



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:57 PM UTC

PDB ID : 1ME8 / pdb_00001me8
Title : Inosine Monophosphate Dehydrogenase (IMPDH) From Tritrichomonas Foetus with RVP bound
Authors : Prosise, G.L.; Wu, J.; Luecke, H.
Deposited on : 2002-08-08
Resolution : 1.90 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)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

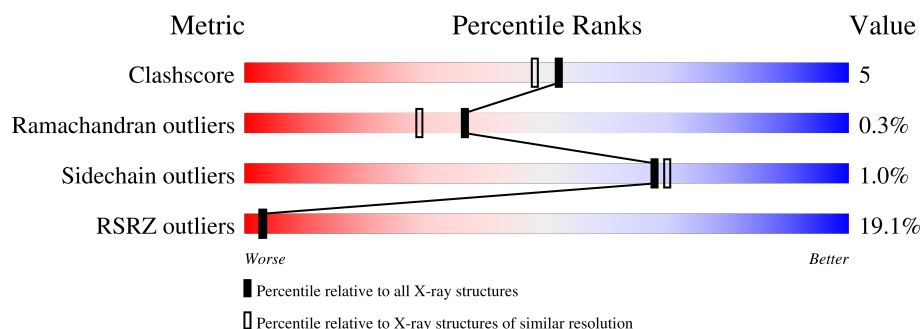
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	503	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2951 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 INOSINE-5'-MONOPHOSPHATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	0	0	0
			2727	1725	466	521	15			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	319	CSO	CYS	modified residue	UNP P50097

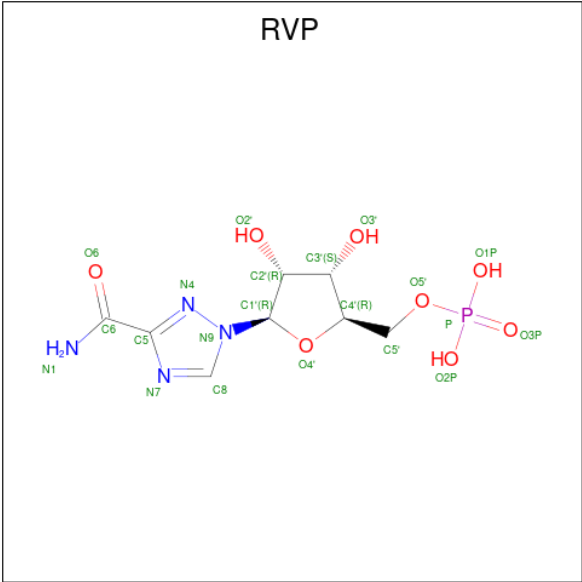
- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is RIBAVIRIN MONOPHOSPHATE (CCD ID: RVP) (formula: C₈H₁₃N₄O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			21	8	4	8	1		

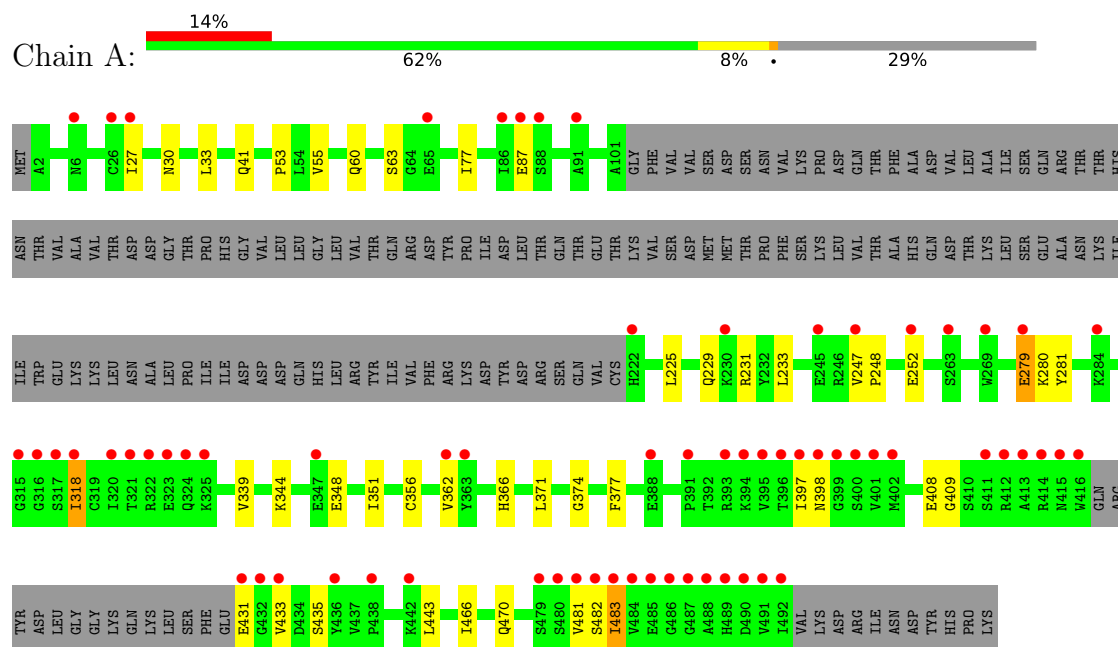
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	201	Total	O	0	0
			201	201		

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: INOSINE-5'-MONOPHOSPHATE DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 3 2	Depositor
Cell constants a, b, c, α , β , γ	154.75Å 154.75Å 154.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.94 – 1.90 48.94 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.94-1.90) 89.6 (48.94-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 1.90Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.243 , 0.258 0.239 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 35.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2951	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% 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: CSO, NA, K, RVP

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	0.34	0/2766	0.85	2/3729 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	63	SER	N-CA-C	6.33	119.69	108.24
1	A	435	SER	N-CA-C	5.93	116.07	108.24

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	2727	0	2716	28	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	21	0	11	0	0
5	A	201	0	0	0	0
All	All	2951	0	2727	28	0

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 5.

All (28) 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:41:GLN:HE22	1:A:351:ILE:HG12	1.24	0.99
1:A:248:PRO:O	1:A:252:GLU:HG2	1.73	0.88
1:A:344:LYS:O	1:A:348:GLU:HG3	1.88	0.73
1:A:41:GLN:NE2	1:A:351:ILE:HG12	2.03	0.70
1:A:362:VAL:H	1:A:366:HIS:HD2	1.44	0.65
1:A:482:SER:O	1:A:483:ILE:HB	1.97	0.64
1:A:280:LYS:O	1:A:280:LYS:HD3	2.02	0.59
1:A:247:VAL:HB	1:A:248:PRO:HD3	1.86	0.58
1:A:397:ILE:HG22	1:A:398:ASN:ND2	2.20	0.56
1:A:318:ILE:HG22	1:A:433:VAL:HG23	1.90	0.51
1:A:443:LEU:C	1:A:443:LEU:HD23	2.35	0.51
1:A:280:LYS:HD2	1:A:281:TYR:CZ	2.46	0.51
1:A:356:CYS:HB2	1:A:377:PHE:CE2	2.48	0.48
1:A:55:VAL:HG12	1:A:77:ILE:HG22	1.95	0.47
1:A:225:LEU:HG	1:A:233:LEU:HD12	1.96	0.47
1:A:33:LEU:HB3	1:A:53:PRO:HD3	1.96	0.47
1:A:229:GLN:OE1	1:A:231:ARG:NH1	2.49	0.45
1:A:339:VAL:HG21	1:A:374:GLY:HA3	1.99	0.45
1:A:87:GLU:H	1:A:87:GLU:CD	2.26	0.43
1:A:482:SER:O	1:A:483:ILE:CB	2.65	0.43
1:A:27:ILE:HG12	1:A:30:ASN:ND2	2.34	0.42
1:A:279:GLU:CD	1:A:279:GLU:C	2.87	0.42
1:A:371:LEU:O	1:A:470:GLN:HG2	2.19	0.42
1:A:409:GLY:O	1:A:431:GLU:HB2	2.20	0.42
1:A:60:GLN:HG3	1:A:408:GLU:OE2	2.20	0.41
1:A:466:ILE:O	1:A:470:GLN:HG3	2.19	0.41
1:A:27:ILE:HG12	1:A:30:ASN:HD22	1.86	0.41
1:A:482:SER:OG	1:A:483:ILE:N	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	350/503 (70%)	332 (95%)	17 (5%)	1 (0%)	36	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	483	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	289/423 (68%)	286 (99%)	3 (1%)	68	70

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	279	GLU
1	A	318	ILE
1	A	481	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	30	ASN
1	A	41	GLN
1	A	49	ASN
1	A	324	GLN
1	A	331	GLN
1	A	366	HIS
1	A	398	ASN
1	A	415	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\# Z > 2$
1	CSO	A	319	3,1	3,6,7	0.65	0	1,6,8	0.47	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
1	CSO	A	319	3,1	-	1/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	319	CSO	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	RVP	A	602	-	22,22,22	2.02	5 (22%)	31,33,33	3.07	9 (29%)

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
4	RVP	A	602	-	-	2/14/30/30	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	RVP	C6-C5	-5.38	1.45	1.49
4	A	602	RVP	C5-N4	3.79	1.39	1.33
4	A	602	RVP	C6-N1	3.74	1.44	1.33
4	A	602	RVP	C1'-N9	3.06	1.51	1.46
4	A	602	RVP	C8-N9	2.87	1.38	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	RVP	C8-N9-N4	-9.24	105.27	109.87
4	A	602	RVP	C6-C5-N7	8.05	131.09	122.67
4	A	602	RVP	O6-C6-C5	7.51	126.62	119.86
4	A	602	RVP	N9-C8-N7	4.55	112.81	110.53
4	A	602	RVP	C6-C5-N4	-3.86	118.63	121.98
4	A	602	RVP	N4-C5-N7	-3.20	110.28	114.90
4	A	602	RVP	O1P-P-O5'	3.05	114.63	106.67
4	A	602	RVP	C8-N7-C5	2.08	106.11	103.46
4	A	602	RVP	C1'-N9-C8	2.08	133.35	128.03

There are no chirality outliers.

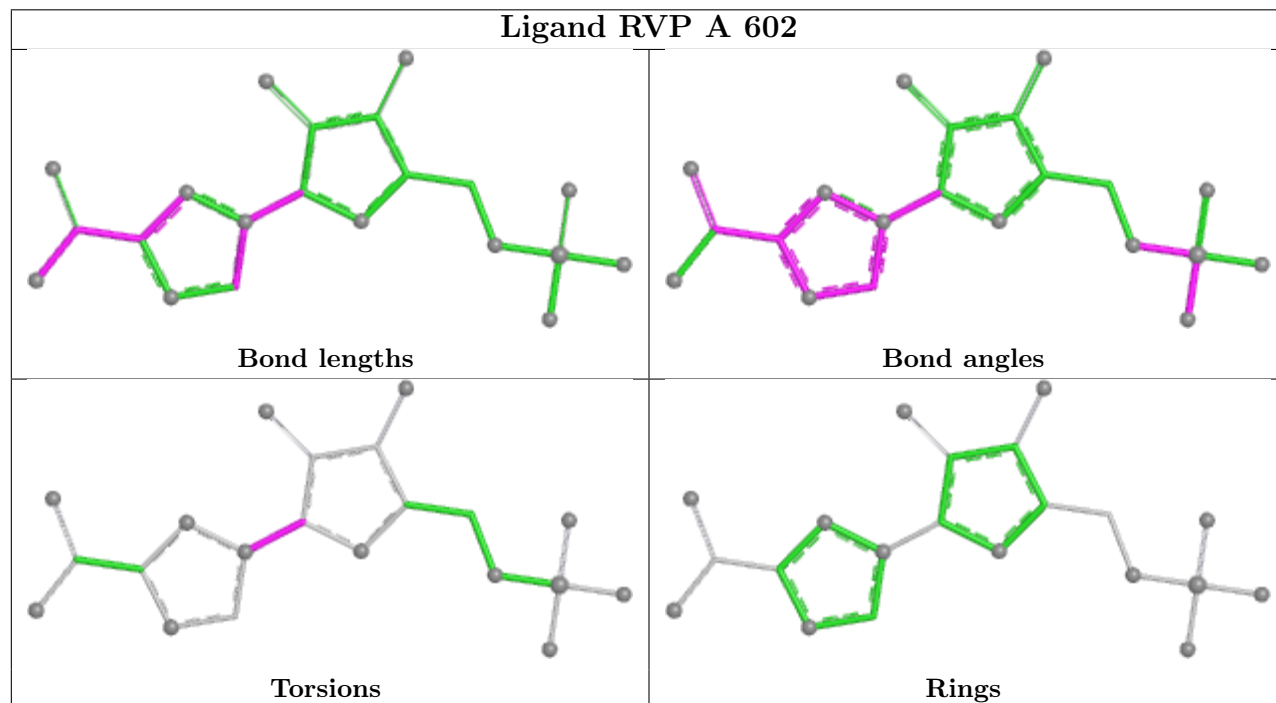
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	602	RVP	C2'-C1'-N9-N4
4	A	602	RVP	C2'-C1'-N9-C8

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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, 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	356/503 (70%)	1.10	68 (19%) 3 3	22, 33, 61, 76	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	483	ILE	8.4
1	A	486	GLY	8.4
1	A	320	ILE	8.4
1	A	487	GLY	8.3
1	A	416	TRP	8.3
1	A	492	ILE	7.4
1	A	488	ALA	7.2
1	A	484	VAL	7.2
1	A	415	ASN	6.7
1	A	481	VAL	6.5
1	A	491	VAL	6.2
1	A	414	ARG	6.2
1	A	482	SER	6.0
1	A	322	ARG	5.7
1	A	433	VAL	5.5
1	A	324	GLN	5.4
1	A	397	ILE	5.2
1	A	480	SER	5.1
1	A	431	GLU	5.1
1	A	222	HIS	4.9
1	A	321	THR	4.6
1	A	398	ASN	4.6
1	A	485	GLU	4.4
1	A	490	ASP	4.2
1	A	87	GLU	4.2
1	A	393	ARG	4.1
1	A	413	ALA	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	318	ILE	4.0
1	A	401	VAL	3.7
1	A	399	GLY	3.7
1	A	325	LYS	3.6
1	A	279	GLU	3.5
1	A	395	VAL	3.4
1	A	284	LYS	3.4
1	A	489	HIS	3.2
1	A	245	GLU	3.2
1	A	432	GLY	3.2
1	A	323	GLU	3.1
1	A	315	GLY	3.0
1	A	27	ILE	3.0
1	A	411	SER	3.0
1	A	412	ARG	3.0
1	A	347	GLU	2.9
1	A	396	THR	2.8
1	A	363	TYR	2.7
1	A	269	TRP	2.7
1	A	88	SER	2.6
1	A	26	CYS	2.6
1	A	394	LYS	2.6
1	A	436	TYR	2.6
1	A	402	MET	2.5
1	A	400	SER	2.4
1	A	252	GLU	2.4
1	A	247	VAL	2.3
1	A	316	GLY	2.3
1	A	442	LYS	2.3
1	A	65	GLU	2.2
1	A	91	ALA	2.2
1	A	438	PRO	2.2
1	A	388	GLU	2.2
1	A	263	SER	2.2
1	A	317	SER	2.2
1	A	391	PRO	2.1
1	A	362	VAL	2.1
1	A	86	ILE	2.0
1	A	479	SER	2.0
1	A	6	ASN	2.0
1	A	230	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	CSO	A	319	7/8	0.72	0.21	56,58,63,64	0

6.3 Carbohydrates [i](#)

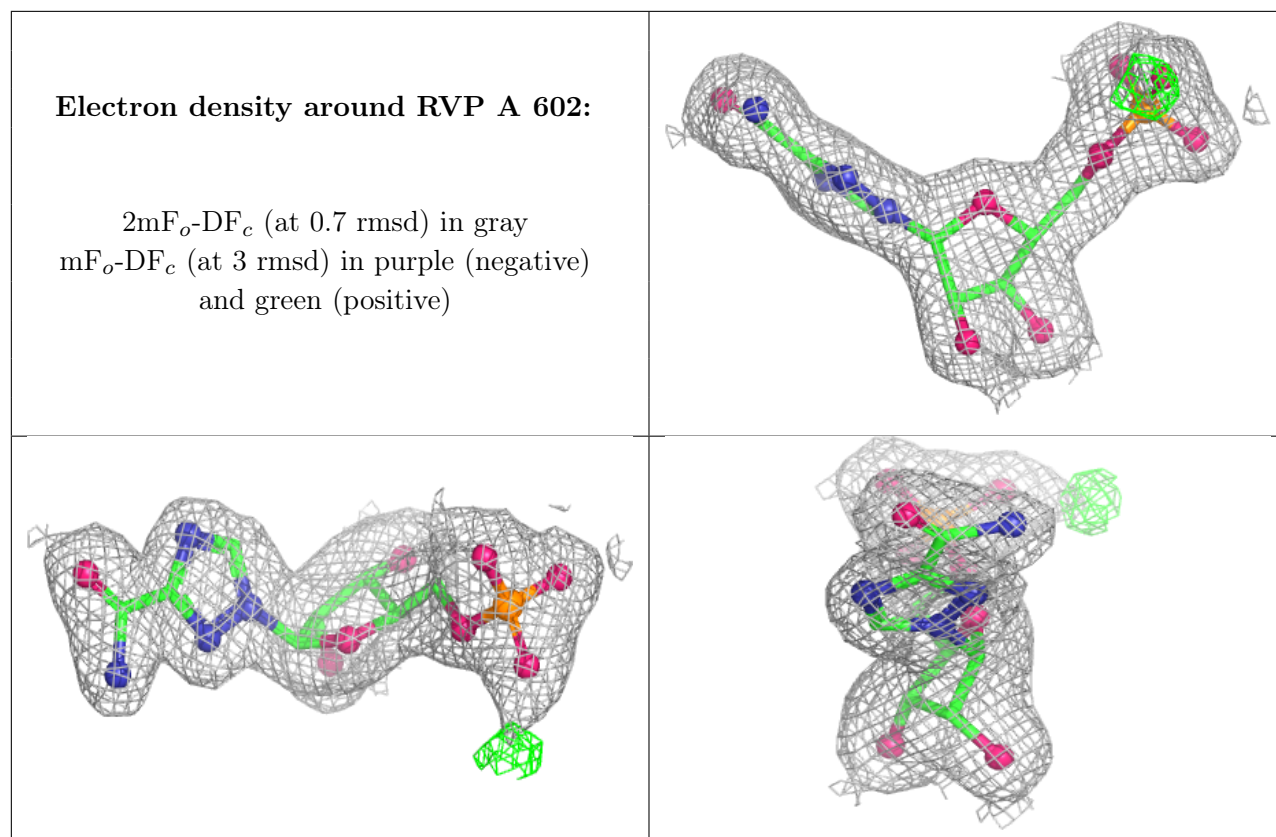
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	A	901	1/1	0.87	0.14	51,51,51,51	0
4	RVP	A	602	21/21	0.96	0.08	28,32,34,35	0
2	K	A	900	1/1	0.99	0.06	33,33,33,33	1

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 [i](#)

There are no such residues in this entry.