



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 11:10 AM EDT

PDB ID : 2FMN
Title : Ala177Val mutant of E. coli Methylenetetrahydrofolate Reductase complex with LY309887
Authors : Pejchal, R.; Campbell, E.; Guenther, B.D.; Lennon, B.W.; Matthews, R.G.; Ludwig, M.L.
Deposited on : 2006-01-09
Resolution : 2.05 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 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)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

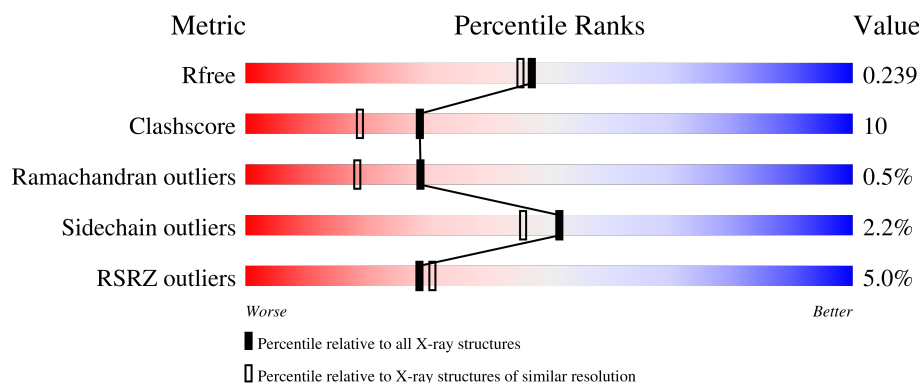
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	304	<div> <div>10%</div> <div> <div></div> <div>74%</div> <div>20%</div> <div>• 5%</div> </div> </div>
1	B	304	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>• 6%</div> </div> </div>
1	C	304	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>16%</div> <div>11%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7066 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 5,10-methylenetetrahydrofolate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2216	1401	388	416	11			
1	B	287	Total	C	N	O	S	0	0	0
			2230	1413	392	414	11			
1	C	271	Total	C	N	O	S	0	0	0
			2087	1327	362	387	11			

There are 27 discrepancies between the modelled and reference sequences:

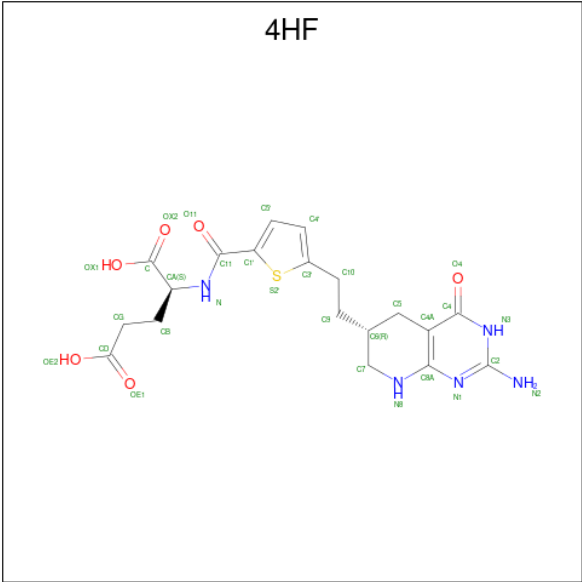
Chain	Residue	Modelled	Actual	Comment	Reference
A	177	VAL	ALA	engineered mutation	UNP P0AEZ1
A	297	LEU	-	cloning artifact	UNP P0AEZ1
A	298	GLU	-	cloning artifact	UNP P0AEZ1
A	299	HIS	-	expression tag	UNP P0AEZ1
A	300	HIS	-	expression tag	UNP P0AEZ1
A	301	HIS	-	expression tag	UNP P0AEZ1
A	302	HIS	-	expression tag	UNP P0AEZ1
A	303	HIS	-	expression tag	UNP P0AEZ1
A	304	HIS	-	expression tag	UNP P0AEZ1
B	177	VAL	ALA	engineered mutation	UNP P0AEZ1
B	297	LEU	-	cloning artifact	UNP P0AEZ1
B	298	GLU	-	cloning artifact	UNP P0AEZ1
B	299	HIS	-	expression tag	UNP P0AEZ1
B	300	HIS	-	expression tag	UNP P0AEZ1
B	301	HIS	-	expression tag	UNP P0AEZ1
B	302	HIS	-	expression tag	UNP P0AEZ1
B	303	HIS	-	expression tag	UNP P0AEZ1
B	304	HIS	-	expression tag	UNP P0AEZ1
C	177	VAL	ALA	engineered mutation	UNP P0AEZ1
C	297	LEU	-	cloning artifact	UNP P0AEZ1
C	298	GLU	-	cloning artifact	UNP P0AEZ1
C	299	HIS	-	expression tag	UNP P0AEZ1
C	300	HIS	-	expression tag	UNP P0AEZ1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	301	HIS	-	expression tag	UNP P0AEZ1
C	302	HIS	-	expression tag	UNP P0AEZ1
C	303	HIS	-	expression tag	UNP P0AEZ1
C	304	HIS	-	expression tag	UNP P0AEZ1

- # FAD

- Molecule 3 is N-[(5-{2-[(6R)-2-AMINO-4-OXO-3,4,5,6,7,8-HEXAHYDROPYRIDO[2,3-D]PYRIMIDIN-6-YL]ETHYL}-2-THIENYL)CARBONYL]-L-GLUTAMIC ACID (three-letter code: 4HF) (formula: C₁₉H₂₃N₅O₆S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			31	19	5	6	1		
3	B	1	Total	C	N	O	S	0	0
			31	19	5	6	1		
3	C	1	Total	C	N	O	S	0	0
			31	19	5	6	1		

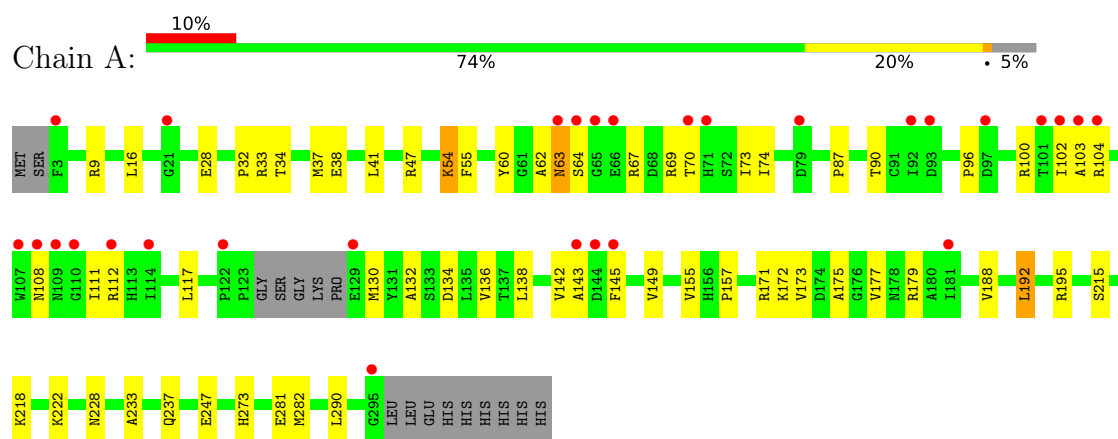
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	62	Total	O	0	0
			62	62		
4	B	124	Total	O	0	0
			124	124		
4	C	95	Total	O	0	0
			95	95		

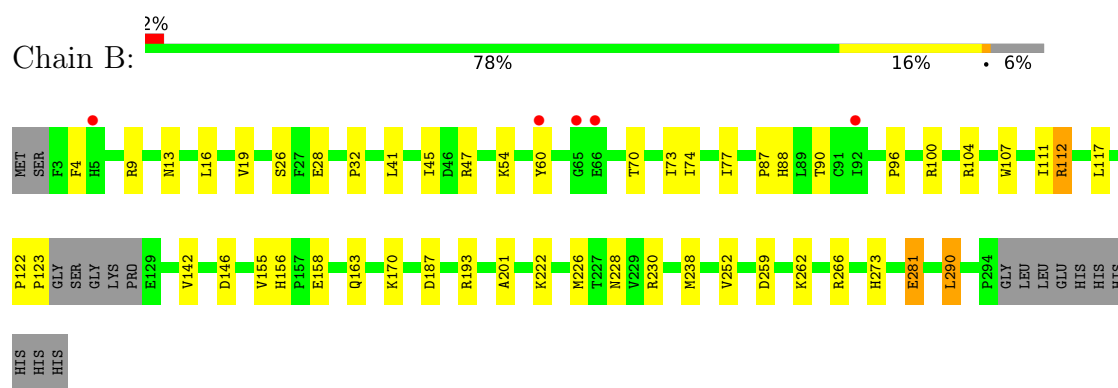
3 Residue-property plots [i](#)

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.

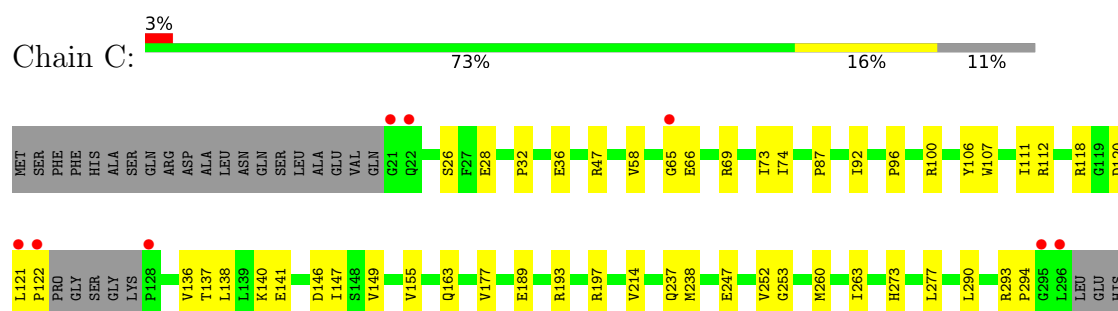
- Molecule 1: 5,10-methylenetetrahydrofolate reductase



- Molecule 1: 5,10-methylenetetrahydrofolate reductase



- Molecule 1: 5,10-methylenetetrahydrofolate reductase



HIS
HIS
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	101.56Å 128.64Å 96.74Å 90.00° 120.87° 90.00°	Depositor
Resolution (Å)	35.78 – 2.05 35.78 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.3 (35.78-2.05) 91.8 (35.78-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.250 0.205 , 0.239	Depositor DCC
R_{free} test set	3161 reflections (4.57%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7066	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% 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: 4HF, 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	0.31	0/2260	0.54	0/3068
1	B	0.36	0/2276	0.59	1/3088 (0.0%)
1	C	0.34	0/2131	0.59	1/2893 (0.0%)
All	All	0.34	0/6667	0.57	2/9049 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	146	ASP	N-CA-C	-5.52	96.09	111.00
1	B	146	ASP	N-CA-C	-5.30	96.67	111.00

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	2216	0	2139	54	0
1	B	2230	0	2173	34	0
1	C	2087	0	2026	46	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	31	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	31	0	21	0	0
3	B	31	0	21	0	0
3	C	31	0	21	1	0
4	A	62	0	0	2	0
4	B	124	0	0	2	0
4	C	95	0	0	2	0
All	All	7066	0	6494	129	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 10.

All (129) 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:C:163:GLN:HE22	1:C:197:ARG:HH22	1.20	0.86
1:C:189:GLU:HB3	1:C:193:ARG:NH2	1.90	0.84
1:A:96:PRO:O	1:A:100:ARG:HG3	1.89	0.72
1:B:16:LEU:HD11	1:B:290:LEU:HD12	1.74	0.70
1:C:92:ILE:HG12	1:C:118:ARG:O	1.91	0.70
1:C:112:ARG:HH11	1:C:112:ARG:HG3	1.58	0.68
1:B:60:TYR:HB2	1:B:88:HIS:O	1.93	0.67
1:B:16:LEU:O	1:B:19:VAL:HG12	1.97	0.65
1:C:238:MET:HG3	1:C:252:VAL:HG11	1.78	0.64
1:A:9:ARG:HG3	1:C:263:ILE:HD11	1.80	0.64
1:B:13:ASN:HD21	1:B:262:LYS:NZ	1.96	0.64
1:B:9:ARG:HD2	1:B:9:ARG:C	2.18	0.63
1:A:149:VAL:HB	1:A:172:LYS:HD3	1.78	0.63
1:C:28:GLU:OE1	1:C:273:HIS:HE1	1.83	0.62
1:B:28:GLU:HB2	1:B:273:HIS:CE1	2.36	0.60
1:B:238:MET:HG3	1:B:252:VAL:HG11	1.82	0.60
1:A:63:ASN:HD22	1:A:64:SER:N	2.00	0.59
1:A:102:ILE:HD12	1:A:103:ALA:N	2.19	0.58
1:C:28:GLU:HB2	1:C:273:HIS:CE1	2.38	0.58
1:C:193:ARG:HH21	1:C:193:ARG:HG3	1.69	0.58
1:A:32:PRO:HD3	1:A:41:LEU:HD22	1.86	0.57
1:A:173:VAL:HA	1:A:177:VAL:HG22	1.86	0.57
1:C:96:PRO:O	1:C:100:ARG:HG3	2.04	0.57
1:A:74:ILE:HG13	1:A:87:PRO:HB3	1.87	0.57
1:A:149:VAL:CB	1:A:172:LYS:HD3	2.34	0.57
1:B:222:LYS:O	1:B:226:MET:HG3	2.05	0.57
1:A:9:ARG:CG	1:C:263:ILE:HD11	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:THR:O	1:C:141:GLU:HG3	2.04	0.57
1:B:96:PRO:O	1:B:100:ARG:HG3	2.05	0.56
1:A:34:THR:HG23	1:A:37:MET:HE3	1.88	0.56
1:B:32:PRO:HD3	1:B:41:LEU:HD22	1.88	0.56
1:A:33:ARG:HB2	1:A:37:MET:HE3	1.88	0.56
1:B:107:TRP:O	1:B:112:ARG:NH1	2.38	0.56
1:C:32:PRO:HG2	4:C:746:HOH:O	2.04	0.56
1:B:32:PRO:HD2	1:B:73:ILE:HD11	1.89	0.55
1:A:54:LYS:HD2	1:A:55:PHE:HD1	1.71	0.55
1:A:281:GLU:OE2	1:C:247:GLU:HG2	2.07	0.55
1:B:156:HIS:CE1	1:B:158:GLU:HB2	2.42	0.55
1:B:28:GLU:OE1	1:B:273:HIS:HE1	1.90	0.54
1:C:107:TRP:CZ3	1:C:112:ARG:HG2	2.43	0.54
1:A:34:THR:HG23	1:A:37:MET:CE	2.39	0.53
1:A:111:ILE:HD12	1:A:111:ILE:N	2.23	0.53
1:C:163:GLN:NE2	1:C:197:ARG:HH22	1.99	0.53
1:C:118:ARG:NH2	4:C:556:HOH:O	2.41	0.52
1:A:9:ARG:HG2	4:A:581:HOH:O	2.10	0.52
1:A:32:PRO:CG	1:A:38:GLU:HG2	2.39	0.52
1:B:193:ARG:HD3	4:B:715:HOH:O	2.10	0.52
1:C:69:ARG:O	1:C:73:ILE:HD13	2.10	0.51
1:A:143:ALA:HB3	1:A:145:PHE:CE1	2.45	0.51
1:B:111:ILE:HD12	1:B:111:ILE:N	2.26	0.51
1:A:16:LEU:HD11	1:A:290:LEU:HD23	1.92	0.50
1:A:132:ALA:HB3	1:A:172:LYS:HE2	1.92	0.50
1:A:157:PRO:HG3	1:A:228:ASN:HB2	1.93	0.50
1:C:47:ARG:HH11	1:C:47:ARG:HG2	1.75	0.50
1:B:238:MET:HG3	1:B:252:VAL:CG1	2.40	0.50
1:A:47:ARG:HG2	1:A:47:ARG:HH21	1.76	0.50
1:C:36:GLU:H	1:C:36:GLU:CD	2.14	0.50
1:C:138:LEU:C	1:C:138:LEU:HD23	2.32	0.50
1:A:112:ARG:HG3	1:A:112:ARG:HH11	1.77	0.49
1:C:74:ILE:HG13	1:C:87:PRO:HB3	1.94	0.49
1:B:266:ARG:NH2	1:C:189:GLU:HB2	2.27	0.49
1:A:90:THR:HA	1:A:117:LEU:O	2.13	0.49
1:C:118:ARG:HD3	1:C:121:LEU:HD21	1.94	0.49
1:A:138:LEU:O	1:A:142:VAL:HG23	2.13	0.49
1:C:277:LEU:HD13	3:C:497:4HF:HG1	1.95	0.48
1:C:238:MET:HG3	1:C:252:VAL:CG1	2.42	0.48
1:B:26:SER:OG	1:B:273:HIS:HD2	1.96	0.48
1:C:47:ARG:HG2	1:C:47:ARG:NH1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:ASN:HD21	1:B:262:LYS:HZ1	1.61	0.48
1:A:63:ASN:O	1:A:67:ARG:HG3	2.14	0.48
1:C:140:LYS:HD3	1:C:147:ILE:HD12	1.95	0.48
1:A:63:ASN:HD22	1:A:64:SER:H	1.60	0.48
1:A:63:ASN:ND2	1:A:64:SER:N	2.62	0.47
1:B:47:ARG:HH11	1:B:47:ARG:HG2	1.79	0.47
1:A:138:LEU:C	1:A:138:LEU:HD23	2.34	0.47
1:A:179:ARG:HG2	1:A:179:ARG:HH11	1.79	0.47
1:A:54:LYS:O	1:A:54:LYS:HD3	2.15	0.47
1:C:26:SER:OG	1:C:273:HIS:HD2	1.97	0.47
1:C:112:ARG:HH11	1:C:112:ARG:CG	2.25	0.47
1:B:156:HIS:ND1	1:B:158:GLU:HB2	2.30	0.47
1:C:106:TYR:HD1	1:C:111:ILE:HG13	1.80	0.47
1:C:293:ARG:HB3	1:C:294:PRO:HD2	1.95	0.46
1:A:60:TYR:HD1	1:A:70:THR:HG21	1.81	0.46
1:B:9:ARG:HD2	1:B:9:ARG:O	2.16	0.46
1:A:173:VAL:HA	1:A:177:VAL:CG2	2.45	0.46
1:A:69:ARG:O	1:A:73:ILE:HG13	2.16	0.46
1:B:104:ARG:HG2	1:B:142:VAL:HG13	1.97	0.45
1:A:132:ALA:O	1:A:136:VAL:HG23	2.17	0.45
1:C:120:ASP:O	1:C:122:PRO:HD3	2.17	0.45
1:B:187:ASP:OD2	1:B:230:ARG:NH2	2.50	0.44
1:C:92:ILE:HG21	1:C:122:PRO:HD2	1.99	0.44
1:C:106:TYR:CD1	1:C:111:ILE:HG13	2.53	0.44
1:A:149:VAL:CG1	1:A:172:LYS:HD3	2.48	0.44
1:A:33:ARG:HB2	1:A:37:MET:CE	2.47	0.44
1:B:45:ILE:HD13	1:B:77:ILE:HG12	2.00	0.43
1:A:215:SER:HB3	1:A:282:MET:CE	2.48	0.43
1:B:281:GLU:HB2	4:B:639:HOH:O	2.19	0.43
1:B:74:ILE:HG13	1:B:87:PRO:HB3	2.00	0.43
1:B:32:PRO:HD2	1:B:73:ILE:CD1	2.48	0.43
1:A:138:LEU:O	1:A:138:LEU:HD23	2.18	0.43
1:B:70:THR:O	1:B:74:ILE:HG12	2.19	0.43
1:B:90:THR:HA	1:B:117:LEU:O	2.19	0.43
1:C:193:ARG:NH2	1:C:193:ARG:HG3	2.33	0.42
1:A:188:VAL:HG12	1:A:192:LEU:HD22	2.02	0.42
1:C:112:ARG:HG3	1:C:112:ARG:NH1	2.31	0.42
1:A:130:MET:HB2	1:A:134:ASP:HB2	2.01	0.42
1:A:233:ALA:O	1:A:237:GLN:HG2	2.20	0.42
1:C:58:VAL:HG21	1:C:73:ILE:HG22	2.01	0.42
1:A:32:PRO:HD2	1:A:73:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ARG:NH2	1:C:260:MET:HG3	2.36	0.41
1:A:218:LYS:O	1:A:222:LYS:HG3	2.21	0.41
1:C:112:ARG:CG	1:C:112:ARG:NH1	2.81	0.41
1:C:189:GLU:OE2	1:C:193:ARG:NH1	2.53	0.41
1:A:28:GLU:HB2	1:A:273:HIS:NE2	2.36	0.41
1:C:189:GLU:HB3	1:C:193:ARG:HH22	1.79	0.41
1:A:281:GLU:HG2	4:A:684:HOH:O	2.21	0.41
1:B:13:ASN:ND2	1:B:262:LYS:NZ	2.67	0.41
1:A:104:ARG:O	1:A:108:ASN:ND2	2.53	0.41
1:A:172:LYS:O	1:A:175:ALA:HB3	2.21	0.41
1:C:136:VAL:O	1:C:140:LYS:HG2	2.21	0.41
1:C:149:VAL:HG22	1:C:177:VAL:HG11	2.02	0.41
1:B:122:PRO:HA	1:B:123:PRO:HD3	1.96	0.40
1:A:149:VAL:HG11	1:A:172:LYS:HD3	2.03	0.40
1:A:179:ARG:HG2	1:A:179:ARG:NH1	2.35	0.40
1:A:62:ALA:HA	1:A:67:ARG:HH11	1.87	0.40
1:A:104:ARG:HE	1:A:104:ARG:HB2	1.60	0.40
1:B:170:LYS:HD2	1:B:201:ALA:O	2.22	0.40
1:C:65:GLY:O	1:C:66:GLU:HB2	2.21	0.40
1:C:214:VAL:O	1:C:253:GLY:HA3	2.21	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	284/304 (93%)	272 (96%)	11 (4%)	1 (0%)	34	24
1	B	283/304 (93%)	278 (98%)	3 (1%)	2 (1%)	22	12
1	C	267/304 (88%)	258 (97%)	8 (3%)	1 (0%)	34	24
All	All	834/912 (91%)	808 (97%)	22 (3%)	4 (0%)	29	18

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	4	PHE
1	C	155	VAL
1	A	155	VAL
1	B	155	VAL

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	228/259 (88%)	222 (97%)	6 (3%)	46	39
1	B	233/259 (90%)	226 (97%)	7 (3%)	41	34
1	C	216/259 (83%)	214 (99%)	2 (1%)	78	79
All	All	677/777 (87%)	662 (98%)	15 (2%)	52	46

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LYS
1	A	63	ASN
1	A	171	ARG
1	A	192	LEU
1	A	195	ARG
1	A	247	GLU
1	B	54	LYS
1	B	112	ARG
1	B	163	GLN
1	B	228	ASN
1	B	259	ASP
1	B	281	GLU
1	B	290	LEU
1	C	237	GLN
1	C	290	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	43	ASN
1	A	63	ASN
1	A	108	ASN
1	A	168	ASN
1	A	219	GLN
1	A	228	ASN
1	B	13	ASN
1	B	14	GLN
1	B	20	GLN
1	B	24	ASN
1	B	109	ASN
1	B	163	GLN
1	B	273	HIS
1	C	39	GLN
1	C	163	GLN
1	C	237	GLN
1	C	273	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FAD	A	395	-	51,58,58	1.88	11 (21%)	60,89,89	2.97	18 (30%)
3	4HF	A	495	-	24,33,33	2.10	7 (29%)	16,46,46	1.65	3 (18%)
3	4HF	B	496	-	24,33,33	2.20	7 (29%)	16,46,46	1.67	4 (25%)
2	FAD	C	397	-	51,58,58	1.79	10 (19%)	60,89,89	2.74	11 (18%)
2	FAD	B	396	-	51,58,58	1.93	12 (23%)	60,89,89	2.79	12 (20%)
3	4HF	C	497	-	24,33,33	2.07	7 (29%)	16,46,46	1.68	4 (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	A	395	-	-	4/30/50/50	0/6/6/6
3	4HF	A	495	-	-	1/13/31/31	0/3/3/3
3	4HF	B	496	-	-	2/13/31/31	0/3/3/3
2	FAD	C	397	-	-	2/30/50/50	0/6/6/6
2	FAD	B	396	-	-	4/30/50/50	0/6/6/6
3	4HF	C	497	-	-	0/13/31/31	0/3/3/3

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	395	FAD	C9A-N10	7.37	1.48	1.38
2	C	397	FAD	C9A-N10	6.70	1.47	1.38
3	B	496	4HF	C10-C3'	6.70	1.53	1.50
2	B	396	FAD	C9A-N10	6.52	1.47	1.38
3	A	495	4HF	C10-C3'	6.21	1.53	1.50
3	C	497	4HF	C10-C3'	5.87	1.53	1.50
2	B	396	FAD	C4X-N5	5.61	1.41	1.33
3	A	495	4HF	C4-N3	4.88	1.41	1.33
3	B	496	4HF	C4-N3	4.72	1.41	1.33
2	A	395	FAD	C4X-N5	4.64	1.40	1.33
3	C	497	4HF	C4-N3	4.60	1.41	1.33
2	C	397	FAD	C4X-N5	4.38	1.39	1.33
2	A	395	FAD	C4-N3	4.21	1.40	1.33
2	B	396	FAD	C4-N3	3.70	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	397	FAD	C10-N1	3.68	1.38	1.33
2	C	397	FAD	C4-N3	3.61	1.39	1.33
3	C	497	4HF	C7-C6	3.60	1.56	1.53
3	B	496	4HF	C7-C6	3.53	1.56	1.53
3	B	496	4HF	C2-N3	3.20	1.41	1.35
3	C	497	4HF	C7-N8	3.18	1.50	1.44
2	C	397	FAD	C8M-C8	3.13	1.57	1.51
2	B	396	FAD	C7M-C7	3.10	1.57	1.51
3	A	495	4HF	C2-N3	3.06	1.40	1.35
2	B	396	FAD	C8M-C8	3.05	1.57	1.51
2	A	395	FAD	C10-N1	3.05	1.37	1.33
2	A	395	FAD	O4B-C1B	3.03	1.45	1.41
2	B	396	FAD	C5X-N5	3.02	1.40	1.35
3	C	497	4HF	C2-N3	2.96	1.40	1.35
3	B	496	4HF	C7-N8	2.92	1.49	1.44
3	A	495	4HF	C7-C6	2.92	1.55	1.53
2	B	396	FAD	C8-C7	2.89	1.48	1.40
2	B	396	FAD	C4-C4X	2.87	1.46	1.41
3	A	495	4HF	C7-N8	2.84	1.49	1.44
2	A	395	FAD	C8-C7	2.81	1.47	1.40
2	C	397	FAD	C8-C7	2.80	1.47	1.40
2	B	396	FAD	C10-N1	2.65	1.36	1.33
3	B	496	4HF	C3'-S2'	2.56	1.79	1.73
2	A	395	FAD	C9-C9A	2.51	1.45	1.40
2	C	397	FAD	C5X-N5	2.48	1.39	1.35
3	C	497	4HF	C3'-S2'	2.46	1.78	1.73
2	B	396	FAD	C2-N1	-2.40	1.33	1.38
3	A	495	4HF	C5-C4A	2.40	1.54	1.51
2	B	396	FAD	C4X-C10	2.37	1.41	1.38
2	A	395	FAD	C8A-N7A	-2.36	1.30	1.34
3	B	496	4HF	C5-C4A	2.27	1.54	1.51
3	A	495	4HF	C3'-S2'	2.23	1.78	1.73
2	B	396	FAD	C9-C9A	2.22	1.45	1.40
3	C	497	4HF	C5-C4A	2.20	1.54	1.51
2	C	397	FAD	C9-C9A	2.18	1.45	1.40
2	A	395	FAD	C6-C5X	2.15	1.45	1.41
2	C	397	FAD	C4-C4X	2.14	1.45	1.41
2	C	397	FAD	C6-C5X	2.07	1.45	1.41
2	A	395	FAD	C5X-N5	2.07	1.38	1.35
2	A	395	FAD	P-O2P	-2.01	1.45	1.55

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	395	FAD	C4-N3-C2	15.50	128.22	115.14
2	B	396	FAD	C4-N3-C2	14.62	127.49	115.14
2	C	397	FAD	C4-N3-C2	14.10	127.04	115.14
2	A	395	FAD	C10-C4X-N5	8.25	126.96	121.26
2	C	397	FAD	C10-C4X-N5	7.03	126.12	121.26
2	A	395	FAD	C4X-C4-N3	-6.99	113.86	123.43
2	B	396	FAD	C10-C4X-N5	6.60	125.82	121.26
2	B	396	FAD	C4X-C4-N3	-6.56	114.46	123.43
2	B	396	FAD	C4-C4X-C10	-6.07	115.94	119.95
2	C	397	FAD	C4X-C4-N3	-5.91	115.35	123.43
2	C	397	FAD	C5X-C9A-N10	-5.42	113.79	117.72
2	C	397	FAD	C4X-C10-N10	-5.23	114.93	120.30
2	A	395	FAD	C4X-C10-N10	-5.09	115.07	120.30
2	C	397	FAD	C4-C4X-C10	-4.94	116.68	119.95
2	A	395	FAD	C5X-C9A-N10	-4.32	114.58	117.72
2	A	395	FAD	C4-C4X-C10	-4.14	117.21	119.95
2	A	395	FAD	C1'-N10-C9A	4.04	121.47	118.29
2	B	396	FAD	C4X-C10-N10	-3.98	116.21	120.30
2	B	396	FAD	C5X-C9A-N10	-3.89	114.89	117.72
3	C	497	4HF	N3-C2-N1	-3.89	119.32	125.42
3	B	496	4HF	N3-C2-N1	-3.87	119.35	125.42
3	A	495	4HF	N3-C2-N1	-3.84	119.39	125.42
2	B	396	FAD	C1'-N10-C9A	3.73	121.22	118.29
3	A	495	4HF	C2-N1-C8A	3.29	121.92	114.54
3	C	497	4HF	C2-N1-C8A	3.22	121.75	114.54
2	C	397	FAD	C1B-N9A-C4A	-3.20	121.02	126.64
2	A	395	FAD	C6-C5X-N5	-3.19	115.54	119.05
3	B	496	4HF	C2-N1-C8A	3.18	121.67	114.54
2	C	397	FAD	O5'-C5'-C4'	2.82	116.88	109.36
2	B	396	FAD	O5'-C5'-C4'	2.79	116.81	109.36
2	A	395	FAD	C4-C4X-N5	-2.60	115.62	118.60
3	C	497	4HF	C4-N3-C2	2.57	120.01	115.93
2	A	395	FAD	C1B-N9A-C4A	-2.54	122.18	126.64
3	B	496	4HF	C4-N3-C2	2.51	119.91	115.93
2	A	395	FAD	C8M-C8-C7	2.46	125.78	120.74
2	C	397	FAD	C1'-N10-C9A	2.41	120.19	118.29
2	C	397	FAD	C6-C5X-N5	-2.40	116.40	119.05
2	A	395	FAD	O2'-C2'-C3'	2.37	114.86	109.10
3	A	495	4HF	C4-N3-C2	2.37	119.69	115.93
2	B	396	FAD	O2'-C2'-C3'	2.34	114.78	109.10
2	A	395	FAD	C4A-C5A-N7A	2.25	111.75	109.40
2	C	397	FAD	O5B-C5B-C4B	2.25	116.73	108.99
2	B	396	FAD	O3'-C3'-C4'	2.22	114.18	108.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	395	FAD	O5B-C5B-C4B	2.18	116.51	108.99
2	B	396	FAD	C8M-C8-C7	2.16	125.17	120.74
2	A	395	FAD	N6A-C6A-N1A	2.14	123.02	118.57
2	A	395	FAD	C8M-C8-C9	-2.13	115.24	120.34
3	B	496	4HF	N2-C2-N1	2.07	120.47	117.25
3	C	497	4HF	N2-C2-N1	2.07	120.47	117.25
2	B	396	FAD	C1B-N9A-C4A	-2.06	123.02	126.64
2	A	395	FAD	C9A-C5X-N5	2.05	125.57	122.36
2	A	395	FAD	O2P-P-O1P	2.01	122.18	112.24

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	396	FAD	O2'-C2'-C3'-C4'
3	A	495	4HF	CB-CA-N-C11
3	B	496	4HF	CB-CA-N-C11
2	A	395	FAD	P-O3P-PA-O2A
2	B	396	FAD	P-O3P-PA-O2A
2	A	395	FAD	O2'-C2'-C3'-C4'
2	B	396	FAD	P-O3P-PA-O1A
3	B	496	4HF	C-CA-N-C11
2	C	397	FAD	O2'-C2'-C3'-C4'
2	A	395	FAD	P-O3P-PA-O1A
2	C	397	FAD	P-O3P-PA-O2A
2	A	395	FAD	C5B-O5B-PA-O1A
2	B	396	FAD	C5B-O5B-PA-O1A

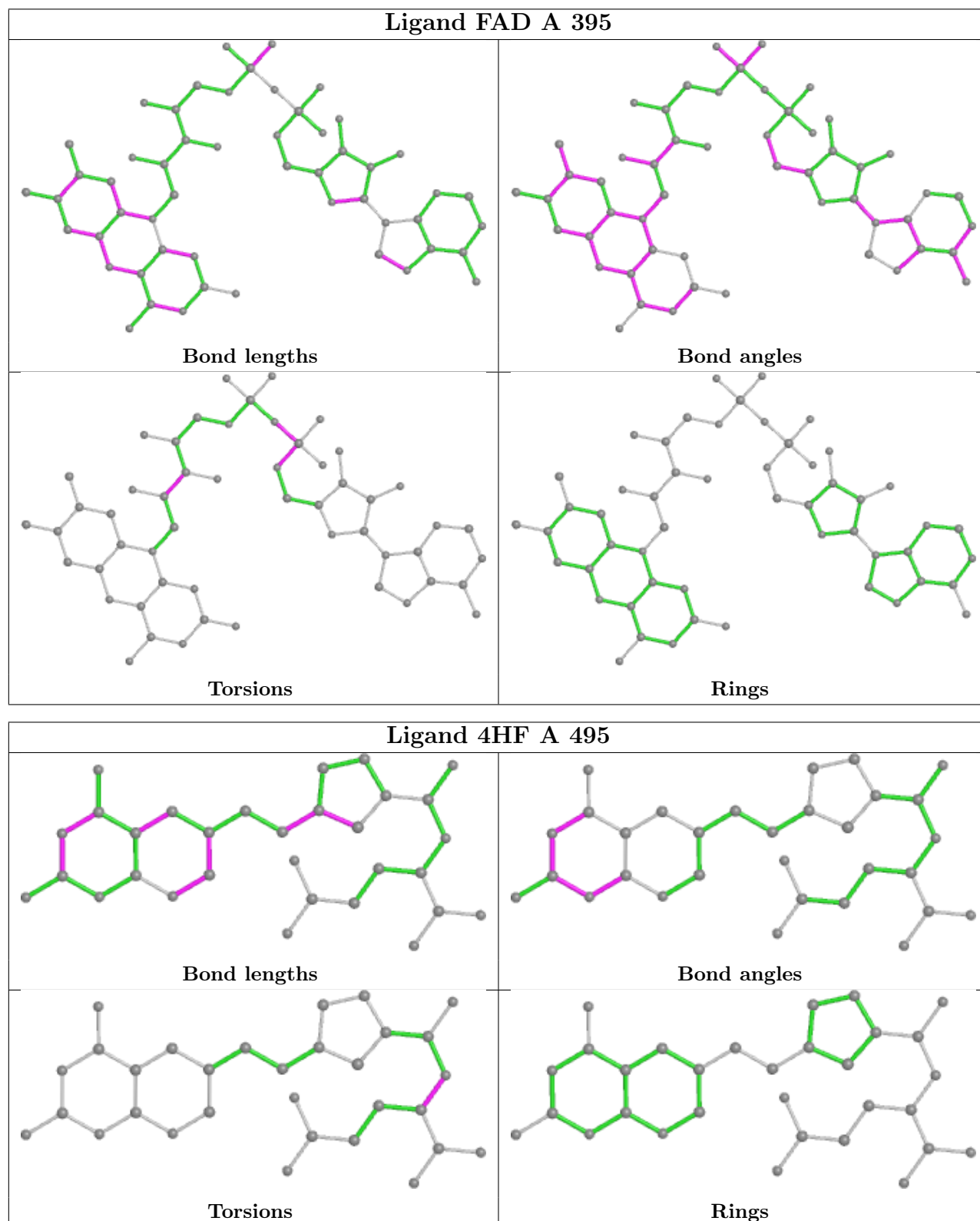
There are no ring outliers.

1 monomer is involved in 1 short contact:

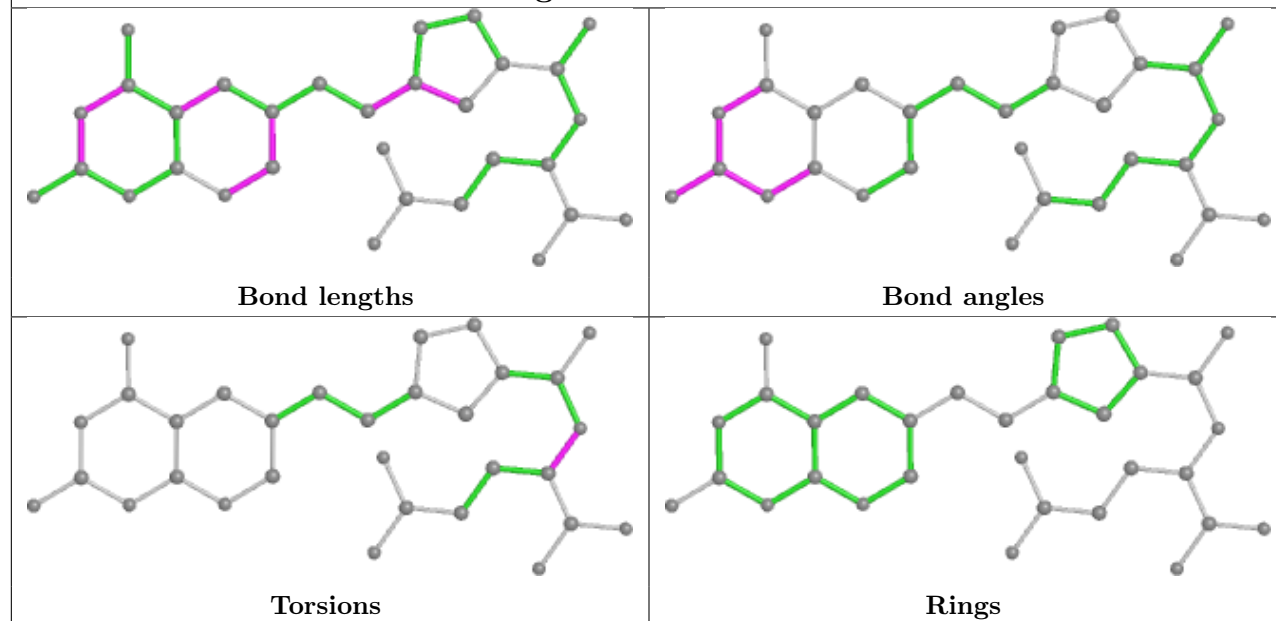
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	497	4HF	1	0

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

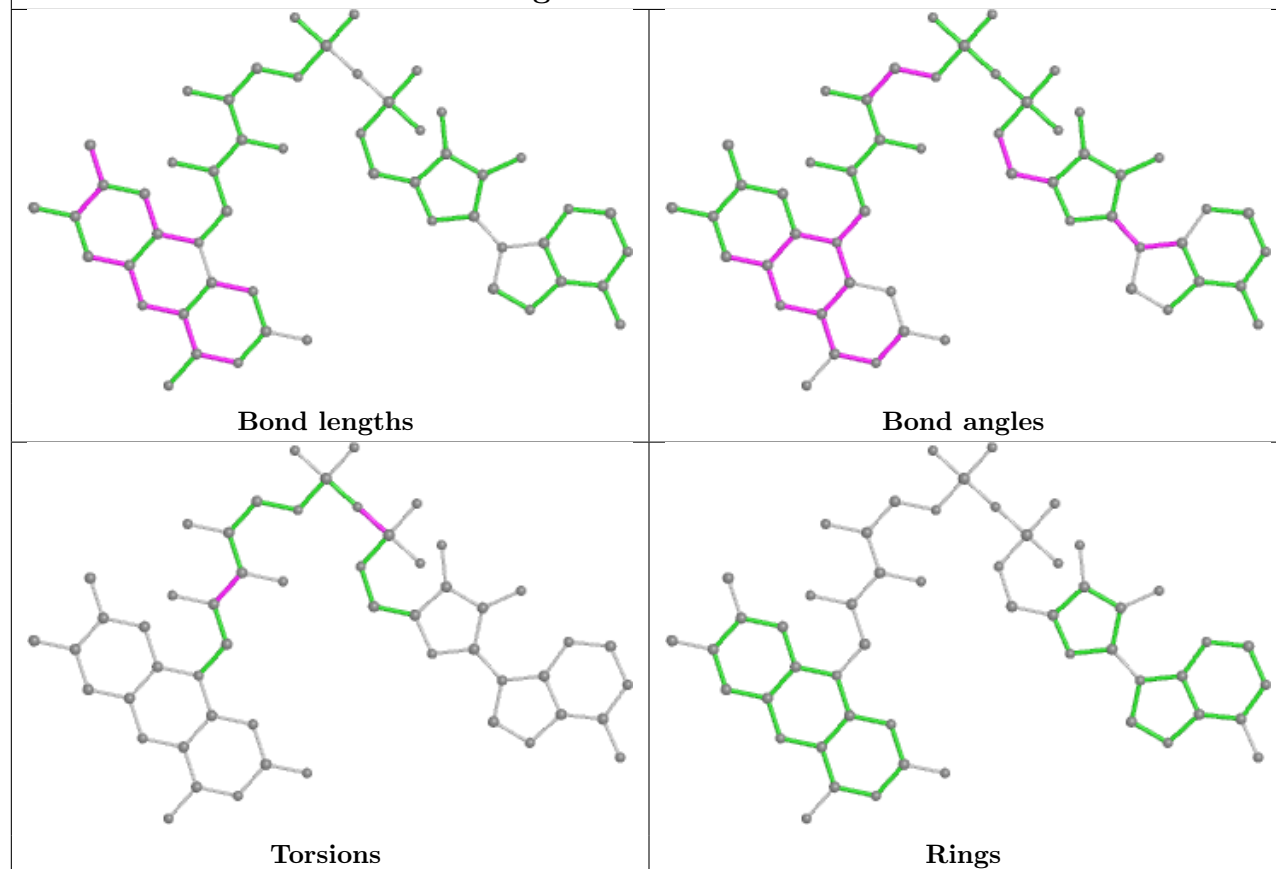
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

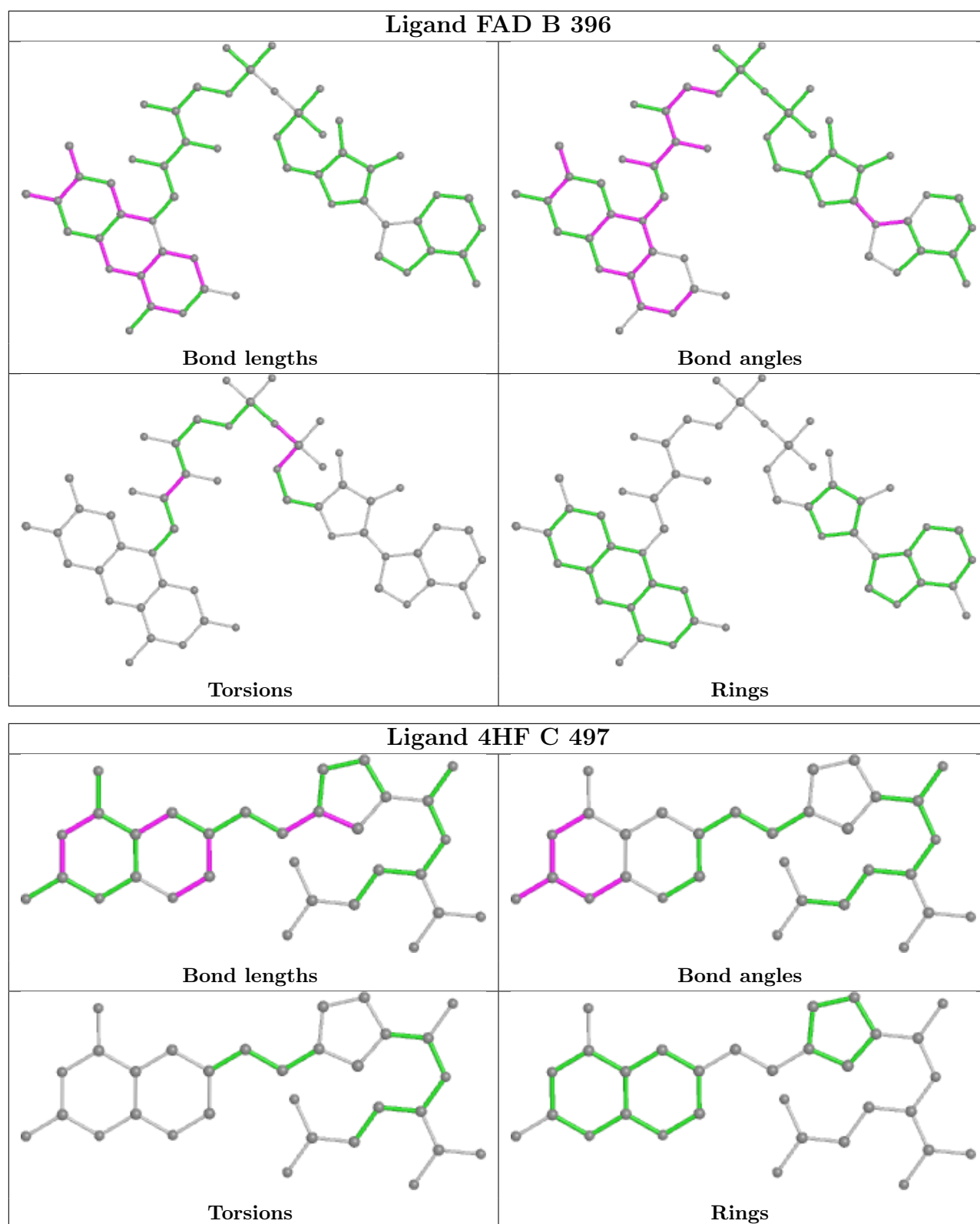


Ligand 4HF B 496



Ligand FAD C 397





5.7 Other polymers [i](#)

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, 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	288/304 (94%)	0.58	29 (10%) 7 7	21, 40, 65, 71	0
1	B	287/304 (94%)	0.02	5 (1%) 70 73	16, 30, 48, 58	0
1	C	271/304 (89%)	-0.03	8 (2%) 50 54	18, 29, 43, 56	0
All	All	846/912 (92%)	0.20	42 (4%) 28 31	16, 32, 58, 71	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	296	LEU	8.7
1	A	295	GLY	7.6
1	A	64	SER	6.3
1	C	128	PRO	4.9
1	A	104	ARG	4.6
1	A	21	GLY	4.6
1	C	21	GLY	4.6
1	A	102	ILE	4.2
1	C	121	LEU	4.1
1	C	295	GLY	4.1
1	A	107	TRP	4.1
1	A	110	GLY	4.0
1	C	122	PRO	3.8
1	A	108	ASN	3.7
1	A	109	ASN	3.6
1	B	65	GLY	3.5
1	A	143	ALA	3.4
1	B	66	GLU	3.4
1	A	92	ILE	3.4
1	A	71	HIS	3.4
1	A	103	ALA	3.3
1	A	112	ARG	3.3
1	A	65	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	66	GLU	3.1
1	A	129	GLU	2.9
1	A	63	ASN	2.9
1	A	145	PHE	2.9
1	A	101	THR	2.8
1	B	92	ILE	2.6
1	A	93	ASP	2.6
1	A	144	ASP	2.6
1	C	22	GLN	2.5
1	C	65	GLY	2.4
1	A	3	PHE	2.3
1	A	79	ASP	2.3
1	A	97	ASP	2.2
1	A	114	ILE	2.2
1	A	122	PRO	2.2
1	B	60	TYR	2.1
1	B	5	HIS	2.1
1	A	181	ILE	2.1
1	A	70	THR	2.1

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 monosaccharides 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(\AA^2)	Q<0.9
3	4HF	A	495	31/31	0.86	0.17	33,42,57,58	0
3	4HF	B	496	31/31	0.87	0.15	28,37,51,52	0
3	4HF	C	497	31/31	0.87	0.17	27,42,58,59	0
2	FAD	B	396	53/53	0.93	0.12	20,24,40,40	0

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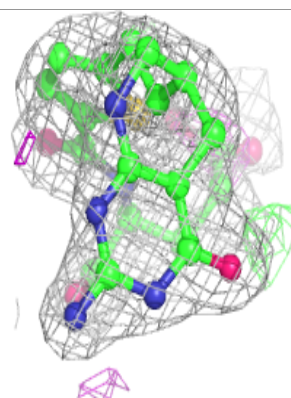
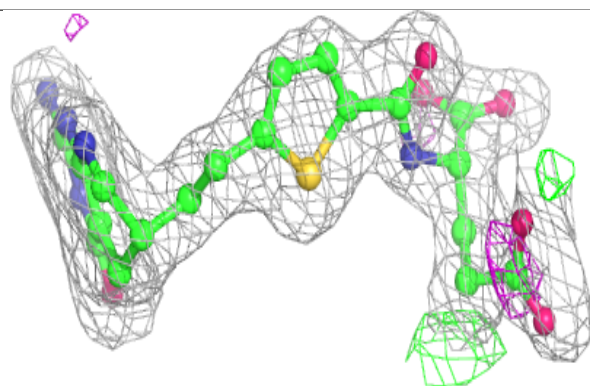
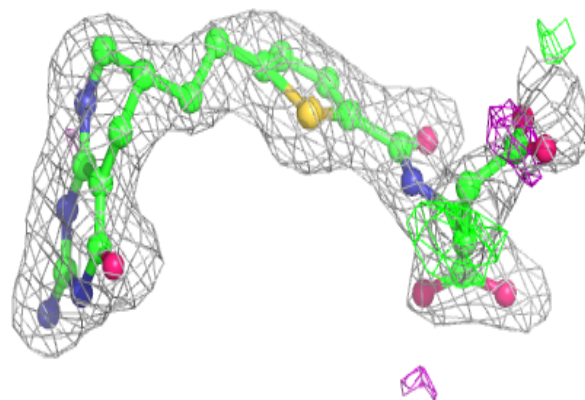
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FAD	A	395	53/53	0.93	0.12	28,31,47,48	0
2	FAD	C	397	53/53	0.95	0.10	20,24,39,40	0

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.

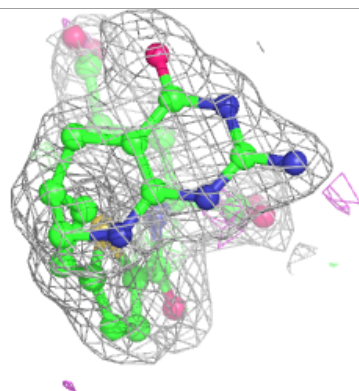
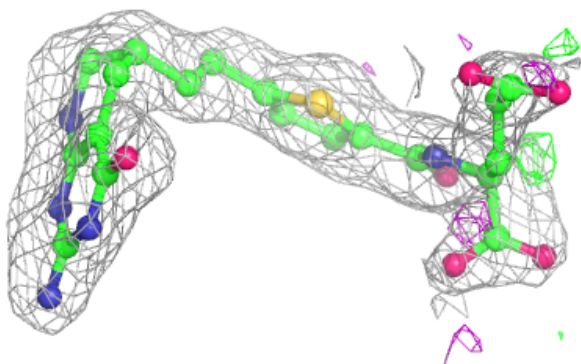
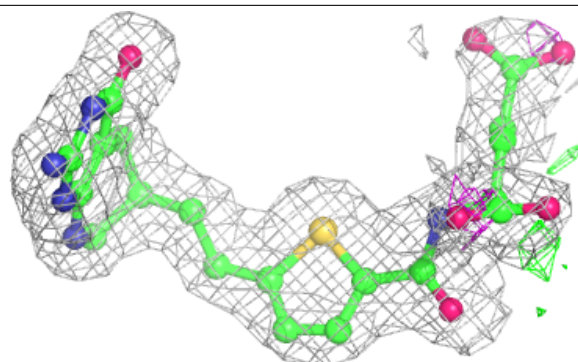
Electron density around 4HF A 495:

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

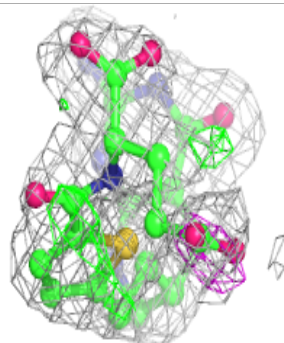
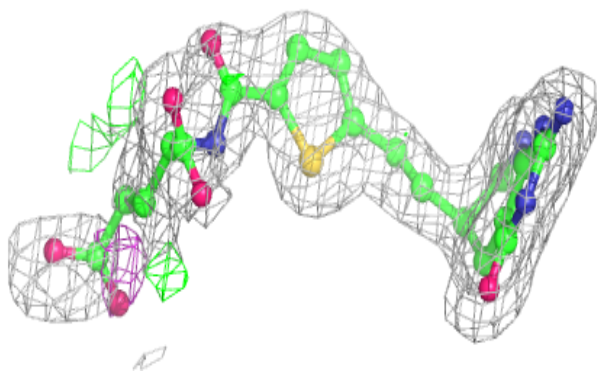
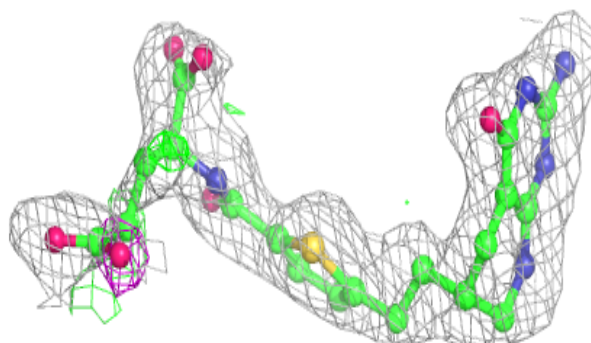


Electron density around 4HF B 496:

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

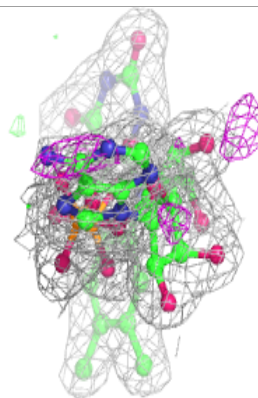
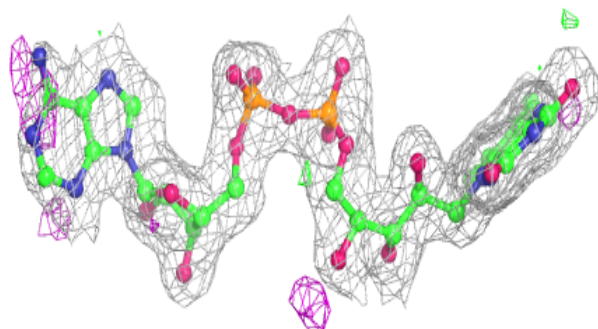
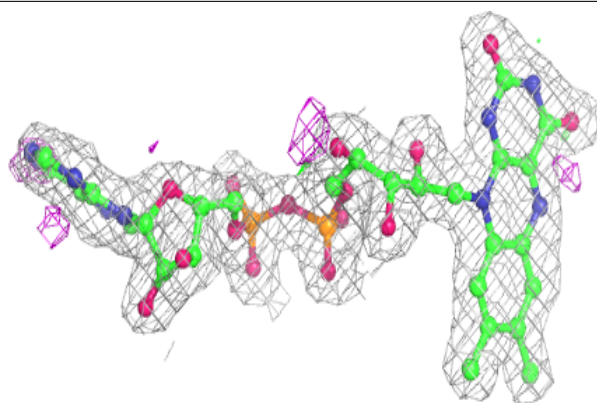
**Electron density around 4HF C 497:**

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

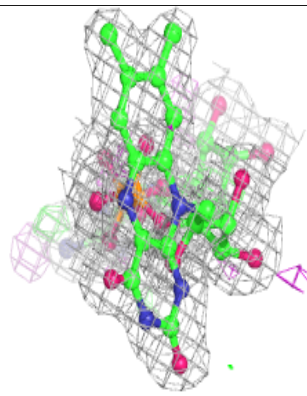
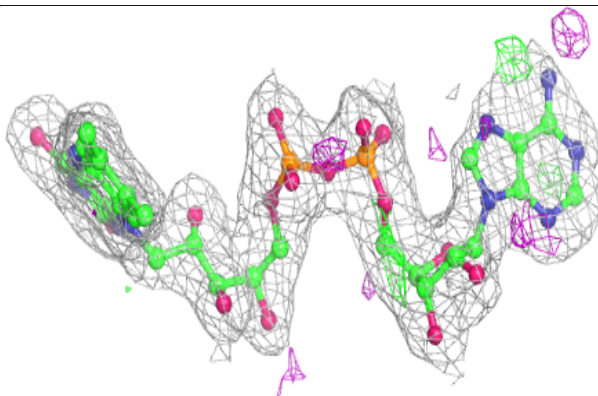
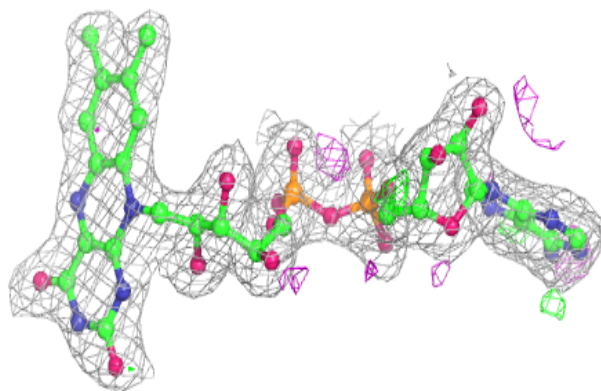


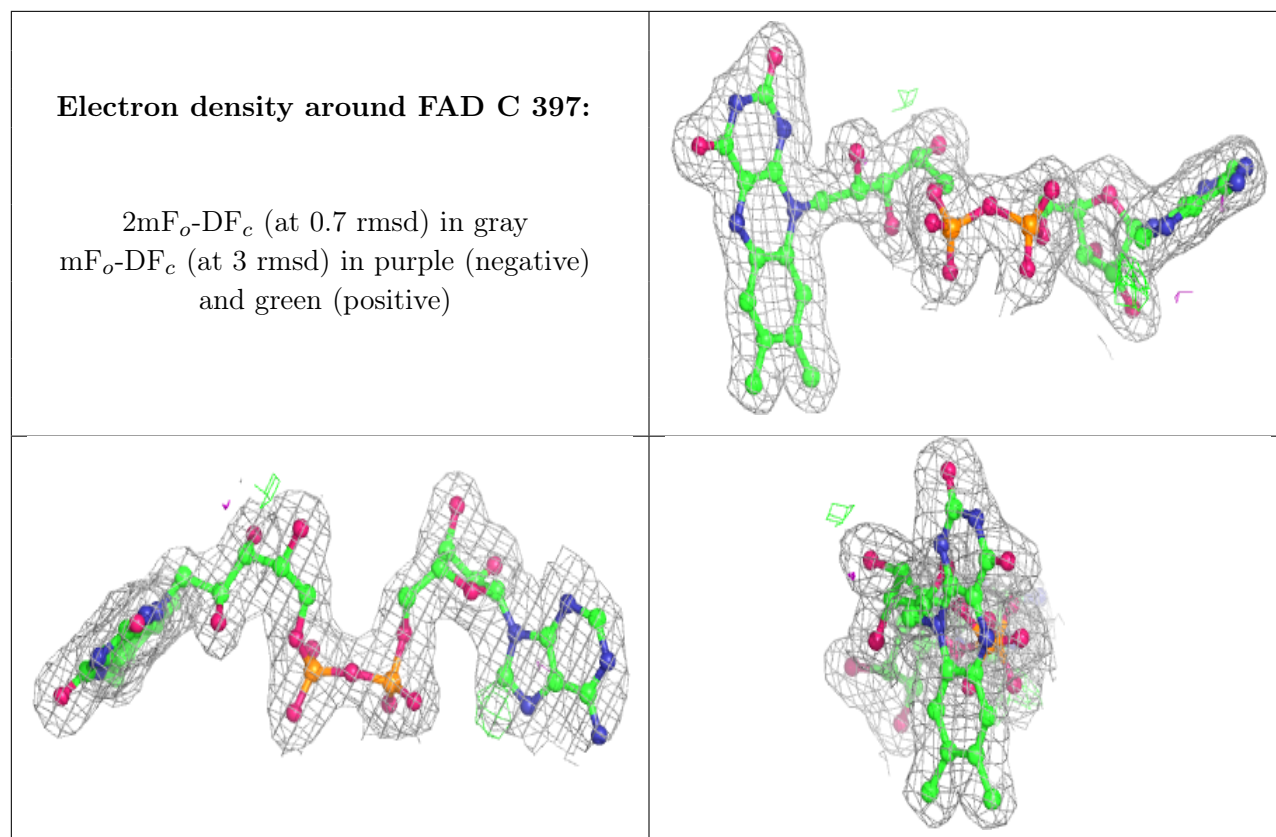
Electron density around FAD B 396:

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

**Electron density around FAD A 395:**

$2mF_o - DF_c$ (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.