



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:06 PM UTC

PDB ID : 5CHO / pdb_00005cho
Title : Crystal Structure of BorF, the Flavin Reductase Component of a Bacterial Two-Component Tryptophan Halogenase
Authors : Ma, Z.; Bellizzi, J.
Deposited on : 2015-07-10
Resolution : 2.37 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

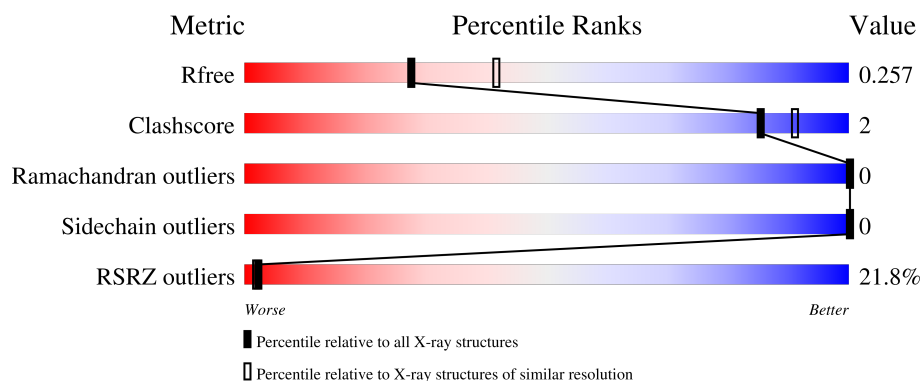
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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.



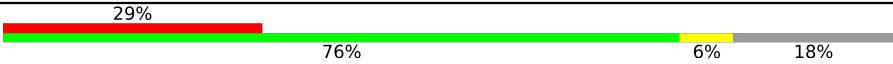
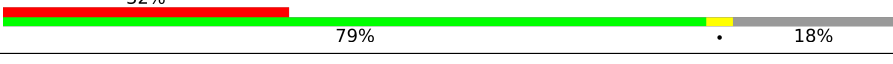
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	196	3% 81% 16%
1	B	196	6% 80% 17%
1	C	196	3% 81% 16%
1	D	196	3% 81% 16%
1	E	196	15% 76% 6% 18%

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Mol	Chain	Length	Quality of chain
1	F	196	
1	G	196	
1	H	196	

2 Entry composition

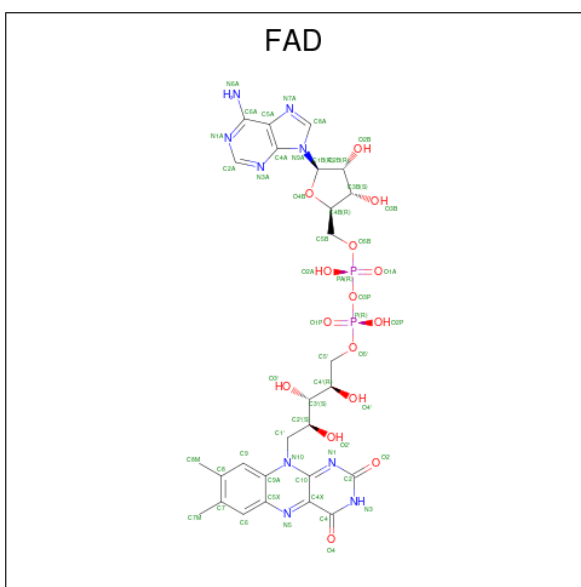
There are 3 unique types of molecules in this entry. The entry contains 10269 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Flavin reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	0	0	0
			1248	787	229	227	5			
1	B	163	Total	C	N	O	S	0	0	0
			1227	773	224	225	5			
1	C	165	Total	C	N	O	S	0	0	0
			1247	786	229	227	5			
1	D	164	Total	C	N	O	S	0	0	0
			1240	781	228	226	5			
1	E	161	Total	C	N	O	S	0	0	0
			1196	755	213	223	5			
1	F	160	Total	C	N	O	S	0	0	0
			1191	752	212	222	5			
1	G	160	Total	C	N	O	S	0	0	0
			1169	741	203	220	5			
1	H	160	Total	C	N	O	S	0	0	0
			1170	742	203	220	5			

- 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	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	D	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	E	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	F	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	G	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	H	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	42	Total O 42 42	0	0
3	B	25	Total O 25 25	0	0
3	C	38	Total O 38 38	0	0
3	D	34	Total O 34 34	0	0

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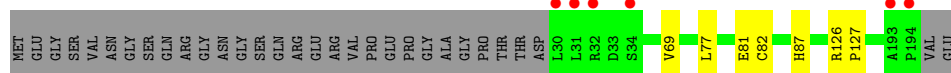
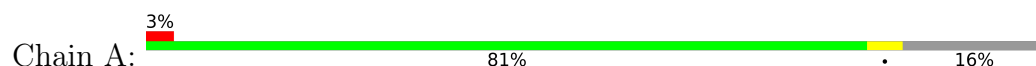
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	10	Total	O	0	0
			10	10		
3	F	4	Total	O	0	0
			4	4		
3	G	4	Total	O	0	0
			4	4		

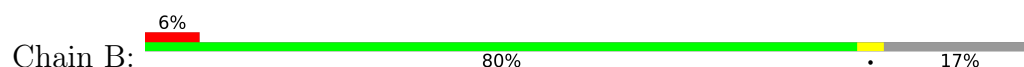
3 Residue-property plots [i](#)

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.

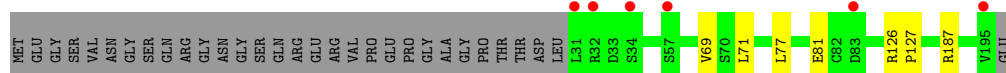
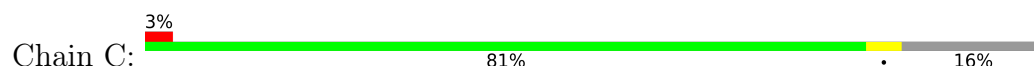
- Molecule 1: Flavin reductase



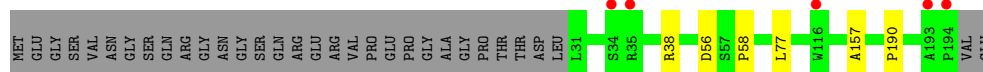
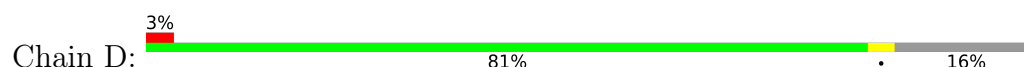
- Molecule 1: Flavin reductase



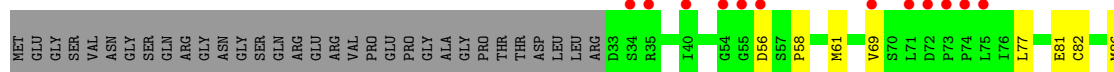
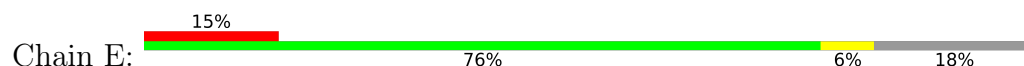
- Molecule 1: Flavin reductase

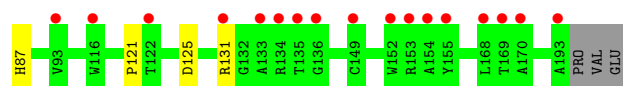


- Molecule 1: Flavin reductase

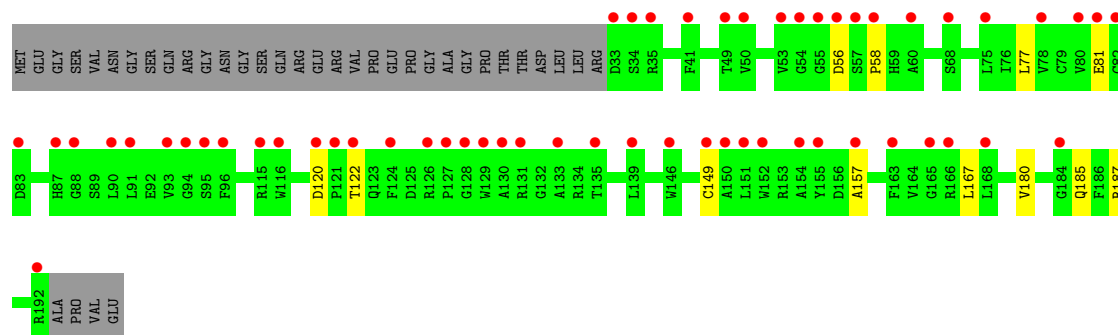
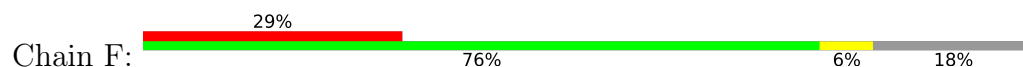


- Molecule 1: Flavin reductase

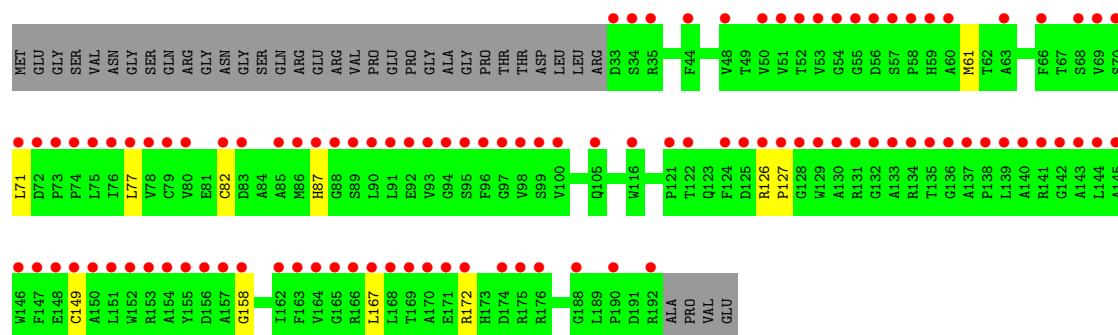
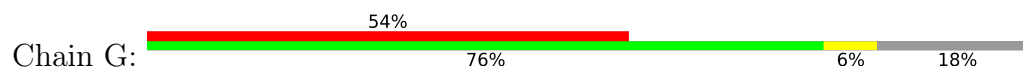




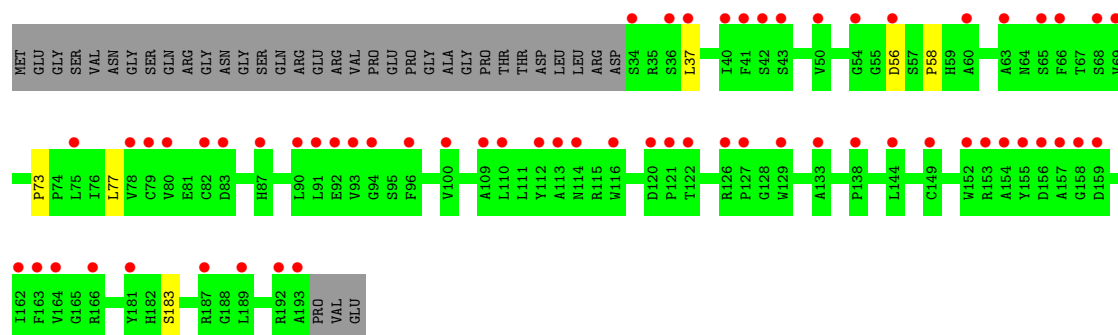
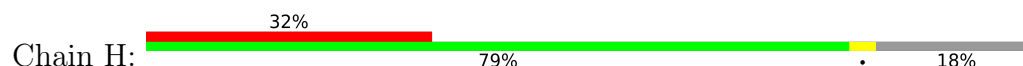
● Molecule 1: Flavin reductase



● Molecule 1: Flavin reductase



● Molecule 1: Flavin reductase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	278.01Å 62.34Å 101.88Å 90.00° 110.84° 90.00°	Depositor
Resolution (Å)	47.61 – 2.37 47.61 – 2.37	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.61-2.37) 100.0 (47.61-2.37)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.10Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.215 , 0.247 0.228 , 0.257	Depositor DCC
R_{free} test set	1989 reflections (1.63%)	wwPDB-VP
Wilson B-factor (Å ²)	42.4	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10269	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% 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: 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	0.34	0/1281	0.70	0/1747
1	B	0.35	0/1259	0.73	0/1717
1	C	0.35	0/1280	0.69	0/1746
1	D	0.35	0/1273	0.67	0/1736
1	E	0.33	0/1228	0.69	0/1678
1	F	0.31	0/1223	0.71	0/1671
1	G	0.33	0/1201	0.73	0/1645
1	H	0.30	0/1202	0.70	0/1646
All	All	0.33	0/9947	0.70	0/13586

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 [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	1248	0	1199	5	0
1	B	1227	0	1170	4	0
1	C	1247	0	1197	6	0
1	D	1240	0	1188	5	0
1	E	1196	0	1124	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1191	0	1119	8	0
1	G	1169	0	1082	8	0
1	H	1170	0	1087	5	0
2	A	53	0	31	2	0
2	B	53	0	31	0	0
2	C	53	0	31	1	0
2	D	53	0	31	0	0
2	E	53	0	31	1	0
2	F	53	0	31	1	0
2	G	53	0	31	1	0
2	H	53	0	31	1	0
3	A	42	0	0	0	0
3	B	25	0	0	0	0
3	C	38	0	0	0	0
3	D	34	0	0	0	0
3	E	10	0	0	0	0
3	F	4	0	0	0	0
3	G	4	0	0	0	0
All	All	10269	0	9414	43	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 2.

All (43) 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:F:185:GLN:OE1	1:F:187:ARG:NH2	2.22	0.71
1:E:125:ASP:OD1	1:E:131:ARG:NH2	2.28	0.67
1:C:71:LEU:HD11	1:D:38:ARG:HE	1.60	0.66
1:A:69:VAL:HG11	1:B:157:ALA:HB1	1.90	0.53
1:G:77:LEU:C	1:G:77:LEU:HD12	2.33	0.53
1:B:126:ARG:HB3	1:B:127:PRO:HD2	1.89	0.53
1:G:71:LEU:HD23	1:H:37:LEU:HD23	1.91	0.53
1:G:149:CYS:SG	1:G:167:LEU:HD23	2.50	0.51
1:F:120:ASP:OD2	1:F:122:THR:HB	2.11	0.51
1:C:126:ARG:HB3	1:C:127:PRO:HD2	1.94	0.49
1:B:56:ASP:OD1	1:B:57:SER:N	2.46	0.49
1:H:77:LEU:HD12	1:H:77:LEU:C	2.38	0.49
1:G:126:ARG:HB3	1:G:127:PRO:HD2	1.95	0.48
1:C:81:GLU:OE2	2:C:201:FAD:O3B	2.30	0.47
1:A:81:GLU:OE2	2:A:201:FAD:O3B	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:LEU:HD12	1:D:77:LEU:C	2.40	0.47
1:F:77:LEU:C	1:F:77:LEU:HD12	2.39	0.46
1:C:187:ARG:NH2	1:D:190:PRO:O	2.32	0.46
1:B:77:LEU:C	1:B:77:LEU:HD12	2.41	0.45
1:G:82:CYS:HA	1:G:87:HIS:CD2	2.52	0.44
1:A:126:ARG:HB3	1:A:127:PRO:HD2	1.99	0.44
1:E:81:GLU:OE2	2:E:201:FAD:O3B	2.24	0.43
1:F:149:CYS:SG	1:F:167:LEU:HD23	2.59	0.43
1:F:81:GLU:OE2	2:F:201:FAD:O3B	2.30	0.43
2:A:201:FAD:H9	2:A:201:FAD:H1'1	1.89	0.43
1:C:77:LEU:C	1:C:77:LEU:HD12	2.43	0.43
1:F:56:ASP:C	1:F:58:PRO:HD3	2.43	0.43
1:C:69:VAL:HG11	1:D:157:ALA:HB1	1.99	0.43
1:E:82:CYS:HA	1:E:87:HIS:CD2	2.54	0.43
1:D:56:ASP:C	1:D:58:PRO:HD3	2.44	0.42
1:E:77:LEU:C	1:E:77:LEU:HD12	2.44	0.42
2:H:201:FAD:H9	2:H:201:FAD:H1'1	1.92	0.42
1:E:56:ASP:C	1:E:58:PRO:HD3	2.44	0.42
1:E:69:VAL:HG11	1:F:157:ALA:HB1	2.02	0.42
1:G:61:MET:HE2	2:G:201:FAD:H5'2	2.00	0.42
1:G:172:ARG:NH2	1:H:183:SER:OG	2.48	0.42
1:A:77:LEU:HD12	1:A:77:LEU:C	2.46	0.41
1:E:58:PRO:HD2	1:E:121:PRO:HB3	2.03	0.41
1:H:56:ASP:C	1:H:58:PRO:HD3	2.45	0.41
1:G:158:GLY:HA3	1:H:73:PRO:HD2	2.02	0.41
1:A:82:CYS:HA	1:A:87:HIS:CD2	2.57	0.40
1:E:61:MET:HG2	1:E:86:MET:HG2	2.03	0.40
1:F:180:VAL:O	1:F:187:ARG:N	2.48	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	163/196 (83%)	161 (99%)	2 (1%)	0	100	100
1	B	161/196 (82%)	159 (99%)	2 (1%)	0	100	100
1	C	163/196 (83%)	161 (99%)	2 (1%)	0	100	100
1	D	162/196 (83%)	160 (99%)	2 (1%)	0	100	100
1	E	159/196 (81%)	157 (99%)	2 (1%)	0	100	100
1	F	158/196 (81%)	155 (98%)	3 (2%)	0	100	100
1	G	158/196 (81%)	156 (99%)	2 (1%)	0	100	100
1	H	158/196 (81%)	156 (99%)	2 (1%)	0	100	100
All	All	1282/1568 (82%)	1265 (99%)	17 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	126/153 (82%)	126 (100%)	0	100	100
1	B	123/153 (80%)	123 (100%)	0	100	100
1	C	126/153 (82%)	126 (100%)	0	100	100
1	D	125/153 (82%)	125 (100%)	0	100	100
1	E	119/153 (78%)	119 (100%)	0	100	100
1	F	119/153 (78%)	119 (100%)	0	100	100
1	G	115/153 (75%)	115 (100%)	0	100	100
1	H	115/153 (75%)	115 (100%)	0	100	100
All	All	968/1224 (79%)	968 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

8 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	B	201	-	58,58,58	2.82	22 (37%)	85,89,89	2.17	23 (27%)
2	FAD	E	201	-	58,58,58	2.84	21 (36%)	85,89,89	2.12	23 (27%)
2	FAD	G	201	-	58,58,58	2.84	22 (37%)	85,89,89	2.16	21 (24%)
2	FAD	F	201	-	58,58,58	2.84	21 (36%)	85,89,89	2.15	24 (28%)
2	FAD	A	201	-	58,58,58	2.84	23 (39%)	85,89,89	2.14	22 (25%)
2	FAD	D	201	-	58,58,58	2.85	21 (36%)	85,89,89	2.13	22 (25%)
2	FAD	H	201	-	58,58,58	2.82	20 (34%)	85,89,89	2.16	24 (28%)
2	FAD	C	201	-	58,58,58	2.85	22 (37%)	85,89,89	2.14	22 (25%)

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	B	201	-	-	5/34/50/50	0/6/6/6
2	FAD	E	201	-	-	4/34/50/50	0/6/6/6
2	FAD	G	201	-	-	0/34/50/50	0/6/6/6
2	FAD	F	201	-	-	4/34/50/50	0/6/6/6
2	FAD	A	201	-	-	0/34/50/50	0/6/6/6
2	FAD	D	201	-	-	3/34/50/50	0/6/6/6
2	FAD	H	201	-	-	5/34/50/50	0/6/6/6
2	FAD	C	201	-	-	2/34/50/50	0/6/6/6

All (172) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	201	FAD	O4B-C1B	8.41	1.61	1.42
2	B	201	FAD	O4B-C1B	8.37	1.61	1.42
2	D	201	FAD	O4B-C1B	8.32	1.61	1.42
2	C	201	FAD	O4B-C1B	8.29	1.61	1.42
2	F	201	FAD	O4B-C1B	8.27	1.61	1.42
2	H	201	FAD	O4B-C1B	8.26	1.61	1.42
2	G	201	FAD	O4B-C1B	8.25	1.61	1.42
2	A	201	FAD	O4B-C1B	8.20	1.60	1.42
2	C	201	FAD	C2B-C1B	-7.86	1.28	1.53
2	E	201	FAD	C2B-C1B	-7.82	1.28	1.53
2	D	201	FAD	C2B-C1B	-7.79	1.29	1.53
2	A	201	FAD	C2B-C1B	-7.78	1.29	1.53
2	B	201	FAD	C2B-C1B	-7.78	1.29	1.53
2	F	201	FAD	C2B-C1B	-7.75	1.29	1.53
2	H	201	FAD	C2B-C1B	-7.75	1.29	1.53
2	G	201	FAD	C2B-C1B	-7.73	1.29	1.53
2	H	201	FAD	O4B-C4B	-7.09	1.29	1.45
2	A	201	FAD	O4B-C4B	-7.08	1.29	1.45
2	G	201	FAD	O4B-C4B	-7.04	1.29	1.45
2	F	201	FAD	O4B-C4B	-7.01	1.29	1.45
2	D	201	FAD	O4B-C4B	-7.01	1.29	1.45
2	E	201	FAD	O4B-C4B	-7.00	1.29	1.45
2	B	201	FAD	O4B-C4B	-6.97	1.29	1.45
2	C	201	FAD	O4B-C4B	-6.88	1.29	1.45
2	A	201	FAD	C4X-N5	5.92	1.43	1.30
2	C	201	FAD	C4X-N5	5.80	1.43	1.30
2	E	201	FAD	C4X-N5	5.78	1.43	1.30
2	D	201	FAD	C4X-N5	5.77	1.43	1.30
2	B	201	FAD	C4X-N5	5.72	1.43	1.30
2	G	201	FAD	C4X-N5	5.61	1.42	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	201	FAD	C4X-N5	5.53	1.42	1.30
2	H	201	FAD	C4X-N5	5.52	1.42	1.30
2	E	201	FAD	C5X-N5	5.23	1.49	1.39
2	C	201	FAD	C5X-N5	5.22	1.49	1.39
2	G	201	FAD	C5X-N5	5.18	1.48	1.39
2	A	201	FAD	C5X-N5	5.13	1.48	1.39
2	D	201	FAD	C5X-N5	5.10	1.48	1.39
2	C	201	FAD	C10-N1	5.06	1.43	1.33
2	F	201	FAD	C5X-N5	5.02	1.48	1.39
2	G	201	FAD	C10-N1	5.02	1.43	1.33
2	F	201	FAD	C10-N1	5.01	1.43	1.33
2	D	201	FAD	C10-N1	5.00	1.43	1.33
2	E	201	FAD	C10-N1	4.99	1.43	1.33
2	B	201	FAD	C5X-N5	4.99	1.48	1.39
2	H	201	FAD	C5X-N5	4.97	1.48	1.39
2	H	201	FAD	C10-N1	4.97	1.43	1.33
2	A	201	FAD	C10-N1	4.95	1.43	1.33
2	B	201	FAD	C10-N1	4.83	1.43	1.33
2	D	201	FAD	C6A-N6A	4.71	1.46	1.34
2	C	201	FAD	O4-C4	-4.69	1.14	1.23
2	B	201	FAD	C6A-N6A	4.67	1.46	1.34
2	G	201	FAD	C6A-N6A	4.65	1.46	1.34
2	E	201	FAD	C6A-N6A	4.64	1.46	1.34
2	C	201	FAD	C6A-N6A	4.64	1.46	1.34
2	H	201	FAD	C6A-N6A	4.63	1.46	1.34
2	F	201	FAD	C6A-N6A	4.61	1.46	1.34
2	A	201	FAD	C6A-N6A	4.60	1.46	1.34
2	B	201	FAD	O4-C4	-4.60	1.14	1.23
2	F	201	FAD	C2-N1	4.54	1.46	1.36
2	D	201	FAD	C2-N1	4.51	1.46	1.36
2	C	201	FAD	C2-N1	4.48	1.46	1.36
2	H	201	FAD	C2-N1	4.48	1.46	1.36
2	G	201	FAD	O4-C4	-4.46	1.15	1.23
2	G	201	FAD	C2-N1	4.45	1.46	1.36
2	F	201	FAD	O4-C4	-4.45	1.15	1.23
2	D	201	FAD	O4-C4	-4.43	1.15	1.23
2	A	201	FAD	C2-N1	4.42	1.46	1.36
2	B	201	FAD	C2-N1	4.42	1.46	1.36
2	E	201	FAD	C2-N1	4.39	1.46	1.36
2	E	201	FAD	O4-C4	-4.38	1.15	1.23
2	H	201	FAD	O4-C4	-4.34	1.15	1.23
2	A	201	FAD	O4-C4	-4.29	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	201	FAD	O2B-C2B	4.24	1.53	1.43
2	E	201	FAD	O2B-C2B	4.24	1.53	1.43
2	D	201	FAD	O2B-C2B	4.21	1.53	1.43
2	G	201	FAD	O2B-C2B	4.20	1.53	1.43
2	B	201	FAD	O2B-C2B	4.17	1.53	1.43
2	A	201	FAD	O2B-C2B	4.16	1.53	1.43
2	H	201	FAD	O2B-C2B	4.14	1.53	1.43
2	F	201	FAD	C10-N10	4.12	1.46	1.37
2	C	201	FAD	O2B-C2B	4.11	1.53	1.43
2	H	201	FAD	C10-N10	4.00	1.46	1.37
2	G	201	FAD	C10-N10	3.79	1.45	1.37
2	A	201	FAD	C10-N10	3.74	1.45	1.37
2	C	201	FAD	C10-N10	3.70	1.45	1.37
2	E	201	FAD	C10-N10	3.67	1.45	1.37
2	D	201	FAD	C10-N10	3.63	1.45	1.37
2	B	201	FAD	C10-N10	3.62	1.45	1.37
2	D	201	FAD	C2-N3	3.46	1.46	1.39
2	E	201	FAD	C2-N3	3.42	1.46	1.39
2	G	201	FAD	C2-N3	3.41	1.46	1.39
2	B	201	FAD	C2-N3	3.38	1.46	1.39
2	G	201	FAD	C8M-C8	3.37	1.57	1.51
2	F	201	FAD	C2-N3	3.37	1.46	1.39
2	C	201	FAD	C2-N3	3.35	1.46	1.39
2	A	201	FAD	C2-N3	3.35	1.46	1.39
2	H	201	FAD	C2-N3	3.34	1.46	1.39
2	F	201	FAD	C9A-N10	3.28	1.46	1.41
2	D	201	FAD	C8M-C8	3.28	1.57	1.51
2	C	201	FAD	C8M-C8	3.24	1.57	1.51
2	H	201	FAD	C9A-N10	3.23	1.46	1.41
2	E	201	FAD	C8M-C8	3.22	1.57	1.51
2	A	201	FAD	C8M-C8	3.21	1.57	1.51
2	B	201	FAD	C8M-C8	3.21	1.57	1.51
2	H	201	FAD	C8M-C8	3.19	1.57	1.51
2	F	201	FAD	C8M-C8	3.16	1.56	1.51
2	D	201	FAD	C9A-N10	3.16	1.46	1.41
2	G	201	FAD	C9A-N10	3.15	1.46	1.41
2	A	201	FAD	C9A-N10	3.13	1.46	1.41
2	C	201	FAD	C9A-N10	3.12	1.46	1.41
2	C	201	FAD	C7M-C7	3.03	1.56	1.51
2	E	201	FAD	C9A-N10	2.97	1.46	1.41
2	B	201	FAD	C9A-N10	2.97	1.46	1.41
2	F	201	FAD	C7M-C7	2.94	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	201	FAD	C7M-C7	2.93	1.56	1.51
2	H	201	FAD	O4'-C4'	-2.93	1.37	1.43
2	E	201	FAD	C7M-C7	2.92	1.56	1.51
2	H	201	FAD	C7M-C7	2.87	1.56	1.51
2	A	201	FAD	C7M-C7	2.86	1.56	1.51
2	G	201	FAD	C7M-C7	2.84	1.56	1.51
2	F	201	FAD	O4'-C4'	-2.84	1.37	1.43
2	B	201	FAD	O4'-C4'	-2.83	1.37	1.43
2	A	201	FAD	O4'-C4'	-2.82	1.37	1.43
2	B	201	FAD	C7M-C7	2.82	1.56	1.51
2	D	201	FAD	O4'-C4'	-2.81	1.37	1.43
2	G	201	FAD	O4'-C4'	-2.79	1.37	1.43
2	C	201	FAD	O4'-C4'	-2.75	1.37	1.43
2	E	201	FAD	O4'-C4'	-2.75	1.37	1.43
2	C	201	FAD	C5'-C4'	2.48	1.55	1.51
2	F	201	FAD	C8A-N7A	2.39	1.36	1.31
2	H	201	FAD	C8A-N7A	2.33	1.36	1.31
2	D	201	FAD	C8A-N7A	2.33	1.36	1.31
2	A	201	FAD	C8A-N7A	2.32	1.36	1.31
2	A	201	FAD	C4-N3	2.31	1.43	1.38
2	G	201	FAD	C4-N3	2.31	1.43	1.38
2	D	201	FAD	C4-N3	2.30	1.43	1.38
2	E	201	FAD	C5'-C4'	2.27	1.54	1.51
2	E	201	FAD	C8A-N7A	2.26	1.36	1.31
2	F	201	FAD	C5B-C4B	2.23	1.58	1.51
2	E	201	FAD	C4-N3	2.23	1.43	1.38
2	C	201	FAD	C8A-N7A	2.23	1.36	1.31
2	G	201	FAD	C5'-C4'	2.22	1.54	1.51
2	G	201	FAD	C8A-N7A	2.22	1.36	1.31
2	B	201	FAD	C8A-N7A	2.21	1.35	1.31
2	F	201	FAD	C4-N3	2.21	1.43	1.38
2	D	201	FAD	C5'-C4'	2.20	1.54	1.51
2	G	201	FAD	C5B-C4B	2.20	1.58	1.51
2	D	201	FAD	C5B-C4B	2.20	1.58	1.51
2	F	201	FAD	C5'-C4'	2.20	1.54	1.51
2	B	201	FAD	C5B-C4B	2.19	1.58	1.51
2	B	201	FAD	C5'-C4'	2.18	1.54	1.51
2	C	201	FAD	C2A-N1A	2.18	1.37	1.33
2	A	201	FAD	C5'-C4'	2.17	1.54	1.51
2	B	201	FAD	C4-N3	2.14	1.42	1.38
2	H	201	FAD	C5B-C4B	2.14	1.58	1.51
2	H	201	FAD	C4-N3	2.14	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	201	FAD	C2A-N1A	2.14	1.37	1.33
2	C	201	FAD	C4-N3	2.13	1.42	1.38
2	B	201	FAD	C2A-N3A	2.12	1.37	1.33
2	C	201	FAD	C2A-N3A	2.12	1.37	1.33
2	C	201	FAD	C6-C5X	2.11	1.43	1.40
2	E	201	FAD	C5B-C4B	2.11	1.57	1.51
2	A	201	FAD	C6-C5X	2.09	1.43	1.40
2	D	201	FAD	C2A-N1A	2.07	1.37	1.33
2	G	201	FAD	C2A-N3A	2.06	1.37	1.33
2	G	201	FAD	C2A-N1A	2.06	1.37	1.33
2	H	201	FAD	C2A-N1A	2.06	1.37	1.33
2	A	201	FAD	C5B-C4B	2.06	1.57	1.51
2	B	201	FAD	C2A-N1A	2.05	1.37	1.33
2	F	201	FAD	C2A-N1A	2.03	1.37	1.33
2	A	201	FAD	C2A-N1A	2.02	1.37	1.33
2	A	201	FAD	C2A-N3A	2.01	1.37	1.33

All (181) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	201	FAD	C7M-C7-C6	-8.50	104.61	119.57
2	B	201	FAD	C7M-C7-C6	-8.05	105.40	119.57
2	H	201	FAD	C7M-C7-C6	-7.96	105.55	119.57
2	F	201	FAD	C7M-C7-C6	-7.91	105.63	119.57
2	E	201	FAD	C7M-C7-C6	-7.81	105.81	119.57
2	D	201	FAD	C7M-C7-C6	-7.73	105.95	119.57
2	A	201	FAD	C7M-C7-C6	-7.45	106.45	119.57
2	C	201	FAD	C7M-C7-C6	-7.39	106.56	119.57
2	G	201	FAD	C7M-C7-C8	7.25	135.57	120.76
2	H	201	FAD	C7M-C7-C8	6.95	134.95	120.76
2	F	201	FAD	C7M-C7-C8	6.94	134.93	120.76
2	B	201	FAD	C7M-C7-C8	6.92	134.88	120.76
2	E	201	FAD	C7M-C7-C8	6.81	134.67	120.76
2	D	201	FAD	C7M-C7-C8	6.68	134.41	120.76
2	A	201	FAD	C7M-C7-C8	6.66	134.35	120.76
2	C	201	FAD	C7M-C7-C8	6.40	133.84	120.76
2	F	201	FAD	N3A-C2A-N1A	-5.77	119.86	128.58
2	A	201	FAD	N3A-C2A-N1A	-5.74	119.90	128.58
2	C	201	FAD	N3A-C2A-N1A	-5.73	119.91	128.58
2	E	201	FAD	N3A-C2A-N1A	-5.64	120.04	128.58
2	D	201	FAD	N3A-C2A-N1A	-5.64	120.05	128.58
2	H	201	FAD	N3A-C2A-N1A	-5.62	120.07	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	201	FAD	N3A-C2A-N1A	-5.60	120.10	128.58
2	B	201	FAD	N3A-C2A-N1A	-5.60	120.11	128.58
2	A	201	FAD	N6A-C6A-N1A	-5.44	106.25	118.38
2	B	201	FAD	N6A-C6A-N1A	-5.41	106.33	118.38
2	B	201	FAD	C5A-C4A-N3A	-5.35	119.34	126.72
2	D	201	FAD	N6A-C6A-N1A	-5.29	106.61	118.38
2	H	201	FAD	N6A-C6A-N1A	-5.27	106.63	118.38
2	C	201	FAD	N6A-C6A-N1A	-5.24	106.71	118.38
2	F	201	FAD	N6A-C6A-N1A	-5.22	106.74	118.38
2	G	201	FAD	C5A-C4A-N3A	-5.20	119.55	126.72
2	G	201	FAD	N6A-C6A-N1A	-5.11	106.99	118.38
2	D	201	FAD	C5A-C4A-N3A	-5.05	119.76	126.72
2	E	201	FAD	N6A-C6A-N1A	-5.01	107.23	118.38
2	H	201	FAD	C5A-C4A-N3A	-4.97	119.88	126.72
2	E	201	FAD	C5A-C4A-N3A	-4.91	119.96	126.72
2	C	201	FAD	C5A-C4A-N3A	-4.83	120.07	126.72
2	F	201	FAD	C5A-C4A-N3A	-4.78	120.13	126.72
2	A	201	FAD	C5A-C4A-N3A	-4.66	120.30	126.72
2	A	201	FAD	N9A-C8A-N7A	-4.28	107.87	113.94
2	A	201	FAD	C5A-C6A-N6A	4.24	133.77	123.29
2	C	201	FAD	N9A-C8A-N7A	-4.19	107.99	113.94
2	B	201	FAD	C5A-C6A-N6A	4.17	133.62	123.29
2	F	201	FAD	N9A-C8A-N7A	-4.16	108.04	113.94
2	C	201	FAD	C8M-C8-C9	4.14	126.87	119.57
2	E	201	FAD	N9A-C8A-N7A	-4.14	108.06	113.94
2	H	201	FAD	C8M-C8-C9	4.14	126.86	119.57
2	H	201	FAD	N9A-C8A-N7A	-4.12	108.09	113.94
2	D	201	FAD	C5A-C6A-N6A	4.12	133.47	123.29
2	C	201	FAD	C5A-C6A-N6A	4.11	133.46	123.29
2	D	201	FAD	N9A-C8A-N7A	-4.09	108.13	113.94
2	H	201	FAD	C5A-C6A-N6A	4.09	133.42	123.29
2	H	201	FAD	C8M-C8-C7	-4.09	112.41	120.76
2	F	201	FAD	C5A-C6A-N6A	4.07	133.36	123.29
2	C	201	FAD	C8M-C8-C7	-4.05	112.49	120.76
2	G	201	FAD	N9A-C8A-N7A	-4.05	108.20	113.94
2	B	201	FAD	N9A-C8A-N7A	-4.03	108.22	113.94
2	D	201	FAD	C8M-C8-C9	3.96	126.55	119.57
2	G	201	FAD	C5A-C6A-N6A	3.92	132.99	123.29
2	E	201	FAD	C5A-C6A-N6A	3.90	132.95	123.29
2	F	201	FAD	C8M-C8-C9	3.85	126.36	119.57
2	D	201	FAD	C8M-C8-C7	-3.81	112.98	120.76
2	F	201	FAD	C8M-C8-C7	-3.77	113.05	120.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	201	FAD	C8M-C8-C9	3.67	126.03	119.57
2	C	201	FAD	C4-N3-C2	-3.61	119.24	125.64
2	E	201	FAD	C8M-C8-C9	3.57	125.86	119.57
2	B	201	FAD	C4-N3-C2	-3.56	119.32	125.64
2	F	201	FAD	C4-N3-C2	-3.52	119.39	125.64
2	E	201	FAD	C8M-C8-C7	-3.50	113.61	120.76
2	D	201	FAD	C4-N3-C2	-3.49	119.45	125.64
2	B	201	FAD	C2A-N3A-C4A	3.46	120.28	111.83
2	H	201	FAD	C4-N3-C2	-3.44	119.53	125.64
2	D	201	FAD	C2A-N3A-C4A	3.42	120.19	111.83
2	A	201	FAD	C4-N3-C2	-3.40	119.60	125.64
2	G	201	FAD	C8M-C8-C7	-3.40	113.82	120.76
2	G	201	FAD	C4-N3-C2	-3.40	119.60	125.64
2	B	201	FAD	N3A-C4A-N9A	3.40	132.95	127.17
2	B	201	FAD	C8M-C8-C9	3.39	125.55	119.57
2	G	201	FAD	C2A-N3A-C4A	3.39	120.11	111.83
2	E	201	FAD	C4-N3-C2	-3.37	119.65	125.64
2	H	201	FAD	C2A-N3A-C4A	3.37	120.07	111.83
2	F	201	FAD	C2A-N3A-C4A	3.36	120.03	111.83
2	A	201	FAD	C8M-C8-C9	3.36	125.49	119.57
2	E	201	FAD	C2A-N3A-C4A	3.34	120.00	111.83
2	G	201	FAD	N3A-C4A-N9A	3.33	132.82	127.17
2	C	201	FAD	C2A-N3A-C4A	3.28	119.85	111.83
2	A	201	FAD	C2A-N3A-C4A	3.28	119.84	111.83
2	B	201	FAD	C8M-C8-C7	-3.27	114.08	120.76
2	A	201	FAD	C8M-C8-C7	-3.24	114.15	120.76
2	D	201	FAD	N3A-C4A-N9A	3.04	132.34	127.17
2	E	201	FAD	N3A-C4A-N9A	3.02	132.31	127.17
2	H	201	FAD	N3A-C4A-N9A	3.02	132.31	127.17
2	A	201	FAD	C5X-C9A-N10	2.99	120.67	117.97
2	A	201	FAD	C9A-C5X-N5	-2.96	119.31	122.45
2	C	201	FAD	N3A-C4A-N9A	2.96	132.20	127.17
2	H	201	FAD	C4X-C10-N10	2.91	120.65	116.48
2	C	201	FAD	C5A-N7A-C8A	2.91	108.02	103.45
2	B	201	FAD	C5A-N7A-C8A	2.89	107.99	103.45
2	A	201	FAD	C5A-N7A-C8A	2.88	107.97	103.45
2	D	201	FAD	C5A-N7A-C8A	2.86	107.94	103.45
2	C	201	FAD	C4X-C4-N3	2.85	120.50	113.25
2	F	201	FAD	N3A-C4A-N9A	2.84	131.99	127.17
2	G	201	FAD	C5A-N7A-C8A	2.81	107.87	103.45
2	H	201	FAD	C5A-N7A-C8A	2.80	107.86	103.45
2	A	201	FAD	N3A-C4A-N9A	2.80	131.94	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	201	FAD	C5A-N7A-C8A	2.80	107.86	103.45
2	F	201	FAD	C4X-C10-N10	2.80	120.49	116.48
2	G	201	FAD	C4X-C10-N10	2.80	120.48	116.48
2	D	201	FAD	C4X-C4-N3	2.78	120.33	113.25
2	F	201	FAD	C5A-N7A-C8A	2.73	107.75	103.45
2	B	201	FAD	C4X-C4-N3	2.72	120.19	113.25
2	E	201	FAD	C10-C4X-N5	-2.68	119.34	124.81
2	C	201	FAD	C4X-C10-N10	2.64	120.26	116.48
2	F	201	FAD	C4X-C4-N3	2.64	119.97	113.25
2	G	201	FAD	C10-C4X-N5	-2.63	119.43	124.81
2	E	201	FAD	C4X-C10-N10	2.63	120.25	116.48
2	C	201	FAD	C9A-C5X-N5	-2.62	119.68	122.45
2	D	201	FAD	C10-C4X-N5	-2.62	119.46	124.81
2	A	201	FAD	C10-C4X-N5	-2.61	119.47	124.81
2	G	201	FAD	C4X-C4-N3	2.61	119.90	113.25
2	E	201	FAD	C9A-C5X-N5	-2.60	119.69	122.45
2	E	201	FAD	C4X-C4-N3	2.59	119.84	113.25
2	B	201	FAD	C4X-C10-N10	2.58	120.18	116.48
2	A	201	FAD	C4X-C4-N3	2.58	119.82	113.25
2	A	201	FAD	C4X-C10-N10	2.57	120.16	116.48
2	D	201	FAD	C4X-C10-N10	2.56	120.15	116.48
2	H	201	FAD	C4X-C4-N3	2.55	119.74	113.25
2	F	201	FAD	C3B-C2B-C1B	2.54	106.27	101.46
2	B	201	FAD	C9A-C5X-N5	-2.54	119.76	122.45
2	C	201	FAD	C5X-C9A-N10	2.54	120.26	117.97
2	H	201	FAD	C10-C4X-N5	-2.52	119.66	124.81
2	A	201	FAD	C4A-N9A-C8A	2.52	108.38	105.74
2	B	201	FAD	C5X-C9A-N10	2.48	120.21	117.97
2	D	201	FAD	C9A-C5X-N5	-2.47	119.83	122.45
2	C	201	FAD	C10-C4X-N5	-2.45	119.81	124.81
2	B	201	FAD	C10-C4X-N5	-2.44	119.82	124.81
2	B	201	FAD	O4-C4-C4X	-2.44	120.10	126.53
2	D	201	FAD	O4-C4-C4X	-2.44	120.10	126.53
2	C	201	FAD	O4-C4-C4X	-2.43	120.11	126.53
2	G	201	FAD	O4-C4-C4X	-2.42	120.14	126.53
2	F	201	FAD	C10-C4X-N5	-2.40	119.90	124.81
2	A	201	FAD	C3B-C2B-C1B	2.38	105.96	101.46
2	C	201	FAD	C4A-N9A-C8A	2.37	108.22	105.74
2	F	201	FAD	O4-C4-C4X	-2.34	120.36	126.53
2	F	201	FAD	C4A-N9A-C8A	2.33	108.19	105.74
2	E	201	FAD	O4-C4-C4X	-2.33	120.39	126.53
2	F	201	FAD	C5X-C9A-N10	2.32	120.07	117.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	201	FAD	C4A-N9A-C8A	2.32	108.17	105.74
2	E	201	FAD	C4A-N9A-C8A	2.30	108.16	105.74
2	E	201	FAD	C5X-C9A-N10	2.30	120.05	117.97
2	B	201	FAD	C6A-C5A-C4A	2.29	120.30	117.18
2	H	201	FAD	O4-C4-C4X	-2.27	120.53	126.53
2	G	201	FAD	C6A-C5A-C4A	2.27	120.27	117.18
2	A	201	FAD	C4A-C5A-N7A	-2.25	108.01	110.58
2	D	201	FAD	C4A-C5A-N7A	-2.24	108.02	110.58
2	C	201	FAD	C4A-C5A-N7A	-2.23	108.03	110.58
2	F	201	FAD	C4X-C10-N1	-2.23	119.13	124.59
2	B	201	FAD	C4A-C5A-N7A	-2.20	108.07	110.58
2	H	201	FAD	C4A-C5A-N7A	-2.20	108.07	110.58
2	G	201	FAD	C4A-N9A-C8A	2.19	108.03	105.74
2	B	201	FAD	C4A-N9A-C8A	2.17	108.02	105.74
2	D	201	FAD	C4A-N9A-C8A	2.16	108.01	105.74
2	B	201	FAD	C4'-C3'-C2'	-2.15	109.99	113.57
2	A	201	FAD	O4-C4-C4X	-2.15	120.86	126.53
2	E	201	FAD	C4'-C3'-C2'	-2.15	110.00	113.57
2	E	201	FAD	C6A-C5A-C4A	2.13	120.09	117.18
2	H	201	FAD	C3B-C2B-C1B	2.12	105.48	101.46
2	F	201	FAD	C4A-C5A-N7A	-2.12	108.16	110.58
2	F	201	FAD	C10-N1-C2	2.10	121.39	116.85
2	H	201	FAD	C4X-C10-N1	-2.09	119.47	124.59
2	H	201	FAD	C4'-C3'-C2'	-2.09	110.09	113.57
2	E	201	FAD	C4A-C5A-N7A	-2.09	108.19	110.58
2	D	201	FAD	C6A-C5A-C4A	2.08	120.02	117.18
2	H	201	FAD	C6A-C5A-C4A	2.05	119.98	117.18
2	C	201	FAD	C6A-C5A-C4A	2.05	119.98	117.18
2	D	201	FAD	C4-C4X-N5	2.04	121.02	118.21
2	H	201	FAD	C4-C4X-C10	2.02	120.41	116.93
2	G	201	FAD	C9A-C5X-N5	-2.02	120.31	122.45
2	F	201	FAD	C4-C4X-C10	2.02	120.40	116.93
2	G	201	FAD	C4A-C5A-N7A	-2.02	108.28	110.58

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	201	FAD	C5'-O5'-P-O2P
2	B	201	FAD	C5'-O5'-P-O3P
2	C	201	FAD	C5'-O5'-P-O2P
2	C	201	FAD	C5'-O5'-P-O3P

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Mol	Chain	Res	Type	Atoms
2	E	201	FAD	C5'-O5'-P-O2P
2	E	201	FAD	C5'-O5'-P-O3P
2	H	201	FAD	C5'-O5'-P-O2P
2	F	201	FAD	O4B-C4B-C5B-O5B
2	H	201	FAD	O4B-C4B-C5B-O5B
2	H	201	FAD	C3B-C4B-C5B-O5B
2	F	201	FAD	C3B-C4B-C5B-O5B
2	F	201	FAD	C2'-C1'-N10-C10
2	H	201	FAD	C5'-O5'-P-O1P
2	H	201	FAD	C5'-O5'-P-O3P
2	D	201	FAD	C2'-C3'-C4'-C5'
2	B	201	FAD	O3'-C3'-C4'-O4'
2	B	201	FAD	C2'-C3'-C4'-O4'
2	D	201	FAD	C2'-C3'-C4'-O4'
2	E	201	FAD	C2'-C3'-C4'-O4'
2	D	201	FAD	O3'-C3'-C4'-O4'
2	E	201	FAD	O3'-C3'-C4'-O4'
2	B	201	FAD	C2'-C3'-C4'-C5'
2	F	201	FAD	P-O3P-PA-O2A

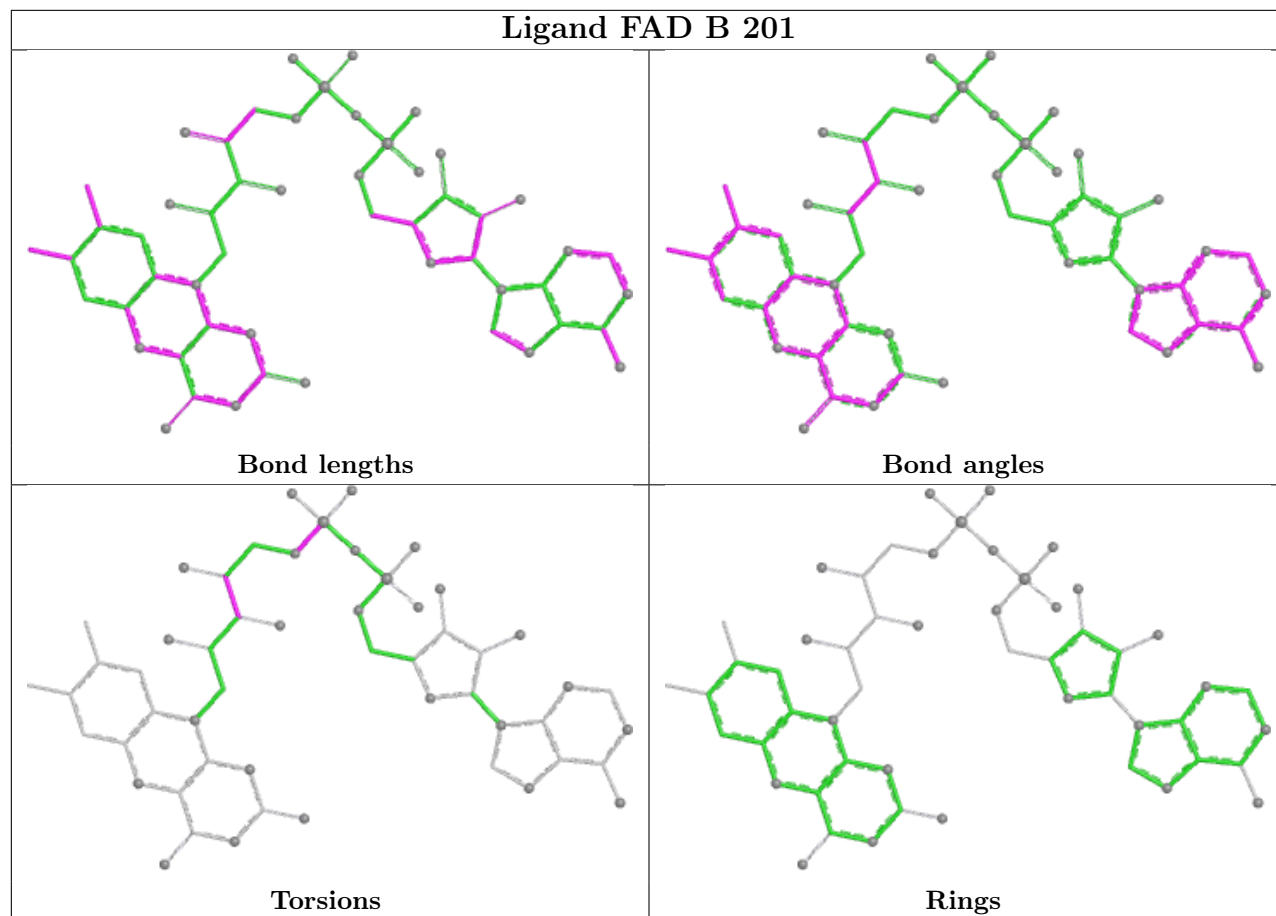
There are no ring outliers.

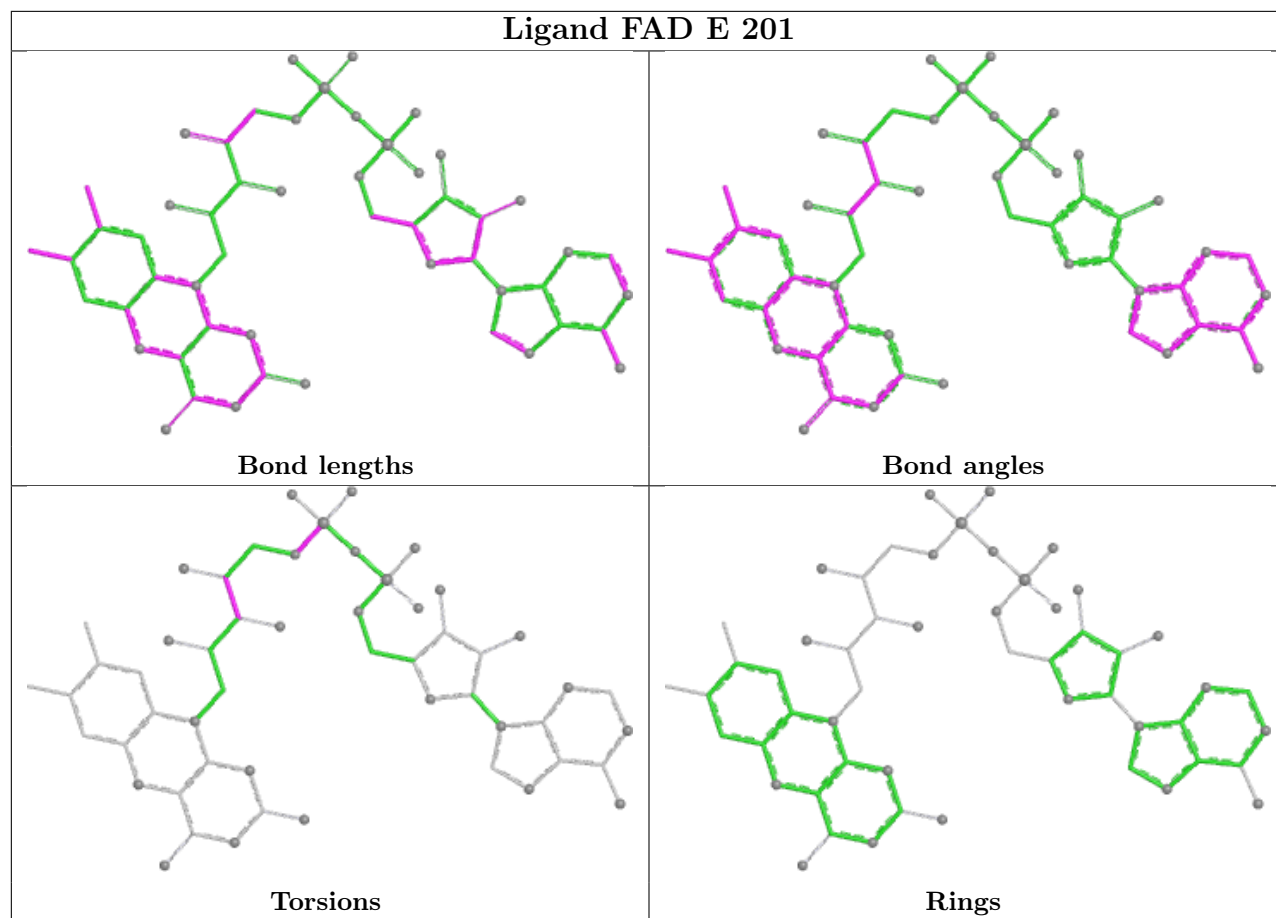
6 monomers are involved in 7 short contacts:

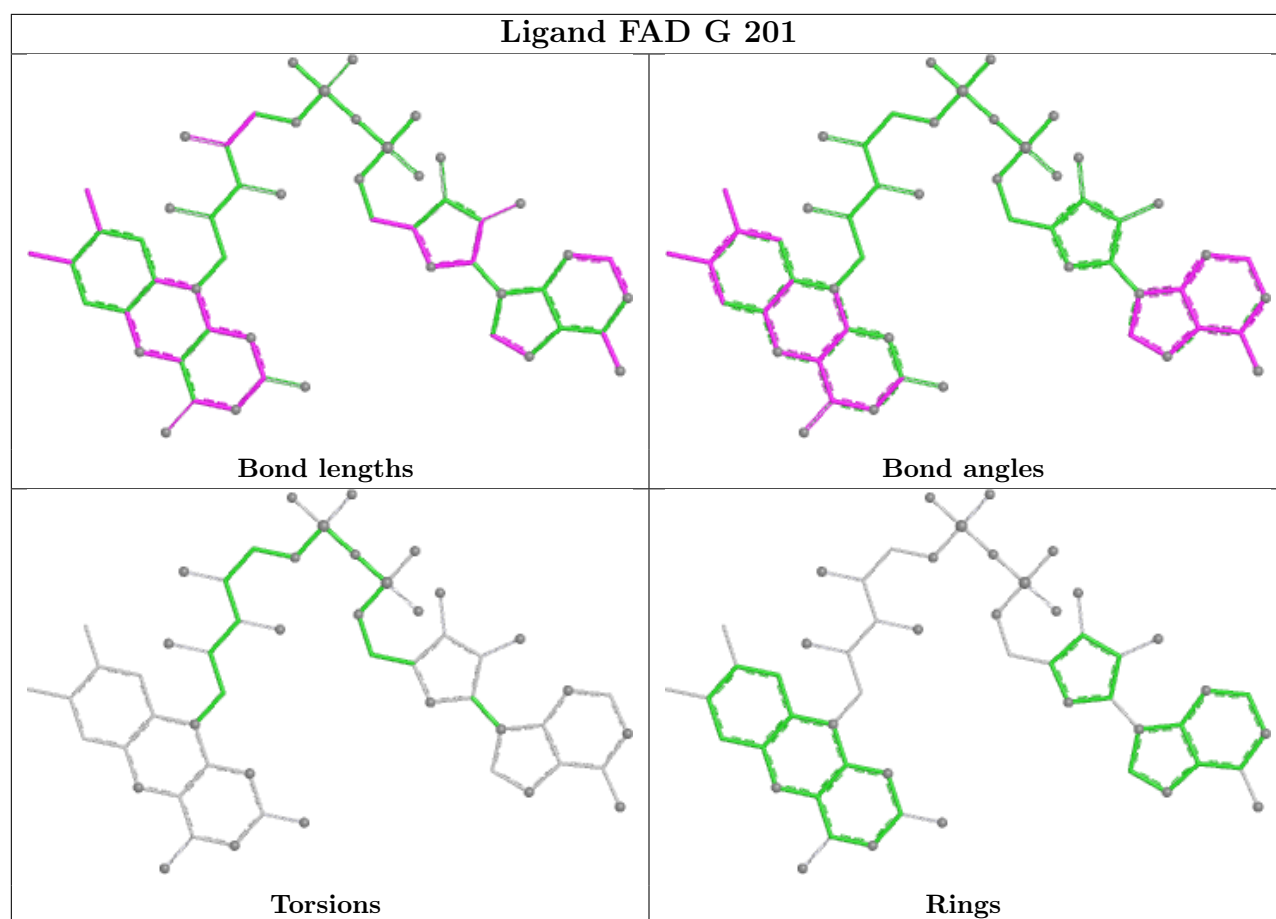
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	201	FAD	1	0
2	G	201	FAD	1	0
2	F	201	FAD	1	0
2	A	201	FAD	2	0
2	H	201	FAD	1	0
2	C	201	FAD	1	0

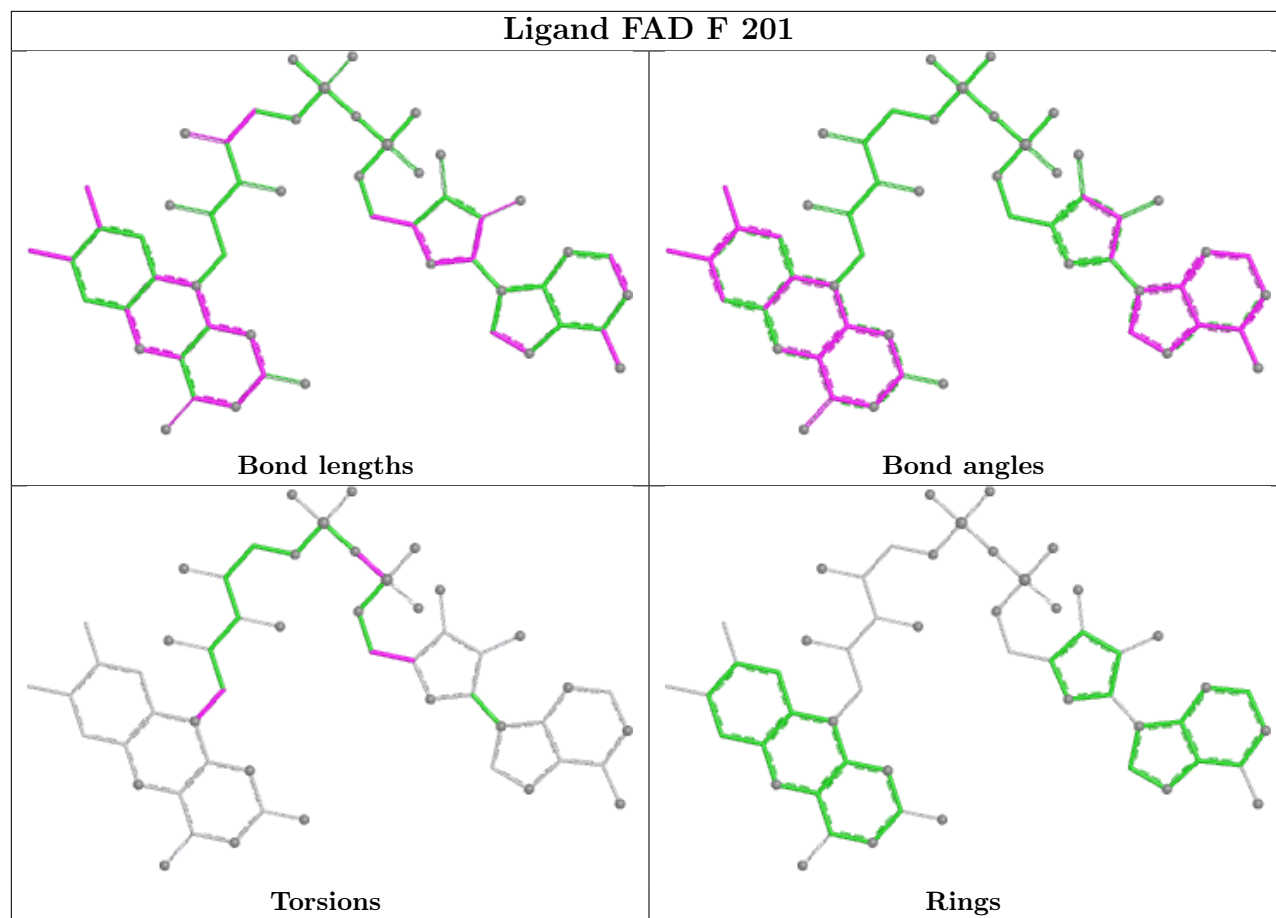
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

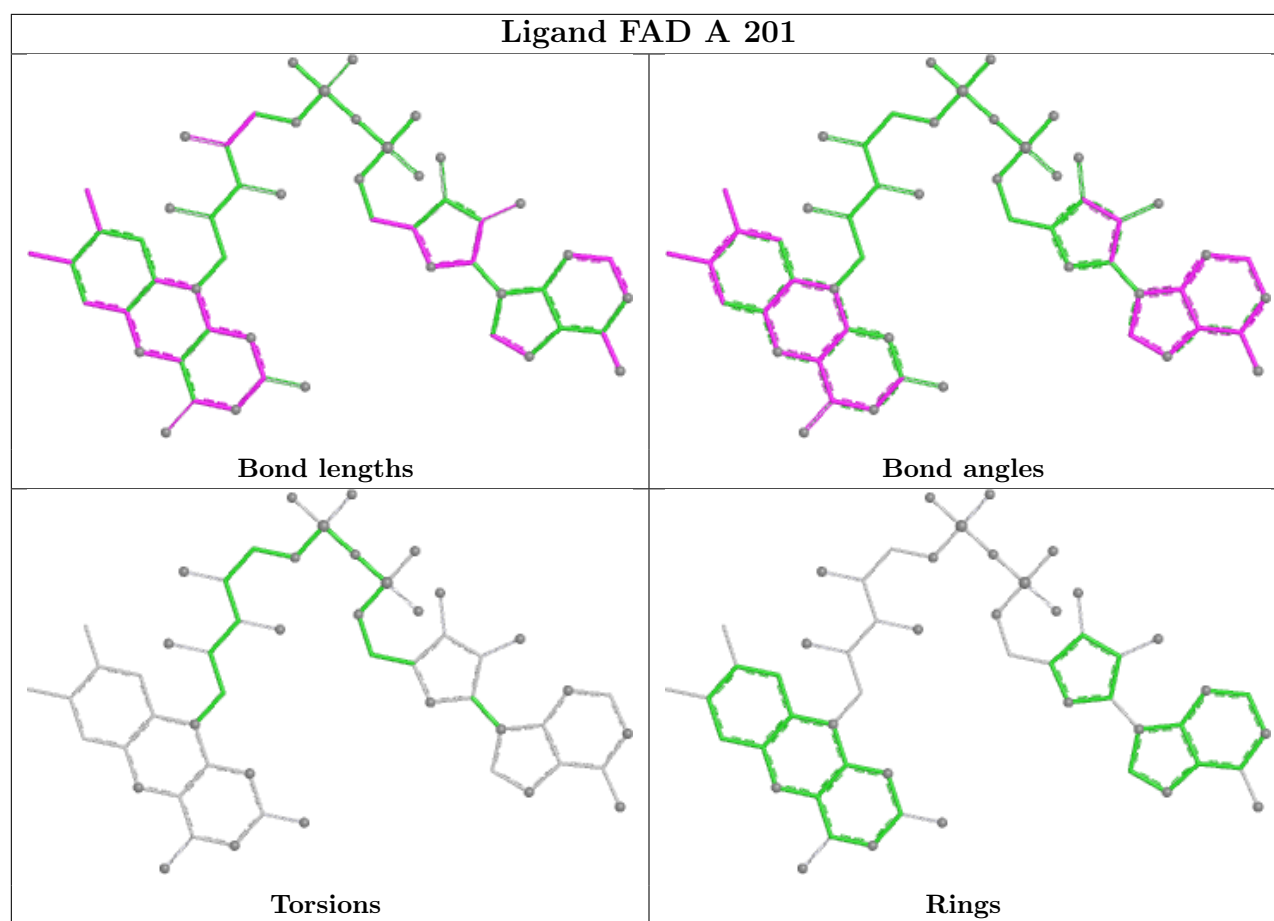
equivalents in the CSD to analyse the geometry.

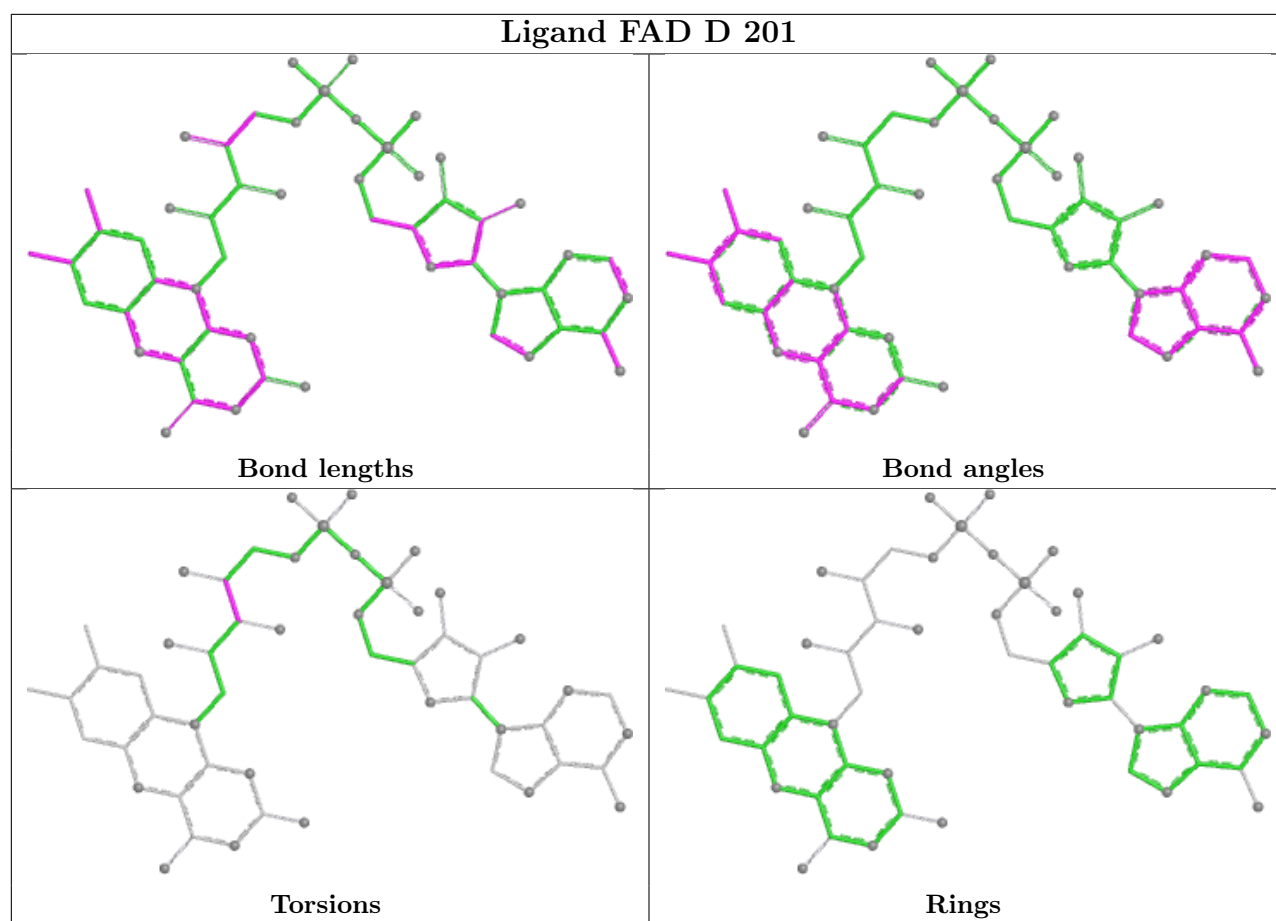


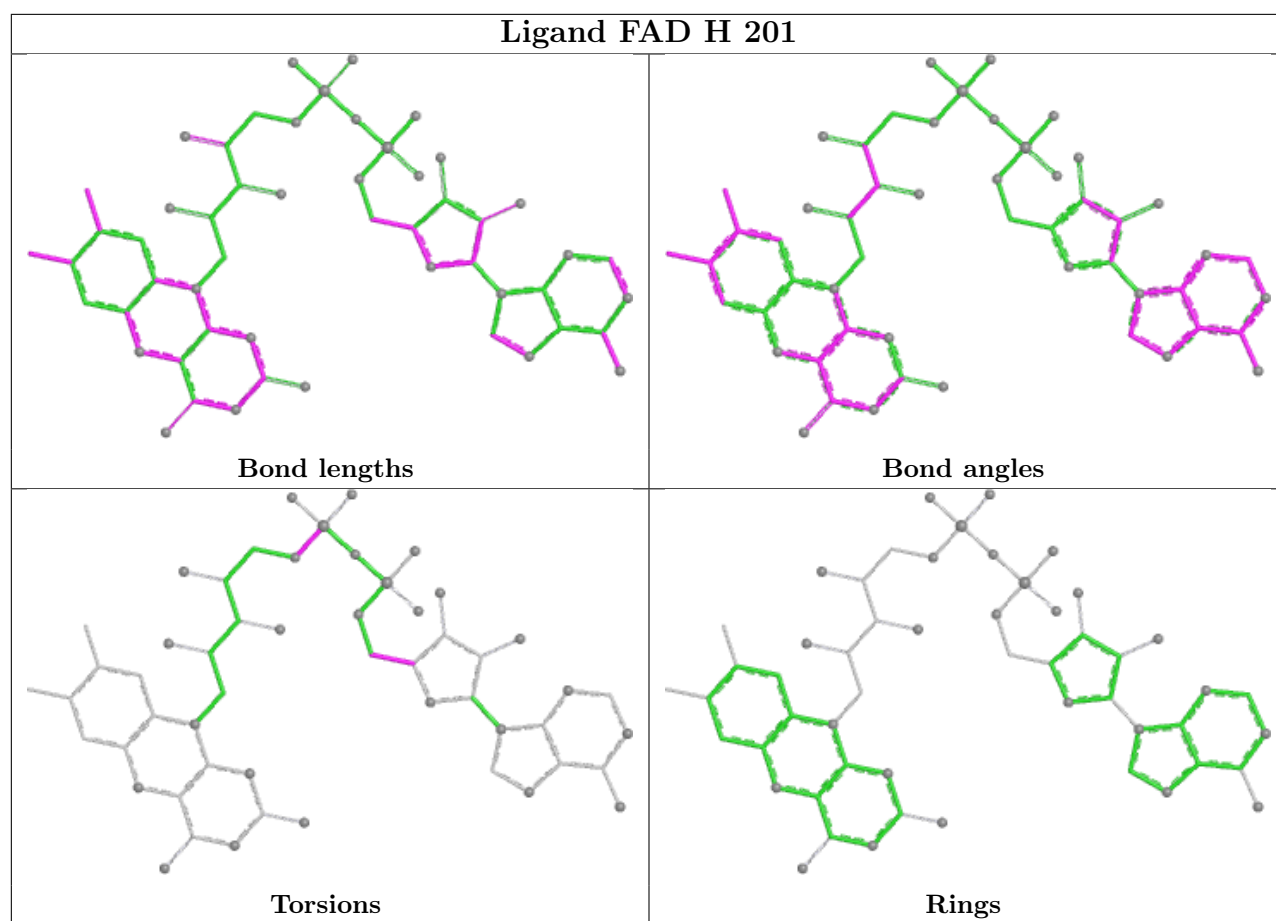


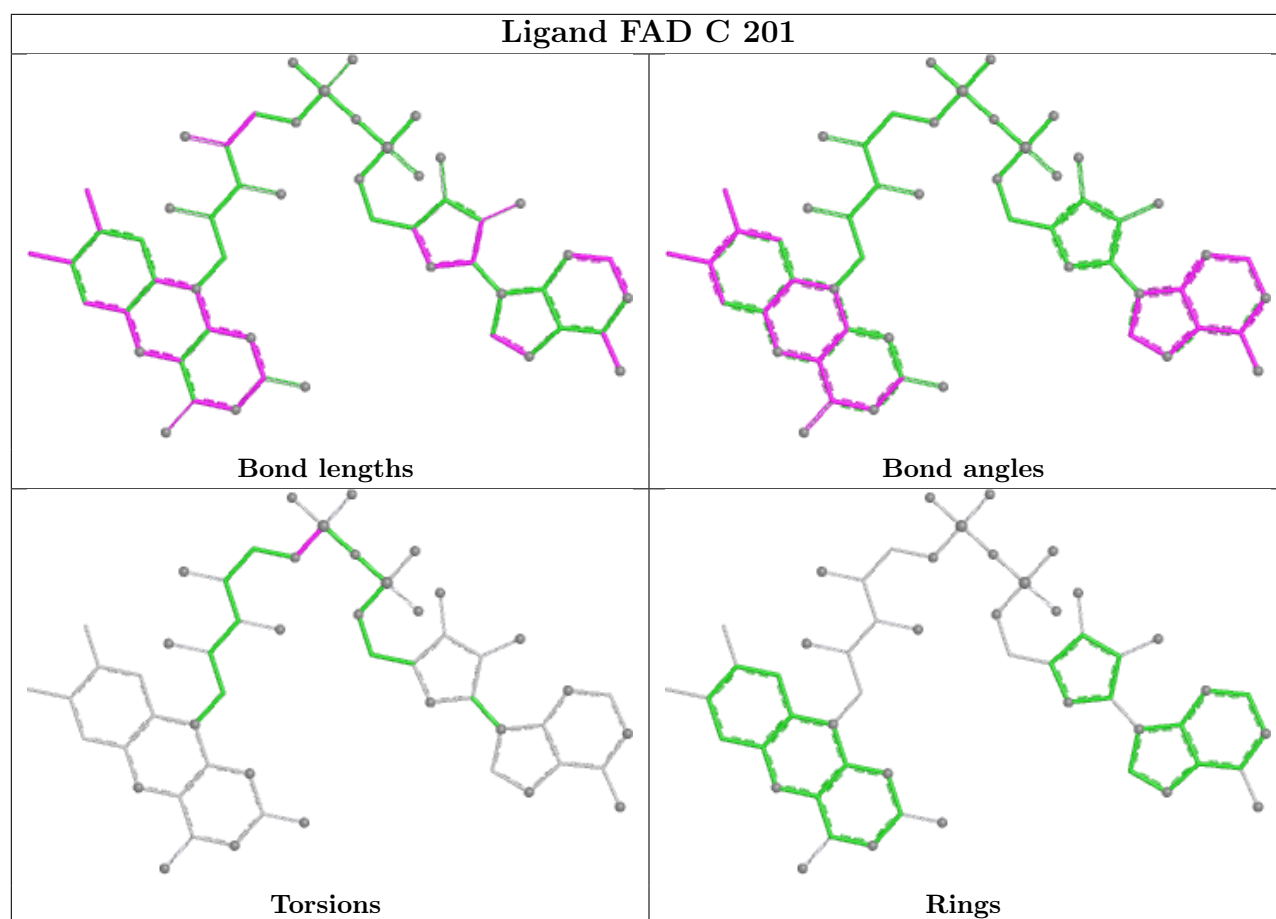












5.7 Other polymers [i](#)

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

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	165/196 (84%)	0.13	6 (3%) 46 46	21, 36, 57, 82	0
1	B	163/196 (83%)	0.29	12 (7%) 20 19	23, 36, 63, 80	0
1	C	165/196 (84%)	0.11	6 (3%) 46 46	23, 34, 54, 80	0
1	D	164/196 (83%)	0.20	5 (3%) 52 52	26, 37, 61, 79	0
1	E	161/196 (82%)	1.22	29 (18%) 3 3	35, 59, 80, 88	0
1	F	160/196 (81%)	1.78	57 (35%) 1 0	49, 75, 90, 100	0
1	G	160/196 (81%)	2.67	105 (65%) 0 0	42, 74, 85, 99	0
1	H	160/196 (81%)	1.89	63 (39%) 1 0	53, 74, 88, 95	0
All	All	1298/1568 (82%)	1.02	283 (21%) 2 2	21, 52, 85, 100	0

All (283) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	152	TRP	7.9
1	G	168	LEU	6.8
1	G	165	GLY	5.5
1	G	167	LEU	5.4
1	G	53	VAL	5.3
1	G	149	CYS	5.1
1	G	163	PHE	5.0
1	G	170	ALA	5.0
1	H	155	TYR	4.9
1	G	54	GLY	4.9
1	G	150	ALA	4.9
1	G	95	SER	4.8
1	G	93	VAL	4.8
1	G	97	GLY	4.7
1	G	164	VAL	4.7
1	G	151	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	G	55	GLY	4.5
1	G	136	GLY	4.5
1	G	147	PHE	4.5
1	G	75	LEU	4.5
1	G	130	ALA	4.3
1	A	194	PRO	4.3
1	G	155	TYR	4.3
1	H	193	ALA	4.2
1	H	37	LEU	4.2
1	G	134	ARG	4.2
1	D	194	PRO	4.2
1	G	169	THR	4.2
1	H	69	VAL	4.1
1	F	127	PRO	4.1
1	G	133	ALA	4.1
1	G	90	LEU	4.1
1	G	146	TRP	4.1
1	G	166	ARG	4.0
1	C	195	VAL	4.0
1	G	91	LEU	4.0
1	G	192	ARG	4.0
1	G	96	PHE	4.0
1	H	41	PHE	4.0
1	G	129	TRP	3.9
1	G	153	ARG	3.9
1	G	138	PRO	3.9
1	G	139	LEU	3.9
1	F	116	TRP	3.8
1	F	151	LEU	3.8
1	H	157	ALA	3.7
1	G	94	GLY	3.7
1	G	141	ARG	3.7
1	F	78	VAL	3.7
1	F	133	ALA	3.7
1	G	89	SER	3.7
1	G	137	ALA	3.6
1	H	34	SER	3.6
1	G	76	ILE	3.6
1	G	92	GLU	3.6
1	F	95	SER	3.5
1	A	30	LEU	3.5
1	H	116	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
1	H	158	GLY	3.5
1	G	74	PRO	3.5
1	B	31	LEU	3.5
1	F	91	LEU	3.5
1	G	80	VAL	3.4
1	H	122	THR	3.4
1	G	51	VAL	3.4
1	G	71	LEU	3.4
1	G	162	ILE	3.4
1	H	90	LEU	3.4
1	H	80	VAL	3.3
1	F	94	GLY	3.3
1	H	149	CYS	3.3
1	F	35	ARG	3.3
1	H	96	PHE	3.3
1	H	43	SER	3.3
1	G	128	GLY	3.3
1	C	32	ARG	3.3
1	G	175	ARG	3.3
1	D	193	ALA	3.3
1	E	193	ALA	3.2
1	G	69	VAL	3.3
1	F	192	ARG	3.2
1	G	85	ALA	3.2
1	H	40	ILE	3.2
1	G	135	THR	3.2
1	H	36	SER	3.2
1	E	122	THR	3.2
1	G	154	ALA	3.2
1	E	170	ALA	3.1
1	E	69	VAL	3.1
1	G	58	PRO	3.1
1	G	66	PHE	3.1
1	G	59	HIS	3.1
1	G	144	LEU	3.1
1	G	122	THR	3.1
1	F	128	GLY	3.1
1	G	86	MET	3.1
1	D	34	SER	3.0
1	H	82	CYS	3.0
1	G	73	PRO	3.0
1	B	32	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	79	CYS	3.0
1	E	134	ARG	3.0
1	H	153	ARG	3.0
1	G	68	SER	3.0
1	G	116	TRP	3.0
1	H	127	PRO	3.0
1	F	139	LEU	3.0
1	G	88	GLY	3.0
1	E	152	TRP	3.0
1	G	140	ALA	2.9
1	G	145	ALA	2.9
1	G	52	THR	2.9
1	H	91	LEU	2.9
1	A	31	LEU	2.9
1	E	75	LEU	2.9
1	F	96	PHE	2.9
1	G	78	VAL	2.9
1	G	132	GLY	2.8
1	F	90	LEU	2.8
1	A	193	ALA	2.8
1	H	154	ALA	2.8
1	F	34	SER	2.8
1	F	163	PHE	2.8
1	F	184	GLY	2.8
1	G	99	SER	2.8
1	H	54	GLY	2.8
1	B	120	ASP	2.8
1	G	56	ASP	2.8
1	H	152	TRP	2.8
1	E	155	TYR	2.8
1	G	60	ALA	2.8
1	H	63	ALA	2.8
1	E	169	THR	2.7
1	G	188	GLY	2.7
1	F	82	CYS	2.7
1	E	168	LEU	2.7
1	F	150	ALA	2.7
1	F	53	VAL	2.7
1	G	98	VAL	2.7
1	H	164	VAL	2.7
1	F	54	GLY	2.7
1	G	82	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	168	LEU	2.7
1	G	176	ARG	2.7
1	H	109	ALA	2.7
1	H	83	ASP	2.7
1	H	94	GLY	2.7
1	E	55	GLY	2.7
1	B	34	SER	2.7
1	E	35	ARG	2.7
1	G	131	ARG	2.7
1	H	113	ALA	2.6
1	B	186	PHE	2.6
1	G	158	GLY	2.6
1	C	31	LEU	2.6
1	B	193	ALA	2.6
1	F	152	TRP	2.6
1	F	154	ALA	2.6
1	F	155	TYR	2.6
1	F	75	LEU	2.6
1	G	72	ASP	2.6
1	F	58	PRO	2.6
1	F	135	THR	2.6
1	E	40	ILE	2.6
1	G	70	SER	2.6
1	G	143	ALA	2.5
1	A	34	SER	2.5
1	F	57	SER	2.5
1	G	50	VAL	2.5
1	H	162	ILE	2.5
1	F	126	ARG	2.5
1	H	75	LEU	2.5
1	E	72	ASP	2.5
1	E	73	PRO	2.5
1	E	74	PRO	2.5
1	B	36	SER	2.5
1	F	93	VAL	2.5
1	G	48	VAL	2.5
1	H	100	VAL	2.5
1	H	56	ASP	2.5
1	H	133	ALA	2.5
1	H	159	ASP	2.5
1	F	149	CYS	2.5
1	G	121	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	116	TRP	2.5
1	H	129	TRP	2.5
1	H	166	ARG	2.5
1	H	112	TYR	2.5
1	G	174	ASP	2.5
1	F	121	PRO	2.5
1	G	127	PRO	2.5
1	F	50	VAL	2.4
1	E	56	ASP	2.4
1	H	60	ALA	2.4
1	F	55	GLY	2.4
1	G	57	SER	2.4
1	F	80	VAL	2.4
1	H	163	PHE	2.4
1	G	87	HIS	2.4
1	F	165	GLY	2.4
1	G	157	ALA	2.4
1	E	135	THR	2.4
1	C	34	SER	2.4
1	G	44	PHE	2.4
1	G	33	ASP	2.4
1	G	142	GLY	2.4
1	F	122	THR	2.4
1	G	148	GLU	2.4
1	E	133	ALA	2.3
1	E	34	SER	2.3
1	G	100	VAL	2.3
1	G	172	ARG	2.3
1	H	92	GLU	2.3
1	F	33	ASP	2.3
1	F	83	ASP	2.3
1	F	49	THR	2.3
1	B	35	ARG	2.3
1	G	171	GLU	2.3
1	H	66	PHE	2.3
1	H	114	ASN	2.3
1	H	120	ASP	2.3
1	F	87	HIS	2.3
1	E	136	GLY	2.3
1	B	192	ARG	2.3
1	G	63	ALA	2.3
1	H	187	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	34	SER	2.3
1	F	88	GLY	2.2
1	H	192	ARG	2.2
1	F	60	ALA	2.2
1	H	110	LEU	2.2
1	F	120	ASP	2.2
1	G	125	ASP	2.2
1	G	35	ARG	2.2
1	F	130	ALA	2.2
1	H	65	SER	2.2
1	F	129	TRP	2.2
1	E	71	LEU	2.2
1	F	56	ASP	2.2
1	H	126	ARG	2.2
1	B	127	PRO	2.2
1	H	42	SER	2.2
1	F	166	ARG	2.2
1	H	189	LEU	2.2
1	H	156	ASP	2.2
1	F	157	ALA	2.2
1	E	93	VAL	2.1
1	G	83	ASP	2.1
1	E	149	CYS	2.1
1	F	68	SER	2.1
1	H	68	SER	2.1
1	G	126	ARG	2.1
1	F	81	GLU	2.1
1	G	156	ASP	2.1
1	B	116	TRP	2.1
1	F	131	ARG	2.1
1	H	79	CYS	2.1
1	C	57	SER	2.1
1	G	105	GLN	2.1
1	G	190	PRO	2.1
1	H	78	VAL	2.1
1	H	138	PRO	2.1
1	F	146	TRP	2.1
1	E	54	GLY	2.1
1	F	115	ARG	2.1
1	E	154	ALA	2.1
1	G	77	LEU	2.1
1	H	121	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	50	VAL	2.1
1	F	124	PHE	2.1
1	D	116	TRP	2.1
1	E	131	ARG	2.1
1	H	144	LEU	2.0
1	H	181	TYR	2.0
1	D	35	ARG	2.0
1	E	153	ARG	2.0
1	H	93	VAL	2.0
1	F	41	PHE	2.0
1	G	124	PHE	2.0
1	B	185	GLN	2.0
1	H	87	HIS	2.0
1	C	83	ASP	2.0
1	A	32	ARG	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](#)

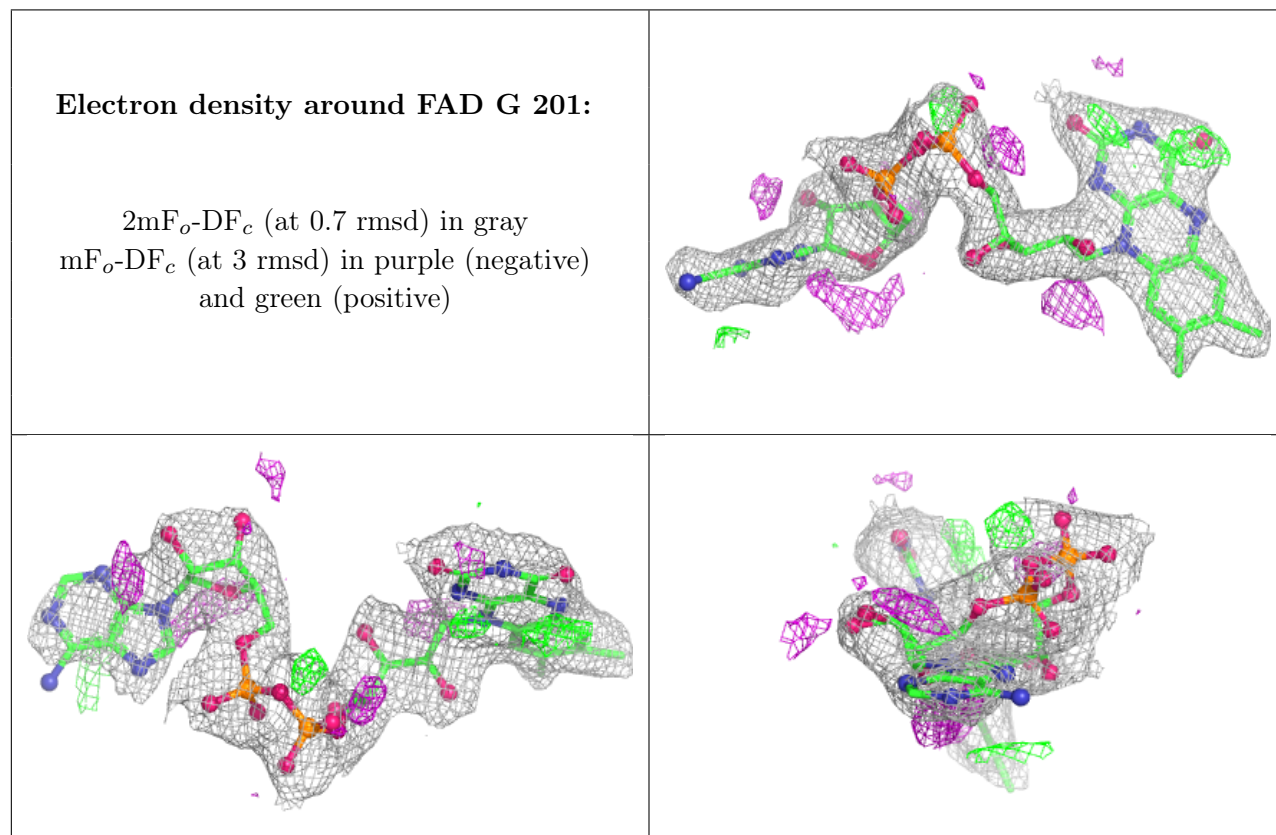
There are no oligosaccharides in this entry.

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.

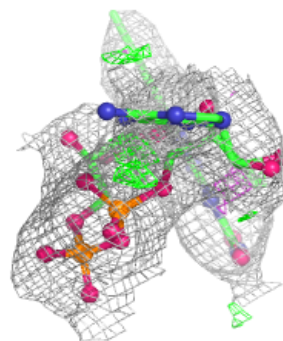
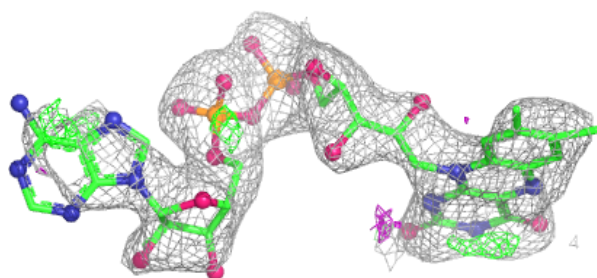
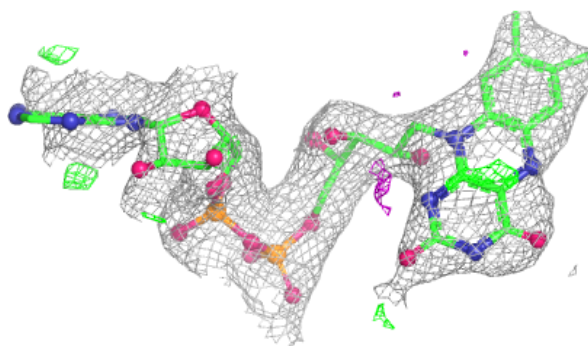
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FAD	G	201	53/53	0.86	0.14	44,60,74,75	0
2	FAD	H	201	53/53	0.86	0.14	56,70,96,98	0
2	FAD	F	201	53/53	0.87	0.13	55,72,91,93	0
2	FAD	E	201	53/53	0.94	0.09	37,50,72,74	0
2	FAD	B	201	53/53	0.95	0.08	27,38,74,78	0
2	FAD	D	201	53/53	0.95	0.08	29,39,68,79	0
2	FAD	A	201	53/53	0.96	0.08	19,28,53,58	0
2	FAD	C	201	53/53	0.97	0.08	20,29,54,59	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.

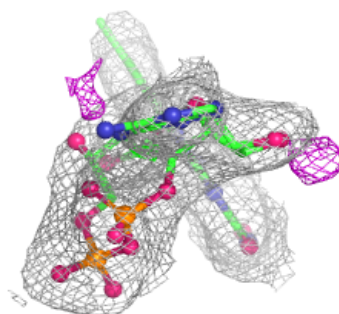
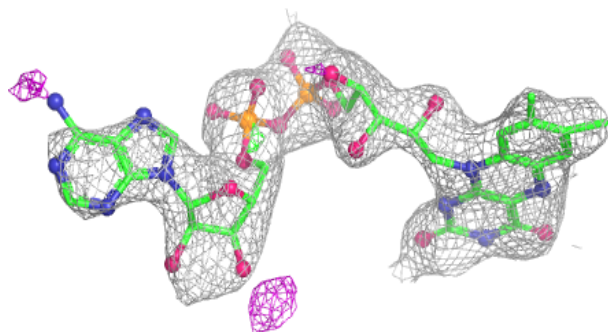
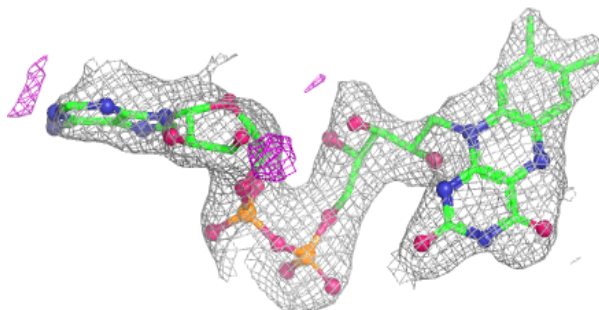


Electron density around FAD H 201:

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

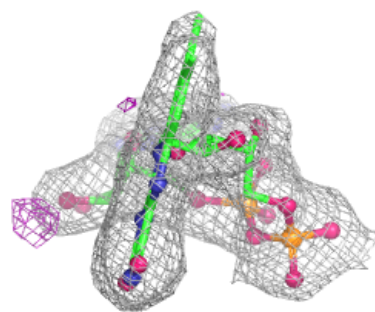
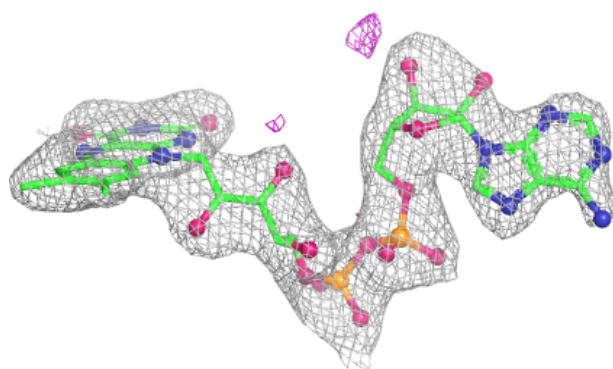
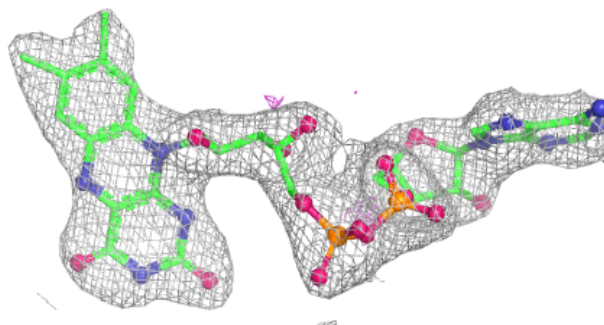
**Electron density around FAD F 201:**

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

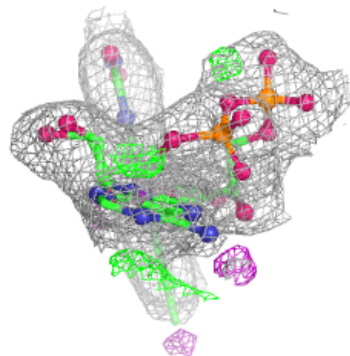
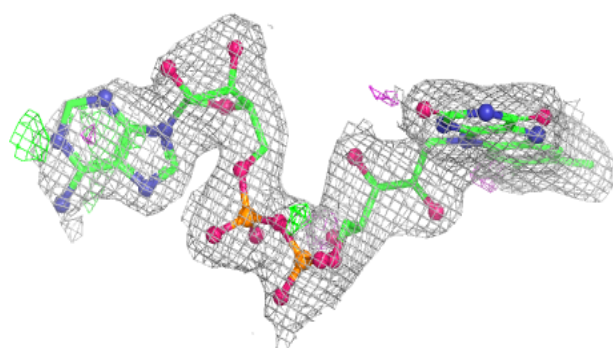
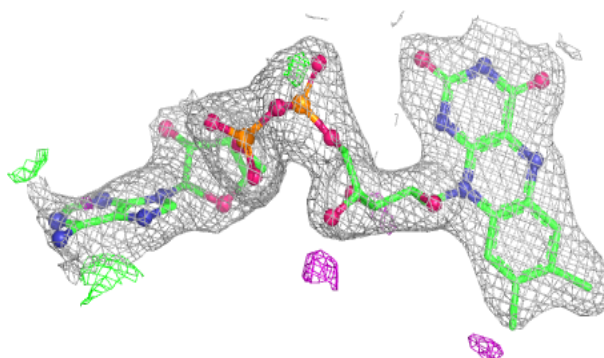


Electron density around FAD E 201:

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

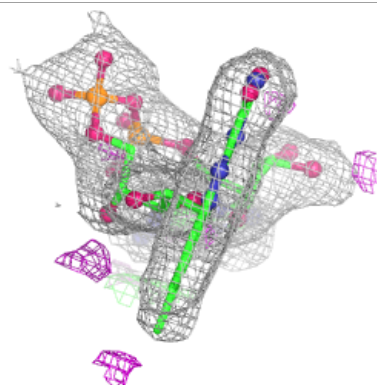
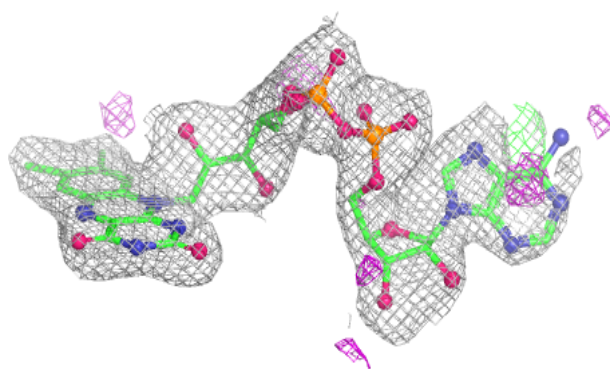
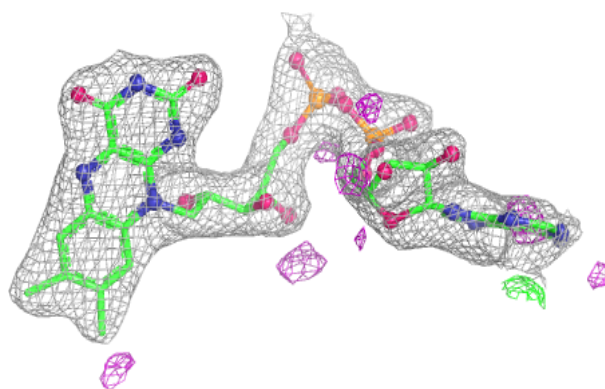
**Electron density around FAD B 201:**

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

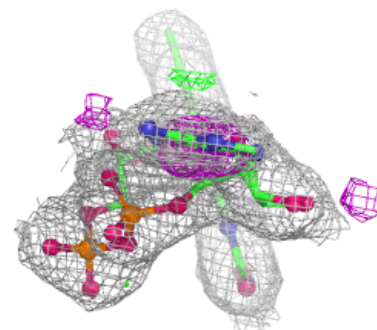
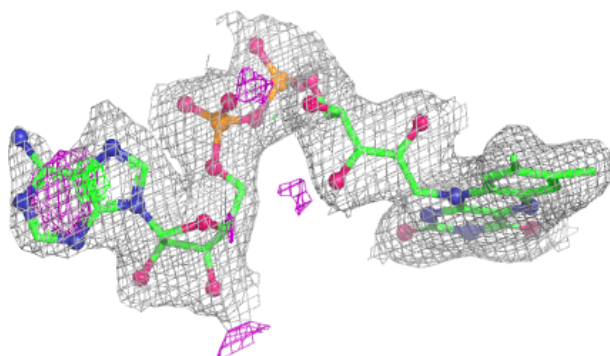
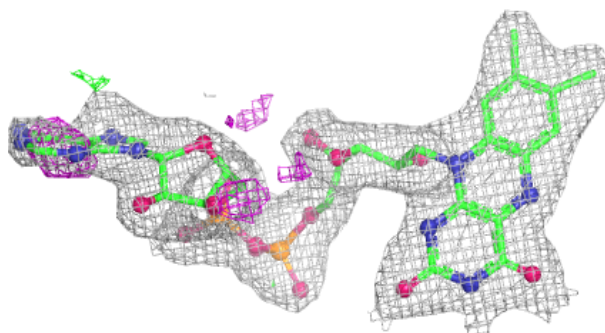


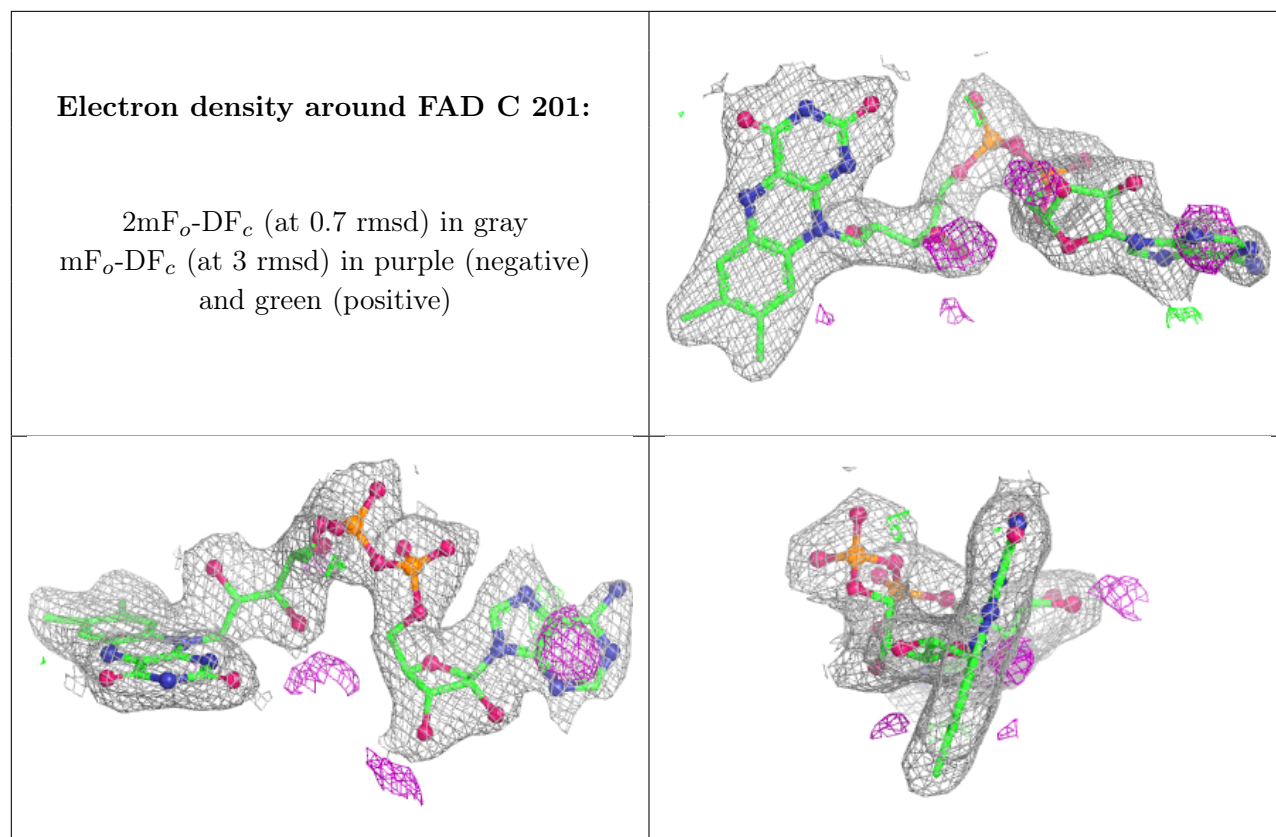
Electron density around FAD D 201:

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

**Electron density around FAD A 201:**

$2mF_o-DF_c$ (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.