



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:57 PM UTC

PDB ID : 9E0A / pdb_00009e0a
Title : Structure of proline utilization A complexed with 1,4-benzenedimethanol
Authors : Tanner, J.J.; Meeks, K.R.
Deposited on : 2024-10-17
Resolution : 1.39 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

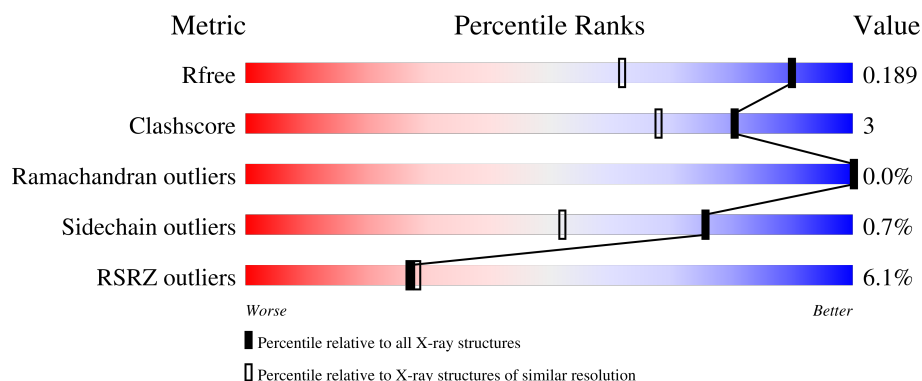
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.39 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	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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	1235	6% 91% 7%
1	B	1235	6% 93% 5%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 21016 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.

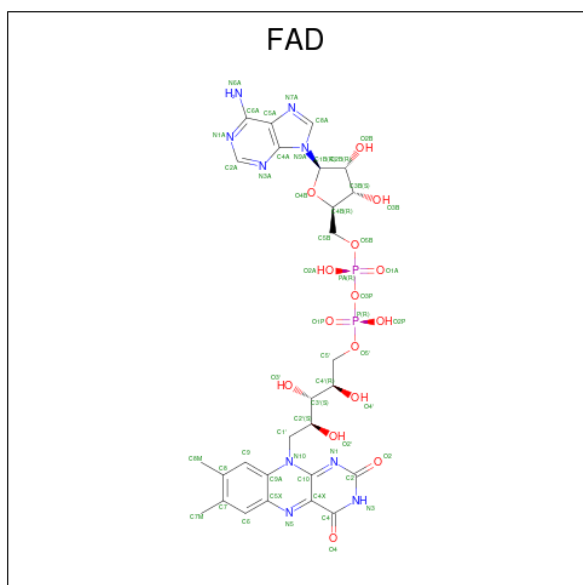
- Molecule 1 is a protein called Bifunctional protein PutA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1216	Total	C	N	O	S	0	25	0
			9117	5758	1631	1693	35			
1	B	1212	Total	C	N	O	S	0	16	0
			9000	5674	1612	1680	34			

There are 4 discrepancies between the modelled and reference sequences:

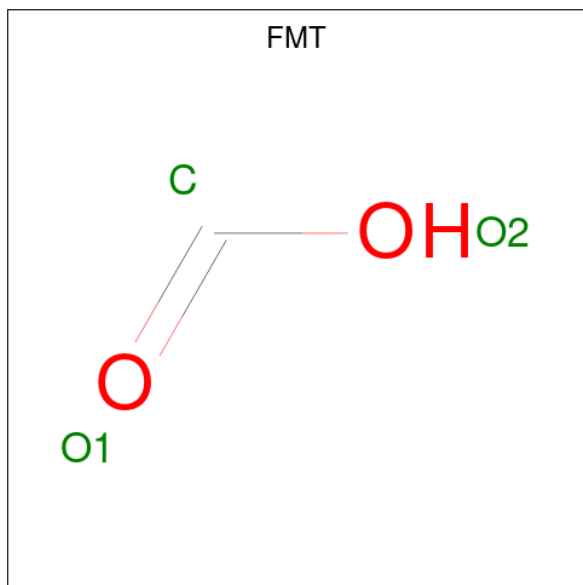
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP F7X6I3
A	0	MET	-	expression tag	UNP F7X6I3
B	-1	SER	-	expression tag	UNP F7X6I3
B	0	MET	-	expression tag	UNP F7X6I3

- 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).



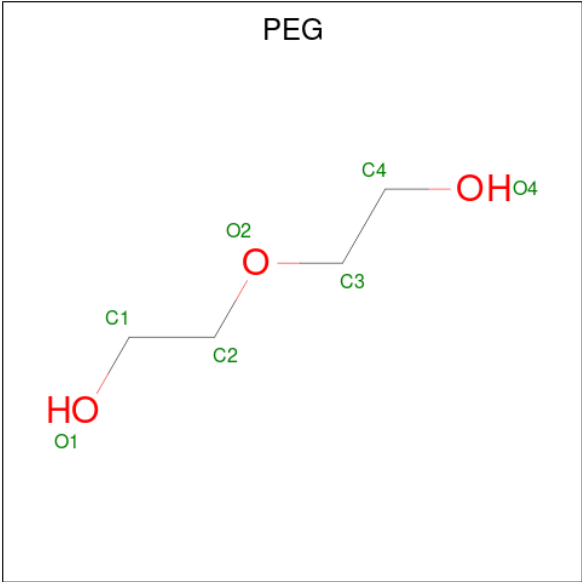
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	
			106	54	18	30	4	
2	B	1	Total	C	N	O	P	
			106	54	18	30	4	

- Molecule 3 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



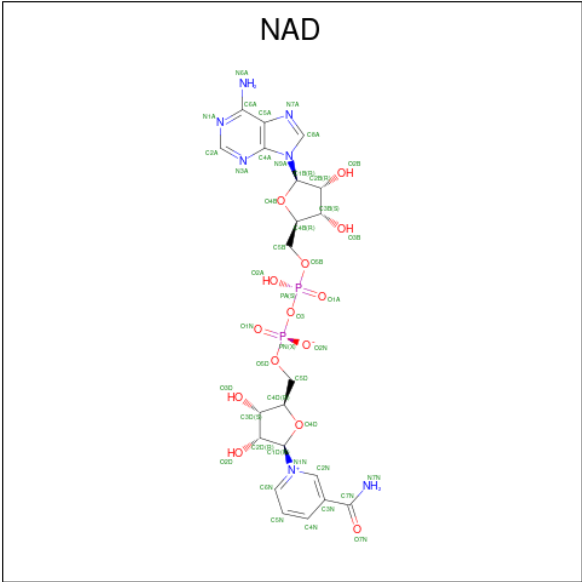
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O		
			3	1	2	0	0
3	B	1	Total	C	O		
			3	1	2	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $\text{C}_4\text{H}_{10}\text{O}_3$).



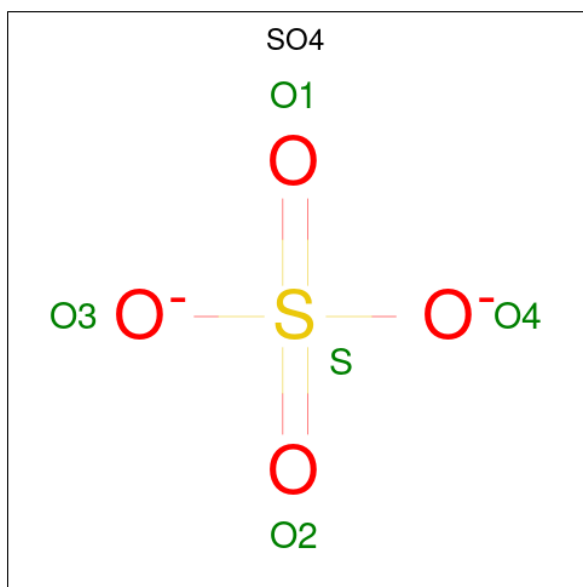
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

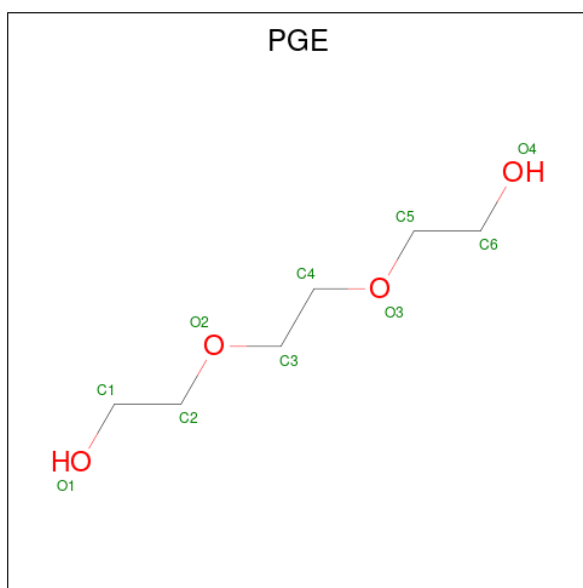


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

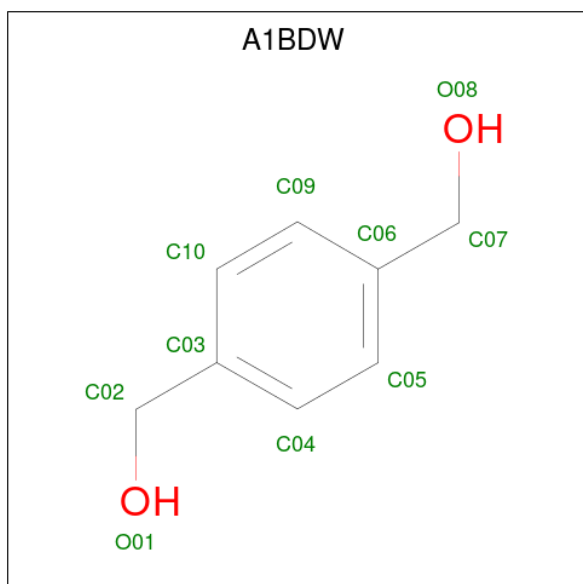
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		
7	B	1	Total	Mg	0	0
			1	1		

- Molecule 8 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 9 is (1,4-phenylene)dimethanol (CCD ID: A1BDW) (formula: $C_8H_{10}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			10	8	2		

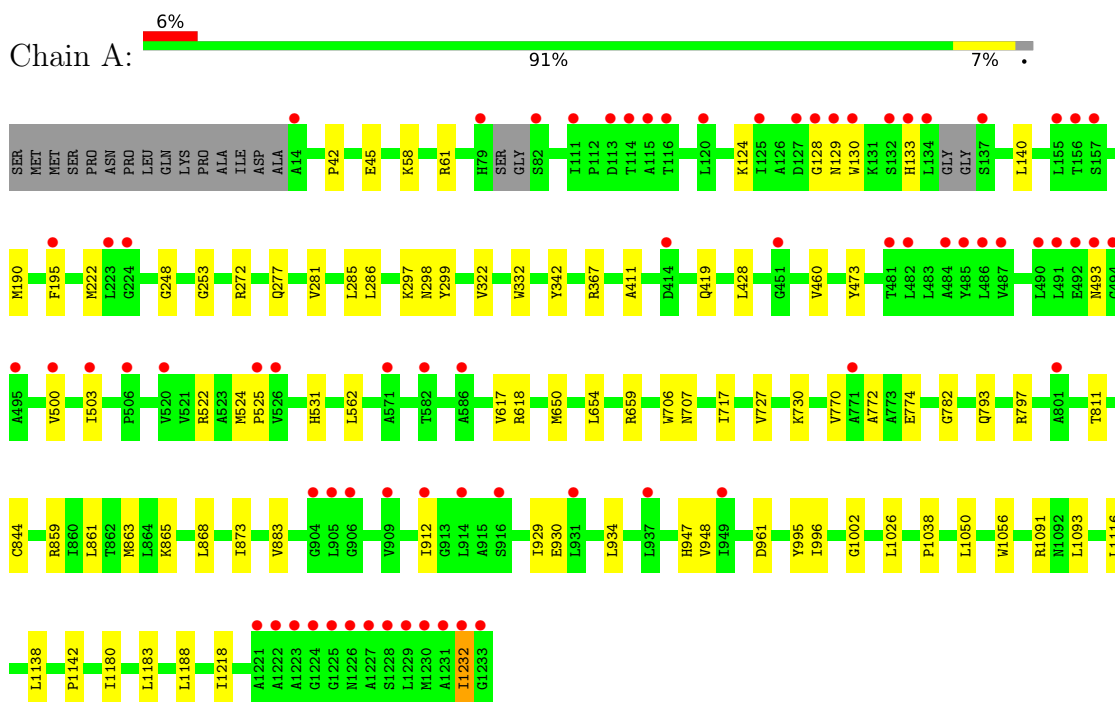
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1234	Total 1234	O 1234	0	0
10	B	1286	Total 1286	O 1286	0	3

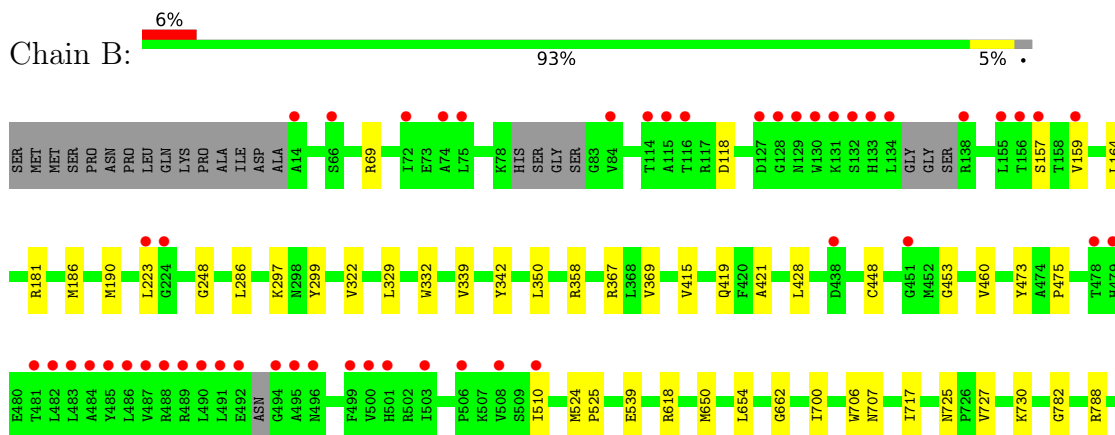
3 Residue-property plots [i](#)

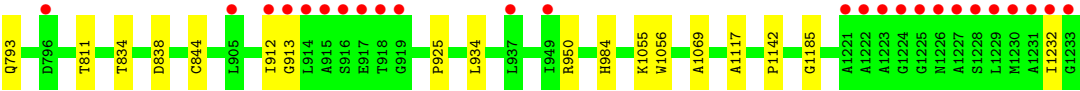
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Bifunctional protein PutA



• Molecule 1: Bifunctional protein PutA





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.72Å 102.07Å 126.18Å 90.00° 106.38° 90.00°	Depositor
Resolution (Å)	47.03 – 1.39 47.03 – 1.39	Depositor EDS
% Data completeness (in resolution range)	97.5 (47.03-1.39) 98.2 (47.03-1.39)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 1.39Å)	Xtriage
Refinement program	PHENIX 1.21rc1_5156	Depositor
R, R_{free}	0.172 , 0.191 (Not available) , 0.189	Depositor DCC
R_{free} test set	24210 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	21016	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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: MG, A1BDW, FAD, PEG, NAD, FMT, SO4, PGE

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	0.25	0/9336	0.45	0/12706
1	B	0.27	0/9209	0.48	0/12535
All	All	0.26	0/18545	0.46	0/25241

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	912	ILE	Peptide

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	9117	0	9187	53	0
1	B	9000	0	8996	37	0
2	A	106	0	62	4	0
2	B	106	0	62	2	0
3	A	3	0	1	0	0
3	B	3	0	1	0	0
4	A	14	0	20	1	0
4	B	7	0	10	0	0
5	A	44	0	26	2	0
5	B	44	0	26	2	0
6	A	25	0	0	1	0
6	B	5	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	B	10	0	14	0	0
9	B	10	0	0	0	0
10	A	1234	0	0	11	0
10	B	1286	0	0	5	0
All	All	21016	0	18405	94	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 3.

All (94) 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:B:844:CYS:SG	5:B:1306:NAD:C4N	2.76	0.73
1:A:873:ILE:HG13	1:A:883:VAL:HB	1.75	0.69
1:A:793:GLN:OE1	10:A:1401:HOH:O	2.12	0.68
1:A:844:CYS:SG	5:A:1305:NAD:C4N	2.81	0.68
1:B:297:LYS:HD2	1:B:329:LEU:HA	1.76	0.68
1:A:996[B]:ILE:HD12	1:A:1218:ILE:HG12	1.76	0.67
1:B:793:GLN:OE1	10:B:1401:HOH:O	2.14	0.66
1:A:861[A]:LEU:HD21	1:A:948:VAL:HG11	1.79	0.65
1:B:339:VAL:HG21	1:B:350:LEU:HD21	1.78	0.65
1:A:1183:LEU:O	10:A:1402:HOH:O	2.14	0.64
1:A:286:LEU:HD21	1:A:322:VAL:HG11	1.79	0.63
1:B:539:GLU:OE1	10:B:1402:HOH:O	2.15	0.63
1:A:961:ASP:OD2	1:B:1055:LYS:NZ	2.31	0.63
1:B:286:LEU:HD21	1:B:322:VAL:HG11	1.83	0.61
1:A:493:ASN:HB3	1:A:500:VAL:HB	1.85	0.59
1:B:650:MET:O	1:B:654:LEU:HG	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:VAL:HG13	1:A:285[B]:LEU:HD23	1.87	0.57
1:A:618:ARG:NH2	10:A:1422:HOH:O	2.38	0.56
1:B:524[A]:MET:HE3	1:B:525:PRO:HD2	1.89	0.54
6:A:1308:SO4:O2	10:A:1404:HOH:O	2.18	0.54
1:B:618:ARG:NH2	10:B:1419:HOH:O	2.41	0.53
1:B:297:LYS:HG3	1:B:332:TRP:HB2	1.91	0.52
1:A:770:VAL:O	1:A:797[A]:ARG:NH1	2.39	0.52
1:B:1056:TRP:CD1	1:B:1142:PRO:HD3	2.45	0.52
1:A:1026:LEU:HD23	1:A:1038:PRO:HG2	1.91	0.52
1:A:42:PRO:HB2	1:A:45:GLU:HG3	1.93	0.51
1:A:1116[B]:LEU:HD11	1:A:1138:LEU:HD11	1.91	0.51
1:A:411:ALA:HA	4:A:1303:PEG:H21	1.94	0.50
1:B:782:GLY:O	1:B:811:THR:HA	2.11	0.50
1:B:950:ARG:NH1	10:B:1407:HOH:O	2.30	0.50
1:B:118:ASP:OD1	1:B:181:ARG:NH2	2.45	0.49
1:B:844:CYS:SG	5:B:1306:NAD:C3N	3.01	0.49
1:A:995:TYR:OH	1:A:1002[A]:GLY:O	2.29	0.48
1:A:524[A]:MET:HE3	1:A:525:PRO:HD2	1.94	0.48
1:A:844:CYS:SG	5:A:1305:NAD:C3N	3.02	0.48
1:A:861[B]:LEU:HG	1:A:865:LYS:HE3	1.96	0.48
1:B:788:ARG:NH2	1:B:1185:GLY:O	2.44	0.48
1:B:706:TRP:CE3	1:B:707:ASN:HA	2.50	0.47
1:B:834:THR:O	1:B:838:ASP:HB3	2.14	0.47
1:A:1056:TRP:CD1	1:A:1142:PRO:HD3	2.49	0.47
1:A:58:LYS:HD3	1:A:61:ARG:NH2	2.30	0.47
1:A:1180:ILE:HG23	1:A:1188:LEU:HD12	1.97	0.47
1:A:782:GLY:O	1:A:811:THR:HA	2.15	0.47
1:A:772:ALA:O	1:A:797[A]:ARG:NH2	2.48	0.46
1:B:223:LEU:HD21	1:B:475:PRO:HB3	1.98	0.46
1:B:69[A]:ARG:HD3	1:B:510:ILE:HG21	1.98	0.46
1:A:617:VAL:HG12	1:A:774:GLU:HB2	1.96	0.46
1:A:650:MET:O	1:A:654:LEU:HG	2.15	0.46
1:B:159:VAL:HG13	1:B:164:LEU:HD12	1.96	0.46
1:A:859:ARG:NE	10:A:1444:HOH:O	2.48	0.46
1:A:428:LEU:HD11	1:A:460:VAL:HG21	1.98	0.46
1:A:562:LEU:HD11	1:A:654:LEU:HD12	1.98	0.45
1:A:706:TRP:CE3	1:A:707:ASN:HA	2.51	0.45
1:A:995:TYR:OH	10:A:1403:HOH:O	2.17	0.45
1:A:473:TYR:HB2	2:A:1301[B]:FAD:HM71	1.97	0.45
1:B:358[A]:ARG:HG3	1:B:415:VAL:HG11	1.98	0.45
1:A:272:ARG:HB3	1:A:277:GLN:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:861[B]:LEU:HD21	1:A:930:GLU:CD	2.43	0.44
1:A:248:GLY:HA3	1:A:299:TYR:CG	2.52	0.44
1:A:298:ASN:ND2	10:A:1423:HOH:O	2.39	0.43
1:B:428:LEU:HD11	1:B:460:VAL:HG21	2.00	0.43
1:B:662:GLY:HA2	10:B:1522:HOH:O	2.18	0.43
1:A:1050:LEU:C	1:A:1050:LEU:HD13	2.43	0.43
1:B:186:MET:O	1:B:190:MET:HG3	2.18	0.43
2:A:1301[A]:FAD:H9	2:A:1301[A]:FAD:H1'1	1.70	0.43
1:A:659:ARG:HD3	10:A:1843:HOH:O	2.18	0.43
1:A:222:MET:HG2	10:A:1480:HOH:O	2.18	0.42
1:A:1091[B]:ARG:HG2	1:A:1093:LEU:HD21	2.01	0.42
1:A:868:LEU:O	1:A:912:ILE:HD11	2.19	0.42
2:A:1301[A]:FAD:HM71	2:A:1301[A]:FAD:HM83	1.83	0.42
1:B:473:TYR:HB2	2:B:1301[B]:FAD:HM71	2.02	0.42
1:B:717:ILE:HG12	1:B:727:VAL:HG11	2.02	0.42
1:B:1069:ALA:HA	1:B:1117:ALA:HB1	2.01	0.42
1:A:297[B]:LYS:HG3	1:A:332:TRP:HB2	2.01	0.42
1:B:367:ARG:HA	1:B:419:GLN:HB2	2.02	0.42
1:A:873:ILE:HD13	1:A:912:ILE:HG21	2.01	0.42
1:A:717:ILE:HG12	1:A:727:VAL:HG11	2.01	0.42
1:B:448:CYS:HB2	1:B:453:GLY:HA3	2.01	0.42
1:B:984:HIS:C	1:B:984:HIS:CD2	2.98	0.41
1:A:124:LYS:HD2	1:A:133:HIS:NE2	2.36	0.41
1:B:369:VAL:HG12	1:B:421:ALA:HB3	2.01	0.41
1:A:929:ILE:O	1:A:947:HIS:HA	2.20	0.41
1:A:128:GLY:O	1:A:130:TRP:N	2.54	0.41
1:A:253:GLY:HA2	10:A:2280:HOH:O	2.20	0.41
1:A:863:MET:HE3	1:A:863:MET:HB2	1.85	0.41
1:A:531:HIS:CE1	1:A:1232:ILE:HG23	2.55	0.41
2:B:1301[B]:FAD:HM73	2:B:1301[B]:FAD:HM81	1.88	0.41
1:B:913:GLY:HA2	1:B:925:PRO:HB3	2.03	0.41
1:A:190:MET:HE2	1:A:195:PHE:CZ	2.56	0.40
2:A:1301[B]:FAD:H8A	10:A:2030:HOH:O	2.21	0.40
1:A:367:ARG:HA	1:A:419:GLN:HB2	2.03	0.40
1:B:248:GLY:HA3	1:B:299:TYR:CG	2.57	0.40
1:B:913:GLY:HA2	1:B:925:PRO:CB	2.52	0.40
1:B:700[B]:ILE:HG12	1:B:725:ASN:HB3	2.03	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	1235/1235 (100%)	1213 (98%)	21 (2%)	1 (0%)	48	21
1	B	1221/1235 (99%)	1199 (98%)	22 (2%)	0	100	100
All	All	2456/2470 (99%)	2412 (98%)	43 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	129	ASN

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	915/951 (96%)	908 (99%)	7 (1%)	73	48
1	B	896/951 (94%)	891 (99%)	5 (1%)	78	56
All	All	1811/1902 (95%)	1799 (99%)	12 (1%)	76	52

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	LEU
1	A	342	TYR
1	A	503	ILE
1	A	522	ARG
1	A	730	LYS

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Mol	Chain	Res	Type
1	A	934	LEU
1	A	1232	ILE
1	B	157	SER
1	B	342	TYR
1	B	730	LYS
1	B	934	LEU
1	B	1232	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	872	HIS
1	A	1040	GLN
1	A	1140	ASN
1	B	440	HIS

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 21 ligands modelled in this entry, 2 are monoatomic - leaving 19 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
6	SO4	A	1309	-	4,4,4	0.68	0	6,6,6	0.11	0
4	PEG	A	1303	-	6,6,6	0.25	0	5,5,5	0.23	0
6	SO4	A	1310	-	4,4,4	0.63	0	6,6,6	0.20	0
6	SO4	A	1306	-	4,4,4	0.57	0	6,6,6	0.30	0
6	SO4	A	1308	-	4,4,4	0.66	0	6,6,6	0.13	0
9	A1BDW	B	1304	-	10,10,10	0.27	0	12,12,12	1.04	0
8	PGE	B	1302	-	9,9,9	0.33	0	8,8,8	0.51	0
6	SO4	A	1307	-	4,4,4	0.69	0	6,6,6	0.21	0
2	FAD	B	1301[B]	-	58,58,58	2.44	16 (27%)	85,89,89	1.65	16 (18%)
3	FMT	B	1303	-	2,2,2	0.81	0	1,1,1	0.23	0
5	NAD	B	1306	7	46,48,48	2.10	6 (13%)	64,73,73	1.77	12 (18%)
2	FAD	A	1301[A]	-	58,58,58	2.24	14 (24%)	85,89,89	1.66	13 (15%)
6	SO4	B	1307	-	4,4,4	0.58	0	6,6,6	0.28	0
3	FMT	A	1302	-	2,2,2	0.48	0	1,1,1	0.24	0
2	FAD	B	1301[A]	-	58,58,58	2.17	13 (22%)	85,89,89	1.56	16 (18%)
4	PEG	A	1304	-	6,6,6	0.27	0	5,5,5	0.23	0
5	NAD	A	1305	7	46,48,48	2.10	11 (23%)	64,73,73	1.69	11 (17%)
2	FAD	A	1301[B]	-	58,58,58	2.28	14 (24%)	85,89,89	1.66	17 (20%)
4	PEG	B	1305	-	6,6,6	0.26	0	5,5,5	0.28	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
4	PEG	A	1303	-	-	2/4/4/4	-
5	NAD	A	1305	7	-	4/30/62/62	0/5/5/5
2	FAD	B	1301[A]	-	-	3/34/50/50	0/6/6/6
2	FAD	B	1301[B]	-	-	8/34/50/50	0/6/6/6
4	PEG	A	1304	-	-	1/4/4/4	-
9	A1BDW	B	1304	-	-	0/4/4/4	0/1/1/1
5	NAD	B	1306	7	-	4/30/62/62	0/5/5/5
8	PGE	B	1302	-	-	2/7/7/7	-
2	FAD	A	1301[A]	-	-	3/34/50/50	0/6/6/6
2	FAD	A	1301[B]	-	-	10/34/50/50	0/6/6/6
4	PEG	B	1305	-	-	1/4/4/4	-

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1301[B]	FAD	PA-O3P	-10.79	1.47	1.59
2	B	1301[A]	FAD	PA-O3P	-9.87	1.48	1.59
2	A	1301[A]	FAD	PA-O3P	-9.55	1.49	1.59
2	A	1301[B]	FAD	PA-O3P	-9.54	1.49	1.59
5	B	1306	NAD	PA-O3	-7.63	1.51	1.59
2	B	1301[B]	FAD	O4-C4	7.39	1.37	1.23
5	A	1305	NAD	PA-O3	-6.95	1.52	1.59
2	A	1301[A]	FAD	O4-C4	6.83	1.36	1.23
2	A	1301[B]	FAD	O4-C4	6.74	1.36	1.23
5	A	1305	NAD	C2N-N1N	6.60	1.42	1.35
2	B	1301[A]	FAD	O4-C4	6.46	1.35	1.23
5	B	1306	NAD	C2N-N1N	6.32	1.41	1.35
2	B	1301[B]	FAD	O2-C2	5.84	1.35	1.24
2	A	1301[B]	FAD	O2-C2	4.97	1.34	1.24
5	B	1306	NAD	C7N-N7N	4.93	1.42	1.33
5	A	1305	NAD	C7N-N7N	4.90	1.42	1.33
2	B	1301[A]	FAD	O2-C2	4.58	1.33	1.24
2	A	1301[A]	FAD	O2-C2	4.35	1.33	1.24
2	A	1301[A]	FAD	C4X-N5	4.21	1.39	1.30
2	B	1301[B]	FAD	C4X-N5	4.05	1.39	1.30
2	B	1301[B]	FAD	C6A-N6A	4.03	1.44	1.34
2	A	1301[B]	FAD	C6A-N6A	4.00	1.44	1.34
2	A	1301[A]	FAD	C6A-N6A	3.99	1.44	1.34
2	B	1301[A]	FAD	C4X-N5	3.97	1.39	1.30
5	B	1306	NAD	C6A-N6A	3.90	1.44	1.34
2	A	1301[B]	FAD	C4X-N5	3.90	1.39	1.30
2	B	1301[A]	FAD	C6A-N6A	3.85	1.44	1.34
5	A	1305	NAD	C6A-N6A	3.72	1.43	1.34
2	A	1301[B]	FAD	P-O3P	3.58	1.63	1.59
2	B	1301[B]	FAD	C2-N1	3.30	1.44	1.36
2	A	1301[A]	FAD	P-O3P	3.18	1.62	1.59
2	A	1301[B]	FAD	C2-N1	3.18	1.43	1.36
2	A	1301[B]	FAD	O2'-C2'	-3.10	1.36	1.43
2	A	1301[A]	FAD	PA-O5B	-2.99	1.47	1.59
2	A	1301[A]	FAD	O2'-C2'	-2.91	1.37	1.43
2	A	1301[B]	FAD	PA-O5B	-2.88	1.48	1.59
2	B	1301[B]	FAD	O2'-C2'	-2.75	1.37	1.43
5	A	1305	NAD	C6N-N1N	2.75	1.41	1.35
2	B	1301[B]	FAD	PA-O5B	-2.69	1.48	1.59
2	A	1301[A]	FAD	O4'-C4'	-2.69	1.37	1.43
2	B	1301[B]	FAD	C10-N1	2.63	1.38	1.33
2	B	1301[A]	FAD	O2'-C2'	-2.55	1.38	1.43
2	B	1301[B]	FAD	O4'-C4'	-2.53	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1301[B]	FAD	P-O3P	2.53	1.62	1.59
2	A	1301[A]	FAD	O4B-C4B	-2.48	1.39	1.45
2	A	1301[A]	FAD	C2-N1	2.48	1.42	1.36
2	A	1301[B]	FAD	O4B-C4B	-2.47	1.39	1.45
5	A	1305	NAD	O3D-C3D	-2.42	1.37	1.43
2	A	1301[B]	FAD	O4'-C4'	-2.39	1.38	1.43
2	B	1301[A]	FAD	O4B-C4B	-2.38	1.39	1.45
2	B	1301[B]	FAD	O4B-C4B	-2.36	1.39	1.45
2	B	1301[B]	FAD	O2B-C2B	-2.36	1.37	1.43
2	B	1301[A]	FAD	C2-N1	2.33	1.41	1.36
2	B	1301[A]	FAD	O4'-C4'	-2.33	1.38	1.43
2	B	1301[A]	FAD	P-O3P	2.32	1.62	1.59
2	A	1301[B]	FAD	C10-N1	2.31	1.37	1.33
5	A	1305	NAD	PA-O5B	-2.30	1.50	1.59
2	B	1301[B]	FAD	PA-O2A	-2.29	1.44	1.55
2	B	1301[A]	FAD	O2B-C2B	-2.25	1.37	1.43
5	B	1306	NAD	C6N-N1N	2.24	1.40	1.35
2	A	1301[B]	FAD	PA-O2A	-2.21	1.45	1.55
2	A	1301[A]	FAD	PA-O2A	-2.21	1.45	1.55
2	B	1301[A]	FAD	PA-O2A	-2.19	1.45	1.55
5	A	1305	NAD	C2D-C3D	-2.17	1.47	1.53
5	B	1306	NAD	C5A-C4A	2.16	1.42	1.39
5	A	1305	NAD	C2B-C3B	-2.14	1.47	1.53
5	A	1305	NAD	O4D-C4D	-2.10	1.40	1.45
2	A	1301[A]	FAD	C10-N1	2.09	1.37	1.33
2	B	1301[B]	FAD	P-O1P	2.09	1.58	1.50
2	A	1301[A]	FAD	O3'-C3'	-2.08	1.37	1.43
5	A	1305	NAD	PA-O2A	-2.06	1.45	1.55
2	B	1301[A]	FAD	P-O1P	2.02	1.57	1.50
2	A	1301[B]	FAD	P-O1P	2.02	1.57	1.50
2	B	1301[B]	FAD	O3'-C3'	-2.02	1.38	1.43

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1306	NAD	N3A-C2A-N1A	-6.50	118.75	128.58
5	A	1305	NAD	N3A-C2A-N1A	-6.28	119.07	128.58
2	A	1301[A]	FAD	N3A-C2A-N1A	-5.71	119.94	128.58
2	A	1301[B]	FAD	N3A-C2A-N1A	-5.64	120.04	128.58
2	B	1301[B]	FAD	N3A-C2A-N1A	-5.48	120.29	128.58
2	B	1301[A]	FAD	N3A-C2A-N1A	-5.16	120.77	128.58
2	A	1301[B]	FAD	C5A-C4A-N3A	-4.99	119.85	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301[A]	FAD	C5A-C4A-N3A	-4.83	120.06	126.72
2	B	1301[B]	FAD	C5A-C4A-N3A	-4.79	120.12	126.72
5	B	1306	NAD	C5A-C4A-N3A	-4.39	120.68	126.72
2	A	1301[B]	FAD	N3A-C4A-N9A	3.98	133.94	127.17
5	B	1306	NAD	C5A-N7A-C8A	3.95	109.66	103.45
2	B	1301[B]	FAD	N3A-C4A-N9A	3.95	133.88	127.17
5	A	1305	NAD	C5A-C4A-N3A	-3.89	121.36	126.72
2	A	1301[B]	FAD	C5A-N7A-C8A	3.81	109.43	103.45
2	A	1301[A]	FAD	N3A-C4A-N9A	3.79	133.61	127.17
2	A	1301[A]	FAD	C5A-N7A-C8A	3.76	109.35	103.45
5	A	1305	NAD	C5A-N7A-C8A	3.75	109.34	103.45
5	B	1306	NAD	N3A-C4A-N9A	3.71	133.47	127.17
5	B	1306	NAD	C2A-N3A-C4A	3.69	120.85	111.83
2	B	1301[A]	FAD	C5A-C4A-N3A	-3.66	121.67	126.72
2	B	1301[B]	FAD	C5A-N7A-C8A	3.66	109.21	103.45
5	B	1306	NAD	N9A-C8A-N7A	-3.65	108.76	113.94
2	A	1301[B]	FAD	C2A-N3A-C4A	3.58	120.58	111.83
2	B	1301[A]	FAD	O2-C2-N1	-3.57	115.87	121.80
2	A	1301[A]	FAD	C2A-N3A-C4A	3.55	120.50	111.83
2	A	1301[A]	FAD	C4-C4X-N5	3.48	123.02	118.21
5	A	1305	NAD	C4D-O4D-C1D	-3.47	106.74	109.92
5	A	1305	NAD	N9A-C8A-N7A	-3.44	109.05	113.94
2	B	1301[B]	FAD	C2A-N3A-C4A	3.43	120.20	111.83
5	A	1305	NAD	N3A-C4A-N9A	3.34	132.85	127.17
5	A	1305	NAD	C2A-N3A-C4A	3.27	119.81	111.83
2	B	1301[A]	FAD	C5A-N7A-C8A	3.21	108.49	103.45
2	A	1301[B]	FAD	O2A-PA-O3P	-3.13	98.82	107.27
2	A	1301[A]	FAD	N9A-C8A-N7A	-3.09	109.55	113.94
2	A	1301[B]	FAD	C4-N3-C2	-3.08	120.18	125.64
2	A	1301[A]	FAD	C9-C9A-N10	-3.05	117.75	121.85
2	A	1301[B]	FAD	N9A-C8A-N7A	-3.05	109.61	113.94
2	A	1301[A]	FAD	C5X-C9A-N10	3.01	120.69	117.97
2	B	1301[A]	FAD	C9-C9A-N10	-3.00	117.82	121.85
2	B	1301[B]	FAD	O2P-P-O3P	-2.98	99.21	107.27
2	A	1301[A]	FAD	C4A-C5A-N7A	-2.93	107.23	110.58
5	B	1306	NAD	C4A-C5A-N7A	-2.93	107.23	110.58
2	A	1301[B]	FAD	C4A-C5A-N7A	-2.92	107.25	110.58
2	B	1301[A]	FAD	C4-C4X-N5	2.91	122.23	118.21
2	A	1301[B]	FAD	O2P-P-O3P	-2.88	99.50	107.27
2	A	1301[B]	FAD	C4-C4X-N5	2.88	122.18	118.21
2	B	1301[A]	FAD	C5X-C9A-N10	2.85	120.55	117.97
2	B	1301[A]	FAD	C4-N3-C2	-2.85	120.58	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1301[B]	FAD	N9A-C8A-N7A	-2.84	109.90	113.94
5	B	1306	NAD	C3N-C7N-N7N	2.83	121.22	117.74
2	B	1301[B]	FAD	O2A-PA-O3P	-2.82	99.65	107.27
2	B	1301[A]	FAD	N3A-C4A-N9A	2.81	131.95	127.17
2	B	1301[A]	FAD	C2A-N3A-C4A	2.80	118.67	111.83
2	B	1301[B]	FAD	C4A-C5A-N7A	-2.79	107.40	110.58
2	A	1301[B]	FAD	C4X-C4-N3	2.76	120.27	113.25
2	B	1301[B]	FAD	C4-N3-C2	-2.75	120.75	125.64
2	A	1301[A]	FAD	C4X-C4-N3	2.73	120.20	113.25
2	A	1301[A]	FAD	C4-N3-C2	-2.72	120.80	125.64
2	B	1301[A]	FAD	C4A-C5A-N7A	-2.67	107.53	110.58
2	B	1301[B]	FAD	C4-C4X-N5	2.66	121.89	118.21
5	A	1305	NAD	C2A-N1A-C6A	2.65	123.09	118.73
5	A	1305	NAD	C4A-C5A-N7A	-2.64	107.56	110.58
5	B	1306	NAD	C4A-N9A-C8A	2.63	108.50	105.74
5	B	1306	NAD	C4D-O4D-C1D	-2.56	107.58	109.92
2	B	1301[B]	FAD	C4X-C4-N3	2.54	119.73	113.25
2	B	1301[A]	FAD	N9A-C8A-N7A	-2.54	110.33	113.94
2	B	1301[A]	FAD	C4X-C10-N10	2.46	120.00	116.48
2	A	1301[B]	FAD	O4-C4-C4X	-2.40	120.21	126.53
5	A	1305	NAD	C4A-N9A-C8A	2.39	108.25	105.74
2	B	1301[A]	FAD	C4X-C4-N3	2.38	119.32	113.25
5	B	1306	NAD	C2A-N1A-C6A	2.32	122.55	118.73
2	B	1301[A]	FAD	C2A-N1A-C6A	2.32	122.54	118.73
2	B	1301[B]	FAD	O3P-P-O1P	2.30	117.62	110.70
2	A	1301[B]	FAD	C5X-C9A-N10	2.29	120.04	117.97
2	A	1301[A]	FAD	O4-C4-C4X	-2.27	120.54	126.53
2	B	1301[B]	FAD	C5X-C9A-N10	2.26	120.01	117.97
5	B	1306	NAD	C6A-C5A-N7A	2.25	136.44	132.09
2	B	1301[B]	FAD	O4-C4-C4X	-2.25	120.59	126.53
2	B	1301[A]	FAD	C2'-C1'-N10	2.21	120.63	110.20
2	B	1301[B]	FAD	C10-C4X-N5	-2.16	120.39	124.81
2	A	1301[B]	FAD	O5'-P-O1P	2.10	117.25	108.94
2	A	1301[B]	FAD	C10-C4X-N5	-2.05	120.61	124.81
5	A	1305	NAD	O2N-PN-O3	2.02	112.74	107.27
2	A	1301[B]	FAD	C4X-C10-N1	-2.01	119.67	124.59

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301[A]	FAD	N10-C1'-C2'-O2'

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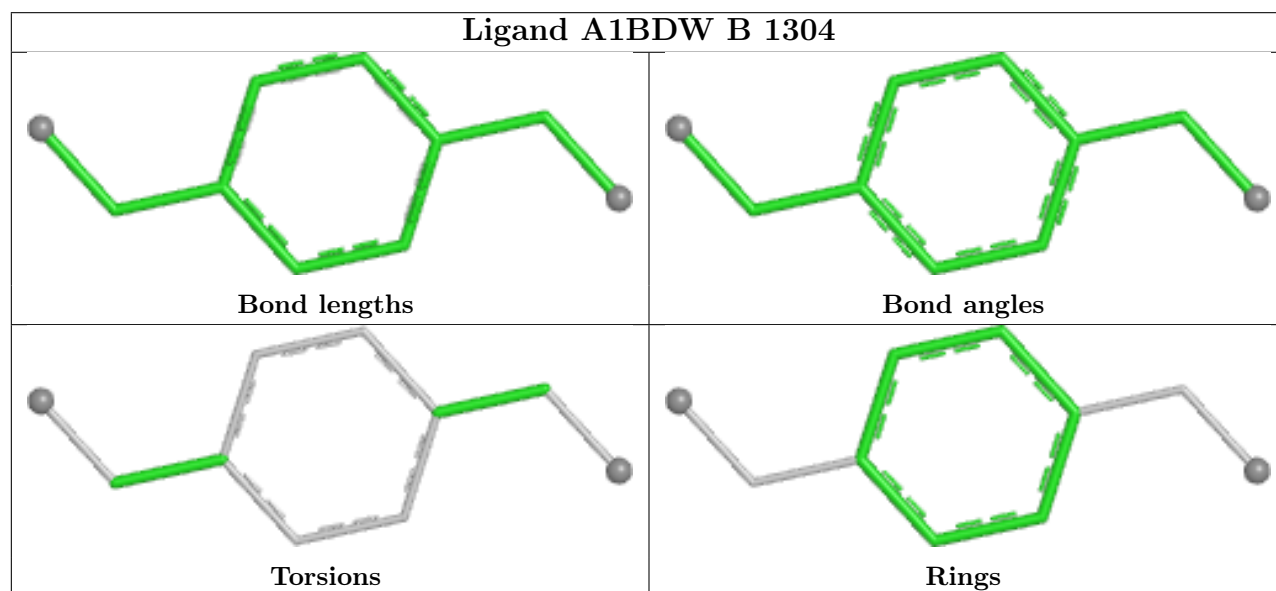
Mol	Chain	Res	Type	Atoms
2	A	1301[A]	FAD	N10-C1'-C2'-C3'
2	A	1301[B]	FAD	C5B-O5B-PA-O3P
2	B	1301[A]	FAD	N10-C1'-C2'-O2'
2	B	1301[A]	FAD	N10-C1'-C2'-C3'
2	B	1301[B]	FAD	C5B-O5B-PA-O3P
2	A	1301[B]	FAD	C2'-C3'-C4'-O4'
2	B	1301[B]	FAD	C3B-C4B-C5B-O5B
4	A	1303	PEG	O2-C3-C4-O4
2	A	1301[B]	FAD	C2'-C3'-C4'-C5'
2	A	1301[B]	FAD	C3B-C4B-C5B-O5B
2	B	1301[B]	FAD	C2'-C3'-C4'-O4'
2	A	1301[B]	FAD	O3'-C3'-C4'-O4'
2	B	1301[B]	FAD	O4B-C4B-C5B-O5B
2	A	1301[A]	FAD	P-O3P-PA-O5B
2	A	1301[B]	FAD	PA-O3P-P-O5'
2	B	1301[A]	FAD	P-O3P-PA-O5B
2	B	1301[B]	FAD	P-O3P-PA-O5B
4	A	1303	PEG	C1-C2-O2-C3
4	A	1304	PEG	O2-C3-C4-O4
2	A	1301[B]	FAD	O3'-C3'-C4'-C5'
8	B	1302	PGE	C4-C3-O2-C2
5	A	1305	NAD	C4D-C5D-O5D-PN
5	A	1305	NAD	C2B-C1B-N9A-C8A
5	B	1306	NAD	C2B-C1B-N9A-C8A
4	B	1305	PEG	O2-C3-C4-O4
8	B	1302	PGE	O1-C1-C2-O2
5	B	1306	NAD	C4D-C5D-O5D-PN
2	B	1301[B]	FAD	O3'-C3'-C4'-O4'
2	A	1301[B]	FAD	C4'-C5'-O5'-P
2	B	1301[B]	FAD	C4'-C5'-O5'-P
2	A	1301[B]	FAD	P-O3P-PA-O5B
2	A	1301[B]	FAD	O4B-C4B-C5B-O5B
5	A	1305	NAD	O4B-C1B-N9A-C8A
5	B	1306	NAD	O4B-C1B-N9A-C8A
2	B	1301[B]	FAD	O3'-C3'-C4'-C5'
5	A	1305	NAD	C2B-C1B-N9A-C4A
5	B	1306	NAD	C2B-C1B-N9A-C4A

There are no ring outliers.

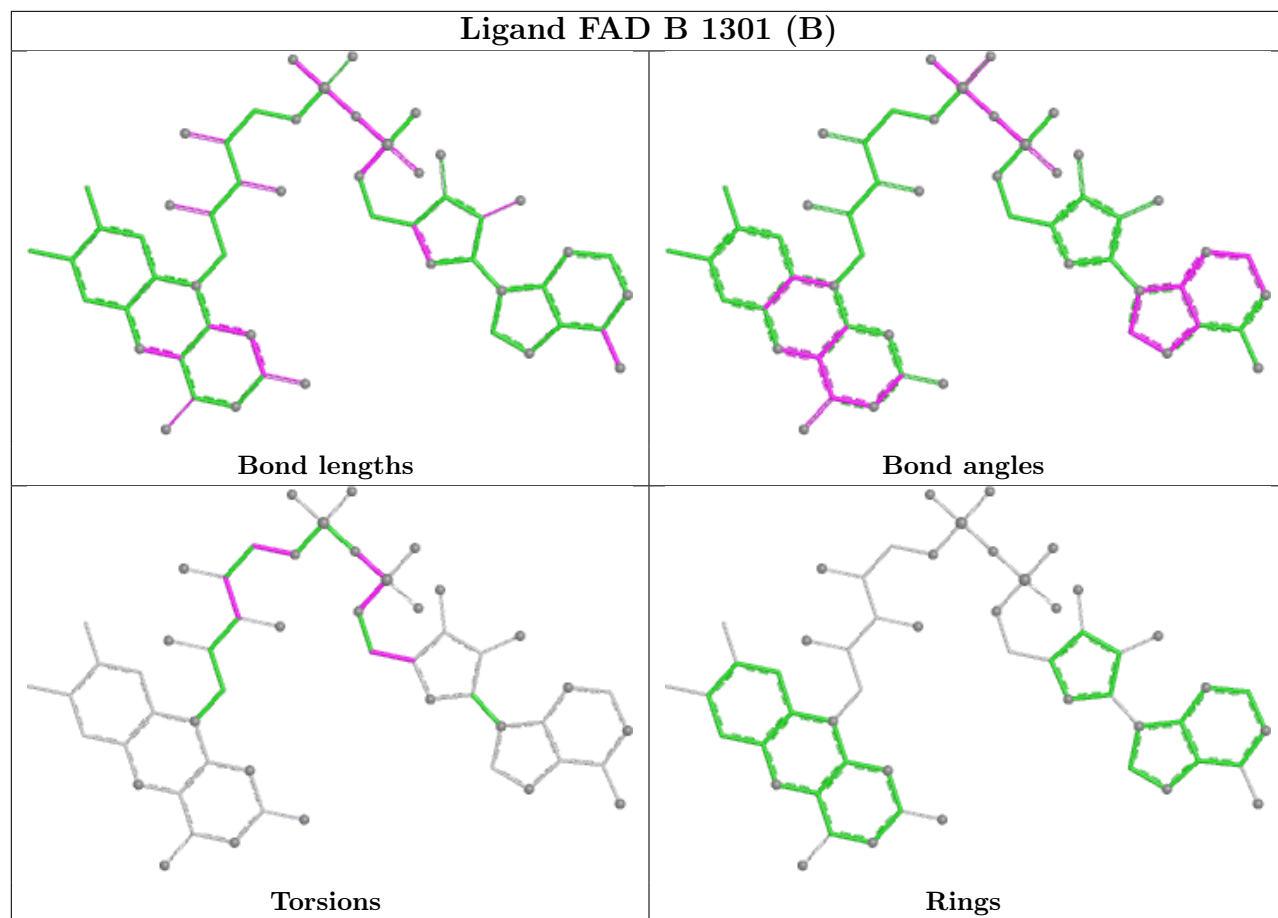
7 monomers are involved in 12 short contacts:

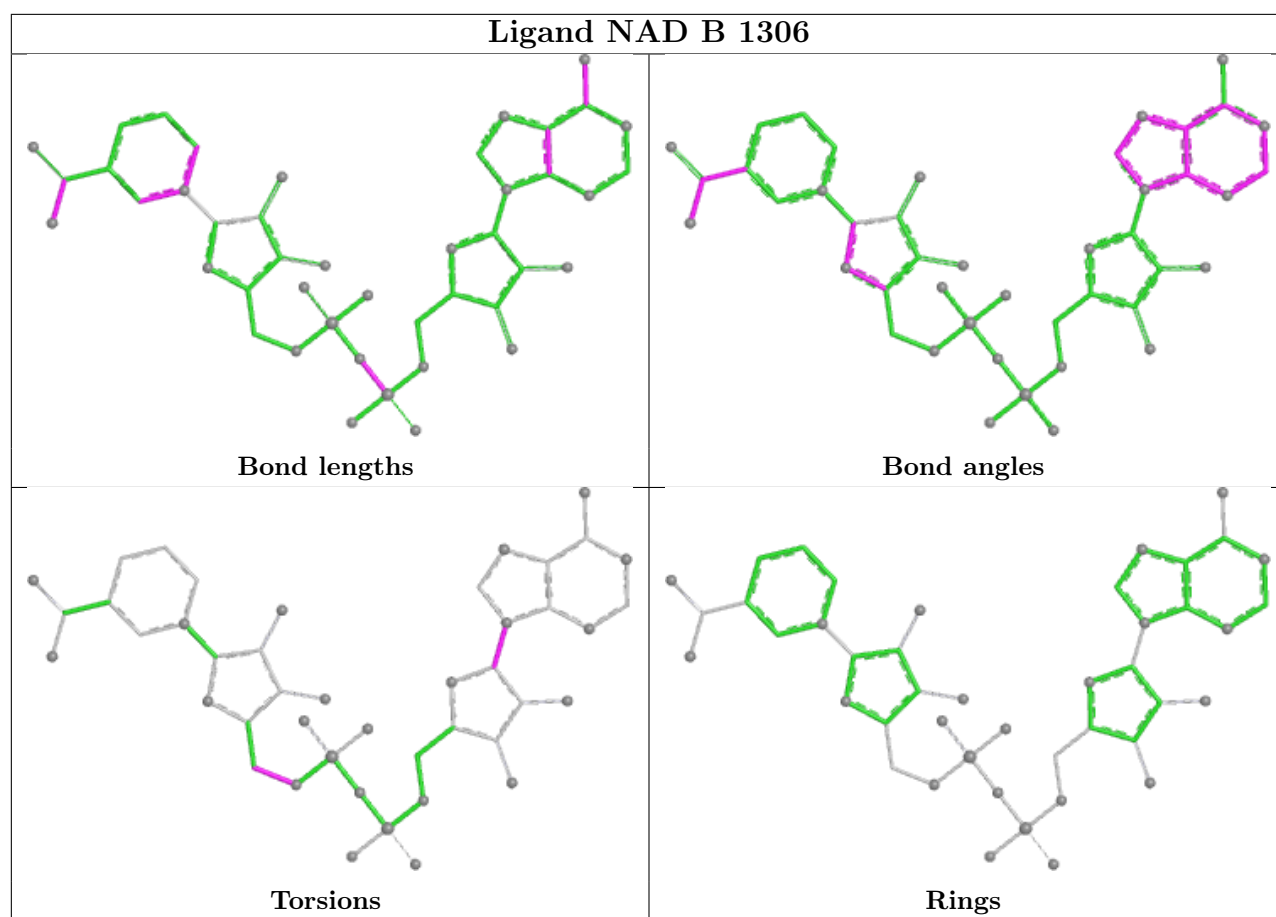
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1303	PEG	1	0
6	A	1308	SO4	1	0
2	B	1301[B]	FAD	2	0
5	B	1306	NAD	2	0
2	A	1301[A]	FAD	2	0
5	A	1305	NAD	2	0
2	A	1301[B]	FAD	2	0

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.

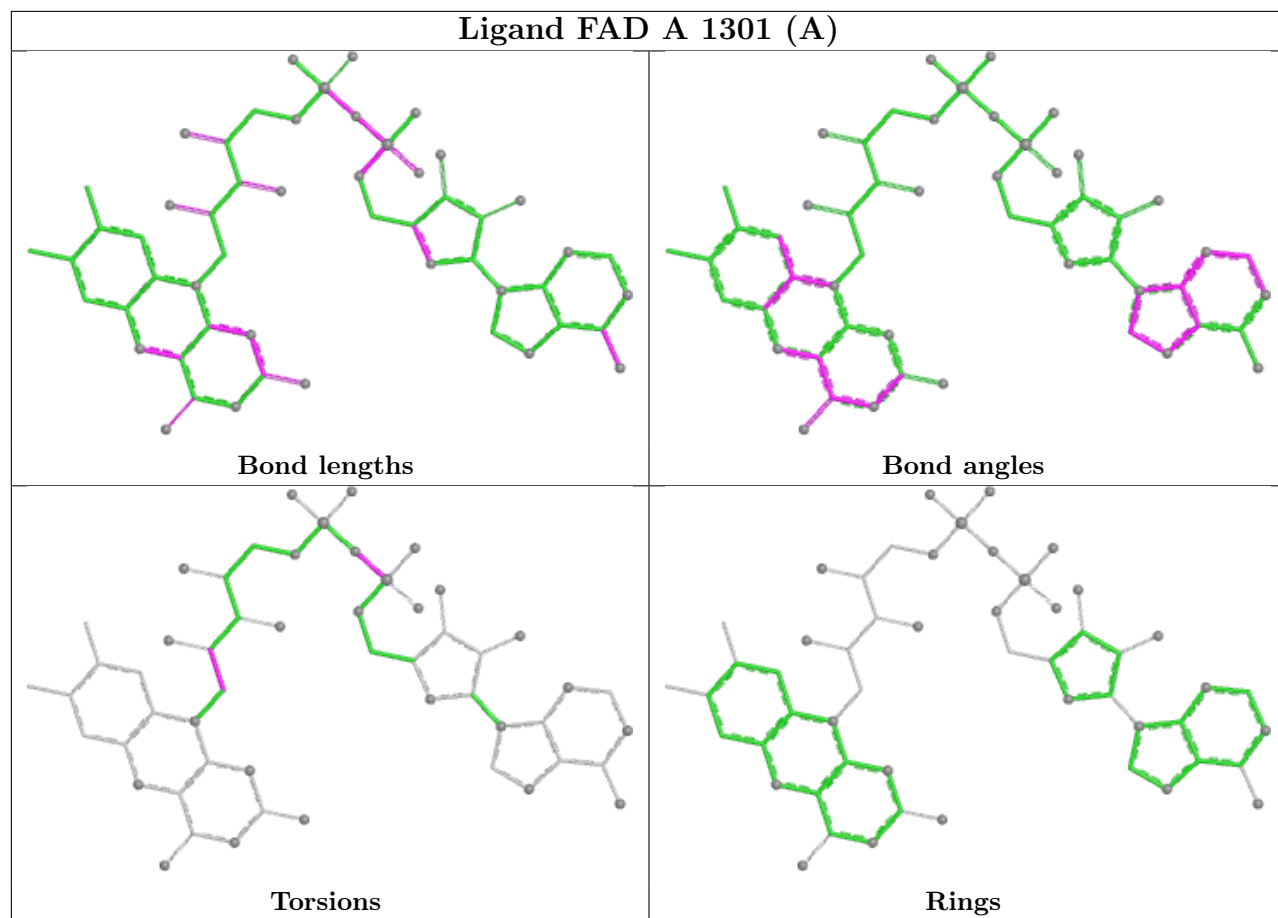


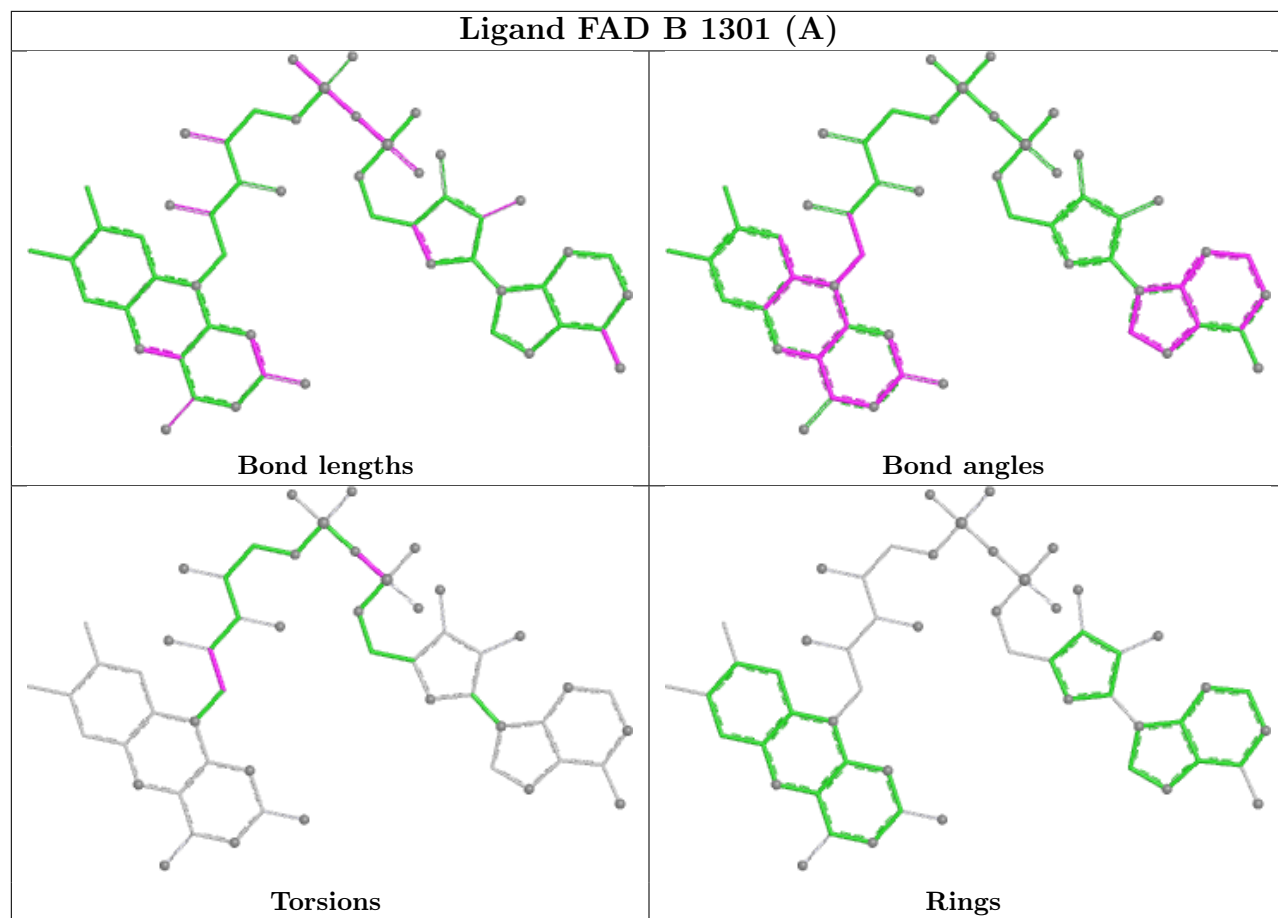
Ligand FAD B 1301 (B)



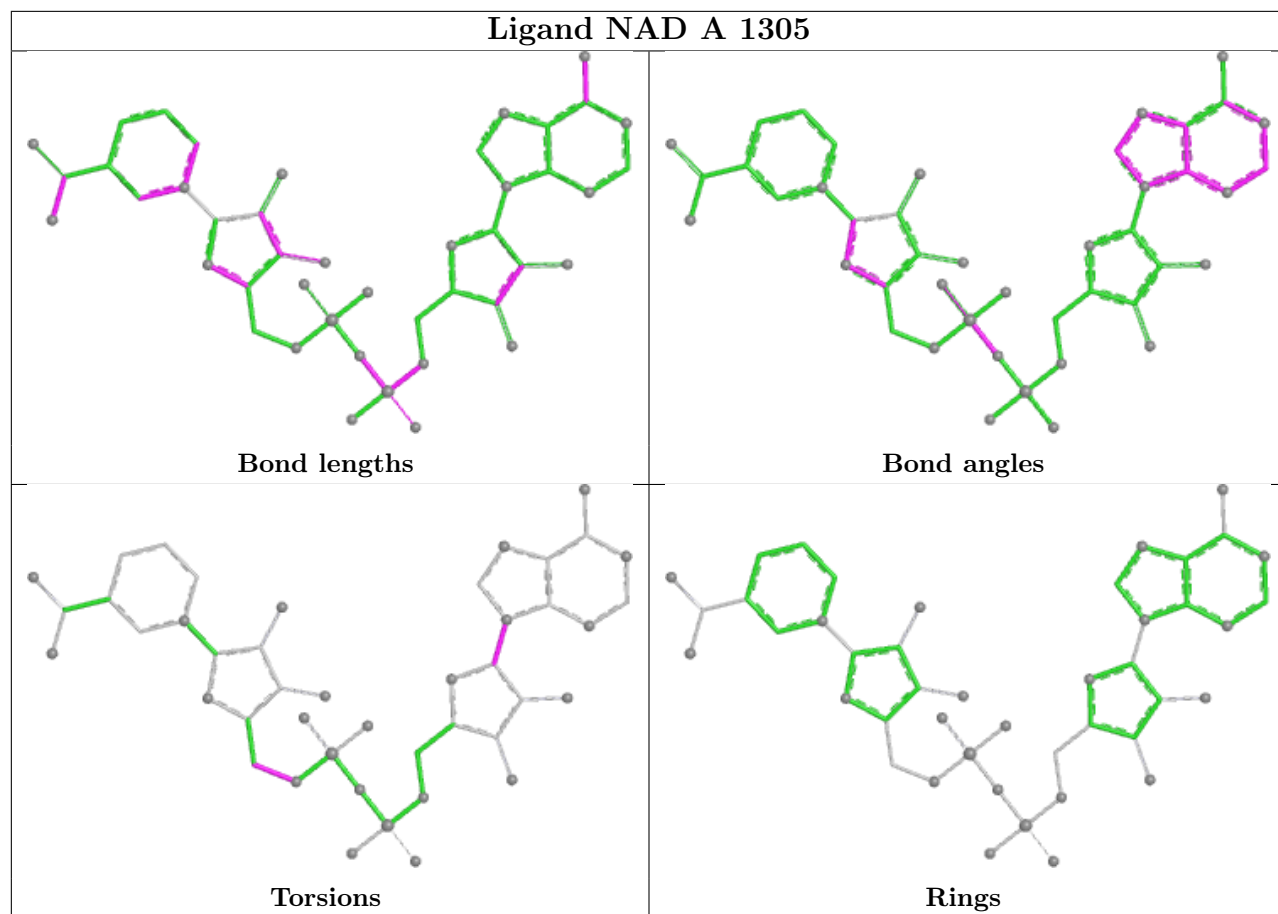


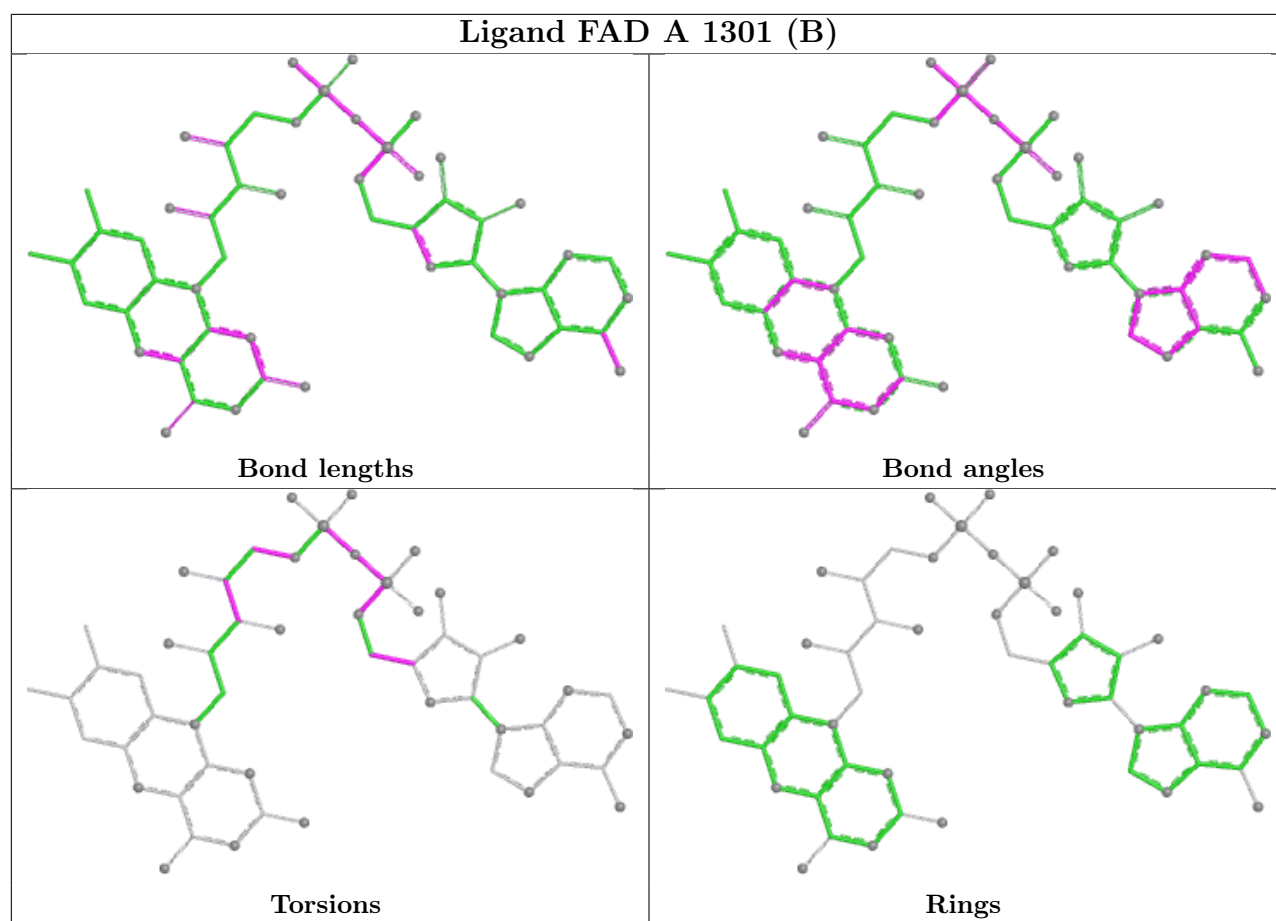
Ligand FAD A 1301 (A)





Ligand NAD A 1305





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	1216/1235 (98%)	0.42	72 (5%) 28 30	8, 23, 40, 62	25 (2%)
1	B	1212/1235 (98%)	0.36	75 (6%) 26 28	9, 21, 42, 69	16 (1%)
All	All	2428/2470 (98%)	0.39	147 (6%) 27 28	8, 22, 41, 69	41 (1%)

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	914	LEU	7.9
1	B	1223	ALA	7.2
1	B	1229	LEU	6.6
1	B	1231	ALA	6.5
1	A	493	ASN	6.5
1	A	156	THR	6.1
1	B	486	LEU	5.9
1	B	1222	ALA	5.9
1	B	494	GLY	5.8
1	B	918	THR	5.8
1	B	1230	MET	5.8
1	B	485	TYR	5.8
1	B	490	LEU	5.8
1	B	491	LEU	5.7
1	B	495	ALA	5.6
1	B	913	GLY	5.5
1	B	1232	ILE	5.2
1	B	915	ALA	5.2
1	A	1223	ALA	5.1
1	A	1227	ALA	5.0
1	A	1222	ALA	5.0
1	A	1232	ILE	4.9
1	B	1227	ALA	4.9
1	A	490	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	223	LEU	4.7
1	B	487	VAL	4.6
1	B	508	VAL	4.5
1	B	912	ILE	4.4
1	A	1229	LEU	4.4
1	A	485	TYR	4.4
1	A	494	GLY	4.3
1	B	500	VAL	4.3
1	B	1225	GLY	4.2
1	B	1228	SER	4.2
1	A	491	LEU	4.2
1	A	1231	ALA	4.1
1	B	482	LEU	4.0
1	B	484	ALA	4.0
1	A	1228	SER	3.9
1	B	156	THR	3.9
1	A	134	LEU	3.8
1	B	134	LEU	3.8
1	A	82	SER	3.8
1	A	137	SER	3.7
1	B	481	THR	3.7
1	B	14	ALA	3.7
1	B	129	ASN	3.6
1	A	492	GLU	3.6
1	A	1226	ASN	3.6
1	B	132	SER	3.5
1	A	481	THR	3.5
1	B	478	THR	3.5
1	A	506	PRO	3.5
1	B	224	GLY	3.5
1	B	492	GLU	3.5
1	B	1226	ASN	3.5
1	B	1224	GLY	3.5
1	B	1233	GLY	3.5
1	A	1230	MET	3.4
1	A	14	ALA	3.4
1	A	905	LEU	3.4
1	B	133	HIS	3.4
1	A	500	VAL	3.4
1	A	495	ALA	3.3
1	A	1225	GLY	3.3
1	A	1233	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	132	SER	3.3
1	A	484	ALA	3.3
1	A	487	VAL	3.2
1	A	451	GLY	3.2
1	A	129	ASN	3.1
1	A	223	LEU	3.1
1	A	912	ILE	3.0
1	B	488	ARG	3.0
1	B	503	ILE	3.0
1	B	127	ASP	2.9
1	B	479	HIS	2.9
1	B	483	LEU	2.9
1	B	510	ILE	2.9
1	A	482	LEU	2.8
1	B	114	THR	2.8
1	B	74	ALA	2.8
1	B	1221	ALA	2.8
1	A	571	ALA	2.8
1	A	79	HIS	2.8
1	B	489	ARG	2.8
1	A	128	GLY	2.7
1	B	128	GLY	2.7
1	A	116	THR	2.7
1	A	503	ILE	2.7
1	B	66	SER	2.6
1	B	496	ASN	2.6
1	A	801	ALA	2.6
1	A	904	GLY	2.6
1	A	133	HIS	2.6
1	A	526	VAL	2.5
1	B	155	LEU	2.5
1	A	414	ASP	2.4
1	B	917	GLU	2.4
1	A	114	THR	2.4
1	A	916	SER	2.4
1	B	916	SER	2.4
1	B	937	LEU	2.4
1	B	501	HIS	2.4
1	B	506	PRO	2.4
1	A	586	ALA	2.4
1	A	125	ILE	2.3
1	B	75	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	84	VAL	2.3
1	B	157	SER	2.3
1	A	127	ASP	2.3
1	A	130	TRP	2.3
1	B	919	GLY	2.3
1	A	115	ALA	2.3
1	A	486	LEU	2.3
1	A	914	LEU	2.3
1	A	931	LEU	2.3
1	A	1224	GLY	2.3
1	A	582	THR	2.3
1	A	155	LEU	2.3
1	A	949	ILE	2.3
1	A	520	VAL	2.3
1	B	115	ALA	2.2
1	A	120	LEU	2.2
1	B	796	ASP	2.2
1	A	525	PRO	2.2
1	A	1221	ALA	2.2
1	A	224	GLY	2.2
1	B	138	ARG	2.2
1	B	451	GLY	2.2
1	A	195	PHE	2.2
1	B	131	LYS	2.2
1	A	113	ASP	2.2
1	A	771	ALA	2.2
1	B	130	TRP	2.1
1	B	949	ILE	2.1
1	B	159	VAL	2.1
1	A	906	GLY	2.1
1	B	116	THR	2.1
1	A	111	ILE	2.1
1	B	438	ASP	2.1
1	B	499	PHE	2.1
1	B	72	ILE	2.1
1	A	909	VAL	2.1
1	A	157	SER	2.0
1	A	937	LEU	2.0
1	B	905	LEU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

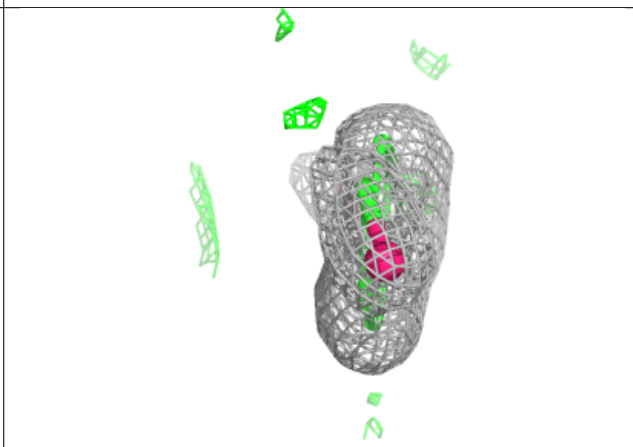
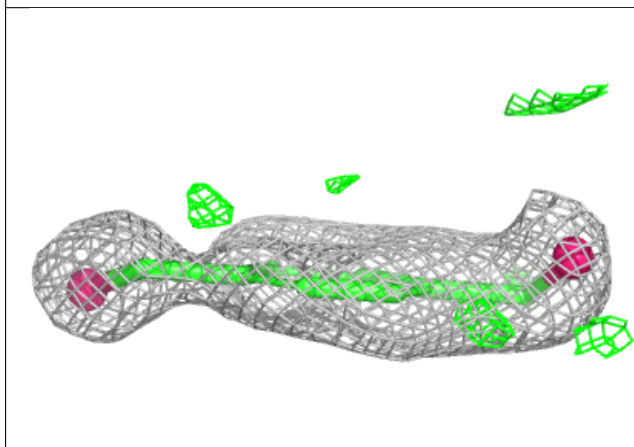
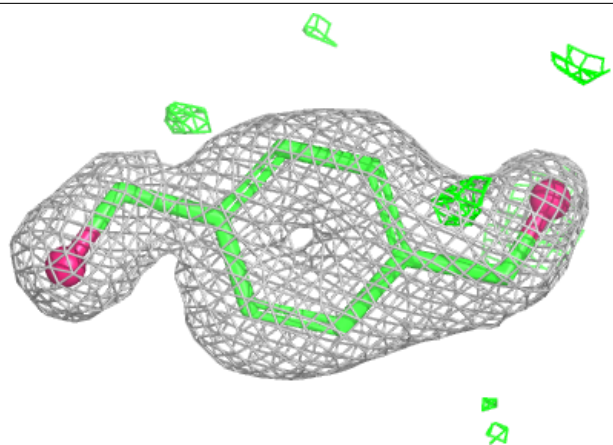
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
6	SO4	A	1309	5/5	0.78	0.15	39,41,45,57	5
4	PEG	A	1304	7/7	0.83	0.14	32,40,46,50	0
4	PEG	B	1305	7/7	0.86	0.13	32,35,36,38	7
4	PEG	A	1303	7/7	0.86	0.13	35,38,41,45	0
6	SO4	A	1307	5/5	0.89	0.12	33,35,40,49	5
8	PGE	B	1302	10/10	0.89	0.11	33,39,43,45	0
6	SO4	A	1308	5/5	0.90	0.10	48,51,52,54	5
9	A1BDW	B	1304	10/10	0.90	0.12	20,23,27,33	10
6	SO4	A	1310	5/5	0.91	0.13	26,28,38,42	5
3	FMT	A	1302	3/3	0.92	0.11	17,17,31,33	3
3	FMT	B	1303	3/3	0.93	0.12	11,11,33,34	3
2	FAD	B	1301[A]	53/53	0.96	0.07	15,19,23,26	53
2	FAD	B	1301[B]	53/53	0.96	0.07	15,18,23,25	53
2	FAD	A	1301[A]	53/53	0.96	0.07	14,20,23,24	53
5	NAD	A	1305	44/44	0.96	0.07	17,21,25,33	0
2	FAD	A	1301[B]	53/53	0.96	0.07	13,20,23,24	53
7	MG	B	1308	1/1	0.97	0.14	23,23,23,23	0
7	MG	A	1311	1/1	0.98	0.07	25,25,25,25	0
5	NAD	B	1306	44/44	0.98	0.05	14,16,19,30	0
6	SO4	A	1306	5/5	0.99	0.05	20,20,24,24	0
6	SO4	B	1307	5/5	0.99	0.05	17,18,22,22	0

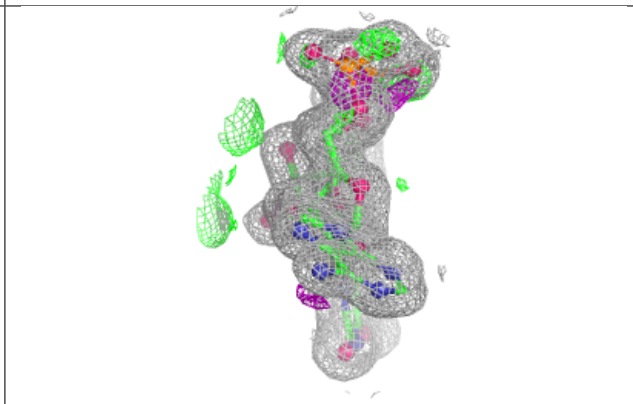
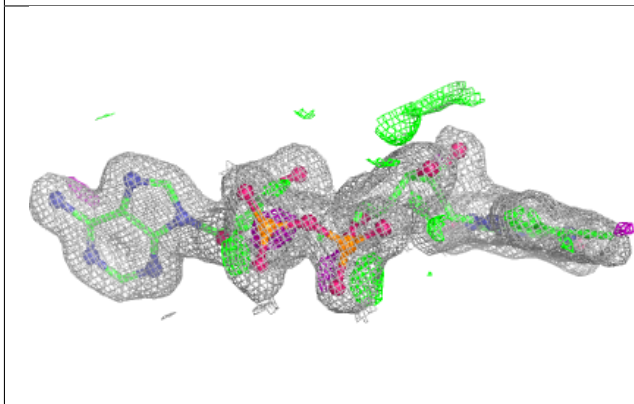
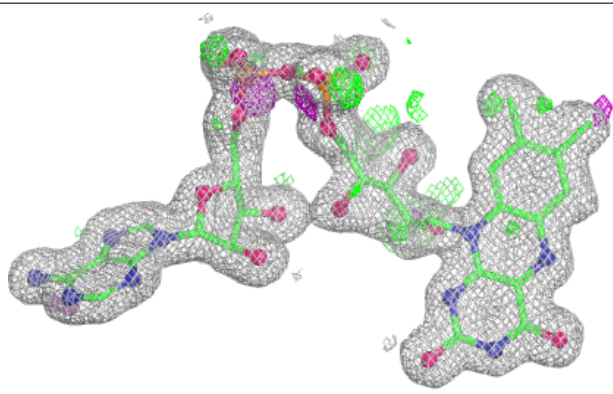
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1BDW B 1304:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

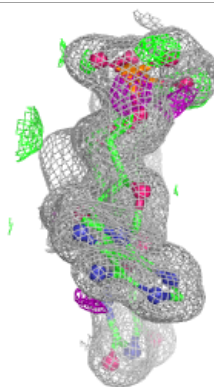
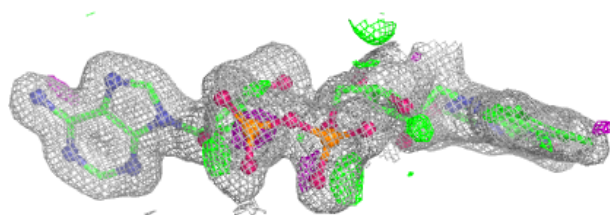
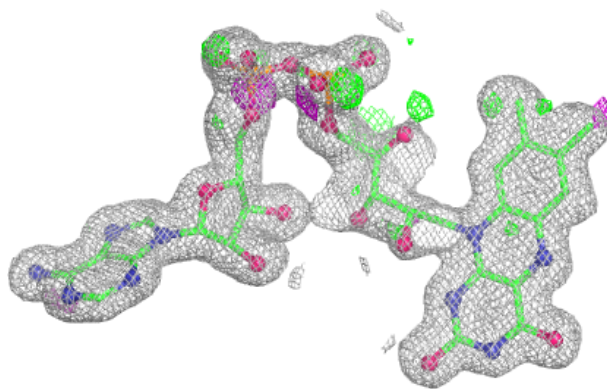
**Electron density around FAD B 1301 (A):**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

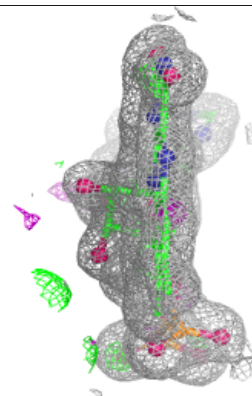
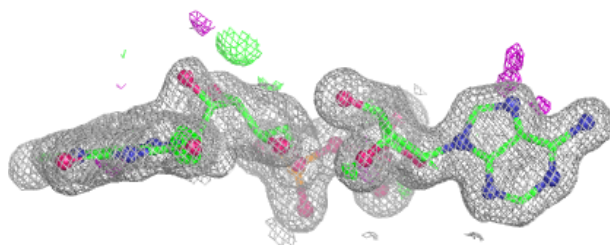
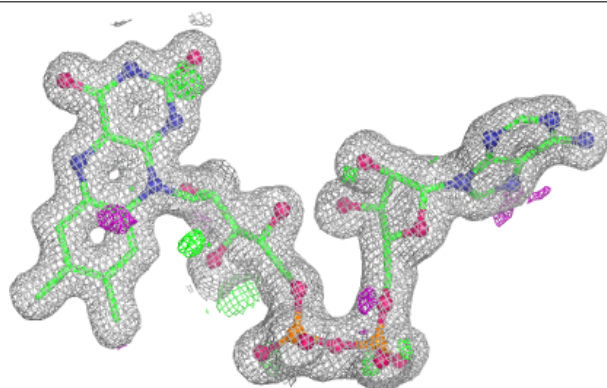


Electron density around FAD B 1301 (B):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

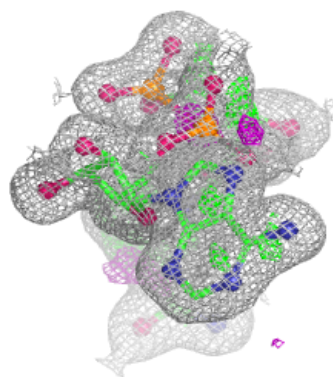
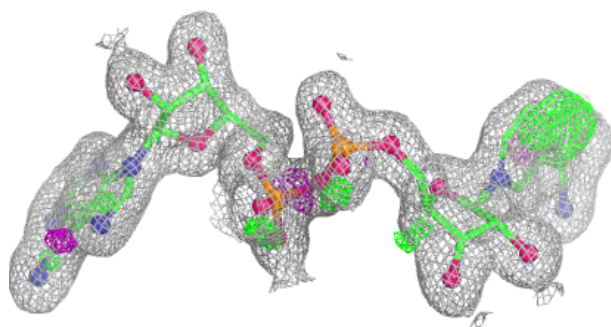
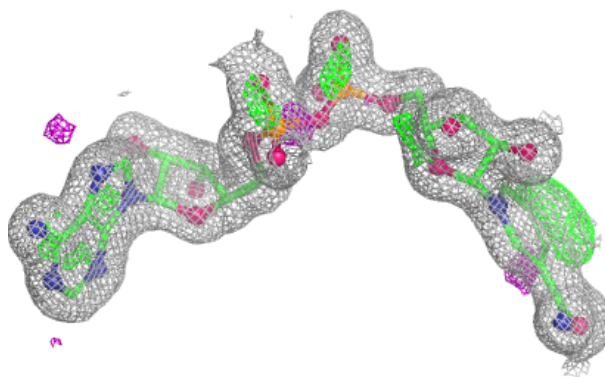
**Electron density around FAD A 1301 (A):**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

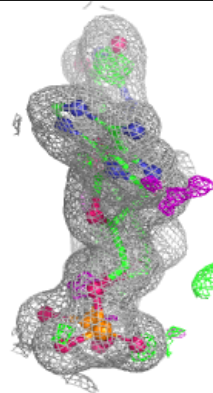
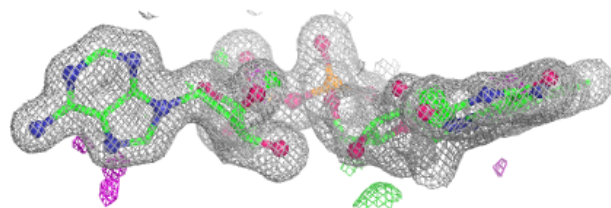
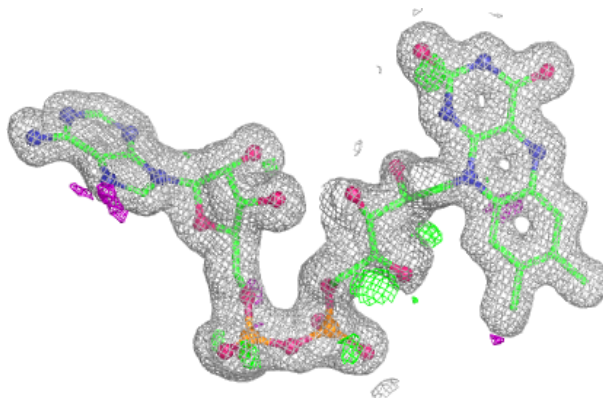


Electron density around NAD A 1305:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

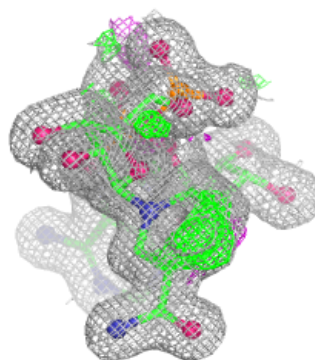
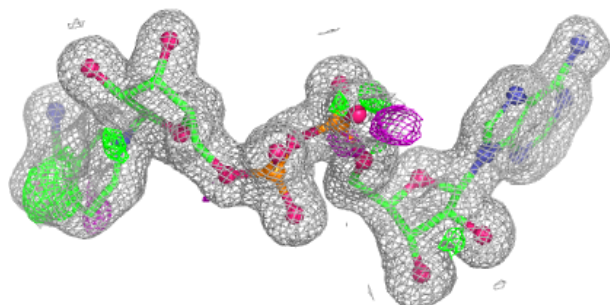
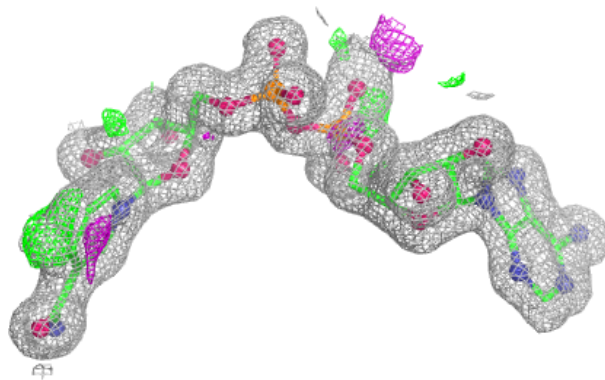
**Electron density around FAD A 1301 (B):**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NAD B 1306:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.