



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 2, 2023 – 05:38 AM EDT

PDB ID : 1EFP
Title : ELECTRON TRANSFER FLAVOPROTEIN (ETF) FROM PARACOCCLUS DENITRIFICANS
Authors : Roberts, D.L.; Salazar, D.; Fulmer, J.P.; Frerman, F.E.; Kim, J.J.-P.
Deposited on : 1998-12-18
Resolution : 2.60 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.34

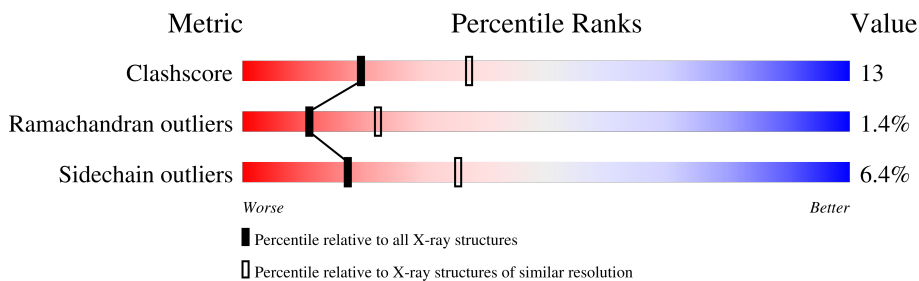
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	307	
1	C	307	
2	B	252	
2	D	252	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8291 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.

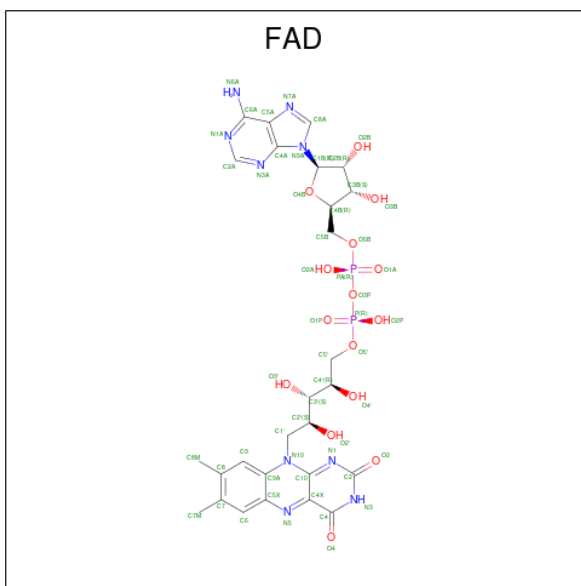
- Molecule 1 is a protein called PROTEIN (ELECTRON TRANSFER FLAVOPROTEIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	307	Total	C	N	O	S	0	0	0
			2193	1380	373	436	4			
1	C	307	Total	C	N	O	S	0	0	0
			2193	1380	373	436	4			

- Molecule 2 is a protein called PROTEIN (ELECTRON TRANSFER FLAVOPROTEIN).

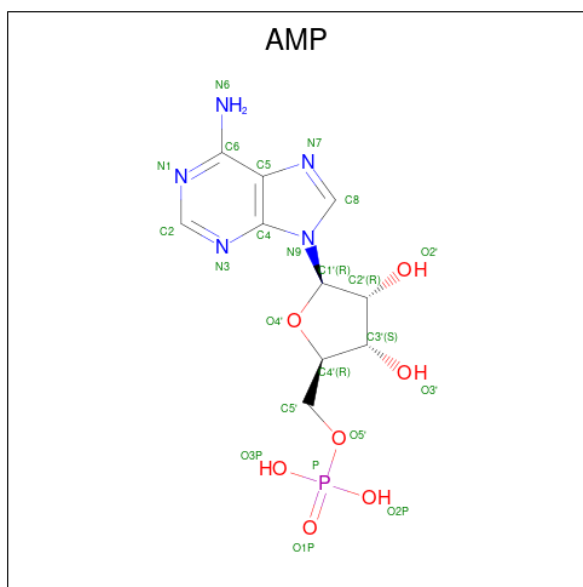
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	246	Total	C	N	O	S	0	0	0
			1826	1148	319	352	7			
2	D	246	Total	C	N	O	S	0	0	0
			1826	1148	319	352	7			

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	23	10	5	7	1	0	0
4	C	1	23	10	5	7	1	0	0

- Molecule 5 is water.

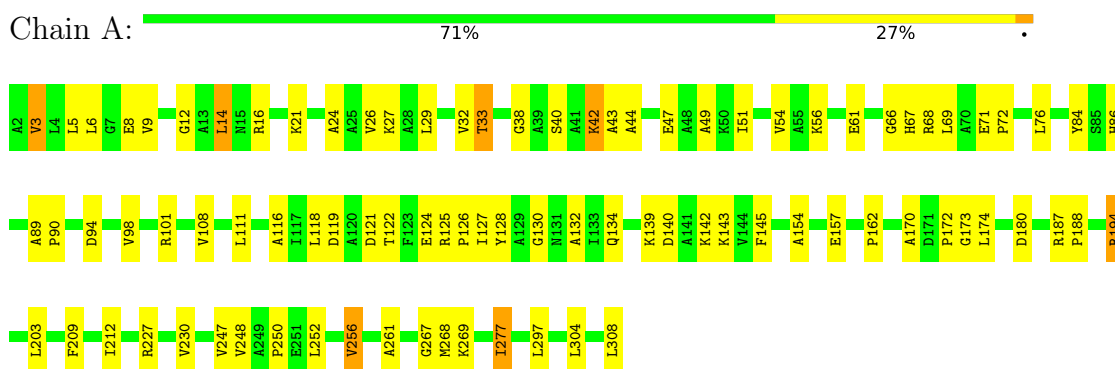
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	28	Total	O	0	0
			28	28		
5	B	23	Total	O	0	0
			23	23		
5	C	31	Total	O	0	0
			31	31		
5	D	19	Total	O	0	0
			19	19		

3 Residue-property plots [i](#)

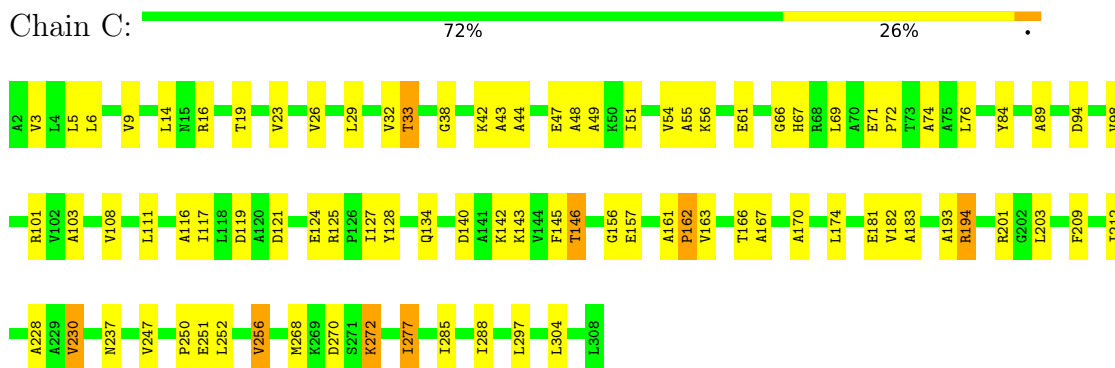
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

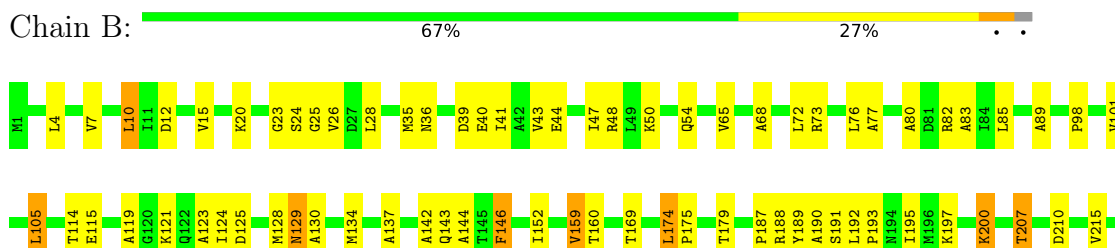
- Molecule 1: PROTEIN (ELECTRON TRANSFER FLAVOPROTEIN)

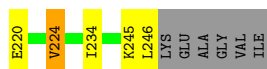


- Molecule 1: PROTEIN (ELECTRON TRANSFER FLAVOPROTEIN)



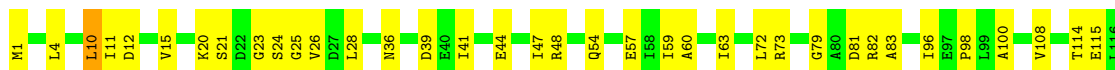
- Molecule 2: PROTEIN (ELECTRON TRANSFER FLAVOPROTEIN)





● Molecule 2: PROTEIN (ELECTRON TRANSFER FLAVOPROTEIN)

Chain D: 66% 29%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.43Å 80.53Å 183.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.60	Depositor
% Data completeness (in resolution range)	87.8 (12.00-2.60)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.193 , 0.286	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	8291	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

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: AMP, 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	0.35	0/2222	0.62	0/3024
1	C	0.35	0/2222	0.62	0/3024
2	B	0.36	0/1841	0.61	0/2488
2	D	0.34	0/1841	0.62	0/2488
All	All	0.35	0/8126	0.62	0/11024

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	2193	0	2226	63	0
1	C	2193	0	2226	59	0
2	B	1826	0	1929	56	0
2	D	1826	0	1929	53	0
3	A	53	0	31	1	0
3	C	53	0	31	0	0
4	A	23	0	12	0	0
4	C	23	0	12	1	0
5	A	28	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	23	0	0	3	0
5	C	31	0	0	2	0
5	D	19	0	0	1	0
All	All	8291	0	8396	213	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 13.

All (213) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:47:ILE:HG21	2:D:188:ARG:HH12	1.28	0.97
2:B:20:LYS:HD2	2:B:24:SER:HB2	1.64	0.80
1:C:3:VAL:HG13	1:C:32:VAL:HA	1.66	0.76
1:C:101:ARG:HH11	2:D:143:GLN:HE21	1.34	0.74
1:C:277:ILE:HD11	1:C:297:LEU:HA	1.69	0.73
1:A:111:LEU:HB2	1:A:145:PHE:HB3	1.72	0.72
2:D:98:PRO:HG2	2:D:128:MET:HG2	1.72	0.71
1:A:101:ARG:HD2	2:B:143:GLN:HE22	1.55	0.71
2:B:197:LYS:O	2:B:200:LYS:HG3	1.91	0.71
1:A:101:ARG:HD2	2:B:143:GLN:NE2	2.07	0.70
2:D:25:GLY:HA2	2:D:224:VAL:HG11	1.74	0.70
1:C:182:VAL:HG22	1:C:183:ALA:H	1.57	0.69
1:A:3:VAL:HG21	1:A:26:VAL:HG21	1.74	0.69
2:B:192:LEU:HD12	2:B:193:PRO:HD3	1.75	0.68
2:B:98:PRO:HG2	2:B:128:MET:HG2	1.75	0.68
1:C:94:ASP:O	1:C:98:VAL:HG12	1.94	0.67
1:C:69:LEU:O	1:C:72:PRO:HD2	1.94	0.67
2:B:25:GLY:HA2	2:B:224:VAL:HG11	1.77	0.67
1:A:94:ASP:O	1:A:98:VAL:HG12	1.94	0.66
1:A:139:LYS:HD2	2:B:220:GLU:HG3	1.77	0.66
2:B:44:GLU:O	2:B:48:ARG:HG3	1.96	0.66
1:C:56:LYS:HA	1:C:162:PRO:HB2	1.78	0.65
1:C:101:ARG:HH11	2:D:143:GLN:NE2	1.94	0.65
1:A:42:LYS:HD2	1:A:43:ALA:N	2.11	0.64
1:A:21:LYS:HG2	1:A:154:ALA:HB2	1.78	0.64
1:A:108:VAL:HG21	1:A:142:LYS:O	1.97	0.64
1:C:111:LEU:HB2	1:C:145:PHE:HB3	1.80	0.64
1:C:71:GLU:HB2	1:C:72:PRO:HD3	1.78	0.64
1:C:42:LYS:HD2	1:C:43:ALA:N	2.14	0.63
2:B:41:ILE:HD13	2:B:187:PRO:HD3	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:72:LEU:HD22	2:B:83:ALA:HB1	1.80	0.62
2:D:119:ALA:O	2:D:179:THR:HA	1.99	0.62
1:A:172:PRO:HB2	1:A:174:LEU:HD13	1.81	0.62
2:D:23:GLY:HA2	2:D:224:VAL:O	1.99	0.62
1:A:51:ILE:O	1:A:54:VAL:HG12	2.00	0.62
1:A:125:ARG:HD3	1:A:134:GLN:HE21	1.65	0.62
1:A:277:ILE:HD11	1:A:297:LEU:HA	1.83	0.60
2:B:119:ALA:O	2:B:179:THR:HA	2.01	0.60
1:A:66:GLY:O	1:A:67:HIS:HB2	2.01	0.60
1:C:116:ALA:HB3	1:C:124:GLU:HB2	1.84	0.60
2:D:12:ASP:HB3	2:D:15:VAL:HG23	1.83	0.60
2:D:144:ALA:CB	2:D:159:VAL:HG11	2.32	0.60
1:A:26:VAL:HG23	1:A:29:LEU:HD12	1.84	0.59
1:A:130:GLY:O	1:A:269:LYS:HE2	2.02	0.59
1:C:66:GLY:O	1:C:67:HIS:HB2	2.02	0.59
1:A:187:ARG:HB2	1:A:188:PRO:HD2	1.84	0.59
1:C:49:ALA:O	1:C:162:PRO:HD2	2.03	0.59
1:C:251:GLU:HA	1:C:272:LYS:HB2	1.85	0.59
1:C:26:VAL:HG23	1:C:29:LEU:HD12	1.85	0.59
1:C:108:VAL:HG23	1:C:140:ASP:CG	2.23	0.59
1:C:108:VAL:HG21	1:C:142:LYS:O	2.02	0.59
1:A:116:ALA:HB3	1:A:124:GLU:HB2	1.85	0.58
2:D:226:GLU:HG3	2:D:227:PRO:HD2	1.85	0.58
1:A:101:ARG:HH11	2:B:143:GLN:NE2	2.02	0.58
2:B:4:LEU:HB2	2:B:114:THR:HG21	1.86	0.58
2:B:144:ALA:HB1	2:B:159:VAL:HG21	1.86	0.57
1:C:101:ARG:HD2	2:D:143:GLN:NE2	2.19	0.57
1:A:71:GLU:HB2	1:A:72:PRO:HD3	1.85	0.57
1:A:14:LEU:HB2	1:A:44:ALA:HB1	1.86	0.56
1:A:33:THR:HG21	1:A:84:TYR:HE2	1.70	0.56
1:A:203:LEU:HD13	1:A:209:PHE:CD1	2.41	0.56
1:A:248:VAL:HB	5:A:607:HOH:O	2.06	0.56
1:A:49:ALA:O	1:A:162:PRO:HD2	2.06	0.55
2:D:26:VAL:O	2:D:28:LEU:HD22	2.05	0.55
1:C:194:ARG:O	1:C:250:PRO:HB2	2.07	0.55
2:D:41:ILE:HD13	2:D:187:PRO:HD3	1.89	0.55
2:D:130:ALA:O	2:D:134:MET:HG3	2.06	0.54
1:A:54:VAL:O	1:A:162:PRO:HG3	2.08	0.54
2:D:36:ASN:HB3	2:D:39:ASP:OD2	2.07	0.54
1:A:56:LYS:HA	1:A:162:PRO:HB2	1.90	0.54
1:A:187:ARG:HB2	1:A:188:PRO:CD	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:ARG:HG3	2:D:137:ALA:HB2	1.90	0.53
1:C:101:ARG:NH1	2:D:143:GLN:HE21	2.02	0.53
2:D:10:LEU:HD21	2:D:36:ASN:HA	1.89	0.53
1:A:3:VAL:HG13	1:A:32:VAL:HA	1.90	0.53
2:B:68:ALA:HB3	2:B:85:LEU:HD11	1.90	0.52
1:C:55:ALA:O	1:C:162:PRO:HB3	2.08	0.52
1:A:108:VAL:HG23	1:A:140:ASP:CG	2.30	0.52
2:B:23:GLY:HA2	2:B:224:VAL:O	2.10	0.52
1:A:121:ASP:HB3	1:A:143:LYS:HE2	1.92	0.52
1:A:111:LEU:HB2	1:A:145:PHE:CB	2.40	0.52
1:C:19:THR:O	1:C:23:VAL:HG23	2.09	0.52
2:D:4:LEU:HB2	2:D:114:THR:HG21	1.92	0.51
1:C:16:ARG:NH2	1:C:156:GLY:HA3	2.25	0.51
1:C:128:TYR:CE1	2:D:26:VAL:HG21	2.45	0.51
1:C:125:ARG:HD3	1:C:134:GLN:HE21	1.75	0.51
1:A:69:LEU:O	1:A:72:PRO:HD2	2.11	0.51
2:B:35:MET:SD	2:B:40:GLU:HG2	2.51	0.50
1:A:5:LEU:HD12	1:A:26:VAL:HG11	1.93	0.50
1:C:49:ALA:HB1	1:C:161:ALA:HA	1.92	0.50
2:B:36:ASN:HB3	2:B:39:ASP:OD2	2.11	0.50
1:C:51:ILE:O	1:C:54:VAL:HG12	2.11	0.50
2:D:209:ALA:HB2	5:D:661:HOH:O	2.11	0.50
1:C:182:VAL:HG22	1:C:183:ALA:N	2.26	0.50
2:D:11:ILE:HD11	2:D:15:VAL:HB	1.94	0.50
2:D:108:VAL:HG12	2:D:211:TYR:CZ	2.47	0.50
1:A:33:THR:HB	1:A:56:LYS:HG3	1.94	0.50
1:A:101:ARG:HH11	2:B:143:GLN:HE21	1.58	0.50
1:A:256:VAL:HB	1:A:277:ILE:HG23	1.93	0.49
1:C:5:LEU:HD12	1:C:26:VAL:HG11	1.94	0.49
1:A:29:LEU:HD13	1:A:86:HIS:CD2	2.48	0.49
2:B:50:LYS:HD2	5:B:664:HOH:O	2.12	0.49
2:B:121:LYS:HG3	2:B:146:PHE:HD1	1.78	0.49
1:C:38:GLY:O	1:C:61:GLU:HA	2.13	0.49
1:C:121:ASP:HB3	1:C:143:LYS:HE2	1.94	0.49
2:B:26:VAL:O	2:B:28:LEU:HD22	2.12	0.48
2:B:191:SER:O	2:B:195:ILE:HG13	2.12	0.48
2:B:192:LEU:CD1	2:B:193:PRO:HD3	2.43	0.48
2:B:68:ALA:HB3	2:B:85:LEU:CD1	2.43	0.48
2:D:153:GLU:HG3	2:D:153:GLU:O	2.14	0.48
2:D:72:LEU:HD22	2:D:83:ALA:HB1	1.96	0.48
2:B:47:ILE:HG21	2:B:188:ARG:NH1	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:VAL:HG12	2:B:89:ALA:O	2.13	0.48
1:A:38:GLY:O	1:A:61:GLU:HA	2.13	0.48
1:C:304:LEU:HD13	2:D:242:LEU:HD23	1.96	0.48
2:D:144:ALA:HB1	2:D:159:VAL:HG11	1.94	0.48
2:D:145:THR:HA	2:D:179:THR:OG1	2.14	0.48
2:B:245:LYS:O	2:B:246:LEU:HB2	2.14	0.48
1:A:68:ARG:HG3	1:A:68:ARG:HH11	1.78	0.48
2:B:76:LEU:HA	2:B:80:ALA:HB3	1.96	0.48
1:A:6:LEU:HB3	1:A:89:ALA:HB2	1.95	0.47
2:B:10:LEU:HD21	2:B:36:ASN:HA	1.96	0.47
2:D:44:GLU:O	2:D:48:ARG:HG3	2.14	0.47
2:B:115:GLU:O	2:B:175:PRO:HA	2.14	0.47
1:A:203:LEU:HD21	1:A:212:ILE:HG12	1.96	0.47
2:D:1:MET:SD	2:D:174:LEU:HD11	2.55	0.47
2:D:174:LEU:O	2:D:176:ALA:N	2.47	0.47
1:C:128:TYR:CD1	2:D:26:VAL:HG21	2.49	0.47
1:A:24:ALA:HA	1:A:27:LYS:HE3	1.97	0.47
2:B:152:ILE:HG22	5:B:630:HOH:O	2.15	0.46
1:C:33:THR:HG21	1:C:84:TYR:HE1	1.80	0.46
2:D:161:ARG:HH11	2:D:168:GLN:NE2	2.13	0.46
2:B:207:THR:HG22	2:B:210:ASP:CG	2.36	0.46
1:A:227:ARG:O	1:A:230:VAL:HG22	2.14	0.46
2:B:101:VAL:HG12	2:B:105:LEU:HD22	1.97	0.46
1:A:127:ILE:HG13	1:A:132:ALA:HB3	1.97	0.46
1:C:42:LYS:HD2	1:C:43:ALA:H	1.77	0.46
2:B:192:LEU:HD12	2:B:193:PRO:CD	2.42	0.46
2:B:12:ASP:HB3	2:B:15:VAL:HG23	1.98	0.46
2:D:59:ILE:N	2:D:59:ILE:HD12	2.31	0.46
1:C:203:LEU:HD13	1:C:209:PHE:CD1	2.51	0.46
1:A:212:ILE:HD13	1:A:212:ILE:HA	1.79	0.45
2:B:25:GLY:HA2	2:B:224:VAL:CG1	2.44	0.45
2:D:161:ARG:NH1	2:D:168:GLN:NE2	2.64	0.45
1:C:212:ILE:HD12	1:C:256:VAL:HG11	1.97	0.45
2:B:77:ALA:HB1	2:B:190:ALA:HB1	1.98	0.45
1:C:193:ALA:O	1:C:250:PRO:HB3	2.17	0.45
2:D:20:LYS:HD2	2:D:24:SER:HB2	1.97	0.45
1:A:261:ALA:CB	3:A:399:FAD:H3'	2.46	0.45
2:D:4:LEU:HB3	2:D:117:ILE:HG12	1.99	0.45
2:B:234:ILE:N	2:B:234:ILE:HD12	2.32	0.45
2:D:152:ILE:HD11	2:D:174:LEU:HD21	1.99	0.45
1:C:270:ASP:HB2	5:C:682:HOH:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:VAL:HG21	1:C:26:VAL:HG21	1.98	0.44
1:C:6:LEU:HB3	1:C:89:ALA:HB2	1.98	0.44
2:D:1:MET:HB2	2:D:115:GLU:OE1	2.17	0.44
2:D:129:ASN:C	2:D:129:ASN:HD22	2.21	0.44
1:C:166:THR:HG22	1:C:167:ALA:H	1.82	0.44
1:C:201:ARG:HB2	1:C:228:ALA:HB1	1.98	0.44
2:B:200:LYS:HD2	2:B:200:LYS:C	2.37	0.44
1:C:48:ALA:O	1:C:54:VAL:HG11	2.17	0.44
1:C:74:ALA:HB2	1:C:98:VAL:HG23	2.00	0.44
1:C:146:THR:CG2	5:C:627:HOH:O	2.65	0.44
1:C:230:VAL:HG21	1:C:237:ASN:HD22	1.81	0.44
1:A:3:VAL:HG21	1:A:26:VAL:CG2	2.42	0.44
2:D:206:LYS:NZ	2:D:210:ASP:HB3	2.32	0.44
2:B:192:LEU:HD13	5:B:694:HOH:O	2.18	0.44
2:D:215:VAL:O	2:D:215:VAL:HG13	2.18	0.44
1:A:16:ARG:HH21	1:A:157:GLU:N	2.16	0.43
1:A:174:LEU:HD23	2:B:142:ALA:N	2.33	0.43
1:C:125:ARG:HH11	1:C:134:GLN:NE2	2.17	0.43
2:D:100:ALA:HB1	2:D:215:VAL:HG23	2.00	0.43
1:A:42:LYS:HD2	1:A:43:ALA:H	1.79	0.43
1:A:118:LEU:HD12	1:A:122:THR:HG22	2.00	0.43
2:B:130:ALA:O	2:B:134:MET:HG3	2.19	0.43
2:B:144:ALA:CB	2:B:159:VAL:HG11	2.49	0.43
1:A:69:LEU:H	1:A:69:LEU:HD22	1.84	0.43
1:A:12:GLY:HA2	1:A:40:SER:O	2.19	0.42
2:D:243:VAL:O	2:D:246:LEU:HG	2.19	0.42
2:B:7:VAL:HG12	2:B:39:ASP:HB3	2.01	0.42
2:B:39:ASP:O	2:B:43:VAL:HG23	2.19	0.42
1:C:29:LEU:HD11	1:C:117:ILE:HG21	2.00	0.42
1:A:8:GLU:HB2	1:A:90:PRO:HG3	2.01	0.42
1:A:128:TYR:CD1	2:B:26:VAL:HG21	2.54	0.42
2:D:63:ILE:HG21	2:D:96:ILE:HD11	2.01	0.42
2:D:194:ASN:HA	2:D:197:LYS:HE2	2.02	0.42
2:B:146:PHE:CD1	2:B:146:PHE:N	2.88	0.42
1:A:247:VAL:HG23	1:A:267:GLY:HA2	2.02	0.42
1:C:14:LEU:HB2	1:C:44:ALA:HB1	2.02	0.42
1:A:101:ARG:HG3	2:B:137:ALA:HB2	2.01	0.41
2:D:57:GLU:HA	2:D:81:ASP:OD2	2.20	0.41
1:A:304:LEU:O	1:A:308:LEU:HD13	2.21	0.41
2:B:123:ALA:O	2:B:125:ASP:N	2.53	0.41
1:C:103:ALA:HB1	1:C:108:VAL:O	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:60:ALA:O	2:D:83:ALA:HA	2.20	0.41
2:D:160:THR:HG22	2:D:169:THR:OG1	2.20	0.41
1:A:194:ARG:O	1:A:250:PRO:HB2	2.20	0.41
2:B:152:ILE:HD11	2:B:174:LEU:HD21	2.02	0.41
1:C:101:ARG:HD2	2:D:143:GLN:HE22	1.84	0.41
1:A:143:LYS:HD2	1:A:143:LYS:N	2.35	0.41
1:C:111:LEU:HB2	1:C:145:PHE:CB	2.50	0.41
2:B:245:LYS:HA	2:B:245:LYS:HD2	1.89	0.41
1:C:16:ARG:HH22	1:C:156:GLY:HA3	1.86	0.41
1:C:111:LEU:HD13	2:D:219:LEU:HD21	2.02	0.41
1:A:16:ARG:HH21	1:A:157:GLU:H	1.68	0.40
2:B:129:ASN:C	2:B:129:ASN:HD22	2.24	0.40
2:D:160:THR:HA	2:D:169:THR:HA	2.03	0.40
1:A:125:ARG:HA	1:A:126:PRO:HD3	1.82	0.40
1:C:285:ILE:O	1:C:288:ILE:HG22	2.22	0.40
2:B:160:THR:HA	2:B:169:THR:HA	2.03	0.40
4:C:400:AMP:H5'2	2:D:122:GLN:HA	2.04	0.40
2:B:174:LEU:HD22	2:B:174:LEU:HA	1.84	0.40
1:C:127:ILE:HD13	1:C:134:GLN:HB3	2.03	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	305/307 (99%)	270 (88%)	32 (10%)	3 (1%)	15	32
1	C	305/307 (99%)	260 (85%)	40 (13%)	5 (2%)	9	19
2	B	244/252 (97%)	221 (91%)	21 (9%)	2 (1%)	19	39
2	D	244/252 (97%)	220 (90%)	19 (8%)	5 (2%)	7	14
All	All	1098/1118 (98%)	971 (88%)	112 (10%)	15 (1%)	11	22

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	ALA
1	C	162	PRO
2	B	124	ILE
1	C	163	VAL
1	C	170	ALA
2	D	232	ALA
1	C	157	GLU
1	A	119	ASP
1	C	119	ASP
2	B	215	VAL
2	D	21	SER
2	D	124	ILE
1	A	173	GLY
2	D	215	VAL
2	D	79	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	218/218 (100%)	205 (94%)	13 (6%)	19	39
1	C	218/218 (100%)	203 (93%)	15 (7%)	15	31
2	B	190/194 (98%)	177 (93%)	13 (7%)	16	32
2	D	190/194 (98%)	179 (94%)	11 (6%)	20	40
All	All	816/824 (99%)	764 (94%)	52 (6%)	17	35

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	9	VAL
1	A	14	LEU
1	A	33	THR
1	A	42	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	47	GLU
1	A	76	LEU
1	A	180	ASP
1	A	194	ARG
1	A	252	LEU
1	A	256	VAL
1	A	268	MET
1	A	277	ILE
2	B	10	LEU
2	B	54	GLN
2	B	73	ARG
2	B	82	ARG
2	B	105	LEU
2	B	129	ASN
2	B	146	PHE
2	B	159	VAL
2	B	174	LEU
2	B	189	TYR
2	B	200	LYS
2	B	207	THR
2	B	224	VAL
1	C	9	VAL
1	C	33	THR
1	C	47	GLU
1	C	76	LEU
1	C	146	THR
1	C	174	LEU
1	C	181	GLU
1	C	194	ARG
1	C	230	VAL
1	C	247	VAL
1	C	252	LEU
1	C	256	VAL
1	C	268	MET
1	C	272	LYS
1	C	277	ILE
2	D	10	LEU
2	D	54	GLN
2	D	73	ARG
2	D	82	ARG
2	D	129	ASN
2	D	146	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	148	SER
2	D	159	VAL
2	D	174	LEU
2	D	200	LYS
2	D	228	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	ASN
1	A	134	GLN
1	A	237	ASN
1	A	240	GLN
2	B	14	ASN
2	B	54	GLN
2	B	129	ASN
2	B	143	GLN
1	C	97	ASN
1	C	134	GLN
1	C	237	ASN
1	C	240	GLN
2	D	54	GLN
2	D	122	GLN
2	D	129	ASN
2	D	143	GLN
2	D	168	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

4 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
4	AMP	A	400	-	22,25,25	1.12	2 (9%)	25,38,38	1.51	5 (20%)
4	AMP	C	400	-	22,25,25	1.56	2 (9%)	25,38,38	1.40	4 (16%)
3	FAD	C	399	-	53,58,58	1.24	6 (11%)	68,89,89	1.53	12 (17%)
3	FAD	A	399	-	53,58,58	1.22	7 (13%)	68,89,89	1.66	10 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AMP	A	400	-	-	0/6/26/26	0/3/3/3
4	AMP	C	400	-	-	0/6/26/26	0/3/3/3
3	FAD	C	399	-	-	1/30/50/50	0/6/6/6
3	FAD	A	399	-	-	1/30/50/50	0/6/6/6

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	400	AMP	O4'-C1'	4.77	1.47	1.41
4	C	400	AMP	C8-N7	-3.87	1.27	1.34
3	C	399	FAD	C10-N10	3.57	1.45	1.37
4	A	400	AMP	O4'-C1'	3.27	1.45	1.41
3	C	399	FAD	C8A-N7A	-2.98	1.29	1.34
3	A	399	FAD	C10-N10	2.83	1.43	1.37
3	A	399	FAD	C9-C8	-2.59	1.35	1.39
3	A	399	FAD	C4X-N5	2.58	1.35	1.30
3	C	399	FAD	C6-C7	-2.58	1.35	1.39
3	A	399	FAD	C6-C7	-2.49	1.35	1.39
3	C	399	FAD	C4X-N5	2.49	1.35	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	399	FAD	C8A-N7A	-2.26	1.30	1.34
3	A	399	FAD	C5X-N5	-2.22	1.35	1.39
4	A	400	AMP	C8-N7	-2.18	1.30	1.34
3	C	399	FAD	O4B-C1B	2.09	1.44	1.41
3	C	399	FAD	C9-C8	-2.05	1.36	1.39
3	A	399	FAD	C6A-C5A	-2.03	1.35	1.43

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	399	FAD	O4B-C1B-C2B	-7.14	96.49	106.93
3	C	399	FAD	O4B-C1B-C2B	-5.40	99.04	106.93
3	A	399	FAD	C9A-C5X-N5	5.11	127.99	122.43
3	C	399	FAD	C9A-C5X-N5	4.75	127.60	122.43
4	C	400	AMP	P-O5'-C5'	3.54	128.06	118.30
4	A	400	AMP	C4-C5-N7	3.52	113.07	109.40
3	A	399	FAD	C4A-C5A-N7A	3.50	113.05	109.40
3	A	399	FAD	C5X-N5-C4X	-3.41	112.40	118.07
3	C	399	FAD	C5X-N5-C4X	-3.40	112.42	118.07
3	C	399	FAD	O2-C2-N3	3.23	124.93	118.65
3	C	399	FAD	C4A-C5A-N7A	2.71	112.23	109.40
3	A	399	FAD	O2B-C2B-C3B	-2.70	103.10	111.82
3	A	399	FAD	C2B-C3B-C4B	-2.65	97.50	102.64
4	C	400	AMP	O5'-C5'-C4'	2.64	118.09	108.99
3	C	399	FAD	N6A-C6A-N1A	2.50	123.76	118.57
4	A	400	AMP	O5'-P-O1P	-2.26	100.13	106.47
3	A	399	FAD	N6A-C6A-N1A	2.26	123.26	118.57
3	A	399	FAD	C6-C5X-N5	-2.25	114.59	118.51
3	A	399	FAD	O4B-C4B-C3B	2.22	109.51	105.11
3	C	399	FAD	O4B-C4B-C3B	2.20	109.47	105.11
4	A	400	AMP	O4'-C4'-C3'	-2.20	100.77	105.11
3	C	399	FAD	O2'-C2'-C1'	2.19	115.09	109.80
3	A	399	FAD	O2P-P-O1P	2.15	122.88	112.24
3	C	399	FAD	C2B-C3B-C4B	-2.12	98.52	102.64
3	C	399	FAD	C4-C4X-N5	-2.12	115.22	118.23
3	C	399	FAD	O2P-P-O1P	2.11	122.70	112.24
4	A	400	AMP	N6-C6-N1	2.11	122.96	118.57
3	C	399	FAD	C6-C5X-N5	-2.09	114.87	118.51
4	A	400	AMP	O5'-C5'-C4'	2.06	116.10	108.99
4	C	400	AMP	N6-C6-N1	2.06	122.86	118.57
4	C	400	AMP	C4-C5-N7	2.02	111.50	109.40

There are no chirality outliers.

All (2) torsion outliers are listed below:

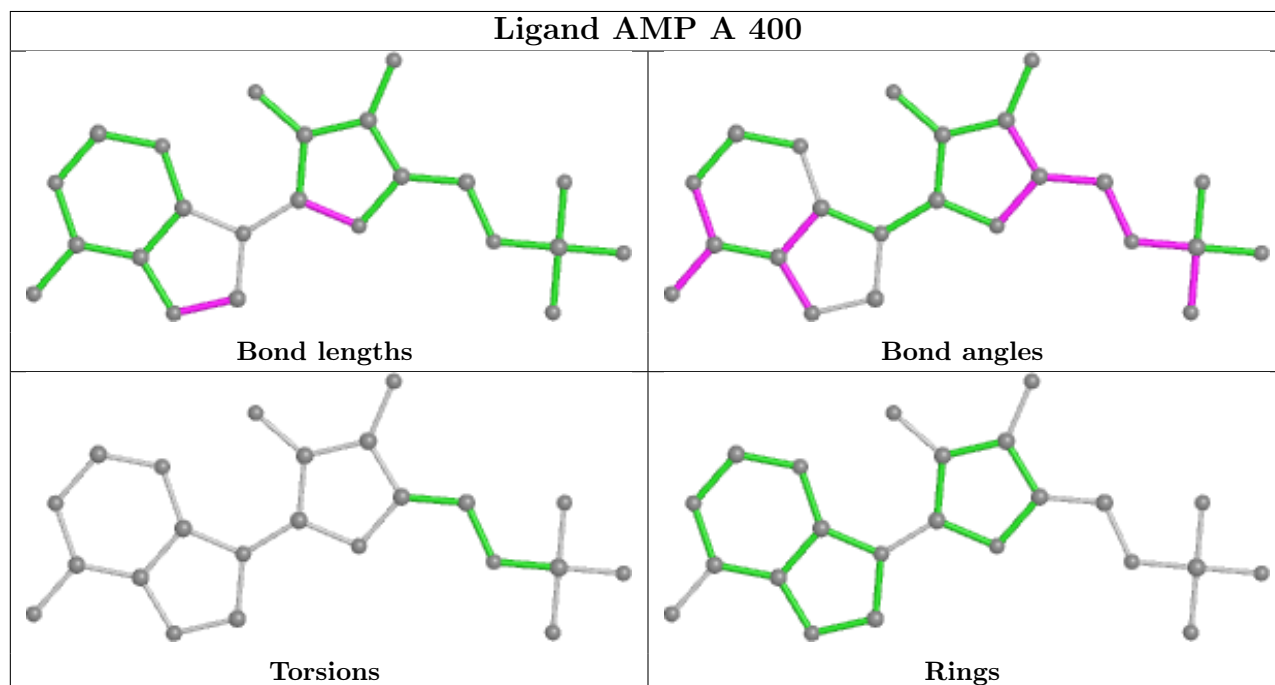
Mol	Chain	Res	Type	Atoms
3	A	399	FAD	O4B-C4B-C5B-O5B
3	C	399	FAD	O4B-C4B-C5B-O5B

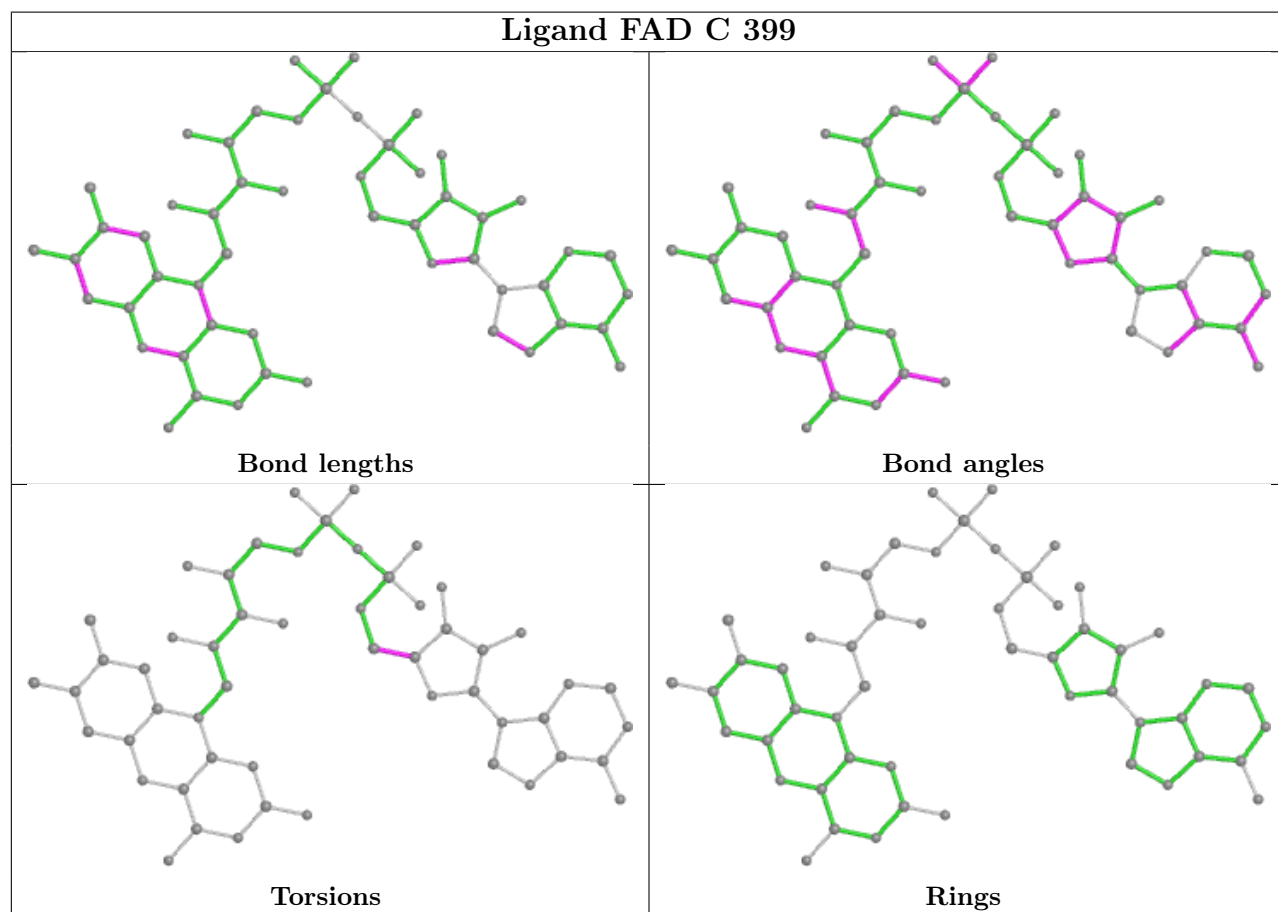
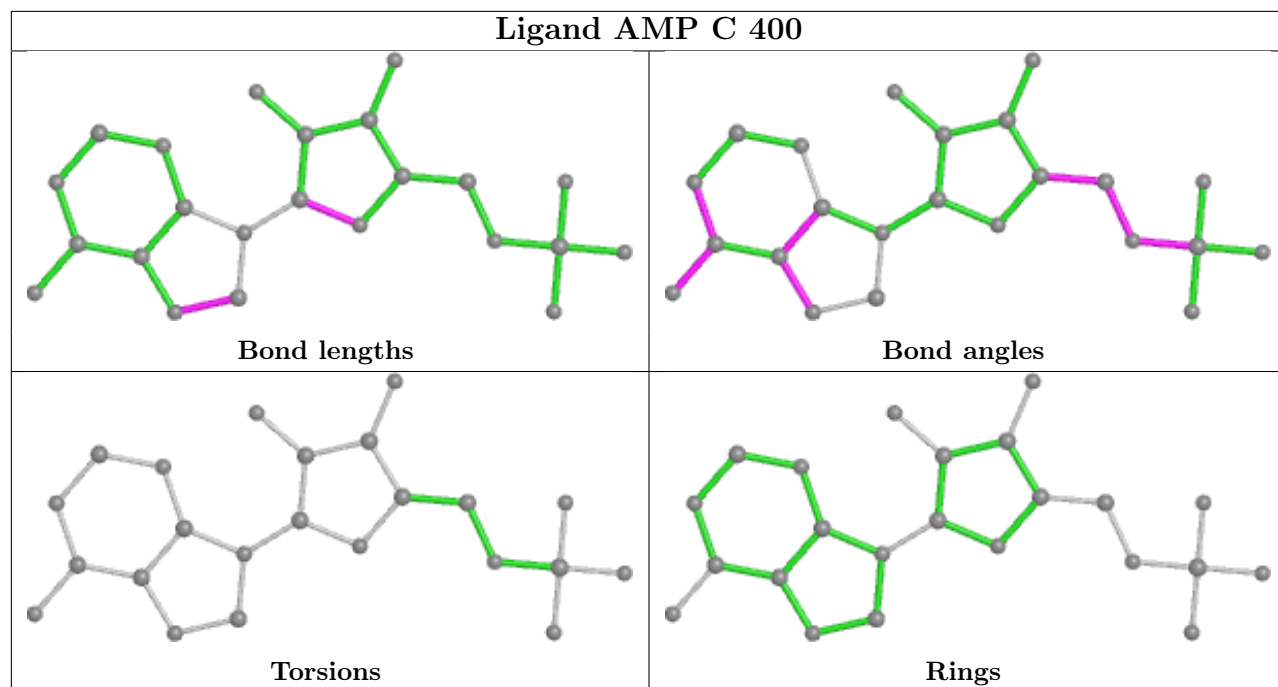
There are no ring outliers.

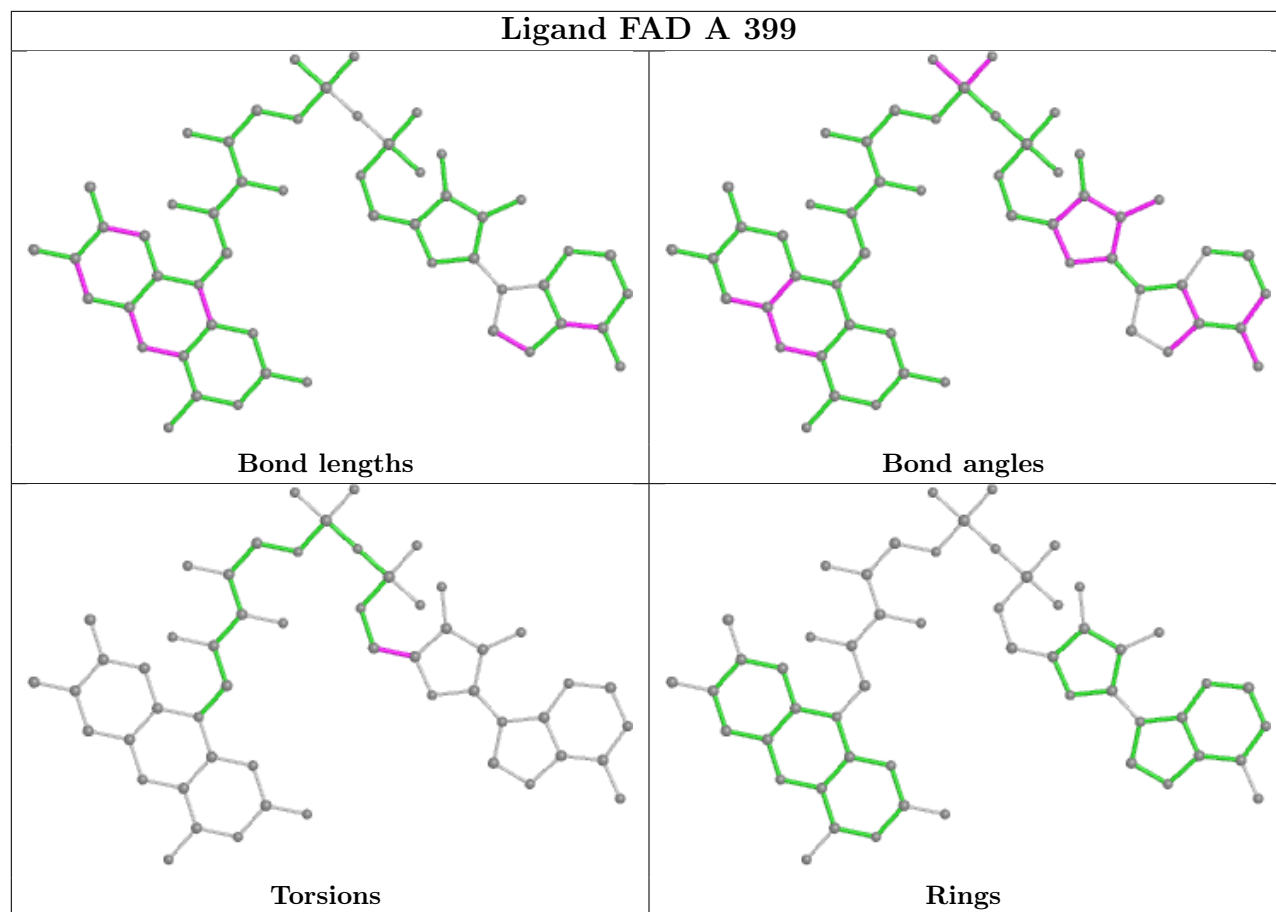
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	400	AMP	1	0
3	A	399	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.