



Full wwPDB Geometry-Only Validation Report ⓘ

Mar 5, 2026 – 09:16 AM UTC

PDB ID : 9V6C / pdb_00009v6c
Title : Neutron crystal structure of the oxidized form of b5R at pD 7.5
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Deposited on : 2025-05-27
Resolution : 1.45 Å(reported)

This is a Full wwPDB Geometry-Only 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)
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

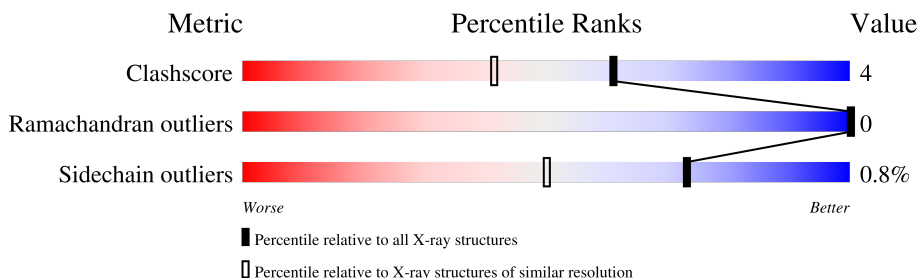
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

NEUTRON DIFFRACTION

The reported resolution of this entry is 1.45 Å.

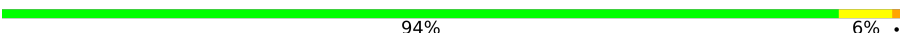
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	272	 94% 6%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6396 atoms, of which 2209 are hydrogens and 1103 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 NADH-cytochrome b5 reductase 3.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	D	H	N	O	S			
1	A	272	5197	1606	491	2186	442	459	13	0	250	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	GLN	GLU	conflict	UNP P83686

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	D	H	N	O	P		
2	A	1	84	27	8	23	9	15	2	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	D	O	0	0
			14	3	8	3		
3	A	1	Total	C	D	O	0	0
			14	3	8	3		
3	A	1	Total	C	D	O	0	0
			14	3	8	3		
3	A	1	Total	C	D	O	0	0
			14	3	8	3		

- Molecule 4 is water.

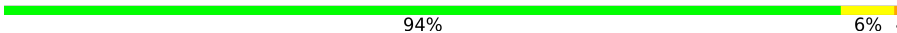
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	456	Total	D	O	0	31
			1059	572	487		

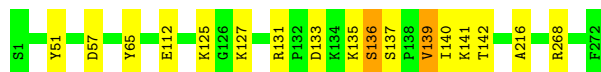
3 Residue-property plots [i](#)

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. 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. 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.

Note EDS was not executed.

- Molecule 1: NADH-cytochrome b5 reductase 3

Chain A:  94% 6% .



4 Model quality [i](#)

4.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, FAD

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	0.68	4/3630 (0.1%)	0.77	0/4915

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	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216[A]	ALA	C-O	5.61	1.30	1.24
1	A	216[B]	ALA	C-O	5.61	1.30	1.24
1	A	125[A]	LYS	CB-CG	5.32	1.68	1.52
1	A	125[B]	LYS	CB-CG	5.32	1.68	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	65[A]	TYR	Sidechain

4.2 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	3011	2186	889	21	0
2	A	61	23	31	0	0
3	A	56	0	32	0	0
4	A	1059	0	0	7	0
All	All	4187	2209	952	21	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 4.

All (21) 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:112[B]:GLU:OE2	4:A:700[B]:HOH:O	1.90	0.88
1:A:57[A]:ASP:OD2	4:A:405:HOH:O	1.98	0.81
1:A:137[A]:SER:O	4:A:404[A]:HOH:O	1.97	0.81
1:A:133[A]:ASP:OD1	1:A:136[A]:SER:HB2	1.83	0.73
1:A:51[A]:TYR:OH	4:A:406:HOH:O	2.06	0.73
1:A:140[A]:ILE:HG12	4:A:594:HOH:O	1.93	0.63
1:A:131[B]:ARG:NH1	1:A:136[B]:SER:O	2.34	0.59
1:A:133[A]:ASP:OD1	1:A:136[A]:SER:CB	2.53	0.56
1:A:141[B]:LYS:HG2	1:A:141[B]:LYS:O	2.05	0.52
1:A:133[A]:ASP:OD1	1:A:135[A]:LYS:C	2.54	0.50
1:A:127[B]:LYS:HG2	1:A:142[B]:THR:OG1	2.10	0.46
1:A:268[B]:ARG:CD	4:A:499:HOH:O	2.66	0.44
1:A:268[B]:ARG:HD2	4:A:499:HOH:O	2.15	0.41

There are no symmetry-related clashes.

4.3 Torsion angles [i](#)

4.3.1 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	439/272 (161%)	431 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

4.3.2 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	390/241 (162%)	386 (99%)	4 (1%)	68	42

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136[A]	SER
1	A	136[B]	SER
1	A	139[A]	VAL
1	A	139[B]	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48[A]	GLN
1	A	182[B]	GLN

4.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

5 ligands are 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	$\# Z > 2$
2	FAD	A	301	-	58,58,58	1.59	8 (13%)	85,89,89	1.21	7 (8%)
3	GOL	A	305	-	5,5,5	0.34	0	5,5,5	0.26	0
3	GOL	A	303	-	5,5,5	0.29	0	5,5,5	0.28	0
3	GOL	A	302	-	5,5,5	0.40	0	5,5,5	0.63	0
3	GOL	A	304	-	5,5,5	0.30	0	5,5,5	0.38	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
2	FAD	A	301	-	-	3/34/50/50	0/6/6/6
3	GOL	A	305	-	-	0/4/4/4	-
3	GOL	A	303	-	-	0/4/4/4	-
3	GOL	A	302	-	-	0/4/4/4	-
3	GOL	A	304	-	-	0/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	FAD	O4B-C1B	5.62	1.55	1.42
2	A	301	FAD	C2B-C1B	-5.31	1.36	1.53
2	A	301	FAD	O4B-C4B	-4.15	1.35	1.45
2	A	301	FAD	P-O3P	3.10	1.62	1.59
2	A	301	FAD	C1'-C2'	2.92	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	FAD	O2B-C2B	2.88	1.50	1.43
2	A	301	FAD	C6A-N6A	2.38	1.40	1.34
2	A	301	FAD	O3B-C3B	-2.02	1.38	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	FAD	C4A-N9A-C8A	4.19	110.14	105.74
2	A	301	FAD	N3A-C2A-N1A	-3.92	122.64	128.58
2	A	301	FAD	N9A-C8A-N7A	-3.44	109.06	113.94
2	A	301	FAD	N6A-C6A-N1A	-3.23	111.17	118.38
2	A	301	FAD	C3B-C2B-C1B	2.94	107.02	101.46
2	A	301	FAD	C5A-C6A-N6A	2.67	129.90	123.29
2	A	301	FAD	N3A-C4A-N9A	2.16	130.85	127.17

There are no chirality outliers.

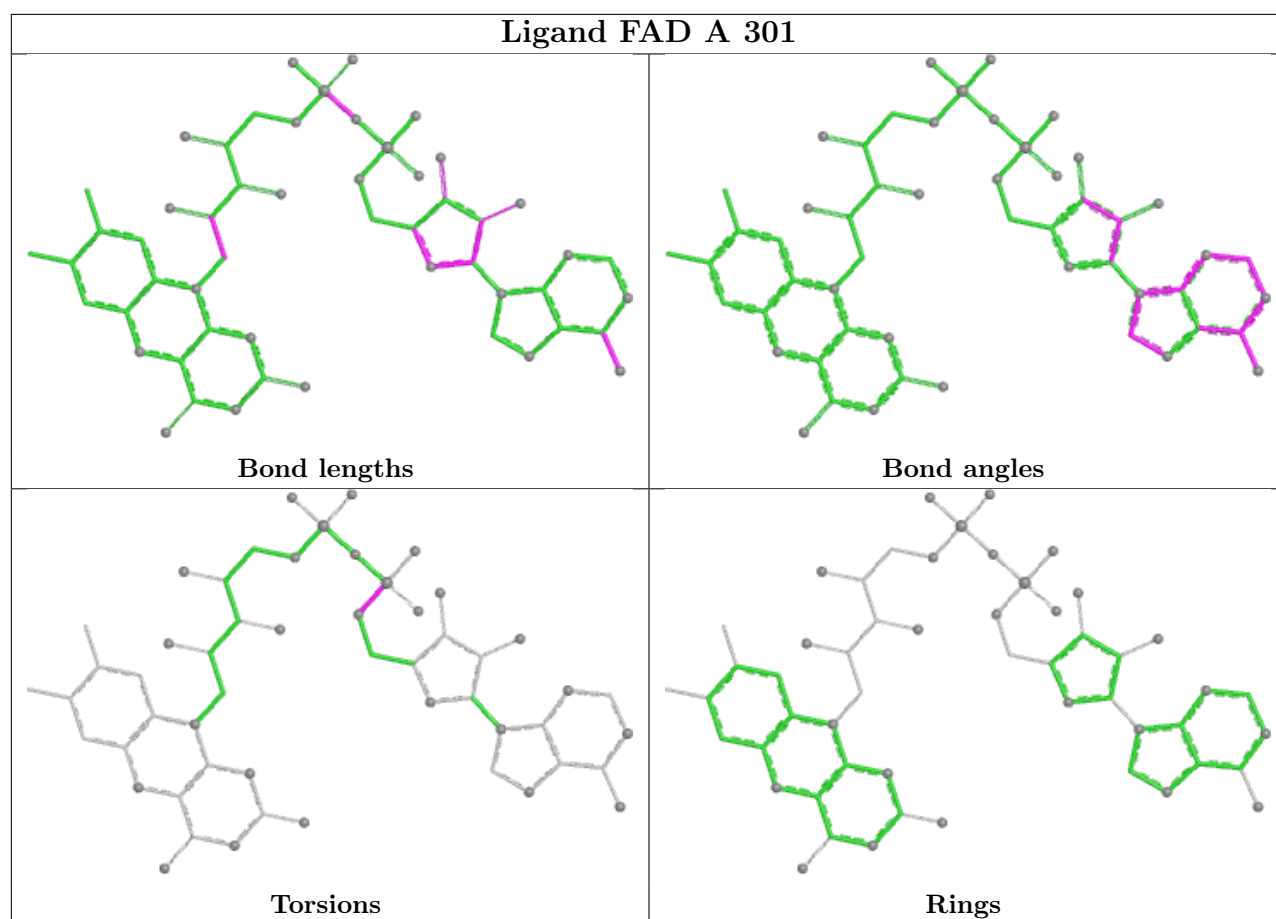
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	FAD	C5B-O5B-PA-O1A
2	A	301	FAD	C5B-O5B-PA-O2A
2	A	301	FAD	C5B-O5B-PA-O3P

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.



4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.