Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:49 PM UTC

PDB ID	:	9E0B / pdb_00009e0b
Title	:	Structure of proline utilization A complexed with (2,3-dihydro-1-benzofuran-5-yl)methanol
Authors	:	Tanner, J.J.; Meeks, K.R.
Deposited on	:	2024-10-17
Resolution	:	1.47 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:

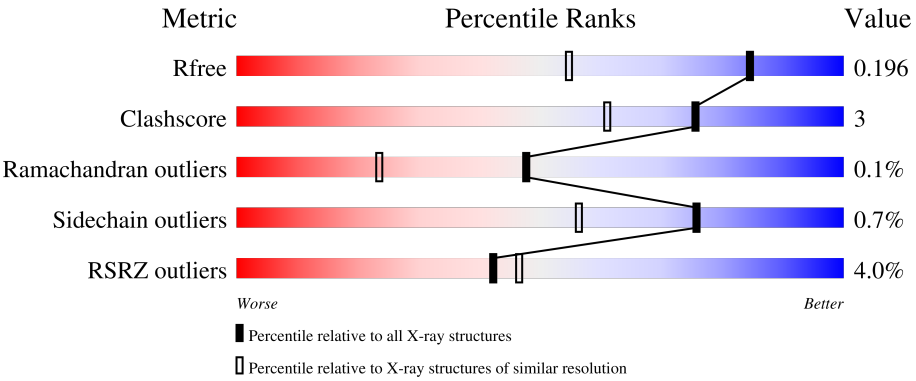
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.47 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	6779 (1.50-1.46)
Clashscore	190562	7025 (1.50-1.46)
Ramachandran outliers	187476	6917 (1.50-1.46)
Sidechain outliers	187428	6914 (1.50-1.46)
RSRZ outliers	180081	6781 (1.50-1.46)

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 <=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	4% 91% 8%
1	B	1235	4% 91% 7%

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
4	FMT	A	1305	-	-	X	-
4	FMT	B	1308	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 20493 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.

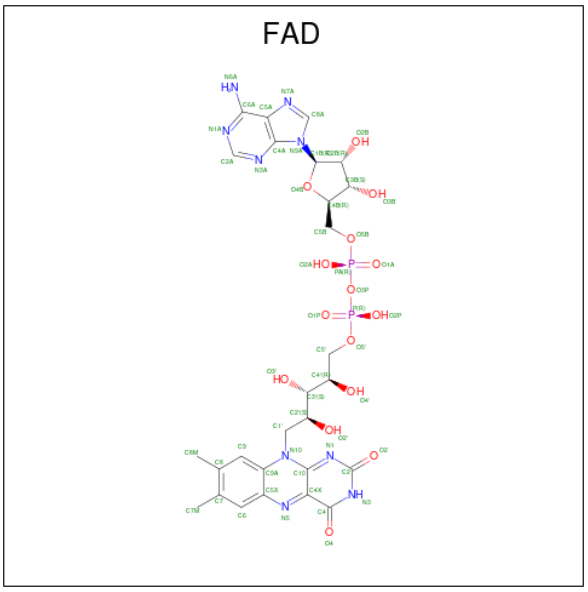
- Molecule 1 is a protein called Bifunctional protein PutA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1213	Total	C	N	O	S	0	21	0
			9043	5703	1624	1680	36			
1	B	1210	Total	C	N	O	S	0	13	0
			8935	5625	1606	1670	34			

There are 4 discrepancies between the modelled and reference sequences:

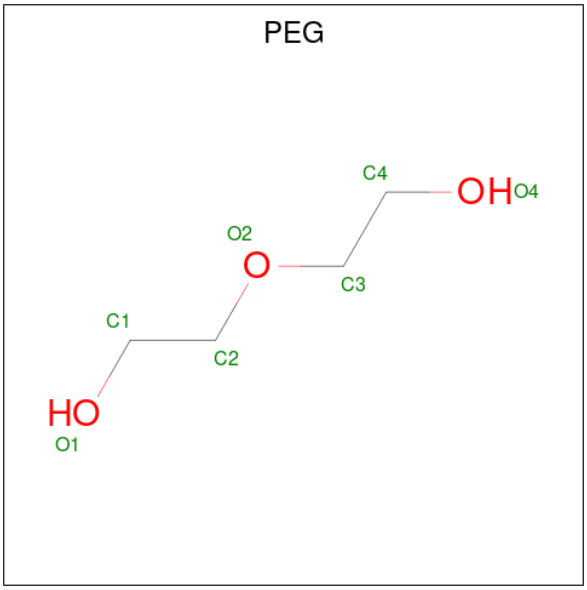
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP F7X6I3
A	0	MET	-	expression tag	UNP F7X6I3
B	-1	SER	-	expression tag	UNP F7X6I3
B	0	MET	-	expression tag	UNP F7X6I3

- 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).



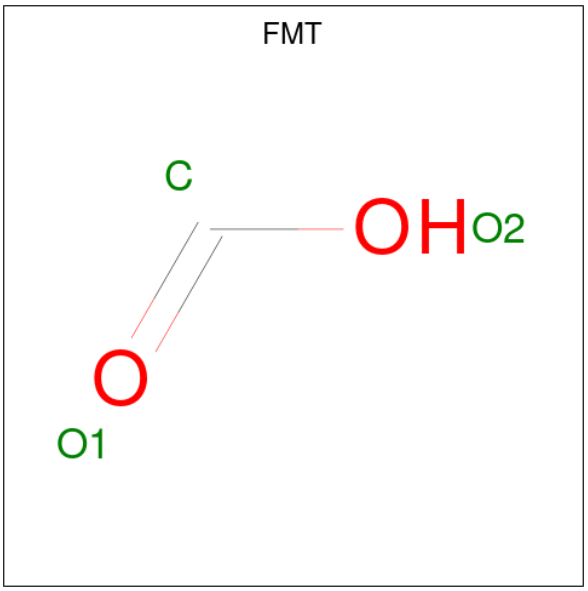
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



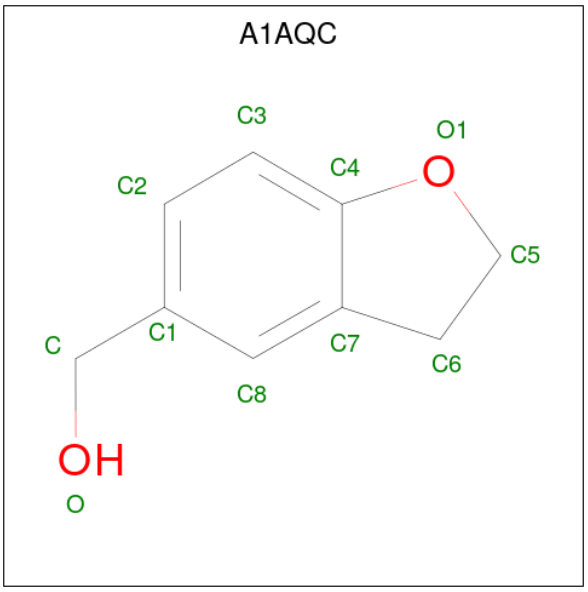
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O		0	0
			7	4	3			
3	B	1	Total	C	O		0	0
			7	4	3			
3	B	1	Total	C	O		0	0
			7	4	3			
3	B	1	Total	C	O		0	0
			7	4	3			
3	B	1	Total	C	O		0	0
			7	4	3			
3	B	1	Total	C	O		0	0
			7	4	3			

- Molecule 4 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



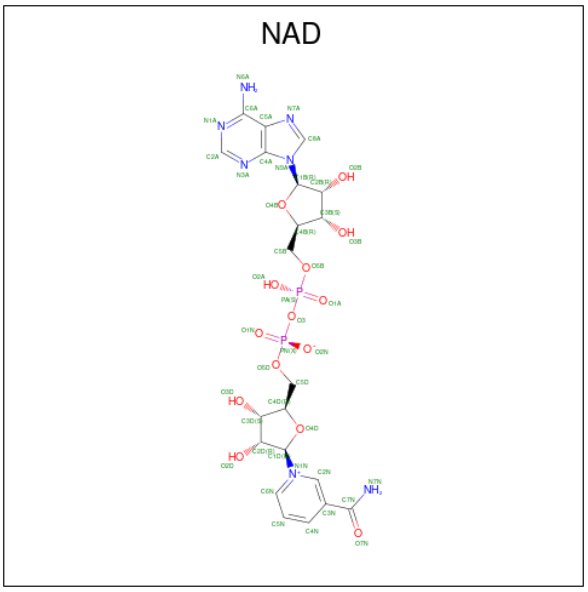
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	1	2		
4	A	1	Total	C	O	0	0
			3	1	2		
4	A	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		

- Molecule 5 is (2,3-dihydro-1-benzofuran-5-yl)methanol (CCD ID: A1AQC) (formula: $C_9H_{10}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	9	2		
5	B	1	Total	C	O	0	0
			11	9	2		

- Molecule 6 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



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

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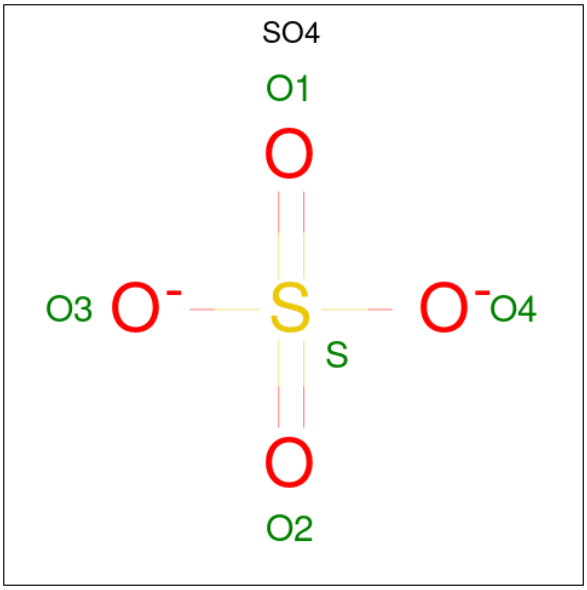
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O_4S).

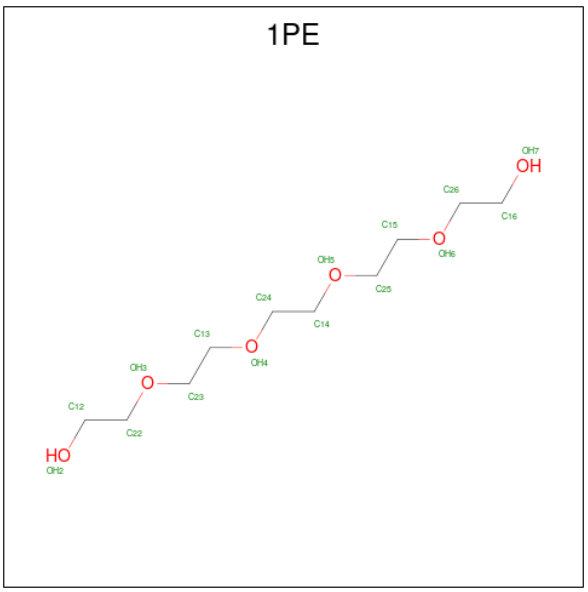


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

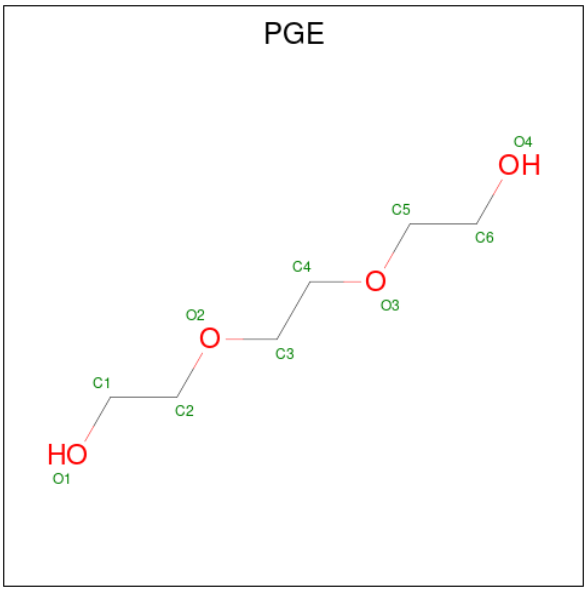
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Mg	0	0
			1	1		
8	B	1	Total	Mg	0	0
			1	1		

- Molecule 9 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O 16 10 6	0	0

- Molecule 10 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 11 is water.

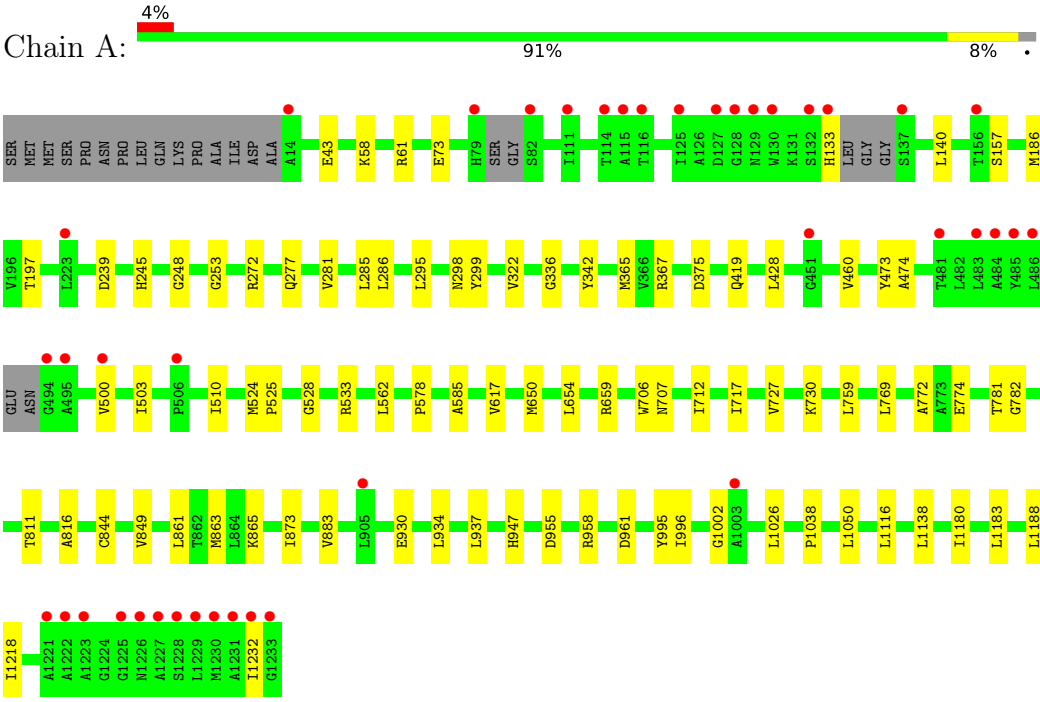
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1067	Total O 1067 1067	0	0
11	B	1114	Total O 1114 1114	0	4

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.

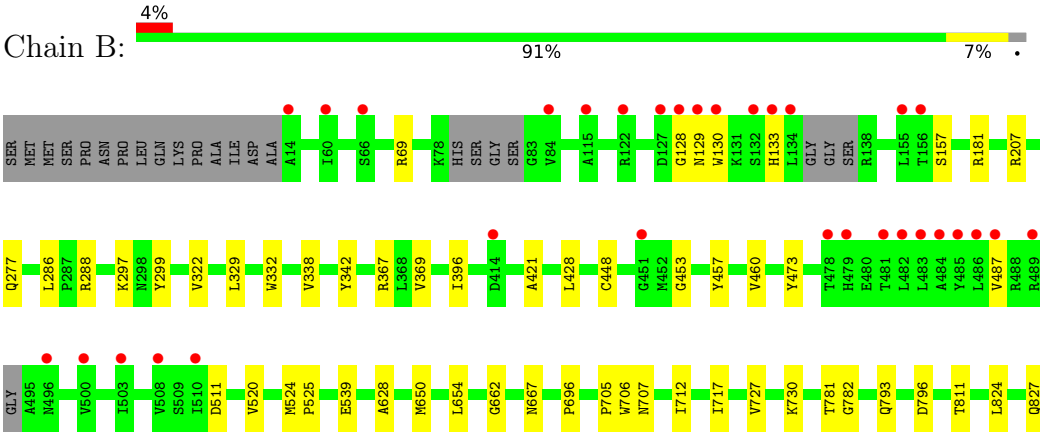
• Molecule 1: Bifunctional protein PutA

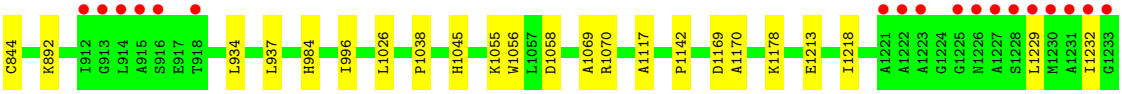
Chain A:



• Molecule 1: Bifunctional protein PutA

Chain B:




C844
K892
I912
G913
L914
A915
S916
E917
T918
L934
L937
H984
I996
L1026
P1038
H1045
K1055
W1056
L1057
D1058
A1069
R1070
A1117
P1142
D1169
A1170
K1178
E1213
I1218
A1221
A1222
A1223
G1224
G1225
N1226
A1227
S1228
L1229
M1230
A1231
I1232
G1233

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	100.53Å 101.76Å 126.02Å 90.00° 106.30° 90.00°	Depositor
Resolution (Å)	45.01 – 1.47 45.01 – 1.47	Depositor EDS
% Data completeness (in resolution range)	96.4 (45.01-1.47) 97.1 (45.01-1.47)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 1.47Å)	Xtriage
Refinement program	PHENIX 1.21rc1_5156	Depositor
R, R_{free}	0.177 , 0.200 0.172 , 0.196	Depositor DCC
R_{free} test set	20111 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	18.9	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 34.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	20493	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 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMT, FAD, PEG, MG, A1AQC, 1PE, PGE, NAD, SO4

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	0.24	0/9262	0.45	0/12601
1	B	0.26	0/9130	0.48	0/12431
All	All	0.25	0/18392	0.46	0/25032

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9043	0	9098	55	0
1	B	8935	0	8893	54	0
2	A	53	0	31	2	0
2	B	53	0	31	2	0
3	A	7	0	10	0	0
3	B	35	0	50	3	0
4	A	9	0	3	2	0
4	B	9	0	3	4	0
5	A	11	0	0	0	0
5	B	11	0	0	0	0
6	A	44	0	26	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	44	0	26	2	0
7	A	25	0	0	0	0
7	B	5	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	B	16	0	22	0	0
10	B	10	0	14	2	0
11	A	1067	0	0	9	0
11	B	1114	0	0	5	0
All	All	20493	0	18207	110	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 (110) 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:793:GLN:OE1	11:B:1401:HOH:O	2.02	0.77
1:A:793:GLN:OE1	11:A:1401:HOH:O	2.08	0.70
1:B:844:CYS:SG	6:B:1312:NAD:C4N	2.79	0.70
1:A:375[B]:ASP:OD1	11:A:1402:HOH:O	2.10	0.69
1:B:539:GLU:OE1	11:B:1402:HOH:O	2.12	0.67
1:A:873:ILE:HG13	1:A:883:VAL:HB	1.77	0.65
1:A:1183:LEU:O	11:A:1404:HOH:O	2.14	0.65
1:A:796:ASP:OD1	11:A:1403:HOH:O	2.14	0.64
1:A:239:ASP:OD1	11:A:1405:HOH:O	2.15	0.64
1:B:1213:GLU:HG3	4:B:1308:FMT:H	1.80	0.63
1:A:844:CYS:SG	6:A:1307:NAD:C4N	2.86	0.63
1:B:838:ASP:HB3	1:B:843:ARG:HH12	1.64	0.62
1:B:286:LEU:HD21	1:B:322:VAL:HG11	1.81	0.62
1:A:286:LEU:HD21	1:A:322:VAL:HG11	1.83	0.61
1:B:1213:GLU:H	4:B:1308:FMT:H	1.66	0.61
1:B:667:ASN:ND2	1:B:838:ASP:OD1	2.33	0.61
1:B:1229:LEU:HD23	1:B:1232:ILE:HD12	1.84	0.60
1:B:824:LEU:HD23	1:B:827:GLN:HG3	1.84	0.59
1:B:1169:ASP:HB2	3:B:1311:PEG:H32	1.85	0.59
1:A:298:ASN:ND2	11:A:1406:HOH:O	2.15	0.58
1:A:996[B]:ILE:HD12	1:A:1218:ILE:HG12	1.87	0.57
1:B:297:LYS:HD2	1:B:329:LEU:HA	1.85	0.57
1:B:297:LYS:HG3	1:B:332:TRP:HB2	1.86	0.57
1:B:1213:GLU:H	4:B:1308:FMT:C	2.17	0.57

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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:B:650:MET:O	1:B:654:LEU:HG	2.04	0.56
1:A:961:ASP:OD2	1:B:1055:LYS:NZ	2.38	0.55
1:B:1213:GLU:CG	4:B:1308:FMT:H	2.38	0.55
1:A:524[A]:MET:HE3	1:A:525:PRO:HD2	1.91	0.53
1:B:524[A]:MET:HE3	1:B:525:PRO:HD2	1.89	0.53
1:B:1045[B]:HIS:CG	10:B:1303:PGE:H1	2.44	0.52
1:A:1116:LEU:HD11	1:A:1138:LEU:HD11	1.93	0.51
1:B:996[B]:ILE:HD12	1:B:1218:ILE:HG12	1.92	0.51
1:A:772:ALA:O	1:A:797[A]:ARG:NH2	2.45	0.50
1:B:1169:ASP:HA	3:B:1311:PEG:H22	1.92	0.50
1:B:838:ASP:OD1	1:B:843:ARG:NH2	2.45	0.50
1:A:995:TYR:OH	1:A:1002:GLY:O	2.29	0.50
1:A:473:TYR:HB2	2:A:1301:FAD:HM72	1.93	0.50
1:A:367:ARG:HA	1:A:419:GLN:HB2	1.95	0.49
1:A:861[B]:LEU:HD21	1:A:930:GLU:CD	2.38	0.48
1:B:396:ILE:HD11	1:B:520:VAL:HB	1.93	0.48
1:A:759[A]:LEU:HD13	1:A:769:LEU:HD21	1.95	0.48
1:B:448:CYS:HB2	1:B:453:GLY:HA3	1.96	0.48
1:B:1170:ALA:H	3:B:1311:PEG:H32	1.78	0.48
1:A:955:ASP:HB3	1:A:958:ARG:HH21	1.79	0.48
1:B:1056:TRP:CD1	1:B:1142:PRO:HD3	2.48	0.48
1:B:288[B]:ARG:NE	11:B:1430:HOH:O	2.47	0.47
1:A:533:ARG:HH21	1:A:1232:ILE:HG12	1.77	0.47
1:A:1205:TYR:H	4:A:1305:FMT:C	2.26	0.47
1:B:128:GLY:O	1:B:130:TRP:N	2.47	0.47
1:A:1026:LEU:HD23	1:A:1038:PRO:HG2	1.95	0.47
1:B:667:ASN:HD21	1:B:838:ASP:CG	2.20	0.47
1:B:844:CYS:SG	6:B:1312:NAD:C3N	3.01	0.47
1:B:1026:LEU:HD23	1:B:1038:PRO:HG2	1.96	0.47
1:A:197[B]:THR:HG21	1:A:474:ALA:HB1	1.95	0.47
2:A:1301:FAD:H1'1	2:A:1301:FAD:H9	1.62	0.47
1:B:1058:ASP:OD2	1:B:1070:ARG:NH1	2.47	0.47
1:A:717:ILE:HG12	1:A:727:VAL:HG11	1.97	0.47
1:B:706:TRP:CE3	1:B:707:ASN:HA	2.50	0.47
1:A:272:ARG:HB3	1:A:277:GLN:HG3	1.97	0.47
1:A:706:TRP:CE3	1:A:707:ASN:HA	2.50	0.46
1:B:473:TYR:HB2	2:B:1301:FAD:HM72	1.97	0.46
1:A:190:MET:HE2	1:A:195:PHE:CZ	2.49	0.46
1:A:650:MET:O	1:A:654:LEU:HG	2.16	0.46
1:A:43:GLU:HB3	1:A:528:GLY:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:782:GLY:O	1:B:811:THR:HA	2.16	0.45
1:A:782:GLY:O	1:A:811:THR:HA	2.17	0.45
2:B:1301:FAD:H9	2:B:1301:FAD:H1'1	1.78	0.45
1:A:245:HIS:CE1	1:A:295:LEU:HD11	2.52	0.44
1:A:1204:ALA:HB3	4:A:1305:FMT:H	1.97	0.44
1:B:1045[B]:HIS:ND1	10:B:1303:PGE:H1	2.32	0.44
1:A:186:MET:HB2	1:A:186:MET:HE2	1.85	0.44
1:A:861[B]:LEU:HG	1:A:865:LYS:HE3	1.99	0.44
1:A:712:ILE:HD13	1:A:781:THR:HG21	1.99	0.44
1:B:338:VAL:HG22	1:B:367:ARG:HB3	2.00	0.43
1:A:336:GLY:HA2	1:A:365:MET:O	2.18	0.43
1:B:428:LEU:HD11	1:B:460:VAL:HG21	2.00	0.43
1:A:253:GLY:HA2	11:A:2243:HOH:O	2.17	0.43
1:B:628:ALA:HB2	1:B:696:PRO:HG3	2.00	0.43
1:A:844:CYS:SG	6:A:1307:NAD:C3N	3.07	0.43
1:B:1069:ALA:HA	1:B:1117:ALA:HB1	2.01	0.43
1:A:578:PRO:HB2	1:A:585:ALA:HB3	2.00	0.43
1:A:1180:ILE:HG23	1:A:1188:LEU:HD12	2.01	0.43
1:A:248:GLY:HA3	1:A:299:TYR:CG	2.53	0.42
1:A:995:TYR:OH	11:A:1407:HOH:O	2.19	0.42
1:B:705:PRO:HD3	1:B:781:THR:HB	2.01	0.42
1:B:717:ILE:HG12	1:B:727:VAL:HG11	2.02	0.42
1:B:487:VAL:O	1:B:491:LEU:N	2.52	0.42
1:B:662:GLY:HA2	11:B:1562:HOH:O	2.19	0.42
1:B:796:ASP:HA	1:B:1178:LYS:HE2	2.01	0.42
1:B:248:GLY:HA3	1:B:299:TYR:CG	2.55	0.42
1:A:617:VAL:HG12	1:A:774:GLU:HB2	2.02	0.42
1:A:863:MET:HB2	1:A:863:MET:HE3	1.73	0.41
1:A:1050:LEU:C	1:A:1050:LEU:HD13	2.44	0.41
1:A:500:VAL:O	1:A:503:ILE:HG22	2.21	0.41
1:B:712:ILE:HD13	1:B:781:THR:HG21	2.01	0.41
1:B:984:HIS:C	1:B:984:HIS:CD2	2.98	0.41
1:A:816:ALA:HA	1:A:849:VAL:O	2.21	0.41
1:A:937:LEU:HD21	1:A:947:HIS:CD2	2.56	0.41
1:A:58:LYS:HD3	1:A:61:ARG:NH2	2.35	0.41
1:A:73:GLU:HG3	1:A:510:ILE:HD13	2.03	0.41
1:B:369:VAL:HG12	1:B:421:ALA:HB3	2.02	0.41
1:A:659:ARG:HD3	11:A:1968:HOH:O	2.20	0.41
1:A:562:LEU:HD11	1:A:654:LEU:HD12	2.02	0.41
1:B:272:ARG:HB3	1:B:277:GLN:HG3	2.04	0.40
1:A:428:LEU:HD11	1:A:460:VAL:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:ARG:NH2	1:B:511:ASP:OD1	2.55	0.40
1:B:448:CYS:HB3	1:B:457:TYR:CE2	2.57	0.40
1:B:892:LYS:NZ	11:B:1468:HOH:O	2.54	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	1226/1235 (99%)	1206 (98%)	20 (2%)	0	100	100
1	B	1215/1235 (98%)	1191 (98%)	22 (2%)	2 (0%)	43	22
All	All	2441/2470 (99%)	2397 (98%)	42 (2%)	2 (0%)	48	23

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	133	HIS
1	B	129	ASN

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	906/951 (95%)	900 (99%)	6 (1%)	76	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	883/951 (93%)	877 (99%)	6 (1%)	76 56
All	All	1789/1902 (94%)	1777 (99%)	12 (1%)	76 56

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

Mol	Chain	Res	Type
1	A	133	HIS
1	A	140	LEU
1	A	157	SER
1	A	342	TYR
1	A	730	LYS
1	A	934	LEU
1	B	157	SER
1	B	181	ARG
1	B	342	TYR
1	B	730	LYS
1	B	934	LEU
1	B	937	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	ASN
1	A	194	GLN
1	A	685	GLN
1	A	793	GLN
1	A	827	GLN
1	A	1040	GLN
1	A	1114	HIS
1	B	419	GLN
1	B	793	GLN
1	B	872	HIS

5.3.3 RNA

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 28 ligands modelled in this entry, 2 are monoatomic - leaving 26 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	FMT	A	1306	-	2,2,2	0.64	0	1,1,1	0.17	0
7	SO4	A	1312	-	4,4,4	0.65	0	6,6,6	0.15	0
6	NAD	A	1307	8	46,48,48	2.15	9 (19%)	64,73,73	1.79	13 (20%)
4	FMT	B	1309	-	2,2,2	0.64	0	1,1,1	0.16	0
5	A1AQC	B	1310	-	12,12,12	1.74	1 (8%)	16,16,16	2.18	3 (18%)
3	PEG	B	1305	-	6,6,6	0.25	0	5,5,5	0.35	0
4	FMT	B	1304	-	2,2,2	0.93	0	1,1,1	0.24	0
10	PGE	B	1303	-	9,9,9	0.33	0	8,8,8	0.45	0
4	FMT	A	1305	-	2,2,2	0.66	0	1,1,1	0.27	0
4	FMT	B	1308	-	2,2,2	0.60	0	1,1,1	0.40	0
2	FAD	B	1301	-	58,58,58	2.06	14 (24%)	85,89,89	1.66	20 (23%)
3	PEG	A	1302	-	6,6,6	0.27	0	5,5,5	0.14	0
3	PEG	B	1315	-	6,6,6	0.26	0	5,5,5	0.20	0
7	SO4	A	1309	-	4,4,4	0.68	0	6,6,6	0.21	0
5	A1AQC	A	1304	-	12,12,12	1.83	1 (8%)	16,16,16	2.21	2 (12%)
6	NAD	B	1312	8	46,48,48	2.10	7 (15%)	64,73,73	1.77	12 (18%)
7	SO4	B	1313	-	4,4,4	0.57	0	6,6,6	0.24	0
2	FAD	A	1301	-	58,58,58	2.24	15 (25%)	85,89,89	1.73	16 (18%)
7	SO4	A	1308	-	4,4,4	0.55	0	6,6,6	0.47	0
3	PEG	B	1307	-	6,6,6	0.25	0	5,5,5	0.24	0
9	1PE	B	1302	-	15,15,15	0.26	0	14,14,14	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	FMT	A	1303	-	2,2,2	0.50	0	1,1,1	0.24	0
3	PEG	B	1311	-	6,6,6	0.25	0	5,5,5	0.20	0
3	PEG	B	1306	-	6,6,6	0.25	0	5,5,5	0.35	0
7	SO4	A	1310	-	4,4,4	0.67	0	6,6,6	0.12	0
7	SO4	A	1311	-	4,4,4	0.67	0	6,6,6	0.15	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
3	PEG	B	1311	-	-	2/4/4/4	-
5	A1AQC	A	1304	-	-	0/2/8/8	0/2/2/2
3	PEG	B	1306	-	-	0/4/4/4	-
6	NAD	B	1312	8	-	3/30/62/62	0/5/5/5
2	FAD	B	1301	-	-	3/34/50/50	0/6/6/6
3	PEG	A	1302	-	-	1/4/4/4	-
2	FAD	A	1301	-	-	5/34/50/50	0/6/6/6
3	PEG	B	1307	-	-	2/4/4/4	-
9	1PE	B	1302	-	-	4/13/13/13	-
3	PEG	B	1315	-	-	0/4/4/4	-
6	NAD	A	1307	8	-	3/30/62/62	0/5/5/5
3	PEG	B	1305	-	-	4/4/4/4	-
5	A1AQC	B	1310	-	-	0/2/8/8	0/2/2/2
10	PGE	B	1303	-	-	1/7/7/7	-

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	FAD	PA-O3P	-9.82	1.48	1.59
2	B	1301	FAD	PA-O3P	-8.24	1.50	1.59
6	B	1312	NAD	PA-O3	-7.82	1.51	1.59
6	A	1307	NAD	PA-O3	-7.32	1.51	1.59
6	A	1307	NAD	C2N-N1N	6.87	1.42	1.35
2	A	1301	FAD	O4-C4	6.34	1.35	1.23
2	B	1301	FAD	O4-C4	6.11	1.35	1.23
6	B	1312	NAD	C2N-N1N	5.76	1.41	1.35
5	A	1304	A1AQC	O1-C4	5.59	1.47	1.38
5	B	1310	A1AQC	O1-C4	5.34	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1307	NAD	C7N-N7N	5.10	1.42	1.33
6	B	1312	NAD	C7N-N7N	5.09	1.42	1.33
2	B	1301	FAD	O2-C2	4.51	1.33	1.24
2	A	1301	FAD	O2-C2	4.32	1.32	1.24
6	B	1312	NAD	C6A-N6A	4.21	1.45	1.34
2	A	1301	FAD	C4X-N5	4.00	1.39	1.30
2	A	1301	FAD	C6A-N6A	3.92	1.44	1.34
2	B	1301	FAD	C4X-N5	3.85	1.39	1.30
2	B	1301	FAD	C6A-N6A	3.82	1.44	1.34
6	A	1307	NAD	C6A-N6A	3.67	1.43	1.34
2	A	1301	FAD	P-O3P	3.66	1.63	1.59
2	A	1301	FAD	O2'-C2'	-2.94	1.37	1.43
2	B	1301	FAD	O2'-C2'	-2.92	1.37	1.43
2	B	1301	FAD	P-O3P	2.84	1.62	1.59
2	A	1301	FAD	PA-O5B	-2.81	1.48	1.59
6	A	1307	NAD	PA-O5B	-2.70	1.48	1.59
2	A	1301	FAD	C1'-C2'	-2.59	1.49	1.52
2	A	1301	FAD	O4'-C4'	-2.55	1.38	1.43
2	A	1301	FAD	C2-N1	2.47	1.42	1.36
2	B	1301	FAD	C2-N1	2.43	1.42	1.36
6	A	1307	NAD	C6N-N1N	2.41	1.40	1.35
6	B	1312	NAD	C6N-N1N	2.36	1.40	1.35
2	A	1301	FAD	O4B-C4B	-2.31	1.39	1.45
2	A	1301	FAD	PA-O2A	-2.28	1.44	1.55
6	A	1307	NAD	O3D-C3D	-2.23	1.37	1.43
2	B	1301	FAD	O4B-C4B	-2.22	1.40	1.45
2	B	1301	FAD	PA-O2A	-2.21	1.45	1.55
2	A	1301	FAD	O3'-C3'	-2.19	1.37	1.43
6	A	1307	NAD	C2B-C3B	-2.16	1.47	1.53
6	A	1307	NAD	PA-O2A	-2.16	1.45	1.55
2	B	1301	FAD	O4'-C4'	-2.13	1.38	1.43
6	B	1312	NAD	PA-O2A	-2.06	1.45	1.55
6	B	1312	NAD	PA-O5B	-2.06	1.51	1.59
2	B	1301	FAD	O3'-C3'	-2.06	1.37	1.43
2	B	1301	FAD	PA-O5B	-2.03	1.51	1.59
2	A	1301	FAD	C10-N1	2.01	1.37	1.33
2	B	1301	FAD	O2B-C2B	-2.00	1.38	1.43

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1312	NAD	N3A-C2A-N1A	-6.48	118.77	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1307	NAD	N3A-C2A-N1A	-6.17	119.25	128.58
5	A	1304	A1AQC	O1-C4-C7	-6.13	109.57	113.19
2	B	1301	FAD	N3A-C2A-N1A	-5.66	120.01	128.58
5	B	1310	A1AQC	C5-C6-C7	5.66	106.60	101.97
5	B	1310	A1AQC	O1-C4-C7	-5.31	110.06	113.19
2	A	1301	FAD	N3A-C2A-N1A	-5.22	120.67	128.58
5	A	1304	A1AQC	C5-C6-C7	5.06	106.11	101.97
2	A	1301	FAD	C5A-C4A-N3A	-4.81	120.10	126.72
6	B	1312	NAD	C5A-C4A-N3A	-4.56	120.44	126.72
6	A	1307	NAD	C4D-O4D-C1D	-4.54	105.77	109.92
6	A	1307	NAD	C5A-C4A-N3A	-4.44	120.60	126.72
6	A	1307	NAD	C5A-N7A-C8A	4.07	109.85	103.45
2	B	1301	FAD	C5A-C4A-N3A	-4.06	121.12	126.72
2	A	1301	FAD	C5A-N7A-C8A	4.01	109.75	103.45
6	B	1312	NAD	C5A-N7A-C8A	3.89	109.57	103.45
6	B	1312	NAD	C2A-N3A-C4A	3.89	121.33	111.83
6	B	1312	NAD	N3A-C4A-N9A	3.73	133.51	127.17
2	A	1301	FAD	C9-C9A-N10	-3.62	116.99	121.85
6	A	1307	NAD	N3A-C4A-N9A	3.60	133.29	127.17
6	B	1312	NAD	N9A-C8A-N7A	-3.59	108.84	113.94
2	A	1301	FAD	N3A-C4A-N9A	3.53	133.18	127.17
6	A	1307	NAD	N9A-C8A-N7A	-3.51	108.96	113.94
2	A	1301	FAD	N9A-C8A-N7A	-3.46	109.03	113.94
6	A	1307	NAD	C2A-N3A-C4A	3.40	120.13	111.83
2	A	1301	FAD	C2A-N3A-C4A	3.39	120.11	111.83
2	B	1301	FAD	O2P-P-O3P	-3.31	98.32	107.27
2	B	1301	FAD	O3P-P-O1P	3.26	120.51	110.70
2	A	1301	FAD	C5X-C9A-N10	3.23	120.89	117.97
2	A	1301	FAD	C4A-C5A-N7A	-3.23	106.89	110.58
2	B	1301	FAD	C5A-N7A-C8A	3.22	108.50	103.45
2	B	1301	FAD	C2A-N3A-C4A	3.15	119.53	111.83
2	B	1301	FAD	O2-C2-N1	-3.06	116.72	121.80
2	A	1301	FAD	C4-C4X-N5	3.05	122.42	118.21
6	A	1307	NAD	C4A-C5A-N7A	-2.94	107.22	110.58
2	A	1301	FAD	C4X-C4-N3	2.94	120.73	113.25
2	B	1301	FAD	C4A-C5A-N7A	-2.92	107.24	110.58
6	B	1312	NAD	C4A-C5A-N7A	-2.90	107.27	110.58
2	B	1301	FAD	N3A-C4A-N9A	2.88	132.06	127.17
2	A	1301	FAD	C4-N3-C2	-2.79	120.70	125.64
2	B	1301	FAD	C4-C4X-N5	2.78	122.05	118.21
2	A	1301	FAD	C1'-C2'-C3'	-2.71	102.31	109.66
6	B	1312	NAD	C4D-O4D-C1D	-2.69	107.46	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1301	FAD	C4-N3-C2	-2.60	121.02	125.64
6	B	1312	NAD	C3N-C7N-N7N	2.60	120.94	117.74
2	A	1301	FAD	C2'-C1'-N10	2.57	122.34	110.20
2	B	1301	FAD	C4X-C10-N10	2.55	120.13	116.48
2	B	1301	FAD	C2'-C1'-N10	2.54	122.20	110.20
2	B	1301	FAD	N9A-C8A-N7A	-2.47	110.43	113.94
6	A	1307	NAD	C2A-N1A-C6A	2.47	122.78	118.73
2	B	1301	FAD	C2A-N1A-C6A	2.47	122.78	118.73
2	B	1301	FAD	C5X-C9A-N10	2.42	120.16	117.97
6	B	1312	NAD	C4A-N9A-C8A	2.42	108.28	105.74
2	A	1301	FAD	O2A-PA-O3P	-2.36	100.89	107.27
2	B	1301	FAD	C4X-C4-N3	2.24	118.97	113.25
6	A	1307	NAD	O2A-PA-O3	-2.21	101.29	107.27
2	B	1301	FAD	C9-C9A-N10	-2.19	118.91	121.85
2	A	1301	FAD	O4-C4-C4X	-2.18	120.77	126.53
5	B	1310	A1AQC	C3-C4-C7	-2.13	120.19	122.92
6	B	1312	NAD	C2A-N1A-C6A	2.11	122.19	118.73
6	B	1312	NAD	C6A-C5A-N7A	2.11	136.15	132.09
6	A	1307	NAD	O5B-PA-O1A	2.09	117.21	108.94
2	B	1301	FAD	C10-C4X-N5	-2.08	120.56	124.81
2	B	1301	FAD	O4-C4-C4X	-2.03	121.17	126.53
6	A	1307	NAD	C4A-N9A-C8A	2.03	107.87	105.74
6	A	1307	NAD	O2N-PN-O3	2.01	112.69	107.27

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301	FAD	N10-C1'-C2'-O2'
2	A	1301	FAD	N10-C1'-C2'-C3'
2	B	1301	FAD	P-O3P-PA-O5B
2	B	1301	FAD	N10-C1'-C2'-O2'
2	B	1301	FAD	N10-C1'-C2'-C3'
3	A	1302	PEG	O2-C3-C4-O4
10	B	1303	PGE	O1-C1-C2-O2
3	B	1311	PEG	O1-C1-C2-O2
2	A	1301	FAD	P-O3P-PA-O5B
2	A	1301	FAD	PA-O3P-P-O5'
6	B	1312	NAD	C2B-C1B-N9A-C8A
3	B	1305	PEG	C1-C2-O2-C3
3	B	1307	PEG	C1-C2-O2-C3
3	B	1311	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
6	A	1307	NAD	C2B-C1B-N9A-C8A
3	B	1305	PEG	O1-C1-C2-O2
9	B	1302	1PE	OH7-C16-C26-OH6
9	B	1302	1PE	C16-C26-OH6-C15
6	A	1307	NAD	C4D-C5D-O5D-PN
6	B	1312	NAD	C4D-C5D-O5D-PN
3	B	1305	PEG	C4-C3-O2-C2
9	B	1302	1PE	C24-C14-OH5-C25
9	B	1302	1PE	C23-C13-OH4-C24
3	B	1307	PEG	C4-C3-O2-C2
6	A	1307	NAD	O4B-C1B-N9A-C8A
3	B	1305	PEG	O2-C3-C4-O4
2	A	1301	FAD	C3B-C4B-C5B-O5B
6	B	1312	NAD	O4B-C1B-N9A-C8A

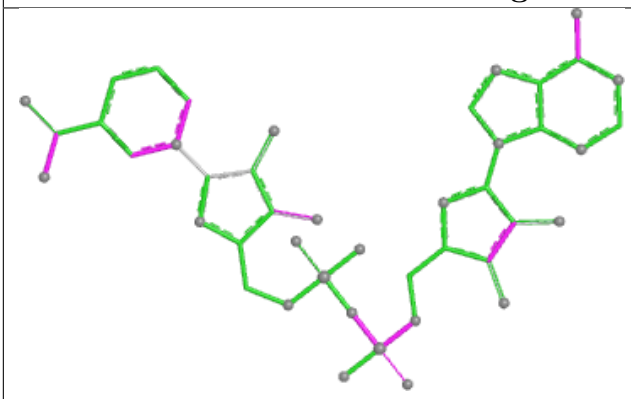
There are no ring outliers.

8 monomers are involved in 19 short contacts:

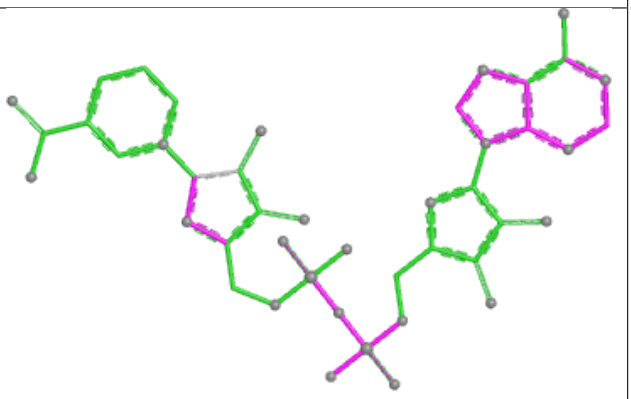
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1307	NAD	2	0
10	B	1303	PGE	2	0
4	A	1305	FMT	2	0
4	B	1308	FMT	4	0
2	B	1301	FAD	2	0
6	B	1312	NAD	2	0
2	A	1301	FAD	2	0
3	B	1311	PEG	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

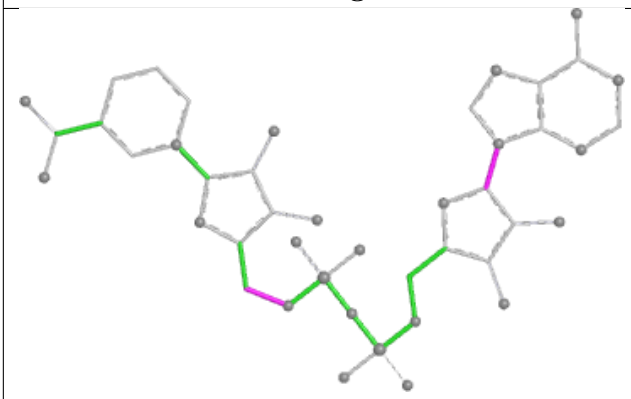
Ligand NAD A 1307



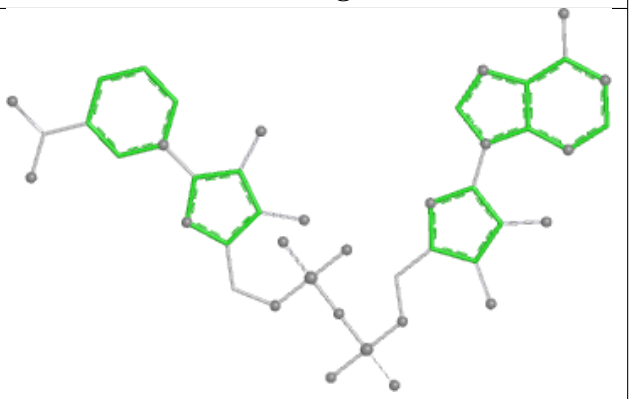
Bond lengths



Bond angles

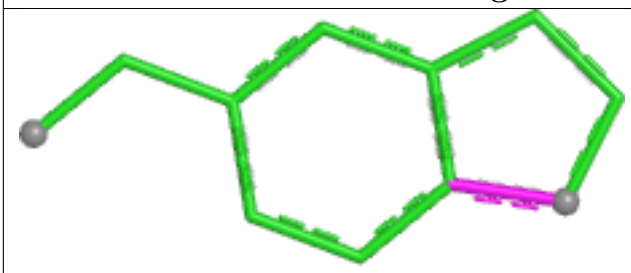


Torsions

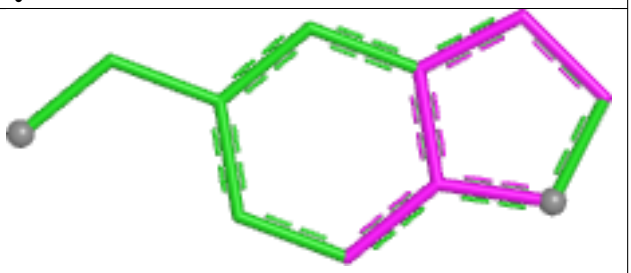


Rings

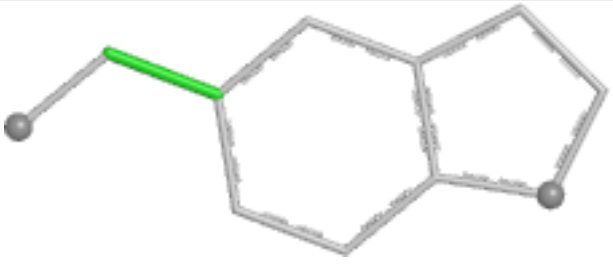
Ligand A1AQC B 1310



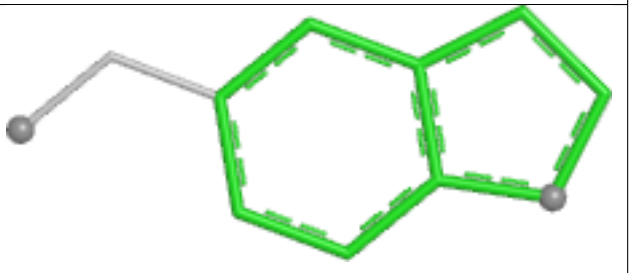
Bond lengths



Bond angles

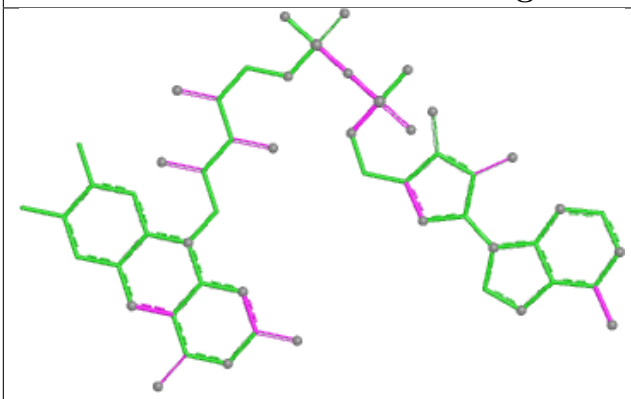


Torsions

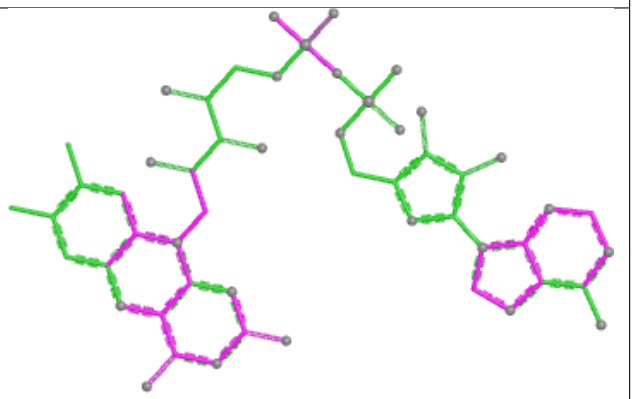


Rings

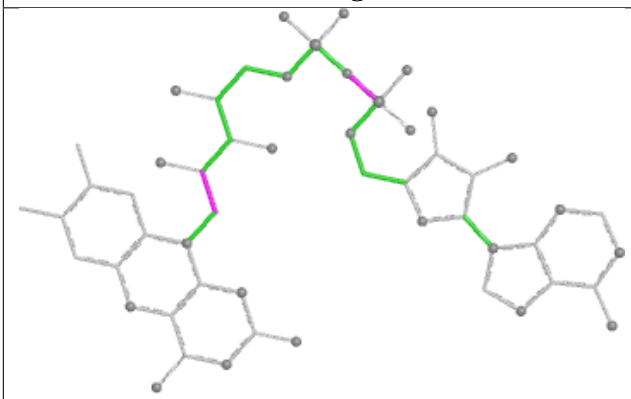
Ligand FAD B 1301



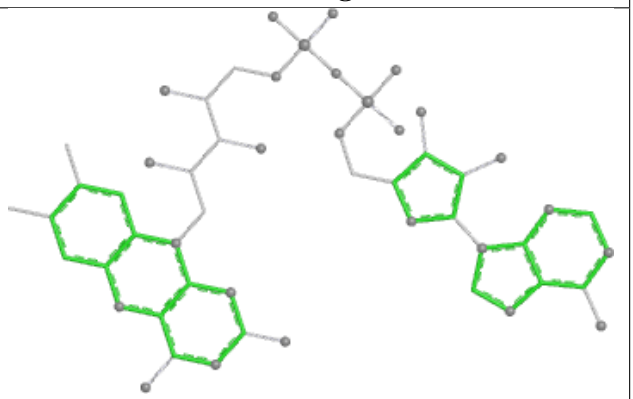
Bond lengths



Bond angles



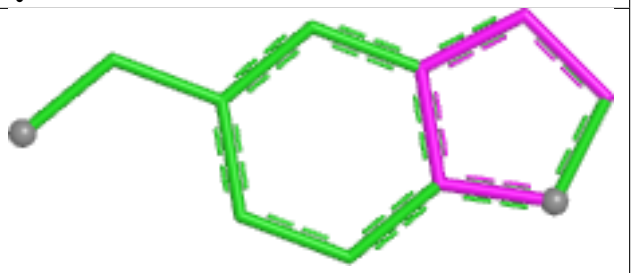
Torsions



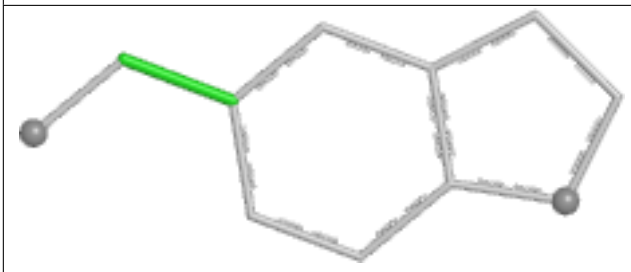
Rings

Ligand A1AQC A 1304

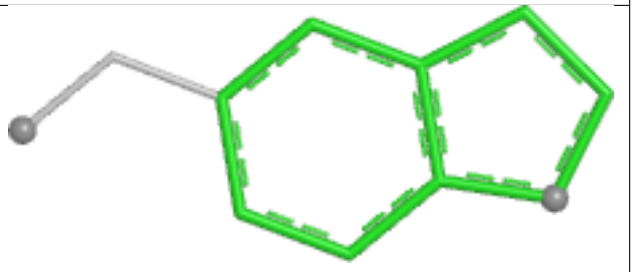
Bond lengths



Bond angles

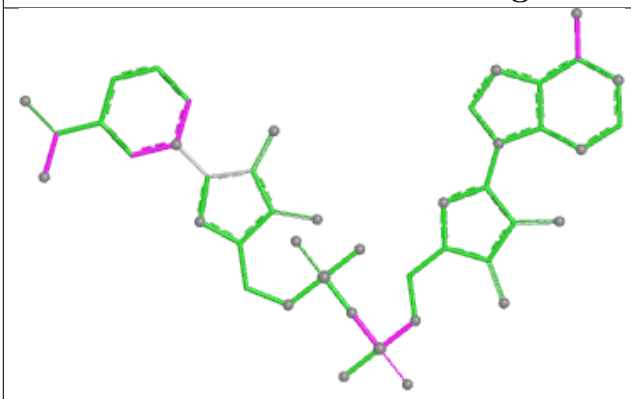


Torsions

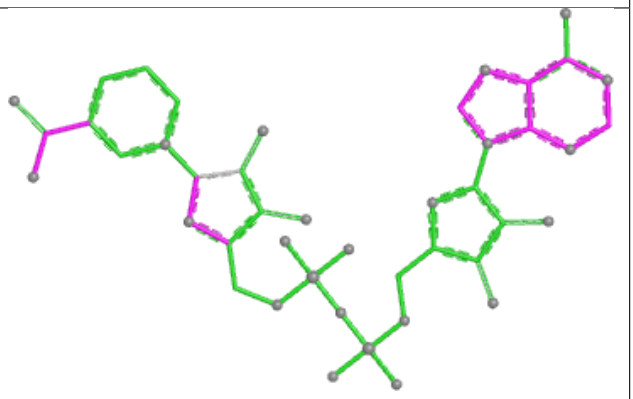


Rings

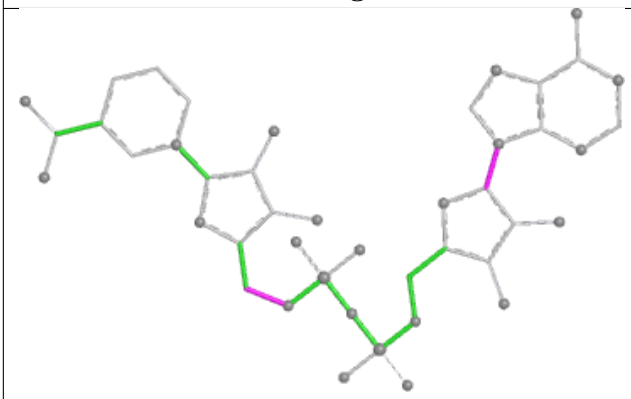
Ligand NAD B 1312



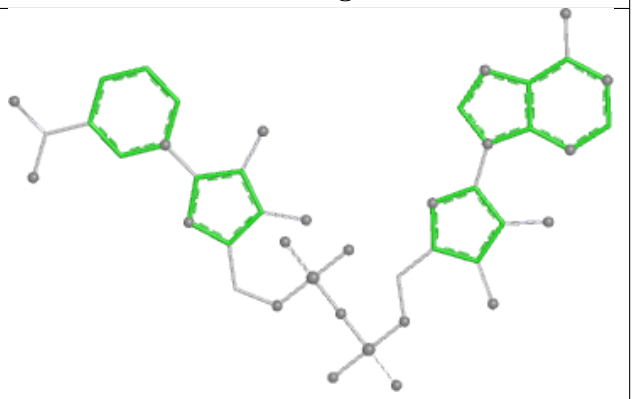
Bond lengths



Bond angles

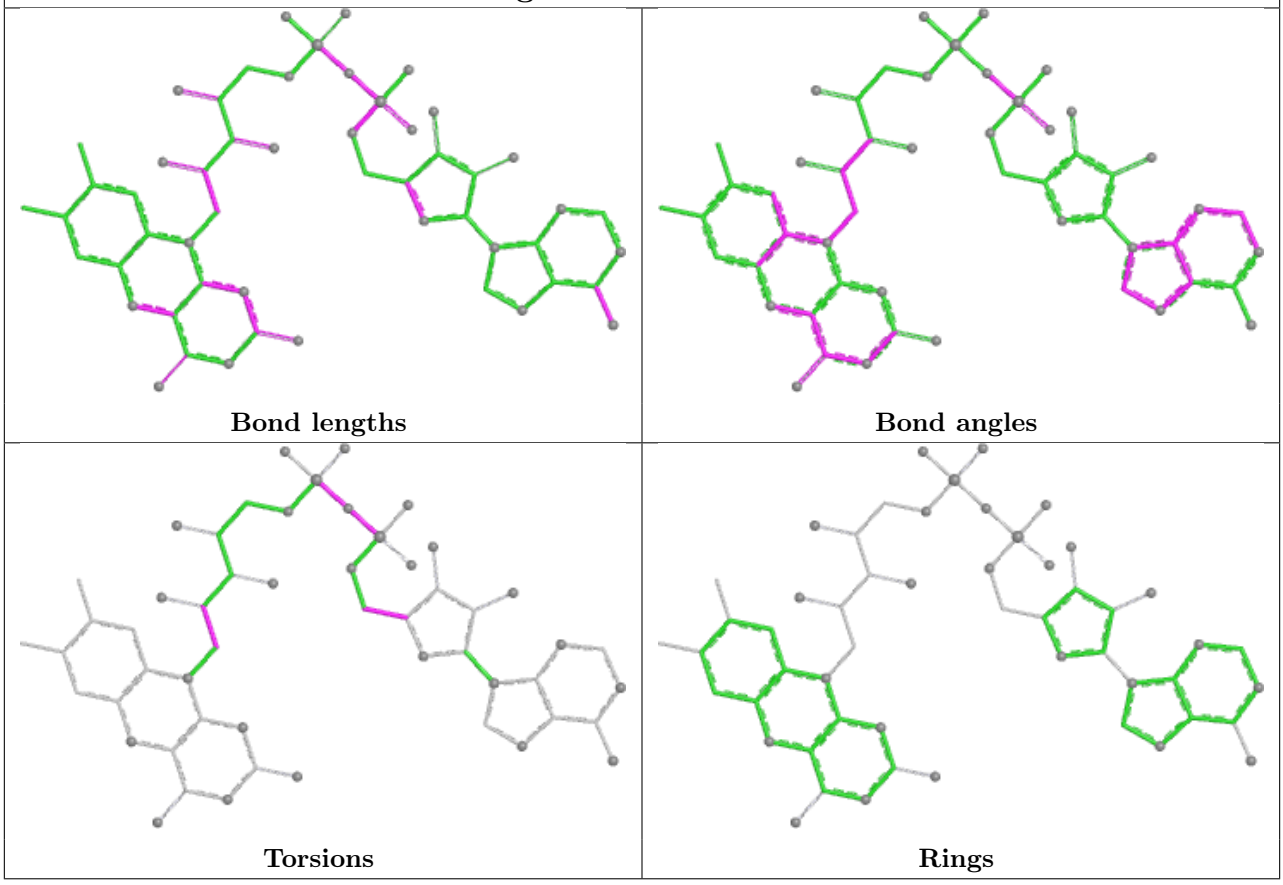


Torsions



Rings

Ligand FAD A 1301



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1213/1235 (98%)	0.14	44 (3%)	46	50	10, 23, 40, 65	21 (1%)
1	B	1210/1235 (97%)	0.11	52 (4%)	40	44	9, 21, 43, 69	13 (1%)
All	All	2423/2470 (98%)	0.13	96 (3%)	42	46	9, 22, 41, 69	34 (1%)

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	491	LEU	7.1
1	B	912	ILE	6.8
1	B	486	LEU	6.7
1	B	1223	ALA	6.4
1	B	487	VAL	5.8
1	B	1230	MET	5.6
1	B	490	LEU	5.6
1	B	1222	ALA	5.5
1	B	918	THR	5.4
1	B	1231	ALA	5.2
1	B	1232	ILE	5.2
1	B	484	ALA	5.1
1	B	1229	LEU	5.1
1	B	481	THR	4.6
1	A	1223	ALA	4.6
1	B	482	LEU	4.5
1	B	485	TYR	4.5
1	A	1222	ALA	4.5
1	A	490	LEU	4.3
1	A	1230	MET	4.3
1	A	491	LEU	4.3
1	B	1227	ALA	4.2
1	B	500	VAL	4.0
1	B	913	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	915	ALA	3.7
1	A	156	THR	3.7
1	B	1233	GLY	3.6
1	A	1226	ASN	3.6
1	B	914	LEU	3.6
1	B	916	SER	3.5
1	B	1228	SER	3.5
1	A	1227	ALA	3.5
1	A	1229	LEU	3.4
1	B	483	LEU	3.4
1	A	1231	ALA	3.4
1	A	494	GLY	3.3
1	A	484	ALA	3.3
1	B	479	HIS	3.3
1	B	129	ASN	3.3
1	B	1225	GLY	3.2
1	A	1225	GLY	3.2
1	A	82	SER	3.2
1	A	1232	ILE	3.2
1	A	130	TRP	3.1
1	B	508	VAL	3.1
1	B	134	LEU	3.1
1	A	481	THR	3.0
1	A	137	SER	3.0
1	B	478	THR	3.0
1	A	127	ASP	3.0
1	A	133	HIS	2.9
1	A	14	ALA	2.8
1	A	79	HIS	2.8
1	A	1228	SER	2.8
1	B	66	SER	2.8
1	A	129	ASN	2.8
1	B	127	ASP	2.7
1	B	14	ALA	2.7
1	A	487	VAL	2.7
1	B	84	VAL	2.7
1	B	451	GLY	2.6
1	A	905	LEU	2.6
1	A	132	SER	2.6
1	A	500	VAL	2.6
1	B	489	ARG	2.6
1	A	486	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1233	GLY	2.5
1	A	116	THR	2.5
1	B	1226	ASN	2.5
1	B	60	ILE	2.5
1	A	1003	ALA	2.4
1	B	155	LEU	2.4
1	A	223	LEU	2.4
1	B	132	SER	2.4
1	B	115	ALA	2.3
1	B	503	ILE	2.3
1	B	510	ILE	2.3
1	B	128	GLY	2.3
1	A	1221	ALA	2.3
1	A	128	GLY	2.3
1	A	485	TYR	2.3
1	B	133	HIS	2.3
1	A	495	ALA	2.3
1	A	114	THR	2.3
1	B	122	ARG	2.2
1	B	130	TRP	2.2
1	A	111	ILE	2.2
1	B	1221	ALA	2.2
1	B	414	ASP	2.2
1	A	506	PRO	2.2
1	A	125	ILE	2.1
1	A	451	GLY	2.1
1	A	115	ALA	2.1
1	B	156	THR	2.1
1	B	496	ASN	2.1
1	A	483	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)

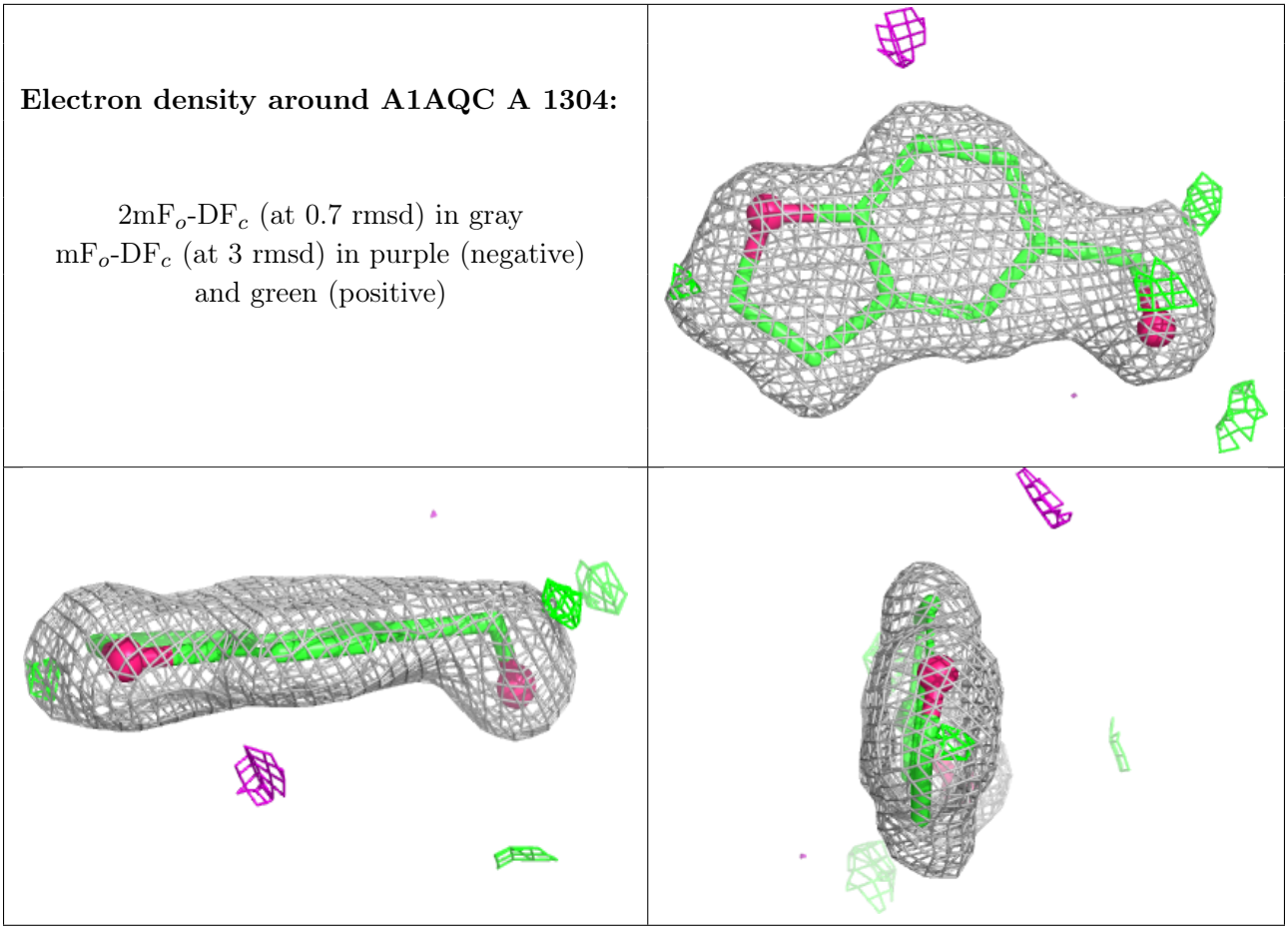
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PEG	B	1305	7/7	0.82	0.15	31,40,44,44	0
3	PEG	B	1315	7/7	0.82	0.13	30,32,42,43	0
4	FMT	A	1306	3/3	0.82	0.15	28,28,31,31	3
3	PEG	B	1306	7/7	0.83	0.14	24,26,28,33	7
7	SO4	A	1311	5/5	0.85	0.14	40,40,42,52	5
3	PEG	B	1311	7/7	0.86	0.13	28,33,40,41	7
3	PEG	B	1307	7/7	0.86	0.11	32,35,40,43	0
4	FMT	B	1309	3/3	0.87	0.10	44,44,47,47	0
7	SO4	A	1309	5/5	0.88	0.11	35,37,41,47	5
3	PEG	A	1302	7/7	0.88	0.11	28,36,42,44	0
4	FMT	B	1308	3/3	0.89	0.14	15,15,22,22	3
9	1PE	B	1302	16/16	0.89	0.12	29,37,39,42	0
5	A1AQC	A	1304	11/11	0.90	0.10	20,22,27,30	11
4	FMT	A	1305	3/3	0.92	0.10	22,22,27,27	3
4	FMT	A	1303	3/3	0.92	0.09	21,21,27,28	3
4	FMT	B	1304	3/3	0.92	0.10	16,16,24,31	3
10	PGE	B	1303	10/10	0.93	0.08	30,35,39,41	0
7	SO4	A	1310	5/5	0.94	0.07	41,41,46,48	5
7	SO4	A	1312	5/5	0.94	0.09	26,31,39,40	5
2	FAD	B	1301	53/53	0.95	0.07	15,19,25,26	0
5	A1AQC	B	1310	11/11	0.95	0.07	20,22,27,30	11
8	MG	B	1314	1/1	0.96	0.10	26,26,26,26	0
2	FAD	A	1301	53/53	0.96	0.07	16,20,27,28	0
6	NAD	A	1307	44/44	0.96	0.07	18,22,24,29	0
6	NAD	B	1312	44/44	0.97	0.05	14,16,20,26	0
8	MG	A	1313	1/1	0.98	0.07	27,27,27,27	0
7	SO4	B	1313	5/5	0.98	0.05	16,18,22,23	0
7	SO4	A	1308	5/5	0.99	0.04	20,20,23,25	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.

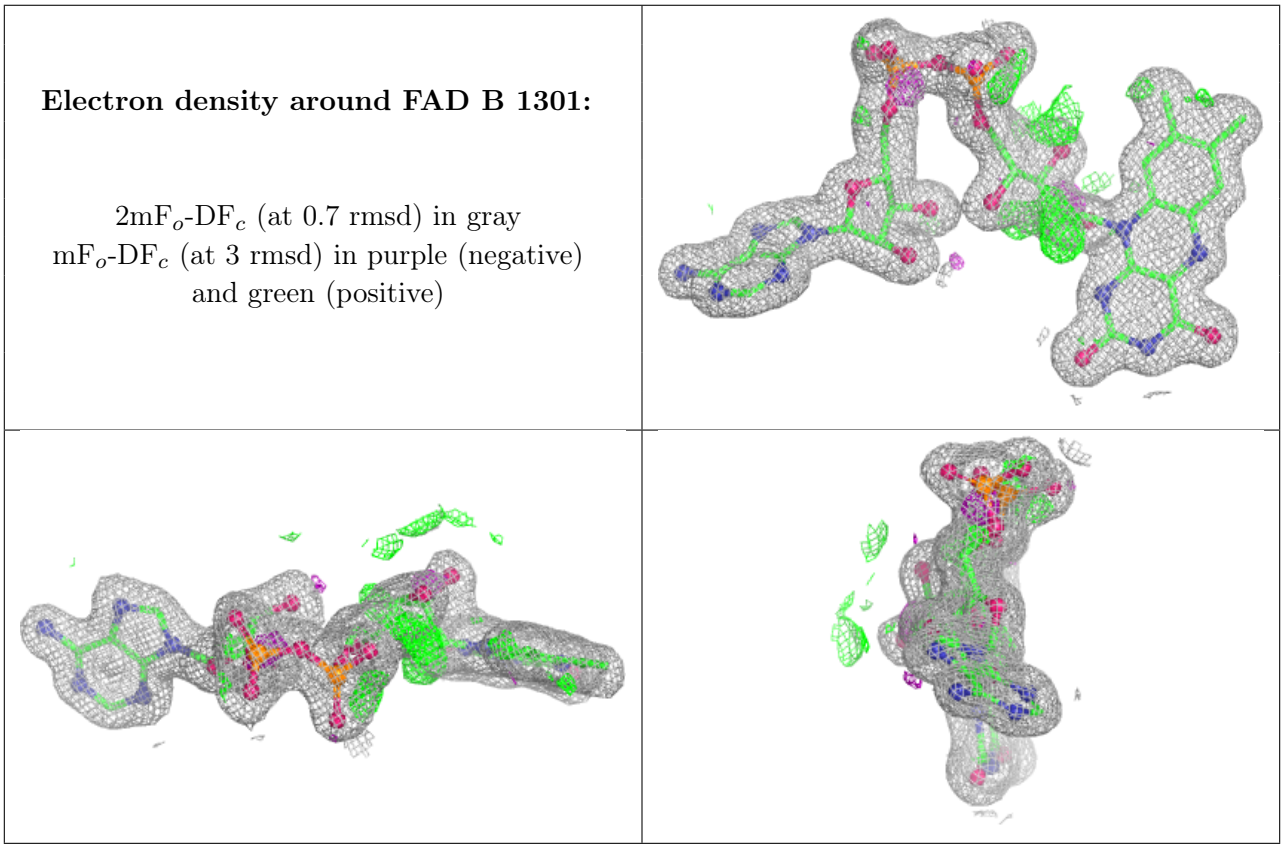
Electron density around A1AQC A 1304:

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



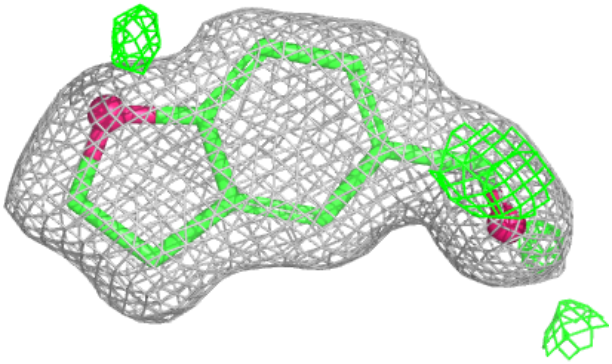
Electron density around FAD B 1301:

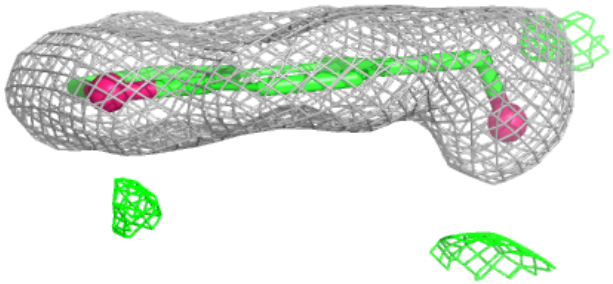
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

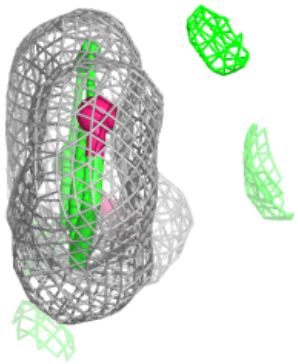


Electron density around A1AQC B 1310:

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

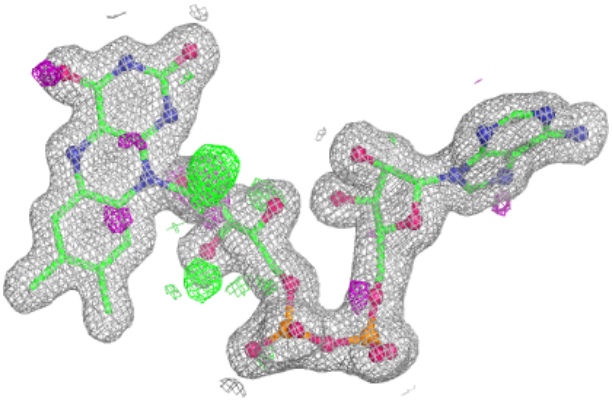


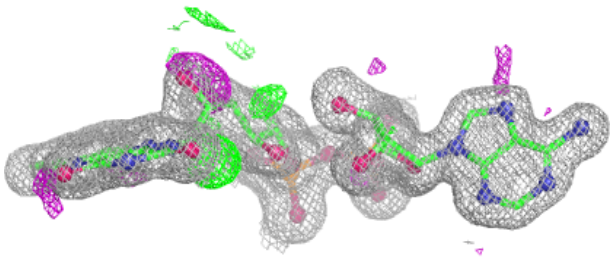


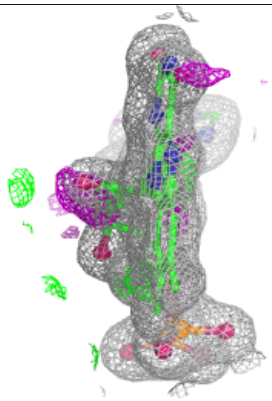


Electron density around FAD A 1301:

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

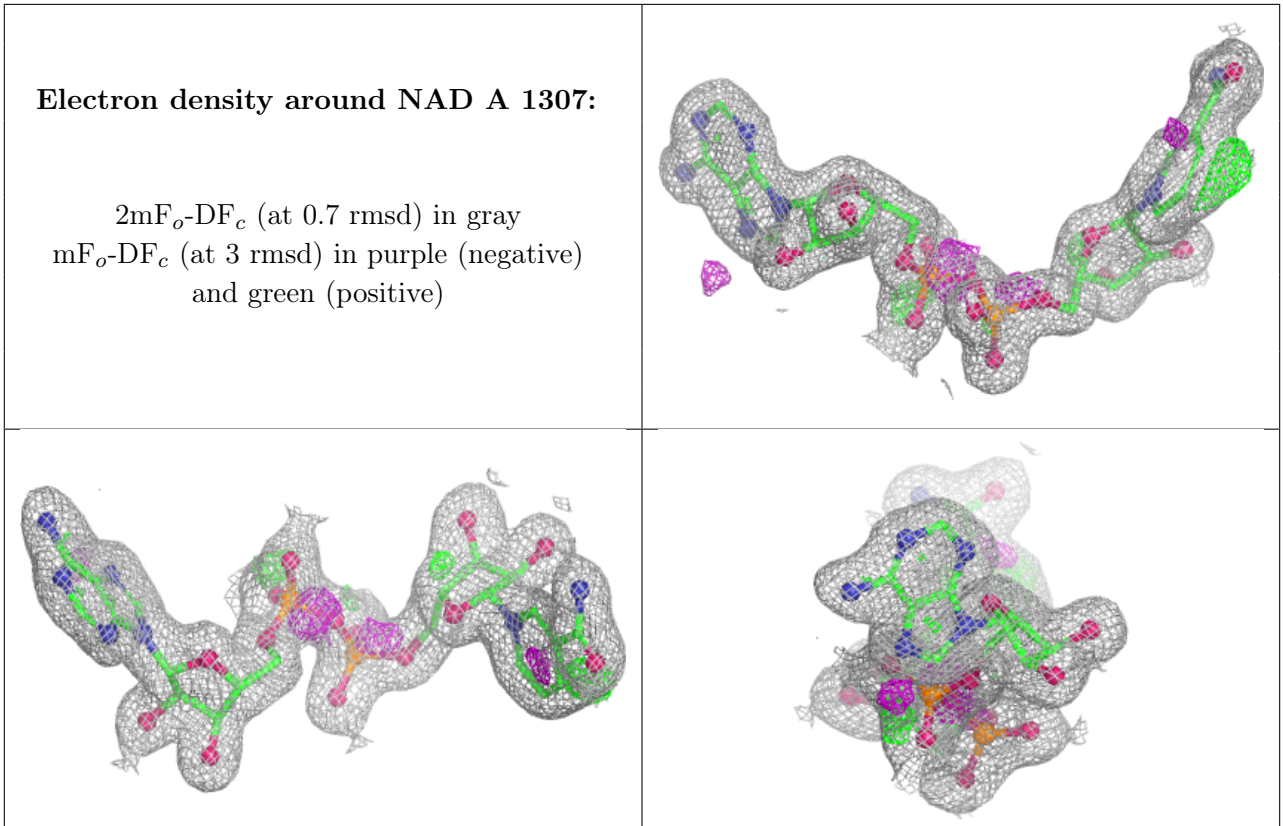






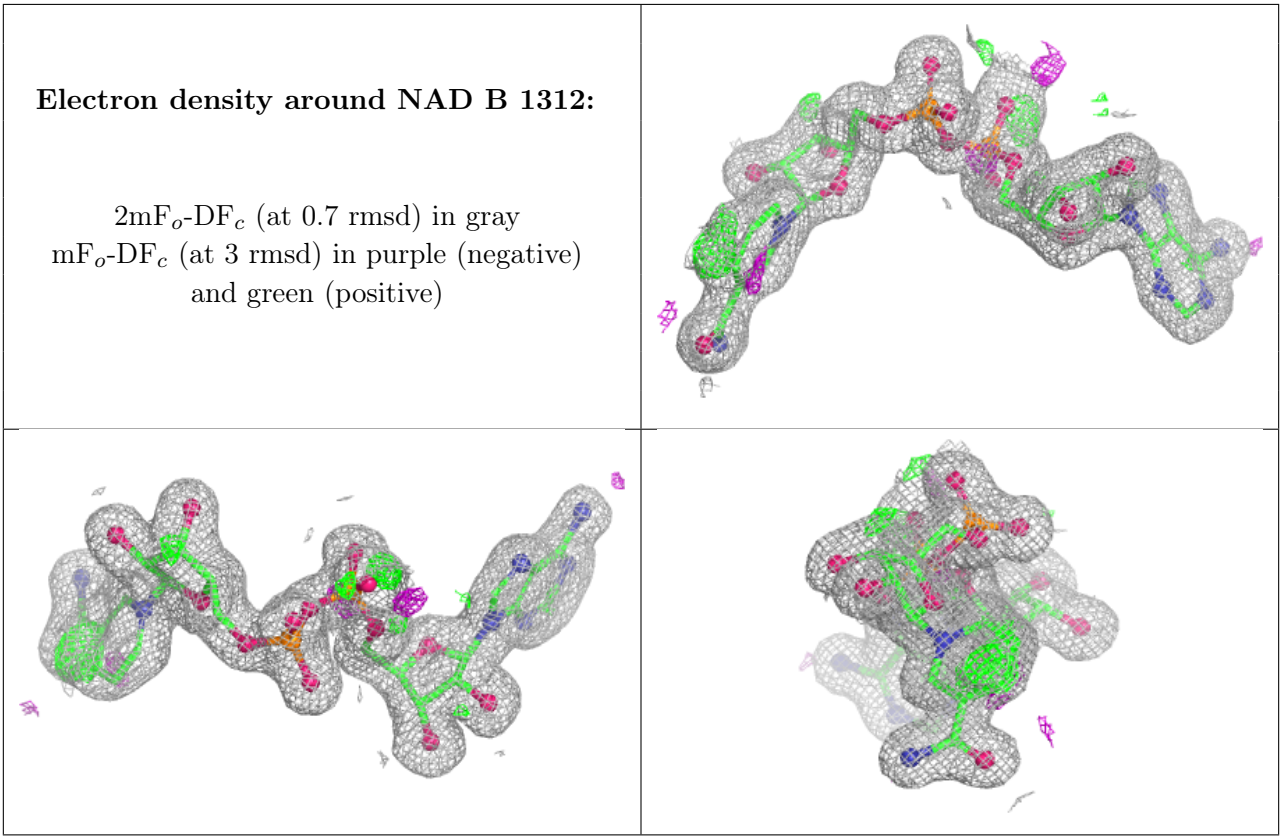
Electron density around NAD A 1307:

$2mF_o$-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 1312:

$2mF_o$-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.