	24.3
1	A	584	THR	24.2
1	A	889	PHE	23.5
1	A	282	GLU	23.3
1	A	420	LYS	23.1
1	A	423	ARG	22.8
1	A	887	LYS	22.7
1	A	406	ASN	22.5
1	A	405	SER	22.3
1	A	806	THR	22.2
1	A	274	LEU	22.0
1	A	570	LYS	21.9
1	A	284	ILE	21.9

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Mol	Chain	Res	Type	RSRZ
1	A	292	TRP	21.8
1	A	309	TYR	21.8
1	A	676	SER	21.8
1	A	453	ASN	21.6
1	A	426	VAL	21.3
1	A	428	ASP	21.1
1	A	444	GLU	21.1
1	A	648	VAL	21.1
1	A	451	VAL	21.0
1	A	589	VAL	21.0
1	A	636	THR	20.9
1	A	296	GLN	20.8
1	A	481	ALA	20.5
1	A	801[A]	HIS	20.5
1	A	291	SER	20.3
1	A	369	GLY	20.2
1	A	410	GLY	20.1
1	A	742	GLN	20.1
1	A	424	GLU	19.9
1	A	289	GLU	19.9
1	A	277	ILE	19.9
1	A	403	VAL	19.7
1	A	740	ILE	19.6
1	A	860	ALA	19.6
1	A	452	TYR	19.3
1	A	564	LEU	19.3
1	A	635	LEU	19.2
1	A	278	GLY	19.2
1	A	303	TRP	19.1
1	A	400	THR	19.1
1	A	285	LYS	19.0
1	A	419	TRP	18.9
1	A	478	TRP	18.9
1	A	579	ARG	18.7
1	A	286	GLN	18.7
1	A	312	LYS	18.7
1	A	741[A]	SER	18.7
1	A	849	SER	18.7
1	A	794	THR	18.5
1	A	882	TYR	18.5
1	A	305	TYR	18.5
1	A	294	TYR	18.4

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Mol	Chain	Res	Type	RSRZ
1	A	311	THR	18.4
1	A	583	PRO	18.4
1	A	298	HIS	18.3
1	A	399	PHE	18.2
1	A	754	LEU	18.2
1	A	314	THR	18.0
1	A	368	GLU	18.0
1	A	544	LEU	17.8
1	A	672	ASP	17.8
1	A	788	VAL	17.7
1	A	281	ILE	17.7
1	A	716	LEU	17.6
1	A	632	ILE	17.5
1	A	858	THR	17.4
1	A	857	ALA	17.3
1	A	631	SER	17.3
1	A	763[A]	SER	17.3
1	A	308	SER	17.2
1	A	302	THR	17.2
1	A	682	ASN	17.2
1	A	872	SER	17.2
1	A	276	ILE	17.1
1	A	404	ARG	17.1
1	A	367	LYS	17.1
1	A	645	ASN	17.1
1	A	664	ASP	17.1
1	A	708	PHE	17.0
1	A	559	GLY	16.9
1	A	572	THR	16.9
1	A	592	ILE	16.8
1	A	633	GLN	16.8
1	A	421	SER	16.8
1	A	787	TRP	16.7
1	A	307	GLY	16.6
1	A	475	TRP	16.5
1	A	273	ASN	16.5
1	A	593	ILE	16.5
1	A	629	PHE	16.5
1	A	880	THR	16.5
1	A	295	ASP	16.5
1	A	535	THR	16.4
1	A	356	LYS	16.4

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Mol	Chain	Res	Type	RSRZ
1	A	293	HIS	16.4
1	A	890	ARG	16.4
1	A	833	TRP	16.3
1	A	398	GLU	16.3
1	A	441	LEU	16.3
1	A	418	LYS	16.3
1	A	446	LYS	16.2
1	A	530	MET	16.2
1	A	357	GLU	16.2
1	A	628	VAL	16.2
1	A	627	GLY	16.1
1	A	665	CYS	16.1
1	A	588	THR	16.0
1	A	558	GLU	16.0
1	A	373	LEU	16.0
1	A	280	ARG	15.9
1	A	634	HIS	15.9
1	A	571	LEU	15.8
1	A	871	ARG	15.8
1	A	531	TYR	15.8
1	A	486	PHE	15.8
1	A	888	ARG	15.8
1	A	835	GLU	15.7
1	A	591	ASP	15.6
1	A	480	GLY	15.6
1	A	790	THR	15.6
1	A	383	LYS	15.5
1	A	875	GLY	15.5
1	A	706	VAL	15.5
1	A	620	ILE	15.5
1	A	746	TRP	15.5
1	A	477	MET	15.4
1	A	582	ARG	15.4
1	A	366	PRO	15.4
1	A	681	LEU	15.4
1	A	455	MET	15.4
1	A	360	ASP	15.3
1	A	850	LEU	15.3
1	A	476	TYR	15.3
1	A	362	ARG	15.3
1	A	396	ARG	15.3
1	A	649	ARG	15.2

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Mol	Chain	Res	Type	RSRZ
1	A	365	GLU	15.2
1	A	864[A]	GLN	15.0
1	A	855	SER	15.0
1	A	569	PHE	14.9
1	A	605	VAL	14.9
1	A	297	ASP	14.9
1	A	575	ASN	14.9
1	A	474	ILE	14.8
1	A	610	ASN	14.8
1	A	886	MET	14.8
1	A	484	LEU	14.8
1	A	374	MET	14.7
1	A	361	THR	14.6
1	A	407	ALA	14.6
1	A	677	ALA	14.6
1	A	603	GLN	14.6
1	A	834	GLU	14.6
1	A	747	SER	14.6
1	A	774	LEU	14.5
1	A	854	THR	14.5
1	A	789	PRO	14.5
1	A	799	ALA	14.5
1	A	881	ASP	14.4
1	A	397	GLU	14.3
1	A	561	HIS	14.2
1	A	786	HIS	14.2
1	A	283	LYS	14.2
1	A	680	ALA	14.1
1	A	679	THR	14.1
1	A	394	CYS	14.1
1	A	748	LEU	14.1
1	A	640	GLU	14.1
1	A	384	GLU	14.1
1	A	532	ALA	14.0
1	A	427	GLU	14.0
1	A	581	GLN	13.9
1	A	344	THR	13.9
1	A	482	ARG	13.9
1	A	574	GLN	13.8
1	A	838	TYR	13.8
1	A	853	LEU	13.8
1	A	613	THR	13.8

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Mol	Chain	Res	Type	RSRZ
1	A	707	PRO	13.8
1	A	566	GLU	13.8
1	A	785[A]	SER	13.7
1	A	876	ASN	13.7
1	A	580	VAL	13.7
1	A	705	GLN	13.7
1	A	873	LEU	13.6
1	A	358	LYS	13.6
1	A	624	GLU	13.5
1	A	594	SER	13.4
1	A	626	GLU	13.4
1	A	719[A]	LYS	13.4
1	A	877	GLU	13.3
1	A	851	ILE	13.3
1	A	557	MET	13.2
1	A	625	GLY	13.1
1	A	487	GLU	13.1
1	A	856	ARG	13.1
1	A	555	ASN	13.0
1	A	601	SER	13.0
1	A	393	MET	13.0
1	A	363	THR	12.9
1	A	440	ASN	12.9
1	A	622	GLN	12.9
1	A	402	LYS	12.9
1	A	879	TYR	12.9
1	A	739	ARG	12.8
1	A	436	ASP	12.8
1	A	551	GLU	12.7
1	A	619	LEU	12.6
1	A	692	GLN	12.6
1	A	310	GLU	12.6
1	A	549	ASN	12.6
1	A	573	TYR	12.5
1	A	422	ALA	12.5
1	A	279	LYS	12.5
1	A	791	SER	12.5
1	A	753	CYS	12.5
1	A	306	HIS	12.4
1	A	621	ARG	12.4
1	A	379	GLU	12.3
1	A	598	GLN	12.2

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Mol	Chain	Res	Type	RSRZ
1	A	545	GLU	12.2
1	A	590	MET	12.2
1	A	687	VAL	12.1
1	A	861	LYS	12.0
1	A	388	LYS	12.0
1	A	454	MET	12.0
1	A	750	GLU	12.0
1	A	606	THR	11.9
1	A	321	VAL	11.9
1	A	568	ILE	11.8
1	A	548	LYS	11.8
1	A	448	GLU	11.6
1	A	751	THR	11.6
1	A	387	LYS	11.6
1	A	409	LEU	11.6
1	A	737	ARG	11.6
1	A	359	VAL	11.6
1	A	600	GLY	11.5
1	A	534	ASP	11.5
1	A	576	LYS	11.4
1	A	401	ARG	11.4
1	A	371	LYS	11.4
1	A	792	ARG	11.4
1	A	599	ARG	11.2
1	A	825	GLU	11.2
1	A	496	HIS	11.1
1	A	301	LYS	11.1
1	A	840	GLY	11.1
1	A	749	ARG	11.1
1	A	556	HIS	11.1
1	A	550	GLU	11.0
1	A	623	MET	11.0
1	A	560	GLU	11.0
1	A	485	GLU	10.9
1	A	821	ASN	10.8
1	A	533	ASP	10.8
1	A	602	GLY	10.7
1	A	845	GLN	10.5
1	A	793	THR	10.3
1	A	604	VAL	10.3
1	A	434	LEU	10.3
1	A	563	LYS	10.2

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Mol	Chain	Res	Type	RSRZ
1	A	432	TRP	10.2
1	A	372	LYS	10.0
1	A	449	THR	10.0
1	A	694	TRP	10.0
1	A	375	LYS	9.9
1	A	512[A]	LEU	9.9
1	A	839	LEU	9.8
1	A	800	THR	9.8
1	A	865	THR	9.7
1	A	842	ARG	9.7
1	A	878	GLU	9.6
1	A	695	GLU	9.6
1	A	779	ILE	9.6
1	A	815	ARG	9.5
1	A	852	GLY	9.5
1	A	644	LYS	9.4
1	A	337	MET	9.2
1	A	841	LYS	9.1
1	A	807	GLU	9.0
1	A	638	THR	8.9
1	A	870	VAL	8.8
1	A	336	PRO	8.8
1	A	652	ARG	8.7
1	A	508	GLU	8.7
1	A	701	ASN	8.6
1	A	318	SER	8.5
1	A	691	ILE	8.4
1	A	288	HIS	8.4
1	A	501	GLU	8.3
1	A	437	LYS	8.3
1	A	597	ASP	8.2
1	A	524	LYS	8.1
1	A	827	LYS	8.1
1	A	885	SER	8.1
1	A	536	ALA	8.1
1	A	493	ASN	7.9
1	A	831	GLU	7.8
1	A	299	PRO	7.8
1	A	673	ARG	7.8
1	A	327	LEU	7.7
1	A	328	LEU	7.7
1	A	609	LEU	7.7

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Mol	Chain	Res	Type	RSRZ
1	A	717	ILE	7.6
1	A	542	ILE	7.5
1	A	541	ARG	7.5
1	A	430	GLY	7.5
1	A	637	VAL	7.4
1	A	319	SER	7.3
1	A	596	ARG	7.3
1	A	525	LYS	7.3
1	A	732	ASP	7.2
1	A	772	LEU	7.2
1	A	433	GLU	7.1
1	A	693	GLN	7.1
1	A	552	MET	7.1
1	A	702	ASP	6.9
1	A	300	TYR	6.9
1	A	660	ILE	6.9
1	A	808	ASP	6.8
1	A	874	ILE	6.8
1	A	820	GLU	6.8
1	A	431	PHE	6.7
1	A	690	ASP	6.7
1	A	803	TRP	6.7
1	A	341	MET	6.7
1	A	757	SER	6.6
1	A	539	ASP	6.6
1	A	340	GLN	6.6
1	A	715	GLU	6.6
1	A	445	GLY	6.6
1	A	630	LYS	6.5
1	A	503	SER	6.5
1	A	764	LEU	6.3
1	A	670	LEU	6.2
1	A	546	ASP	6.2
1	A	521	ASP	6.1
1	A	683	ASP	6.1
1	A	720	ASP	6.0
1	A	343	MET	6.0
1	A	776	ALA	6.0
1	A	439	ARG	5.9
1	A	685	GLY	5.9
1	A	723	VAL	5.9
1	A	663	ASP	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	650	VAL	5.8
1	A	567	ALA	5.8
1	A	497	TRP	5.8
1	A	642	ALA	5.7
1	A	730	ASN	5.7
1	A	509	GLY	5.7
1	A	538	TRP	5.7
1	A	704	THR	5.6
1	A	816	VAL	5.6
1	A	540	THR	5.6
1	A	611	THR	5.6
1	A	483	PHE	5.6
1	A	523	SER	5.6
1	A	826	ASP	5.6
1	A	830	VAL	5.5
1	A	802	GLU	5.5
1	A	828	THR	5.5
1	A	819	GLN	5.5
1	A	646	TRP	5.5
1	A	479	LEU	5.5
1	A	810	LEU	5.5
1	A	781	SER	5.5
1	A	867	ILE	5.5
1	A	507	VAL	5.4
1	A	780	CYS	5.4
1	A	866	ALA	5.3
1	A	647	LEU	5.3
1	A	386	GLY	5.3
1	A	495	ASP	5.3
1	A	578	VAL	5.3
1	A	554	THR	5.3
1	A	498	PHE	5.3
1	A	674	PHE	5.2
1	A	738	ALA	5.2
1	A	450	CYS	5.1
1	A	537	GLY	5.1
1	A	381	LEU	5.1
1	A	836	ILE	5.1
1	A	832	SER	5.0
1	A	829	PRO	5.0
1	A	671	ASP	5.0
1	A	447	CYS	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	783	VAL	4.9
1	A	814	ASN	4.9
1	A	758	TYR	4.9
1	A	805	THR	4.9
1	A	320	MET	4.8
1	A	615	MET	4.8
1	A	811	THR	4.8
1	A	595	ARG	4.8
1	A	639	GLU	4.7
1	A	726	VAL	4.7
1	A	334	ILE	4.7
1	A	443	LEU	4.7
1	A	710	SER	4.7
1	A	562	LYS	4.7
1	A	729	ARG	4.7
1	A	438	GLU	4.6
1	A	494	GLU	4.6
1	A	491	PHE	4.6
1	A	769	ARG	4.6
1	A	370	THR	4.5
1	A	698	ARG	4.5
1	A	616	GLU	4.5
1	A	435	VAL	4.5
1	A	733	GLU	4.5
1	A	338	VAL	4.5
1	A	612	PHE	4.5
1	A	818	ILE	4.4
1	A	725	VAL	4.4
1	A	728	CYS	4.4
1	A	329	THR	4.4
1	A	378	ALA	4.4
1	A	804	MET	4.3
1	A	678	LEU	4.3
1	A	520	ARG	4.3
1	A	868	ASN	4.3
1	A	824	MET	4.2
1	A	656	SER	4.2
1	A	339	THR	4.2
1	A	392	ARG	4.2
1	A	492	LEU	4.1
1	A	377	THR	4.1
1	A	884	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	848	GLY	4.1
1	A	529	ALA	4.1
1	A	514	LYS	4.1
1	A	862	ASN	4.1
1	A	711	HIS	4.1
1	A	499	SER	4.1
1	A	863	ILE	4.0
1	A	325	VAL	4.0
1	A	518	ILE	4.0
1	A	510	GLU	3.9
1	A	658	MET	3.9
1	A	390	THR	3.9
1	A	837	PRO	3.9
1	A	823	TRP	3.9
1	A	342	ALA	3.8
1	A	442	HIS	3.8
1	A	724	LEU	3.7
1	A	755	GLY	3.7
1	A	380	TRP	3.7
1	A	721	GLY	3.7
1	A	395	THR	3.7
1	A	504	LEU	3.7
1	A	607	TYR	3.6
1	A	502	ASN	3.6
1	A	777	ASN	3.6
1	A	768	HIS	3.5
1	A	736	GLY	3.5
1	A	759	ALA	3.5
1	A	784	PRO	3.4
1	A	762	TRP	3.4
1	A	376	ILE	3.4
1	A	713	PHE	3.4
1	A	766	TYR	3.4
1	A	577	VAL	3.4
1	A	513	HIS	3.4
1	A	651	GLY	3.4
1	A	846	TRP	3.4
1	A	684	MET	3.3
1	A	547	LEU	3.3
1	A	697	SER	3.2
1	A	519	LEU	3.2
1	A	330	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	883	MET	3.2
1	A	382	TRP	3.2
1	A	765	MET	3.2
1	A	812	VAL	3.2
1	A	735	ILE	3.2
1	A	515	LEU	3.2
1	A	655	LEU	3.2
1	A	689	LYS	3.1
1	A	565	ALA	3.1
1	A	734	LEU	3.1
1	A	669	PRO	3.1
1	A	699	GLY	3.1
1	A	718	MET	3.1
1	A	522	VAL	3.0
1	A	869	GLN	3.0
1	A	324	VAL	3.0
1	A	662	GLY	3.0
1	A	526	GLU	2.9
1	A	809	MET	2.9
1	A	675	ALA	2.9
1	A	618	GLN	2.9
1	A	760	GLN	2.9
1	A	847	CYS	2.9
1	A	659	ALA	2.9
1	A	335	ILE	2.9
1	A	332	TRP	2.8
1	A	657	ARG	2.8
1	A	517	TYR	2.8
1	A	686	LYS	2.8
1	A	527	GLY	2.8
1	A	553	VAL	2.7
1	A	643	VAL	2.7
1	A	654	ARG	2.7
1	A	389	LYS	2.7
1	A	767	PHE	2.7
1	A	722	ARG	2.7
1	A	516	GLY	2.6
1	A	500	ARG	2.6
1	A	489	LEU	2.6
1	A	703	TRP	2.6
1	A	775	ALA	2.6
1	A	490	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	331	PRO	2.5
1	A	714	HIS	2.4
1	A	326	ARG	2.4
1	A	756	LYS	2.4
1	A	653	GLU	2.4
1	A	488	ALA	2.3
1	A	322	ASN	2.2
1	A	782	ALA	2.2
1	A	709	CYS	2.2
1	A	859	TRP	2.2
1	A	333	ASP	2.1
1	A	844	ASP	2.1
1	A	696	PRO	2.1
1	A	385	LEU	2.0
1	A	817	TRP	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
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
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

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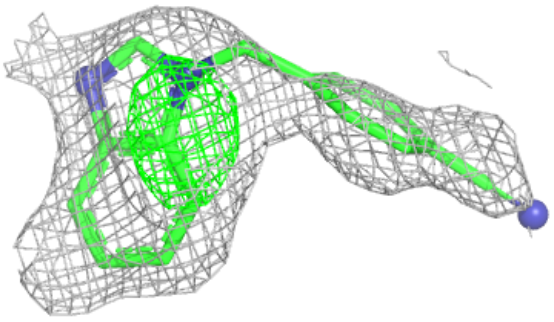
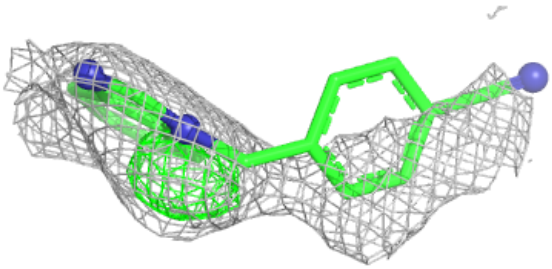
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	CL	A	1011	1/1	0.90	0.16	2,2,2,2	1
2	ZN	A	1001	1/1	0.97	0.04	39,39,39,39	0
2	ZN	A	1002	1/1	0.99	0.07	77,77,77,77	0

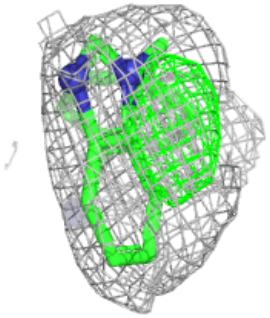
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around RYM A 1009:

$2mF_o$-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.