



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:38 PM UTC

PDB ID : 1QX4 / pdb_00001qx4
Title : Structrue of S127P mutant of cytochrome b5 reductase
Authors : Bewley, M.C.; Davis, C.A.; Marohnic, C.C.; Taormina, D.; Barber, M.J.
Deposited on : 2003-09-04
Resolution : 1.80 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
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

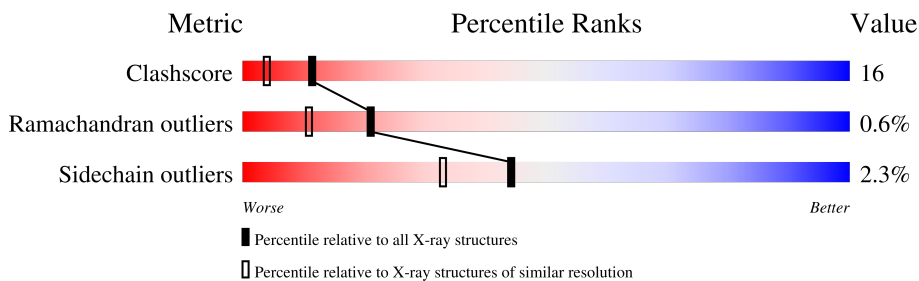
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)

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	274	
1	B	274	

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:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FAD	B	302	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4588 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 NADH-cytochrome b5 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2113	1355	365	381	12			
1	B	264	Total	C	N	O	S	0	0	0
			2113	1355	365	381	12			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MET	-	cloning artifact	UNP P20070
A	28	HIS	-	cloning artifact	UNP P20070
A	29	HIS	-	cloning artifact	UNP P20070
A	30	HIS	-	cloning artifact	UNP P20070
A	31	HIS	-	cloning artifact	UNP P20070
A	32	MET	-	cloning artifact	UNP P20070
A	52	LEU	ILE	conflict	UNP P20070
A	115	GLU	ASP	conflict	UNP P20070
A	127	PRO	SER	engineered mutation	UNP P20070
B	27	MET	-	cloning artifact	UNP P20070
B	28	HIS	-	cloning artifact	UNP P20070
B	29	HIS	-	cloning artifact	UNP P20070
B	30	HIS	-	cloning artifact	UNP P20070
B	31	HIS	-	cloning artifact	UNP P20070
B	32	MET	-	cloning artifact	UNP P20070
B	52	LEU	ILE	conflict	UNP P20070
B	115	GLU	ASP	conflict	UNP P20070
B	127	PRO	SER	engineered mutation	UNP P20070

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

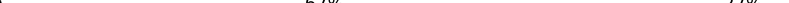


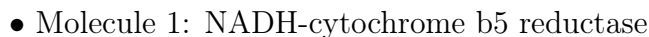
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	53	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	125	Total O 125 125	0	0
3	B	131	Total O 131 131	0	0

Note EDS was not executed.

- Chain A:  67% 27% ...



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.24Å 48.00Å 77.25Å 90.00° 107.69° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-1.80)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.207 , 0.241	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4588	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.82	0/2166	1.18	15/2935 (0.5%)
1	B	0.80	0/2166	1.16	15/2935 (0.5%)
All	All	0.81	0/4332	1.17	30/5870 (0.5%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	GLY	N-CA-C	-7.96	105.91	114.67
1	B	108	VAL	N-CA-C	-7.02	97.74	107.99
1	B	58	ARG	N-CA-C	-6.83	98.11	109.24
1	A	108	VAL	N-CA-C	-6.83	98.03	107.99
1	B	182	GLY	N-CA-C	-6.67	107.00	114.40
1	A	96	VAL	N-CA-C	-6.62	105.08	113.22
1	B	69	ILE	N-CA-C	-6.55	99.66	108.96
1	A	97	SER	N-CA-C	-6.47	102.19	110.53
1	B	96	VAL	N-CA-C	-6.29	105.48	113.22
1	A	63	LEU	N-CA-C	-6.29	102.90	110.13
1	B	97	SER	N-CA-C	-6.07	102.71	110.53
1	A	167	VAL	N-CA-C	-5.92	99.17	108.23
1	A	69	ILE	N-CA-C	-5.89	100.60	108.96
1	A	114	LYS	N-CA-C	5.88	123.33	110.80
1	A	160	ALA	N-CA-C	-5.81	104.95	111.28
1	A	100	ASP	N-CA-C	-5.79	106.05	113.23
1	A	287	LEU	N-CA-C	-5.55	105.23	111.28
1	B	160	ALA	N-CA-C	-5.53	105.25	111.28
1	A	80	LEU	N-CA-C	-5.47	100.79	109.76
1	B	80	LEU	N-CA-C	-5.43	100.85	109.76
1	B	100	ASP	N-CA-C	-5.33	106.62	113.23
1	A	65	SER	N-CA-C	-5.18	103.46	108.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206	LEU	N-CA-C	-5.18	97.27	107.69
1	B	63	LEU	N-CA-C	-5.18	102.51	110.07
1	B	274	GLY	CA-C-N	5.18	123.44	119.66
1	B	274	GLY	C-N-CA	5.18	123.44	119.66
1	B	287	LEU	N-CA-C	-5.17	105.65	111.28
1	A	175	GLY	N-CA-C	-5.11	103.40	112.54
1	B	237	THR	N-CA-C	-5.10	101.32	109.23
1	B	206	LEU	N-CA-C	-5.09	97.45	107.69

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	2113	0	2124	62	0
1	B	2113	0	2124	80	0
2	A	53	0	30	0	0
2	B	53	0	30	5	0
3	A	125	0	0	1	0
3	B	131	0	0	3	0
All	All	4588	0	4308	138	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 16.

All (138) 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)
2:B:302:FAD:H4B	2:B:302:FAD:H8A	1.26	1.10
1:B:58:ARG:HH11	1:B:58:ARG:HG2	1.14	1.08
2:B:302:FAD:H4B	2:B:302:FAD:C8A	1.89	0.99
1:B:58:ARG:HH11	1:B:58:ARG:CG	1.79	0.94
1:B:91:ARG:HH21	1:B:125:LYS:HE2	1.33	0.93
1:A:52:LEU:HG	1:A:57:ARG:HA	1.67	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ILE:HD12	1:B:32:MET:HE2	1.71	0.72
1:B:169:ARG:NH2	1:B:266:GLU:HG3	2.05	0.72
2:B:302:FAD:C8A	2:B:302:FAD:C4B	2.68	0.71
1:A:56:THR:C	1:A:57:ARG:HD2	2.16	0.70
1:B:91:ARG:NH2	1:B:125:LYS:HE2	2.06	0.70
1:A:114:LYS:HB2	1:A:115:GLU:OE2	1.93	0.68
1:B:88:LEU:HD21	1:B:90:ILE:HD11	1.76	0.67
1:B:33:ILE:HG23	1:B:36:GLU:HG2	1.75	0.67
1:B:78:ILE:C	1:B:78:ILE:HD12	2.20	0.65
1:B:123:GLY:HA3	1:B:125:LYS:HZ1	1.61	0.65
1:B:58:ARG:CG	1:B:58:ARG:NH1	2.46	0.65
1:A:240:LYS:O	1:A:240:LYS:HD3	1.96	0.65
1:A:79:TYR:HB2	1:A:142:ARG:HG2	1.79	0.64
1:A:223:GLU:O	1:A:227:GLU:HG3	1.98	0.64
1:B:58:ARG:HG2	1:B:58:ARG:NH1	1.96	0.63
1:B:123:GLY:HA3	1:B:125:LYS:NZ	2.12	0.62
1:A:32:MET:HE2	1:B:40:ILE:HD12	1.81	0.61
1:B:143:GLY:HA2	1:B:145:ASN:ND2	2.15	0.61
1:B:216:LEU:HG	1:B:217:LEU:HG	1.83	0.61
1:A:216:LEU:HG	1:A:217:LEU:HG	1.82	0.61
1:A:258:ARG:HG3	1:A:290:VAL:HG22	1.81	0.60
1:B:79:TYR:HB2	1:B:142:ARG:HG2	1.83	0.60
1:B:258:ARG:HG3	1:B:290:VAL:HG22	1.83	0.60
1:B:54:HIS:CE1	1:B:214:ASP:OD2	2.56	0.59
1:A:40:ILE:CD1	1:B:32:MET:HE2	2.33	0.59
1:A:52:LEU:HG	1:A:57:ARG:CA	2.34	0.57
1:B:292:HIS:HE1	3:B:317:HOH:O	1.88	0.57
1:A:54:HIS:CE1	1:A:214:ASP:OD2	2.57	0.57
1:B:50:GLU:HB3	1:B:58:ARG:HB2	1.87	0.56
1:B:58:ARG:HD3	1:B:108:VAL:HG22	1.85	0.56
1:A:115:GLU:CD	1:A:115:GLU:N	2.63	0.56
1:A:52:LEU:CD2	1:A:58:ARG:HD2	2.36	0.56
1:A:293:PRO:HG2	1:A:296:ARG:HB2	1.88	0.56
1:A:90:ILE:HD12	1:A:142:ARG:CZ	2.37	0.55
1:A:78:ILE:C	1:A:78:ILE:HD12	2.32	0.54
1:A:114:LYS:HD2	1:A:114:LYS:C	2.32	0.54
1:B:33:ILE:HD11	3:B:383:HOH:O	2.07	0.54
1:A:209:ASN:O	1:A:238:VAL:HA	2.08	0.53
1:A:143:GLY:HA2	1:A:145:ASN:ND2	2.23	0.53
1:A:184:THR:OG1	1:A:185:PRO:HD3	2.09	0.53
1:B:204:TYR:CG	1:B:262:PRO:HD3	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:PRO:HG3	1:A:296:ARG:HD2	1.91	0.52
1:B:184:THR:OG1	1:B:185:PRO:HD3	2.09	0.52
1:A:292:HIS:HE1	3:A:311:HOH:O	1.92	0.52
1:B:81:SER:HA	1:B:89:VAL:O	2.10	0.52
1:B:148:LEU:C	1:B:148:LEU:HD23	2.36	0.51
1:B:33:ILE:HG23	1:B:36:GLU:CG	2.40	0.51
1:B:88:LEU:CD2	1:B:90:ILE:HD11	2.40	0.51
1:A:126:MET:SD	1:A:139:ILE:HD11	2.51	0.51
1:A:241:ALA:H	1:A:249:GLN:HE21	1.59	0.51
1:A:32:MET:HG3	1:B:40:ILE:HD11	1.92	0.50
1:A:204:TYR:CG	1:A:262:PRO:HD3	2.46	0.50
1:B:225:ARG:HD3	1:B:234:LEU:HB3	1.94	0.50
1:A:52:LEU:CD1	1:A:58:ARG:HD2	2.41	0.50
1:B:54:HIS:HE1	1:B:214:ASP:OD2	1.94	0.50
1:A:153:LYS:HB2	1:A:155:LYS:HZ2	1.78	0.49
1:B:114:LYS:NZ	1:B:115:GLU:OE1	2.46	0.49
1:A:177:ILE:HG22	1:A:278:MET:HE2	1.95	0.48
1:B:114:LYS:O	1:B:115:GLU:C	2.56	0.48
1:B:209:ASN:O	1:B:238:VAL:HA	2.13	0.48
1:A:46:LEU:HD21	1:A:49:LYS:HG2	1.96	0.48
1:B:181:THR:C	1:B:183:ILE:N	2.70	0.48
1:A:181:THR:C	1:A:183:ILE:N	2.72	0.48
1:B:96:VAL:HG21	1:B:108:VAL:HG23	1.96	0.48
1:B:241:ALA:H	1:B:249:GLN:HE21	1.61	0.48
1:A:33:ILE:HG23	1:A:71:GLY:HA3	1.96	0.47
1:A:126:MET:HB3	1:A:127:PRO:HD3	1.95	0.47
1:B:33:ILE:HD11	1:B:35:LEU:O	2.14	0.47
1:A:36:GLU:OE1	1:B:36:GLU:OE1	2.33	0.47
1:B:194:LEU:HD12	1:B:224:LEU:HD22	1.97	0.47
1:B:181:THR:C	1:B:183:ILE:H	2.21	0.47
1:A:81:SER:HA	1:A:89:VAL:O	2.15	0.47
1:B:182:GLY:O	1:B:185:PRO:HD2	2.15	0.47
1:B:58:ARG:HD2	1:B:106:ASP:OD1	2.15	0.47
1:B:56:THR:C	1:B:57:ARG:HD2	2.40	0.46
1:B:126:MET:SD	1:B:139:ILE:HD11	2.54	0.46
1:A:32:MET:HE2	1:B:40:ILE:CD1	2.46	0.46
1:A:50:GLU:O	1:A:57:ARG:CB	2.64	0.46
1:A:52:LEU:HD21	1:A:58:ARG:N	2.30	0.46
1:B:296:ARG:HD2	3:B:368:HOH:O	2.14	0.46
1:B:126:MET:HB3	1:B:127:PRO:HD3	1.97	0.45
1:B:169:ARG:HH21	1:B:266:GLU:HA	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:GLY:HA2	1:B:209:ASN:OD1	2.16	0.45
1:A:181:THR:C	1:A:183:ILE:H	2.24	0.45
1:B:169:ARG:HH11	1:B:169:ARG:HG3	1.80	0.45
1:A:48:ASP:OD2	1:A:60:ARG:HB3	2.16	0.45
1:B:78:ILE:C	1:B:78:ILE:CD1	2.88	0.45
1:B:183:ILE:HB	1:B:207:PHE:CZ	2.51	0.45
1:B:208:ALA:HB1	2:B:302:FAD:O2B	2.16	0.45
1:B:76:GLN:NE2	1:B:144:PRO:HB2	2.31	0.45
1:A:183:ILE:HB	1:A:207:PHE:CZ	2.51	0.45
1:B:204:TYR:CE2	1:B:233:LYS:HG3	2.52	0.45
1:A:54:HIS:HE1	1:A:214:ASP:OD2	1.98	0.44
1:B:177:ILE:HG22	1:B:278:MET:HE2	1.98	0.44
1:A:240:LYS:HD3	1:A:240:LYS:C	2.42	0.44
1:B:124:GLY:C	1:B:127:PRO:HD2	2.41	0.44
1:A:47:ILE:HD11	1:A:60:ARG:HG2	1.99	0.44
1:B:93:TYR:HA	2:B:302:FAD:N5	2.33	0.44
1:B:196:ASP:HB3	1:B:199:ASP:HB2	2.00	0.43
1:B:177:ILE:HG12	1:B:261:LEU:HD11	2.00	0.43
1:A:32:MET:HB2	1:A:68:HIS:HA	2.00	0.43
1:A:96:VAL:HG21	1:A:108:VAL:HG23	1.99	0.43
1:A:180:GLY:HA2	1:A:209:ASN:OD1	2.17	0.43
1:A:204:TYR:CD1	1:A:262:PRO:HD3	2.54	0.43
1:B:61:PHE:CD2	1:B:141:PHE:HZ	2.36	0.43
1:B:223:GLU:O	1:B:227:GLU:HG3	2.19	0.42
1:A:57:ARG:HG2	1:A:59:PHE:CE2	2.54	0.42
1:B:73:PRO:HD2	1:B:76:GLN:HE21	1.83	0.42
1:B:276:PRO:N	1:B:277:PRO:HD2	2.33	0.42
1:B:293:PRO:HG2	1:B:296:ARG:HB2	2.00	0.42
1:A:40:ILE:HD11	1:B:32:MET:HG3	2.00	0.42
1:B:183:ILE:HB	1:B:207:PHE:CE1	2.55	0.42
1:B:55:ASP:OD1	1:B:56:THR:HG23	2.19	0.42
1:B:204:TYR:CD1	1:B:262:PRO:HD3	2.54	0.42
1:A:183:ILE:HB	1:A:207:PHE:CE1	2.54	0.42
1:A:276:PRO:N	1:A:277:PRO:HD2	2.34	0.42
1:B:237:THR:HA	1:B:248:SER:O	2.20	0.42
1:A:46:LEU:HD21	1:A:49:LYS:HD3	2.01	0.42
1:B:81:SER:HB2	1:B:90:ILE:HG12	2.00	0.42
1:A:41:LYS:HD3	1:A:142:ARG:NH2	2.35	0.41
1:B:190:ILE:O	1:B:194:LEU:HG	2.20	0.41
1:B:169:ARG:HG3	1:B:169:ARG:NH1	2.36	0.41
1:B:32:MET:HB2	1:B:68:HIS:HA	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:LEU:HD23	1:A:52:LEU:N	2.36	0.41
1:A:148:LEU:HD23	1:A:148:LEU:C	2.46	0.41
1:B:72:LEU:CD2	1:B:95:PRO:HD2	2.51	0.41
1:A:56:THR:HG21	1:A:216:LEU:HD13	2.02	0.41
1:B:54:HIS:NE2	1:B:213:LYS:HE3	2.37	0.40
1:A:263:PRO:HA	1:A:264:PRO:HD3	1.96	0.40
1:A:293:PRO:CG	1:A:296:ARG:HD2	2.51	0.40
1:B:41:LYS:HD3	1:B:41:LYS:N	2.35	0.40
1:A:46:LEU:HD21	1:A:49:LYS:CG	2.51	0.40

There are no symmetry-related clashes.

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	260/274 (95%)	253 (97%)	6 (2%)	1 (0%)	30	19
1	B	260/274 (95%)	253 (97%)	5 (2%)	2 (1%)	16	6
All	All	520/548 (95%)	506 (97%)	11 (2%)	3 (1%)	21	11

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	LYS
1	B	114	LYS
1	B	123	GLY

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	235/245 (96%)	228 (97%)	7 (3%)	36	24
1	B	235/245 (96%)	231 (98%)	4 (2%)	53	45
All	All	470/490 (96%)	459 (98%)	11 (2%)	44	33

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	LYS
1	A	52	LEU
1	A	57	ARG
1	A	64	PRO
1	A	114	LYS
1	A	115	GLU
1	A	294	LYS
1	B	33	ILE
1	B	41	LYS
1	B	58	ARG
1	B	125	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	HIS
1	A	76	GLN
1	A	249	GLN
1	A	292	HIS
1	B	76	GLN
1	B	128	GLN
1	B	151	GLN
1	B	200	HIS
1	B	210	GLN
1	B	226	ASN
1	B	228	HIS
1	B	249	GLN
1	B	292	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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	3.55	23 (39%)	85,89,89	3.01	21 (24%)
2	FAD	B	302	-	58,58,58	2.94	22 (37%)	85,89,89	2.74	24 (28%)

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	-	-	10/34/50/50	0/6/6/6
2	FAD	B	302	-	1/1/9/9	10/34/50/50	0/6/6/6

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	FAD	P-O3P	-16.03	1.42	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	302	FAD	PA-O3P	10.68	1.71	1.59
2	A	301	FAD	C1'-C2'	9.29	1.65	1.52
2	A	301	FAD	PA-O3P	8.63	1.68	1.59
2	B	302	FAD	C1'-C2'	8.36	1.64	1.52
2	B	302	FAD	P-O3P	-7.89	1.51	1.59
2	A	301	FAD	PA-O5B	-7.04	1.31	1.59
2	A	301	FAD	C2'-C3'	-6.69	1.41	1.53
2	B	302	FAD	PA-O5B	-6.03	1.35	1.59
2	A	301	FAD	O5B-C5B	-5.68	1.23	1.44
2	B	302	FAD	PA-O2A	-5.22	1.31	1.55
2	B	302	FAD	C2'-C3'	-5.20	1.44	1.53
2	A	301	FAD	PA-O2A	-4.82	1.33	1.55
2	A	301	FAD	O4B-C1B	3.97	1.51	1.42
2	A	301	FAD	C5'-C4'	3.92	1.57	1.51
2	B	302	FAD	O4B-C1B	3.75	1.50	1.42
2	B	302	FAD	O4B-C4B	3.73	1.53	1.45
2	A	301	FAD	C4X-N5	3.49	1.38	1.30
2	B	302	FAD	C9A-C5X	3.46	1.46	1.41
2	A	301	FAD	C9A-C5X	3.34	1.46	1.41
2	B	302	FAD	C5A-C4A	3.19	1.44	1.39
2	B	302	FAD	C4X-N5	3.04	1.37	1.30
2	B	302	FAD	O5B-C5B	-2.80	1.34	1.44
2	B	302	FAD	C5A-C6A	2.76	1.48	1.41
2	A	301	FAD	P-O5'	-2.75	1.48	1.59
2	A	301	FAD	C5A-C4A	2.69	1.43	1.39
2	A	301	FAD	C5A-C6A	2.67	1.48	1.41
2	A	301	FAD	C1B-N9A	2.65	1.53	1.46
2	B	302	FAD	C1B-N9A	2.63	1.53	1.46
2	B	302	FAD	P-O2P	-2.61	1.43	1.55
2	A	301	FAD	C3B-C4B	2.51	1.59	1.53
2	B	302	FAD	C2A-N1A	2.46	1.38	1.33
2	A	301	FAD	C6-C5X	2.40	1.43	1.40
2	B	302	FAD	C8-C7	2.33	1.46	1.40
2	B	302	FAD	C5'-C4'	2.30	1.54	1.51
2	A	301	FAD	C8-C7	2.29	1.46	1.40
2	B	302	FAD	C4A-N3A	2.27	1.38	1.34
2	A	301	FAD	C4A-N3A	2.24	1.38	1.34
2	B	302	FAD	O2-C2	-2.16	1.20	1.24
2	A	301	FAD	C10-N1	2.15	1.37	1.33
2	A	301	FAD	O2B-C2B	-2.13	1.37	1.43
2	A	301	FAD	C2A-N1A	2.12	1.37	1.33
2	A	301	FAD	P-O2P	-2.10	1.45	1.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	302	FAD	O4-C4	-2.09	1.19	1.23
2	B	302	FAD	O2B-C2B	-2.04	1.37	1.43

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	FAD	O5B-C5B-C4B	10.93	146.22	108.99
2	A	301	FAD	O5'-C5'-C4'	10.68	137.88	109.36
2	B	302	FAD	O3B-C3B-C4B	10.13	140.19	111.08
2	B	302	FAD	O3'-C3'-C4'	-9.79	86.68	108.93
2	A	301	FAD	O3'-C3'-C4'	-9.53	87.29	108.93
2	B	302	FAD	C4B-O4B-C1B	-8.74	90.17	109.47
2	B	302	FAD	C5'-C4'-C3'	-7.85	97.40	112.22
2	A	301	FAD	C5'-C4'-C3'	-7.43	98.20	112.22
2	A	301	FAD	PA-O5B-C5B	7.06	161.81	121.35
2	A	301	FAD	C4'-C3'-C2'	-6.80	102.25	113.57
2	A	301	FAD	O4'-C4'-C3'	6.53	124.54	109.25
2	A	301	FAD	O4B-C4B-C5B	6.46	130.01	109.33
2	B	302	FAD	O3P-PA-O1A	-5.43	94.36	110.70
2	B	302	FAD	PA-O5B-C5B	4.94	149.67	121.35
2	A	301	FAD	O2A-PA-O1A	4.85	135.03	112.44
2	B	302	FAD	O2A-PA-O1A	4.84	134.97	112.44
2	A	301	FAD	O2P-P-O3P	4.69	119.94	107.27
2	B	302	FAD	O5'-P-O1P	4.24	125.75	108.94
2	A	301	FAD	O4B-C1B-N9A	4.05	115.86	108.09
2	A	301	FAD	O2A-PA-O3P	4.04	118.19	107.27
2	B	302	FAD	O5'-C5'-C4'	3.81	119.54	109.36
2	B	302	FAD	O4B-C4B-C5B	-3.77	97.26	109.33
2	B	302	FAD	O4B-C1B-N9A	3.54	114.89	108.09
2	B	302	FAD	O5B-C5B-C4B	-3.51	97.03	108.99
2	B	302	FAD	P-O5'-C5'	3.27	140.07	121.35
2	A	301	FAD	O3P-PA-O1A	-3.15	101.22	110.70
2	B	302	FAD	O5B-PA-O1A	-3.04	96.91	108.94
2	A	301	FAD	O2P-P-O5'	-3.00	93.96	107.57
2	A	301	FAD	C1'-C2'-C3'	-2.98	101.58	109.66
2	B	302	FAD	C1'-C2'-C3'	-2.94	101.69	109.66
2	B	302	FAD	O4'-C4'-C3'	-2.89	102.49	109.25
2	A	301	FAD	O2A-PA-O5B	-2.88	94.51	107.57
2	B	302	FAD	C2B-C3B-C4B	-2.79	97.21	102.61
2	B	302	FAD	O2P-P-O5'	-2.76	95.07	107.57
2	B	302	FAD	C5X-C9A-N10	-2.73	115.50	117.97
2	A	301	FAD	P-O5'-C5'	2.62	136.38	121.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	302	FAD	C4'-C3'-C2'	-2.61	109.23	113.57
2	B	302	FAD	C4-N3-C2	-2.34	121.48	125.64
2	A	301	FAD	C2A-N1A-C6A	2.29	122.50	118.73
2	A	301	FAD	C5X-C9A-N10	-2.26	115.93	117.97
2	B	302	FAD	C5B-C4B-C3B	-2.22	107.23	115.21
2	A	301	FAD	O2P-P-O1P	-2.16	102.40	112.44
2	B	302	FAD	C2A-N1A-C6A	2.16	122.27	118.73
2	A	301	FAD	O3P-P-O1P	-2.06	104.52	110.70
2	B	302	FAD	C4X-C10-N10	2.03	119.39	116.48

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	302	FAD	C4B

All (20) torsion outliers are listed below:

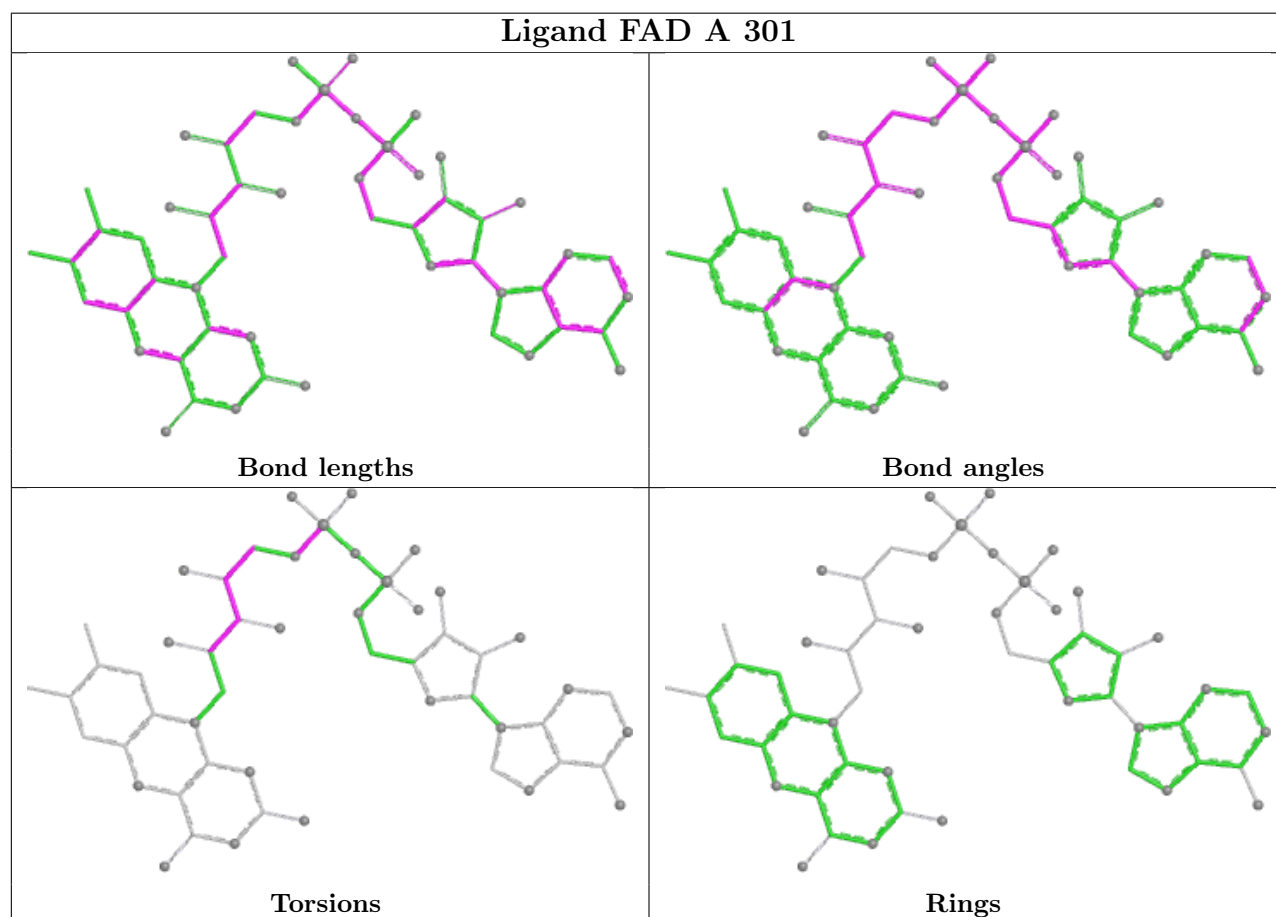
Mol	Chain	Res	Type	Atoms
2	A	301	FAD	C2'-C3'-C4'-O4'
2	A	301	FAD	C2'-C3'-C4'-C5'
2	A	301	FAD	O3'-C3'-C4'-O4'
2	A	301	FAD	C3'-C4'-C5'-O5'
2	A	301	FAD	O4'-C4'-C5'-O5'
2	A	301	FAD	C5'-O5'-P-O1P
2	A	301	FAD	C5'-O5'-P-O3P
2	B	302	FAD	C5B-O5B-PA-O1A
2	B	302	FAD	C5B-O5B-PA-O2A
2	B	302	FAD	C5B-O5B-PA-O3P
2	B	302	FAD	C2'-C3'-C4'-O4'
2	B	302	FAD	O3'-C3'-C4'-O4'
2	A	301	FAD	O3'-C3'-C4'-C5'
2	B	302	FAD	O3'-C3'-C4'-C5'
2	B	302	FAD	C2'-C3'-C4'-C5'
2	B	302	FAD	C3B-C4B-C5B-O5B
2	A	301	FAD	O2'-C2'-C3'-C4'
2	B	302	FAD	O4B-C4B-C5B-O5B
2	B	302	FAD	O2'-C2'-C3'-C4'
2	A	301	FAD	C5'-O5'-P-O2P

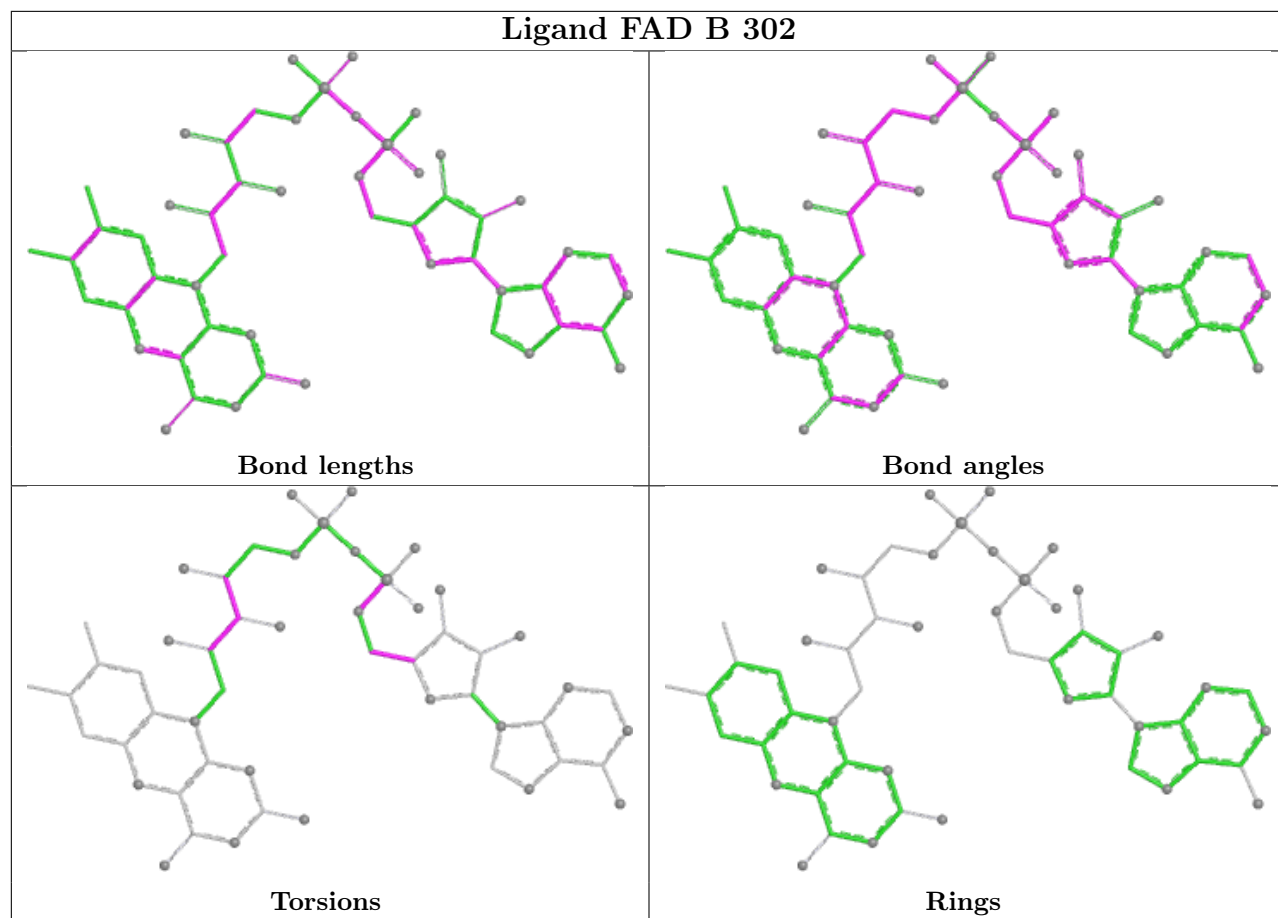
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	302	FAD	5	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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.