Full wwPDB X-ray Structure Validation Report ⓘ

Jan 4, 2024 – 05:16 pm GMT

PDB ID	:	5AE1
Title	:	Ether Lipid-Generating Enzyme AGPS in complex with inhibitor ZINC69435460
Authors	:	Piano, V.; Benjamin, D.I.; Valente, S.; Nenci, S.; Marrocco, B.; Mai, A.; Aliverti, A.; Nomura, D.K.; Mattevi, A.
Deposited on	:	2015-08-25
Resolution	:	2.10 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:

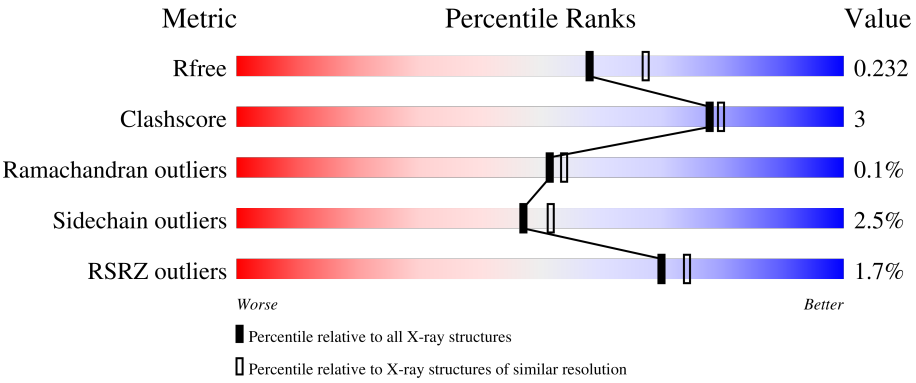
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	658	2% 78% 7% 15%
1	B	658	75% 7% 18%
1	C	658	76% 8% 15%
1	D	658	2% 79% 6% 14%

2 Entry composition (i)

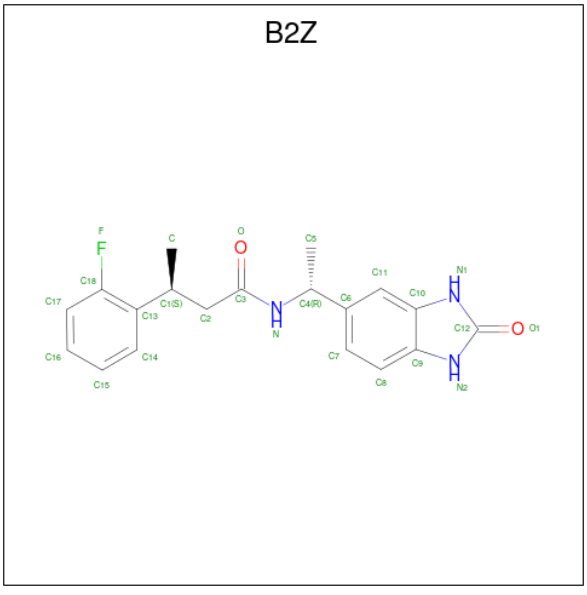
There are 5 unique types of molecules in this entry. The entry contains 18358 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE, PEROXISOMAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	560	Total	C	N	O	S	0	1	0
			4410	2810	761	815	24			
1	B	539	Total	C	N	O	S	0	0	0
			4254	2703	740	787	24			
1	C	559	Total	C	N	O	S	0	2	0
			4407	2800	761	822	24			
1	D	564	Total	C	N	O	S	0	0	0
			4395	2786	765	820	24			

- Molecule 2 is (3-(2-FLUOROPHENYL)-N-(1-(2-OXO-2,3-DIHYDRO-1H-BENZO[D]IMIDAZOL-5-YL)ETHYL)BUTANAMIDE) (three-letter code: B2Z) (formula: $C_{19}H_{20}FN_3O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			25	19	1	3	2		

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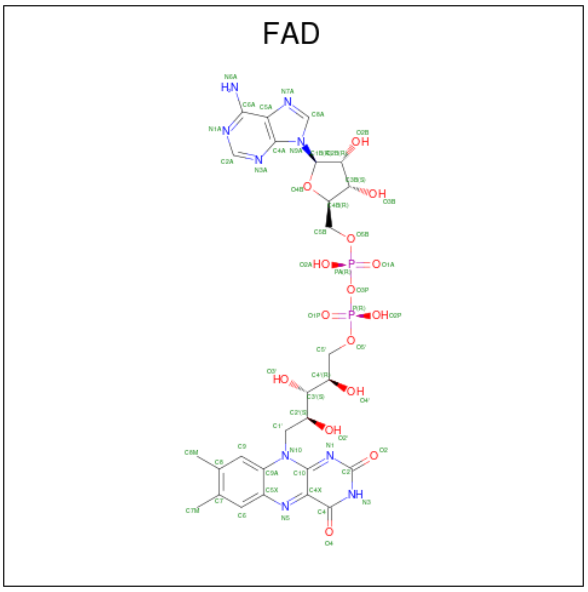
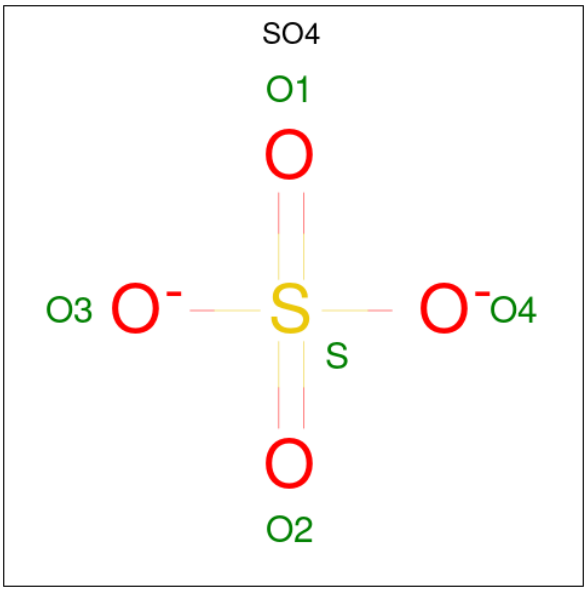
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	F	N	O	0	0
			25	19	1	3	2		
2	C	1	Total	C	F	N	O	0	0
			25	19	1	3	2		
2	D	1	Total	C	F	N	O	0	0
			25	19	1	3	2		

- 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
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is water.

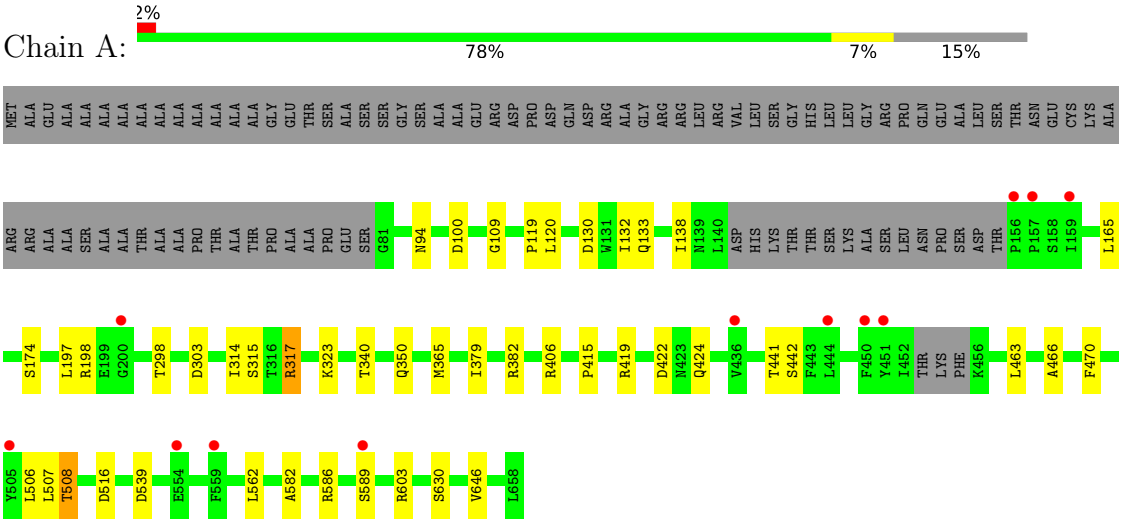
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	150	Total O 150 150	0	0
5	B	123	Total O 123 123	0	0
5	C	171	Total O 171 171	0	0
5	D	116	Total O 116 116	0	0

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.

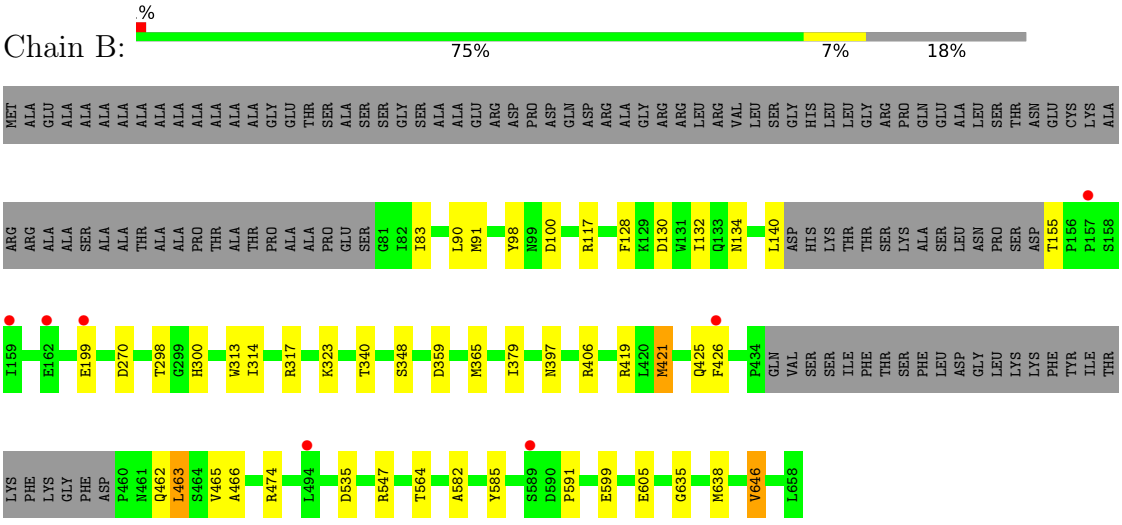
• Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE, PEROXISOMAL

Chain A:



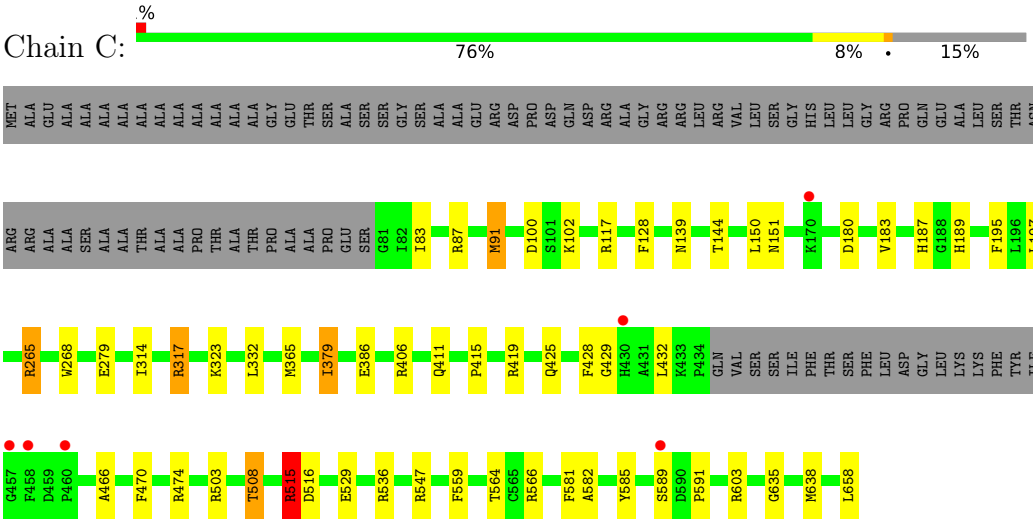
• Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE, PEROXISOMAL

Chain B:



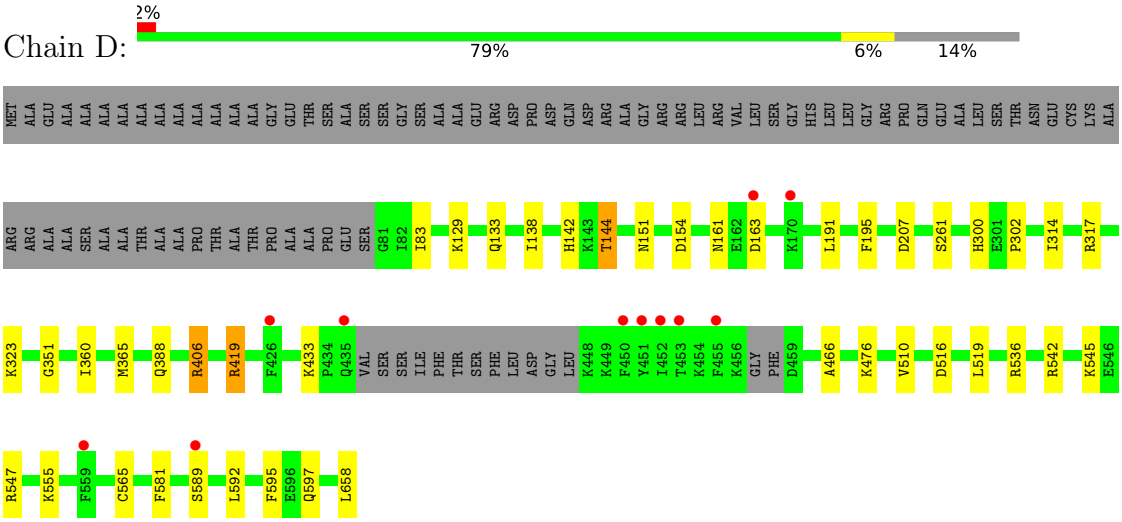
• Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE, PEROXISOMAL

Chain C:



• Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE, PEROXISOMAL

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	60.79Å 99.02Å 107.02Å 90.64° 89.96° 95.49°	Depositor
Resolution (Å)	107.01 – 2.10 40.14 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.6 (107.01-2.10) 93.6 (40.14-2.10)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, R_{free}	0.186 , 0.229 0.193 , 0.232	Depositor DCC
R_{free} test set	1484 reflections (1.09%)	wwPDB-VP
Wilson B-factor (Å^2)	26.9	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 45.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18358	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, SO4, B2Z

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	0.80	2/4514 (0.0%)	0.92	11/6103 (0.2%)
1	B	0.80	0/4350	0.87	7/5882 (0.1%)
1	C	0.83	0/4515	0.93	14/6110 (0.2%)
1	D	0.80	0/4493	0.90	7/6084 (0.1%)
All	All	0.81	2/17872 (0.0%)	0.90	39/24179 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	315	SER	CB-OG	-5.66	1.34	1.42
1	A	174	SER	CB-OG	-5.39	1.35	1.42

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	515	ARG	NE-CZ-NH2	-13.12	113.74	120.30
1	A	317	ARG	NE-CZ-NH1	10.85	125.73	120.30
1	C	317	ARG	NE-CZ-NH1	10.27	125.44	120.30
1	D	317	ARG	NE-CZ-NH1	9.51	125.05	120.30
1	C	515	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	B	317	ARG	NE-CZ-NH1	8.61	124.60	120.30
1	C	204	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	A	603	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	A	603	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	C	100	ASP	CB-CG-OD1	7.04	124.64	118.30
1	D	547	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	B	359	ASP	CB-CG-OD1	6.49	124.14	118.30
1	D	536	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	C	265	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	A	317	ARG	NE-CZ-NH2	-6.20	117.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	87	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	D	516	ASP	CB-CG-OD1	6.18	123.86	118.30
1	D	317	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	A	422	ASP	CB-CG-OD1	6.07	123.76	118.30
1	C	117	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	B	474	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	B	535	ASP	CB-CG-OD1	5.87	123.58	118.30
1	C	536	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	100	ASP	CB-CG-OD1	5.79	123.51	118.30
1	D	406	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	382	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	463	LEU	CA-CB-CG	5.59	128.15	115.30
1	A	516	ASP	CB-CG-OD1	5.53	123.27	118.30
1	C	516	ASP	CB-CG-OD1	5.45	123.20	118.30
1	B	359	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	A	539	ASP	CB-CG-OD1	5.24	123.02	118.30
1	C	547	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	C	603	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	C	603	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	D	207	ASP	CB-CG-OD2	5.11	122.90	118.30
1	C	91	MET	CG-SD-CE	-5.09	92.05	100.20
1	B	270	ASP	CB-CG-OD1	5.01	122.81	118.30
1	A	303	ASP	CB-CG-OD1	5.01	122.81	118.30
1	B	100	ASP	CB-CG-OD1	5.00	122.80	118.30

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	4410	0	4328	21	0
1	B	4254	0	4191	21	0
1	C	4407	0	4318	36	0
1	D	4395	0	4270	18	0
2	A	25	0	20	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	25	0	20	3	0
2	C	25	0	20	3	0
2	D	25	0	20	3	0
3	A	53	0	31	2	0
3	B	53	0	31	2	0
3	C	53	0	31	2	0
3	D	53	0	31	3	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	A	150	0	0	2	0
5	B	123	0	0	2	0
5	C	171	0	0	9	0
5	D	116	0	0	1	0
All	All	18358	0	17311	101	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (101) 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:411:GLN:HG2	5:C:2127:HOH:O	1.65	0.95
2:A:888:B2Z:H51C	3:A:999:FAD:HM82	1.58	0.84
1:D:300:HIS:ND1	1:D:302:PRO:HD3	1.99	0.78
1:C:150:LEU:HD22	1:C:180:ASP:HA	1.74	0.70
1:C:386:GLU:CD	5:C:2120:HOH:O	2.31	0.68
1:A:133:GLN:HG2	1:A:138:ILE:O	1.94	0.67
2:A:888:B2Z:C5	3:A:999:FAD:HM82	2.22	0.67
2:D:888:B2Z:H51C	3:D:999:FAD:HM82	1.79	0.65
1:C:246:MET:SD	5:C:2071:HOH:O	2.55	0.64
1:B:425:GLN:HG3	1:B:564:THR:OG1	1.99	0.63
1:C:515:ARG:HD3	5:C:2141:HOH:O	1.99	0.63
1:C:428:PHE:CZ	1:C:432:LEU:HD21	2.34	0.62
1:C:635:GLY:HA2	1:C:638:MET:CE	2.29	0.62
1:C:582:ALA:HB2	2:C:888:B2Z:H17	1.82	0.61
1:D:658:LEU:C	5:D:2109:HOH:O	2.38	0.61
2:C:888:B2Z:C5	3:C:999:FAD:HM82	2.31	0.61
1:C:635:GLY:HA2	1:C:638:MET:HE3	1.83	0.61
2:C:888:B2Z:H51C	3:C:999:FAD:HM82	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:MET:HB2	1:B:425:GLN:HB2	1.83	0.60
2:D:888:B2Z:C5	3:D:999:FAD:HM82	2.32	0.59
1:C:317:ARG:NH2	5:C:2092:HOH:O	2.37	0.57
1:C:411:GLN:CG	5:C:2127:HOH:O	2.36	0.57
1:C:332:LEU:HB3	1:C:379:ILE:CD1	2.35	0.56
2:B:888:B2Z:H51C	3:B:999:FAD:HM82	1.88	0.56
1:A:415:PRO:HB3	1:A:470:PHE:CE2	2.41	0.55
1:D:129:LYS:O	1:D:133:GLN:HG3	2.07	0.55
1:B:582:ALA:HB2	2:B:888:B2Z:H17	1.89	0.54
1:C:314:ILE:HG23	1:C:365:MET:HG2	1.89	0.54
1:A:314:ILE:HG23	1:A:365:MET:HG2	1.90	0.54
1:B:397:ASN:HA	1:B:462:GLN:O	2.08	0.54
1:D:161:ASN:OD1	1:D:163:ASP:N	2.41	0.53
1:D:314:ILE:HG23	1:D:365:MET:HG2	1.90	0.53
1:D:144:THR:HG21	1:D:519:LEU:O	2.10	0.52
1:B:314:ILE:HG23	1:B:365:MET:HG2	1.92	0.51
1:B:635:GLY:HA2	1:B:638:MET:HE3	1.93	0.51
1:D:133:GLN:HG2	1:D:138:ILE:O	2.10	0.51
1:A:94:ASN:HA	1:A:197:LEU:HD13	1.92	0.51
1:A:119:PRO:HG2	1:A:506:LEU:HD22	1.93	0.50
1:D:300:HIS:CE1	1:D:302:PRO:HD3	2.46	0.50
1:A:138:ILE:O	1:A:138:ILE:HD12	2.12	0.50
1:C:150:LEU:CD1	1:C:183:VAL:HG11	2.42	0.49
1:B:298:THR:HG21	1:B:379:ILE:HD12	1.94	0.49
1:B:340:THR:HB	1:B:646:VAL:HG13	1.95	0.49
1:A:424:GLN:NE2	1:A:562:LEU:HD12	2.28	0.49
1:C:83:ILE:HG23	1:C:91:MET:CE	2.43	0.49
1:A:298:THR:HG21	1:A:379:ILE:HD12	1.94	0.48
1:C:425:GLN:HG3	1:C:564:THR:OG1	2.13	0.48
1:C:429:GLY:O	1:C:503:ARG:NH2	2.47	0.47
1:B:585:TYR:HB2	1:B:591:PRO:HB3	1.95	0.47
1:A:132:ILE:HG22	1:A:138:ILE:HD11	1.95	0.47
1:B:155:THR:N	5:B:2024:HOH:O	2.47	0.47
1:A:317:ARG:NH1	5:A:2070:HOH:O	2.48	0.47
2:D:888:B2Z:C7	3:D:999:FAD:HM72	2.44	0.47
1:B:83:ILE:HD12	5:B:2058:HOH:O	2.15	0.47
1:B:300:HIS:HD2	1:B:313:TRP:CE3	2.33	0.47
1:B:426:PHE:CD1	1:B:465:VAL:HG21	2.49	0.47
1:A:419:ARG:O	1:A:466:ALA:HA	2.15	0.46
1:A:109:GLY:HA3	1:C:268:TRP:CE3	2.50	0.46
1:C:265:ARG:HD3	1:C:279:GLU:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:419:ARG:O	1:C:466:ALA:HA	2.15	0.46
1:A:582:ALA:HB2	2:A:888:B2Z:H17	1.98	0.45
1:C:515:ARG:CD	5:C:2141:HOH:O	2.61	0.45
5:C:2144:HOH:O	1:D:351:GLY:N	2.49	0.45
1:A:419:ARG:HH22	1:A:508:THR:HG21	1.82	0.44
1:C:658:LEU:C	5:C:2163:HOH:O	2.56	0.44
1:B:419:ARG:O	1:B:466:ALA:HA	2.17	0.44
1:B:463:LEU:C	1:B:463:LEU:HD23	2.38	0.44
1:A:119:PRO:CG	1:A:506:LEU:HD22	2.48	0.44
1:A:442:SER:HB3	1:D:542:ARG:NH1	2.32	0.44
1:C:425:GLN:HE22	1:C:566:ARG:CD	2.31	0.44
1:D:555:LYS:NZ	1:D:597:GLN:OE1	2.46	0.44
1:D:191:LEU:HD23	1:D:595:PHE:CD2	2.53	0.43
1:D:151:ASN:HB3	1:D:154:ASP:OD2	2.18	0.43
1:B:635:GLY:HA2	1:B:638:MET:CE	2.47	0.43
1:C:150:LEU:HD11	1:C:183:VAL:HG21	2.00	0.43
2:B:888:B2Z:C5	3:B:999:FAD:HM82	2.48	0.43
1:C:585:TYR:HB2	1:C:591:PRO:HB3	2.01	0.43
1:C:332:LEU:HB3	1:C:379:ILE:HD13	2.01	0.43
1:B:547:ARG:NH1	1:B:605:GLU:OE1	2.48	0.43
1:D:360:ILE:HD13	1:D:360:ILE:HG21	1.75	0.43
1:C:386:GLU:OE1	1:C:474:ARG:NH1	2.52	0.42
1:B:83:ILE:HG23	1:B:91:MET:CE	2.50	0.42
1:C:635:GLY:HA2	1:C:638:MET:HE2	2.02	0.42
1:D:545:LYS:HE3	1:D:565:CYS:SG	2.59	0.42
1:B:98:TYR:CD2	1:B:117:ARG:HD3	2.55	0.42
1:C:189:HIS:O	1:C:515:ARG:NH2	2.52	0.42
1:A:630:SER:HA	1:B:348:SER:OG	2.20	0.42
1:C:150:LEU:HG	1:C:151:ASN:N	2.34	0.42
1:C:415:PRO:HB3	1:C:470:PHE:CD1	2.55	0.41
1:C:187:HIS:CE1	1:C:197:LEU:HD11	2.55	0.41
1:D:419:ARG:O	1:D:466:ALA:HA	2.21	0.41
1:C:425:GLN:HE22	1:C:566:ARG:HD3	1.85	0.41
1:B:128:PHE:O	1:B:132:ILE:HG13	2.21	0.40
1:A:350:GLN:HA	5:A:2080:HOH:O	2.20	0.40
1:C:83:ILE:HG23	1:C:91:MET:HE3	2.02	0.40
1:A:340:THR:HB	1:A:646:VAL:HG13	2.03	0.40
1:A:442:SER:CB	1:D:542:ARG:NH1	2.85	0.40
1:D:83:ILE:HB	1:D:261:SER:HB2	2.04	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	555/658 (84%)	543 (98%)	10 (2%)	2 (0%)	34	32
1	B	533/658 (81%)	522 (98%)	11 (2%)	0	100	100
1	C	557/658 (85%)	547 (98%)	10 (2%)	0	100	100
1	D	558/658 (85%)	549 (98%)	9 (2%)	0	100	100
All	All	2203/2632 (84%)	2161 (98%)	40 (2%)	2 (0%)	51	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	ARG
1	A	586	ARG

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	471/545 (86%)	462 (98%)	9 (2%)	57	63
1	B	457/545 (84%)	446 (98%)	11 (2%)	49	53
1	C	474/545 (87%)	460 (97%)	14 (3%)	41	44
1	D	465/545 (85%)	452 (97%)	13 (3%)	43	47
All	All	1867/2180 (86%)	1820 (98%)	47 (2%)	47	52

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	LEU
1	A	130	ASP
1	A	165	LEU
1	A	323	LYS
1	A	406	ARG
1	A	441	THR
1	A	507	LEU
1	A	508	THR
1	A	589	SER
1	B	90	LEU
1	B	130	ASP
1	B	134	ASN
1	B	140	LEU
1	B	199	GLU
1	B	323	LYS
1	B	406	ARG
1	B	421	MET
1	B	463	LEU
1	B	599	GLU
1	B	646	VAL
1	C	102	LYS
1	C	128	PHE
1	C	139	ASN
1	C	144	THR
1	C	195	PHE
1	C	323	LYS
1	C	379	ILE
1	C	406	ARG
1	C	508	THR
1	C	515	ARG
1	C	529	GLU
1	C	559	PHE
1	C	581	PHE
1	C	589	SER
1	D	142	HIS
1	D	144	THR
1	D	195	PHE
1	D	323	LYS
1	D	388	GLN
1	D	406	ARG
1	D	419	ARG
1	D	433	LYS
1	D	476	LYS

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Mol	Chain	Res	Type
1	D	510	VAL
1	D	581	PHE
1	D	589	SER
1	D	592	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	290	GLN
1	A	335	HIS
1	A	424	GLN
1	B	290	GLN
1	B	430	HIS
1	C	423	ASN
1	C	425	GLN
1	C	427	GLN
1	D	388	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 (i)

12 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	B2Z	C	888	-	27,27,27	1.05	3 (11%)	36,38,38	2.35	6 (16%)
3	FAD	D	999	-	53,58,58	1.25	6 (11%)	68,89,89	1.49	13 (19%)
3	FAD	B	999	-	53,58,58	1.57	11 (20%)	68,89,89	1.36	11 (16%)
3	FAD	A	999	-	53,58,58	1.60	6 (11%)	68,89,89	1.54	17 (25%)
2	B2Z	A	888	-	27,27,27	1.52	5 (18%)	36,38,38	2.00	6 (16%)
4	SO4	A	1659	-	4,4,4	0.31	0	6,6,6	0.64	0
2	B2Z	D	888	-	27,27,27	1.53	3 (11%)	36,38,38	2.30	11 (30%)
4	SO4	B	1659	-	4,4,4	0.68	0	6,6,6	0.86	0
3	FAD	C	999	-	53,58,58	1.52	10 (18%)	68,89,89	1.58	17 (25%)
2	B2Z	B	888	-	27,27,27	1.54	6 (22%)	36,38,38	2.08	9 (25%)
4	SO4	C	1659	-	4,4,4	0.36	0	6,6,6	0.92	0
4	SO4	D	1659	-	4,4,4	0.53	0	6,6,6	0.90	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	B2Z	C	888	-	-	0/16/16/16	0/3/3/3
3	FAD	D	999	-	-	2/30/50/50	0/6/6/6
3	FAD	B	999	-	-	3/30/50/50	0/6/6/6
3	FAD	A	999	-	-	2/30/50/50	0/6/6/6
2	B2Z	A	888	-	-	0/16/16/16	0/3/3/3
2	B2Z	D	888	-	-	0/16/16/16	0/3/3/3
3	FAD	C	999	-	-	2/30/50/50	0/6/6/6
2	B2Z	B	888	-	-	0/16/16/16	0/3/3/3

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	FAD	C9A-C5X	7.99	1.54	1.41
3	C	999	FAD	C9A-C5X	5.14	1.49	1.41
3	B	999	FAD	C9A-C5X	4.41	1.48	1.41
3	A	999	FAD	C8-C7	4.08	1.51	1.40
2	A	888	B2Z	C10-N1	-3.82	1.31	1.38
3	C	999	FAD	C4-N3	-3.74	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	999	FAD	C4-N3	-3.73	1.31	1.38
2	D	888	B2Z	C10-N1	-3.72	1.32	1.38
2	B	888	B2Z	C12-N1	-3.52	1.31	1.37
3	D	999	FAD	C4-N3	-3.50	1.32	1.38
2	B	888	B2Z	C10-N1	-3.49	1.32	1.38
2	D	888	B2Z	C12-N1	-3.47	1.32	1.37
2	D	888	B2Z	O1-C12	3.34	1.30	1.23
2	A	888	B2Z	C12-N1	-3.33	1.32	1.37
3	D	999	FAD	C9A-C5X	3.29	1.46	1.41
3	A	999	FAD	C4-N3	-3.17	1.33	1.38
2	B	888	B2Z	C13-C1	-3.10	1.47	1.52
3	B	999	FAD	C2-N3	-3.00	1.32	1.39
2	A	888	B2Z	O1-C12	2.97	1.29	1.23
3	B	999	FAD	C5X-N5	-2.95	1.33	1.39
3	B	999	FAD	O4B-C1B	2.79	1.45	1.41
2	A	888	B2Z	C7-C6	2.77	1.43	1.39
2	B	888	B2Z	C12-N2	-2.63	1.33	1.37
3	C	999	FAD	PA-O2A	-2.56	1.43	1.55
3	A	999	FAD	C4X-N5	2.56	1.35	1.30
3	B	999	FAD	C8-C7	2.51	1.47	1.40
3	B	999	FAD	C2-N1	-2.49	1.30	1.36
3	D	999	FAD	O2-C2	2.48	1.28	1.24
2	C	888	B2Z	C7-C6	2.47	1.43	1.39
3	C	999	FAD	C6-C5X	2.45	1.43	1.40
2	B	888	B2Z	C7-C6	2.43	1.43	1.39
3	D	999	FAD	C9-C8	-2.38	1.36	1.39
2	B	888	B2Z	O1-C12	2.38	1.28	1.23
3	B	999	FAD	C1'-C2'	2.36	1.56	1.52
3	C	999	FAD	O2'-C2'	2.35	1.48	1.43
3	B	999	FAD	C5A-C4A	2.33	1.47	1.40
3	B	999	FAD	C2A-N3A	2.33	1.35	1.32
2	C	888	B2Z	O1-C12	2.28	1.28	1.23
3	C	999	FAD	C5A-C4A	2.26	1.46	1.40
3	D	999	FAD	C5X-N5	-2.26	1.35	1.39
3	C	999	FAD	C10-N1	2.23	1.37	1.33
3	C	999	FAD	C8-C7	2.19	1.46	1.40
2	A	888	B2Z	C13-C1	-2.18	1.49	1.52
2	C	888	B2Z	C10-N1	-2.13	1.34	1.38
3	C	999	FAD	C2'-C3'	-2.11	1.49	1.53
3	C	999	FAD	C2-N3	-2.10	1.34	1.39
3	A	999	FAD	C5A-C4A	2.10	1.46	1.40
3	D	999	FAD	C2B-C1B	-2.10	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	FAD	C4X-C10	2.03	1.50	1.44
3	B	999	FAD	PA-O2A	-2.00	1.45	1.55

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	888	B2Z	N2-C12-N1	7.37	115.18	106.57
2	C	888	B2Z	C9-N2-C12	-7.08	102.64	110.12
2	D	888	B2Z	O1-C12-N1	-6.86	118.93	126.72
2	C	888	B2Z	O1-C12-N1	-6.47	119.37	126.72
2	D	888	B2Z	C9-N2-C12	-5.84	103.96	110.12
2	A	888	B2Z	C9-N2-C12	-5.69	104.11	110.12
2	A	888	B2Z	N2-C12-N1	5.41	112.89	106.57
2	D	888	B2Z	N2-C12-N1	5.17	112.61	106.57
2	B	888	B2Z	N2-C12-N1	5.04	112.46	106.57
2	A	888	B2Z	O1-C12-N1	-4.97	121.08	126.72
2	B	888	B2Z	C9-N2-C12	-4.86	104.98	110.12
2	B	888	B2Z	O1-C12-N1	-4.81	121.26	126.72
2	C	888	B2Z	C10-N1-C12	-4.04	105.85	110.12
3	C	999	FAD	C1B-N9A-C4A	-3.97	119.67	126.64
3	C	999	FAD	C4-C4X-N5	3.93	123.83	118.23
2	B	888	B2Z	C17-C18-C13	-3.87	119.41	123.72
2	D	888	B2Z	C17-C18-C13	-3.82	119.47	123.72
3	C	999	FAD	C9A-C5X-N5	-3.46	118.67	122.43
2	A	888	B2Z	C17-C18-C13	-3.43	119.90	123.72
3	D	999	FAD	C1B-N9A-C4A	-3.42	120.64	126.64
3	B	999	FAD	C4-C4X-N5	3.41	123.09	118.23
3	B	999	FAD	O2A-PA-O1A	3.39	128.98	112.24
2	B	888	B2Z	C14-C13-C18	3.31	120.38	116.13
2	D	888	B2Z	C1-C2-C3	-3.30	108.44	113.03
2	A	888	B2Z	C14-C13-C18	3.30	120.37	116.13
2	D	888	B2Z	C4-N-C3	-3.29	118.21	122.90
3	A	999	FAD	C9A-C5X-N5	-3.26	118.89	122.43
3	A	999	FAD	C5X-C9A-N10	3.25	121.31	117.95
3	A	999	FAD	C8M-C8-C9	-3.17	113.62	119.49
3	A	999	FAD	N3A-C2A-N1A	-3.16	123.73	128.68
2	B	888	B2Z	C2-C1-C13	-3.14	103.26	110.75
3	D	999	FAD	N3A-C2A-N1A	-3.11	123.82	128.68
3	D	999	FAD	C4-C4X-N5	3.10	122.64	118.23
3	A	999	FAD	C4X-C10-N10	3.06	120.95	116.48
3	A	999	FAD	C5'-C4'-C3'	3.01	118.02	112.20
3	C	999	FAD	O2P-P-O1P	3.00	127.05	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	999	FAD	C4X-C10-N1	-2.89	118.02	124.73
3	B	999	FAD	N3A-C2A-N1A	-2.80	124.31	128.68
2	C	888	B2Z	C4-N-C3	-2.80	118.91	122.90
3	D	999	FAD	C2A-N1A-C6A	2.79	123.53	118.75
3	D	999	FAD	C10-N1-C2	2.69	122.28	116.90
2	B	888	B2Z	C5-C4-C6	2.64	118.28	112.25
2	B	888	B2Z	C4-N-C3	-2.63	119.15	122.90
3	C	999	FAD	O2A-PA-O1A	2.63	125.26	112.24
3	C	999	FAD	C4X-C10-N1	-2.62	118.65	124.73
3	A	999	FAD	O2A-PA-O1A	2.62	125.17	112.24
3	C	999	FAD	O2-C2-N1	-2.60	117.52	121.83
3	A	999	FAD	C1B-N9A-C4A	-2.60	122.08	126.64
3	D	999	FAD	C4X-C10-N10	2.58	120.26	116.48
3	A	999	FAD	C9A-N10-C10	-2.58	116.75	120.77
2	D	888	B2Z	C2-C1-C13	-2.55	104.66	110.75
3	B	999	FAD	C10-N1-C2	2.53	121.96	116.90
3	D	999	FAD	C5X-C9A-N10	2.53	120.56	117.95
3	B	999	FAD	O2P-P-O1P	2.51	124.64	112.24
2	D	888	B2Z	F-C18-C13	2.46	122.22	118.23
3	C	999	FAD	C4X-C4-N3	2.44	119.38	113.19
2	A	888	B2Z	C2-C1-C13	-2.43	104.95	110.75
3	A	999	FAD	C8M-C8-C7	2.42	125.69	120.74
3	A	999	FAD	O2P-P-O1P	2.41	124.14	112.24
3	C	999	FAD	C5X-N5-C4X	2.37	122.02	118.07
3	A	999	FAD	C1'-N10-C9A	2.37	124.46	120.51
3	D	999	FAD	C9A-N10-C10	-2.34	117.13	120.77
3	B	999	FAD	C1B-N9A-C4A	-2.33	122.54	126.64
3	D	999	FAD	O3'-C3'-C4'	2.33	114.44	108.81
2	B	888	B2Z	C5-C4-N	-2.31	104.98	109.05
3	A	999	FAD	P-O3P-PA	-2.30	124.93	132.83
3	C	999	FAD	C5X-C9A-N10	2.30	120.33	117.95
3	A	999	FAD	C4-C4X-N5	2.30	121.50	118.23
3	C	999	FAD	C2A-N1A-C6A	2.26	122.62	118.75
3	C	999	FAD	N3A-C2A-N1A	-2.25	125.16	128.68
3	C	999	FAD	N6A-C6A-N1A	2.24	123.22	118.57
3	A	999	FAD	C4X-C10-N1	-2.22	119.57	124.73
3	B	999	FAD	C9A-C5X-N5	-2.21	120.03	122.43
3	D	999	FAD	O2A-PA-O1A	2.17	122.97	112.24
2	D	888	B2Z	C16-C17-C18	2.16	122.00	118.46
3	C	999	FAD	C4X-C10-N10	2.15	119.63	116.48
3	D	999	FAD	C4X-C10-N1	-2.12	119.80	124.73
3	B	999	FAD	C4X-C4-N3	2.12	118.58	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	999	FAD	C10-N1-C2	2.11	121.13	116.90
3	A	999	FAD	O2'-C2'-C1'	2.11	114.89	109.80
3	B	999	FAD	C8M-C8-C9	-2.10	115.61	119.49
3	A	999	FAD	C2A-N1A-C6A	2.10	122.35	118.75
3	B	999	FAD	C5X-C9A-N10	2.09	120.11	117.95
2	D	888	B2Z	C14-C13-C18	2.09	118.81	116.13
3	C	999	FAD	C5'-C4'-C3'	2.07	116.20	112.20
2	C	888	B2Z	C10-C9-N2	2.06	109.32	106.42
3	D	999	FAD	C4X-C4-N3	2.06	118.42	113.19
2	D	888	B2Z	C10-N1-C12	-2.06	107.94	110.12
3	D	999	FAD	C4A-C5A-N7A	-2.02	107.29	109.40
3	C	999	FAD	O4-C4-C4X	-2.00	121.29	126.60

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	999	FAD	N10-C1'-C2'-O2'
3	A	999	FAD	N10-C1'-C2'-C3'
3	B	999	FAD	N10-C1'-C2'-O2'
3	B	999	FAD	N10-C1'-C2'-C3'
3	C	999	FAD	N10-C1'-C2'-O2'
3	C	999	FAD	N10-C1'-C2'-C3'
3	D	999	FAD	N10-C1'-C2'-O2'
3	D	999	FAD	N10-C1'-C2'-C3'
3	B	999	FAD	PA-O3P-P-O2P

There are no ring outliers.

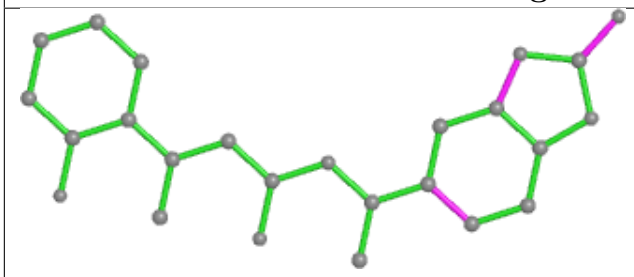
8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	888	B2Z	3	0
3	D	999	FAD	3	0
3	B	999	FAD	2	0
3	A	999	FAD	2	0
2	A	888	B2Z	3	0
2	D	888	B2Z	3	0
3	C	999	FAD	2	0
2	B	888	B2Z	3	0

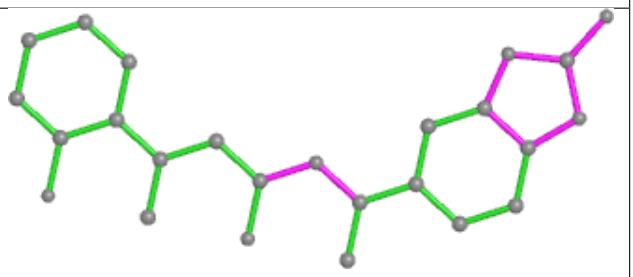
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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

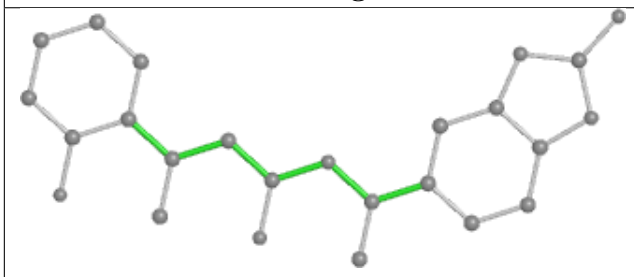
Ligand B2Z C 888



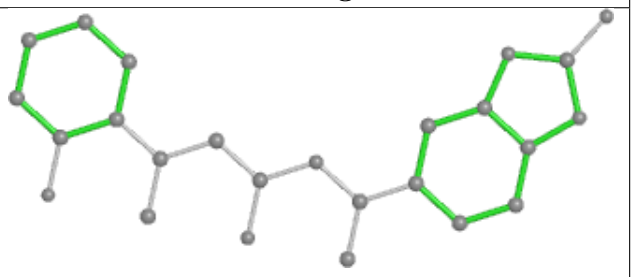
Bond lengths



Bond angles

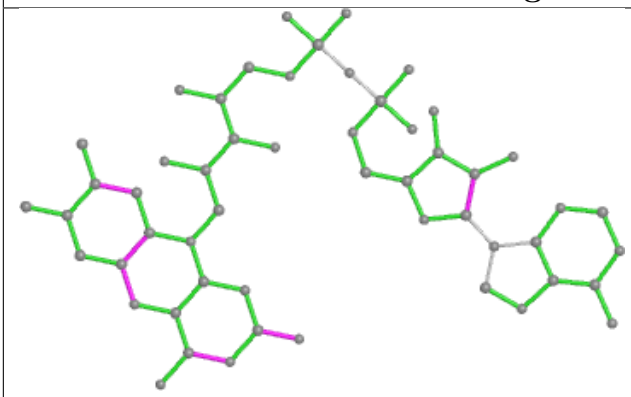


Torsions

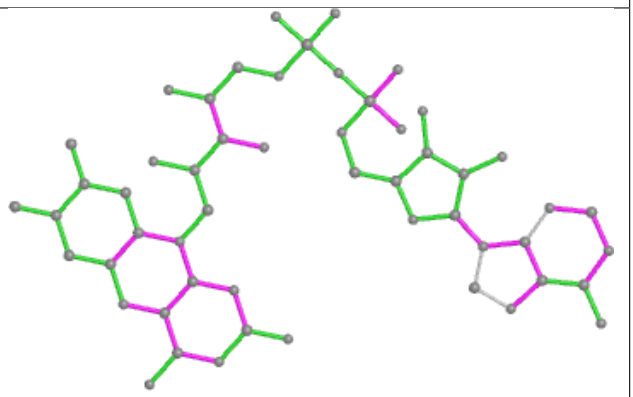


Rings

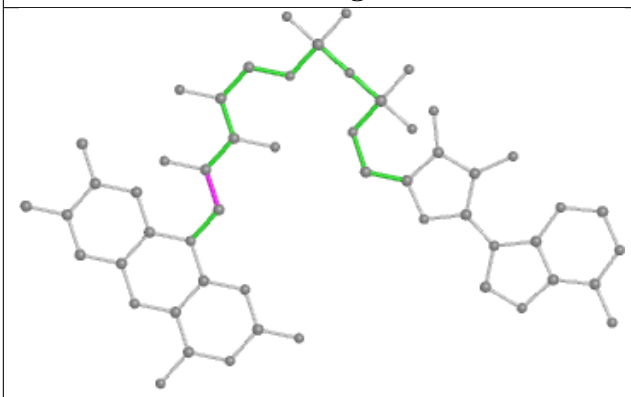
Ligand FAD D 999



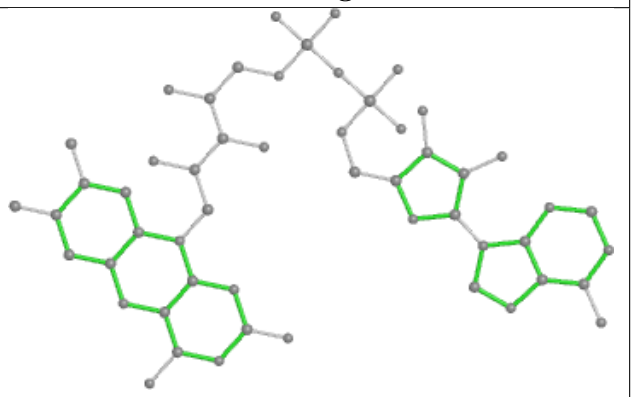
Bond lengths



Bond angles

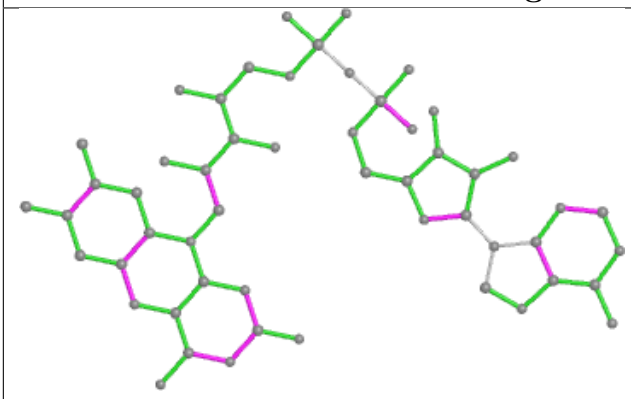


Torsions

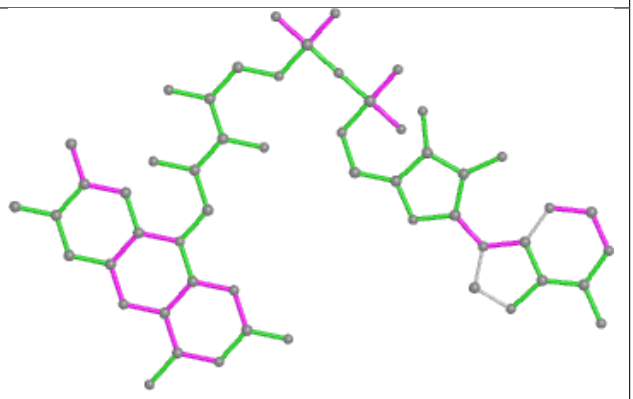


Rings

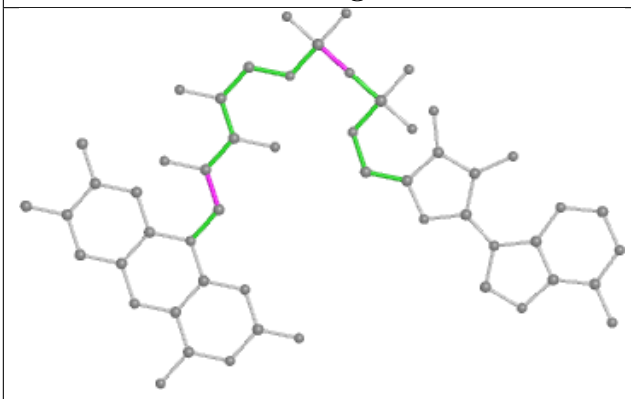
Ligand FAD B 999



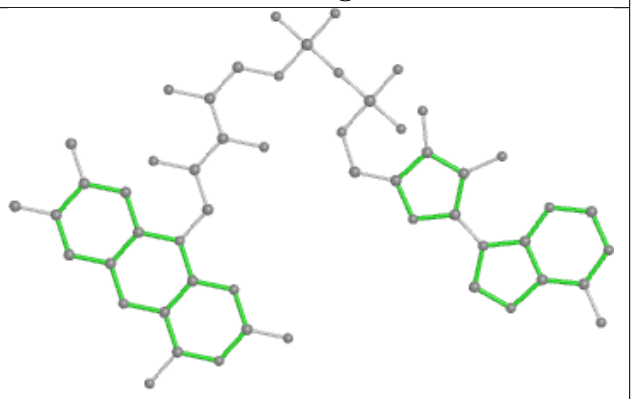
Bond lengths



Bond angles

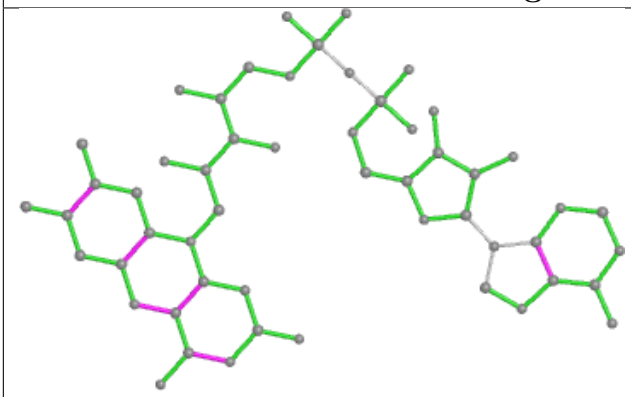


Torsions

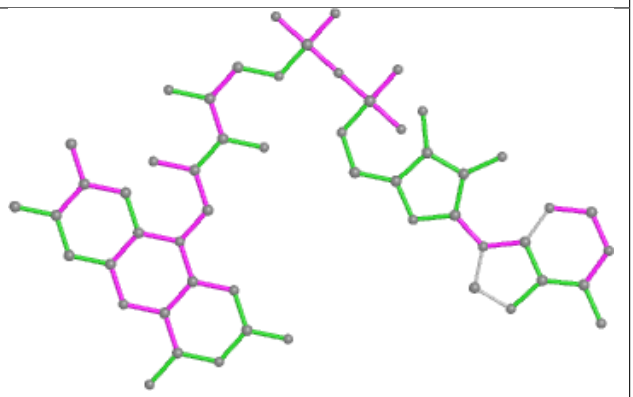


Rings

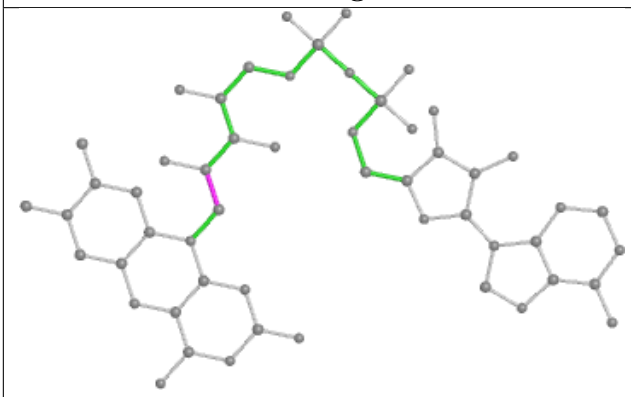
Ligand FAD A 999



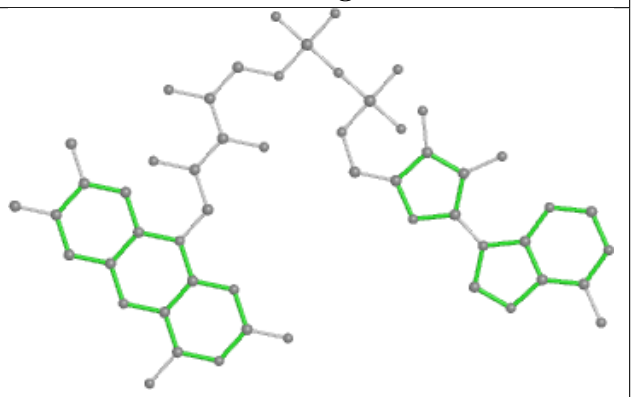
Bond lengths



Bond angles

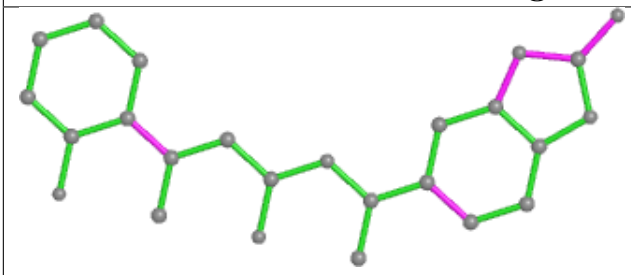


Torsions

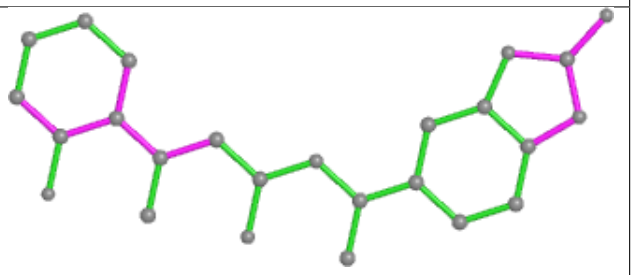


Rings

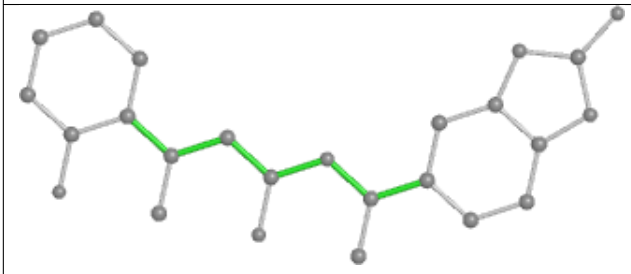
Ligand B2Z A 888



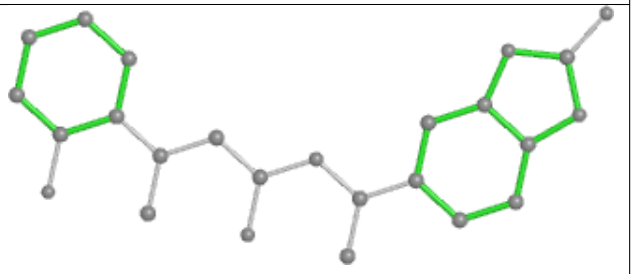
Bond lengths



Bond angles

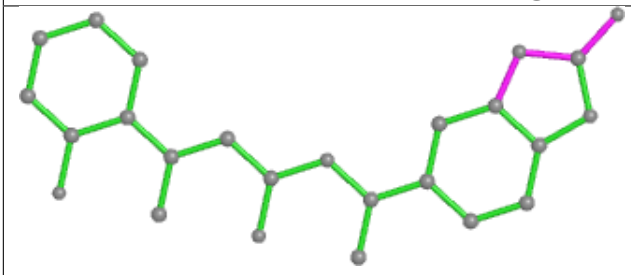


Torsions

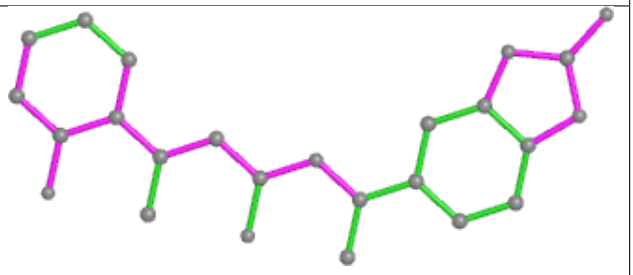


Rings

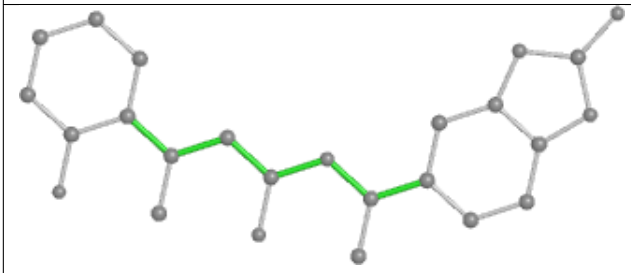
Ligand B2Z D 888



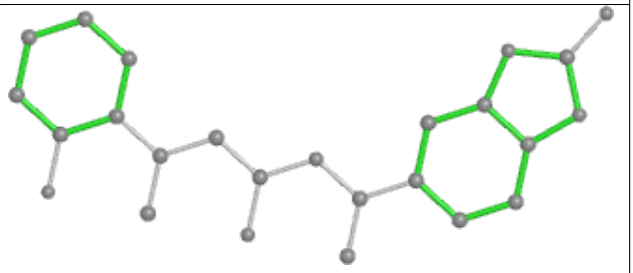
Bond lengths



Bond angles

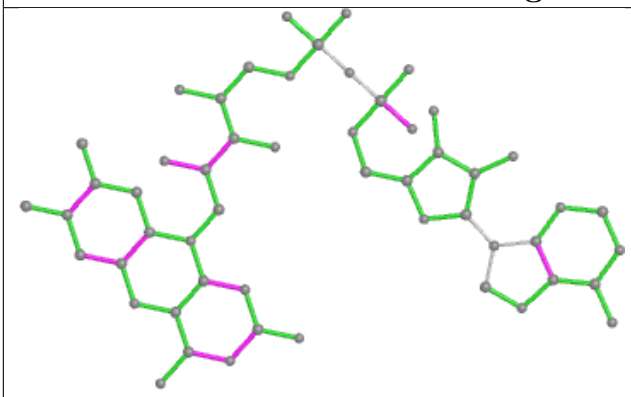


Torsions

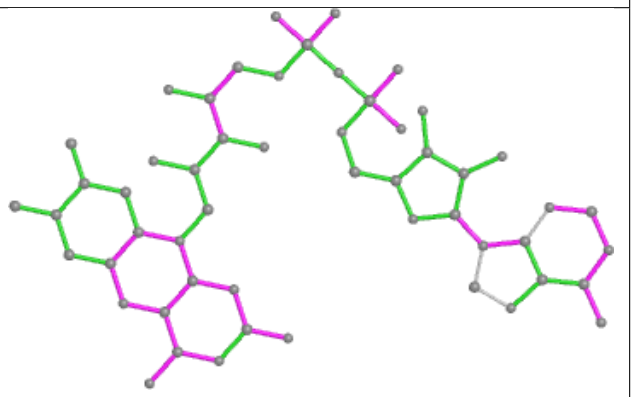


Rings

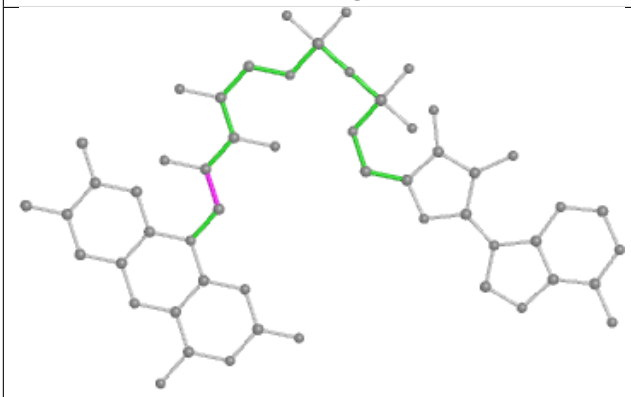
Ligand FAD C 999



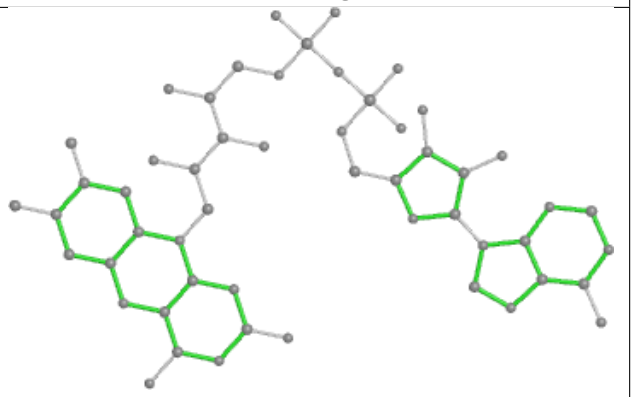
Bond lengths



Bond angles

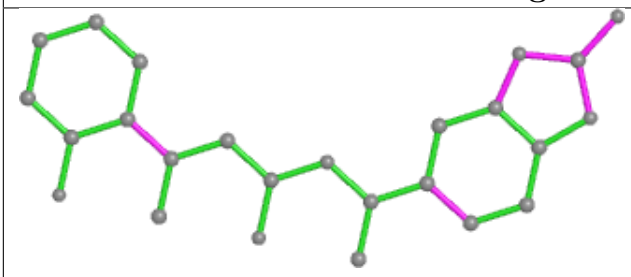


Torsions

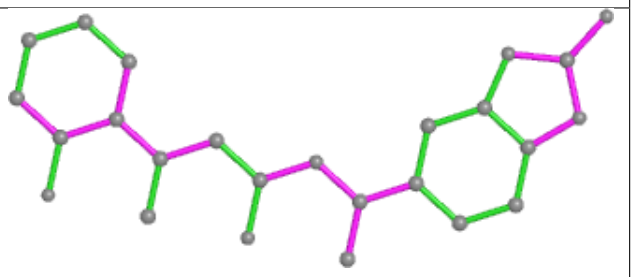


Rings

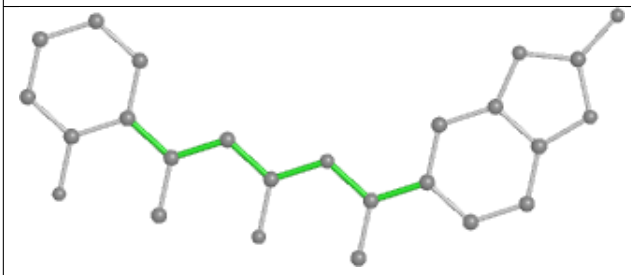
Ligand B2Z B 888



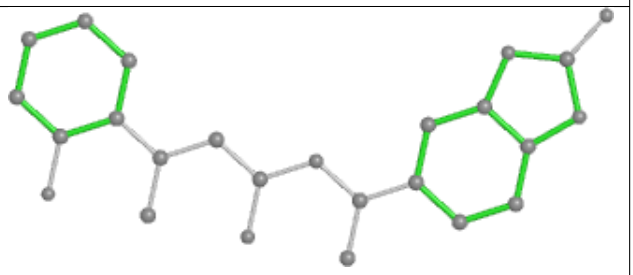
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	560/658 (85%)	-0.12	12 (2%)	63	68	15, 31, 57, 74	0
1	B	539/658 (81%)	-0.18	7 (1%)	77	80	17, 30, 53, 72	0
1	C	559/658 (84%)	-0.16	8 (1%)	75	78	15, 28, 50, 77	1 (0%)
1	D	564/658 (85%)	-0.12	11 (1%)	65	69	16, 31, 57, 78	0
All	All	2222/2632 (84%)	-0.14	38 (1%)	70	74	15, 30, 55, 78	1 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	159	ILE	4.8
1	D	453	THR	4.5
1	C	455	PHE	3.8
1	C	458	PHE	3.3
1	B	494	LEU	3.2
1	B	157	PRO	3.0
1	A	589	SER	3.0
1	A	451	TYR	3.0
1	D	455	PHE	2.9
1	A	444	LEU	2.9
1	B	199	GLU	2.9
1	C	460	PRO	2.8
1	B	589	SER	2.7
1	B	162	GLU	2.7
1	C	456	LYS	2.7
1	D	450	PHE	2.7
1	A	505[A]	TYR	2.7
1	D	452	ILE	2.6
1	D	451	TYR	2.6
1	A	156	PRO	2.5
1	A	450	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	457	GLY	2.4
1	D	170	LYS	2.4
1	D	163	ASP	2.4
1	D	426	PHE	2.4
1	C	430	HIS	2.4
1	D	559	PHE	2.2
1	A	436	VAL	2.2
1	A	157	PRO	2.2
1	C	170	LYS	2.1
1	D	589	SER	2.1
1	A	200	GLY	2.1
1	A	554	GLU	2.1
1	A	159	ILE	2.0
1	B	426	PHE	2.0
1	C	589	SER	2.0
1	D	435	GLN	2.0
1	A	559	PHE	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 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	B	1659	5/5	0.92	0.21	51,52,58,63	0
2	B2Z	C	888	25/25	0.93	0.13	23,32,39,53	0
4	SO4	D	1659	5/5	0.93	0.26	42,50,58,76	0
2	B2Z	D	888	25/25	0.94	0.14	31,38,51,56	0
2	B2Z	B	888	25/25	0.94	0.13	33,38,58,70	0
2	B2Z	A	888	25/25	0.94	0.13	30,34,57,65	0

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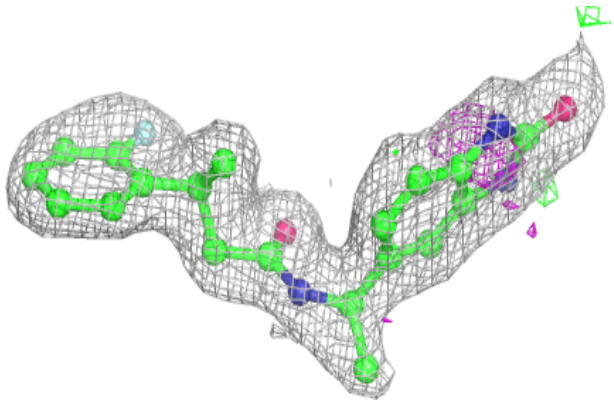
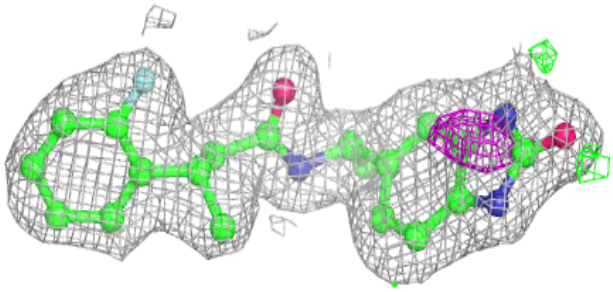
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	A	1659	5/5	0.96	0.10	52,54,60,60	0
4	SO4	C	1659	5/5	0.97	0.12	35,45,53,58	0
3	FAD	B	999	53/53	0.98	0.13	15,18,20,24	0
3	FAD	D	999	53/53	0.98	0.13	15,17,20,21	0
3	FAD	C	999	53/53	0.99	0.12	12,15,17,18	0
3	FAD	A	999	53/53	0.99	0.14	15,19,21,22	0

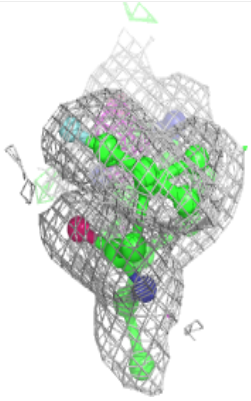
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around B2Z C 888:

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

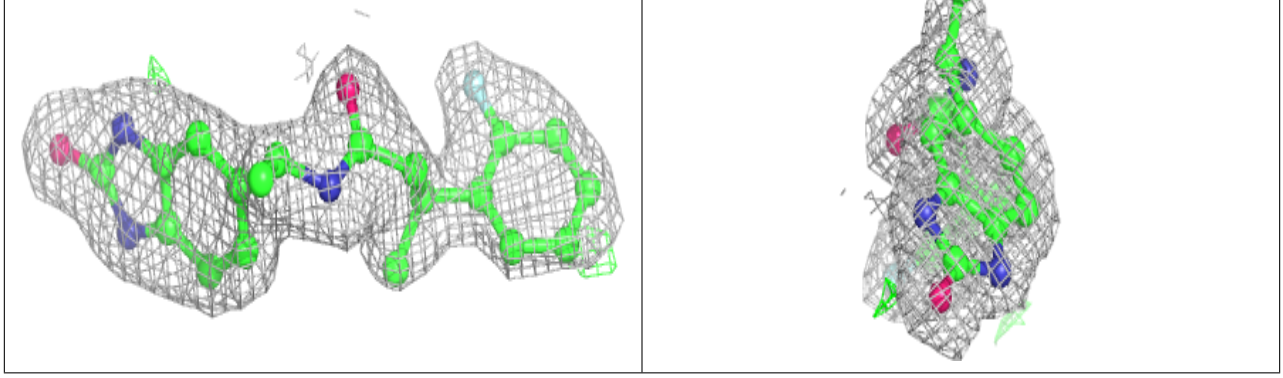






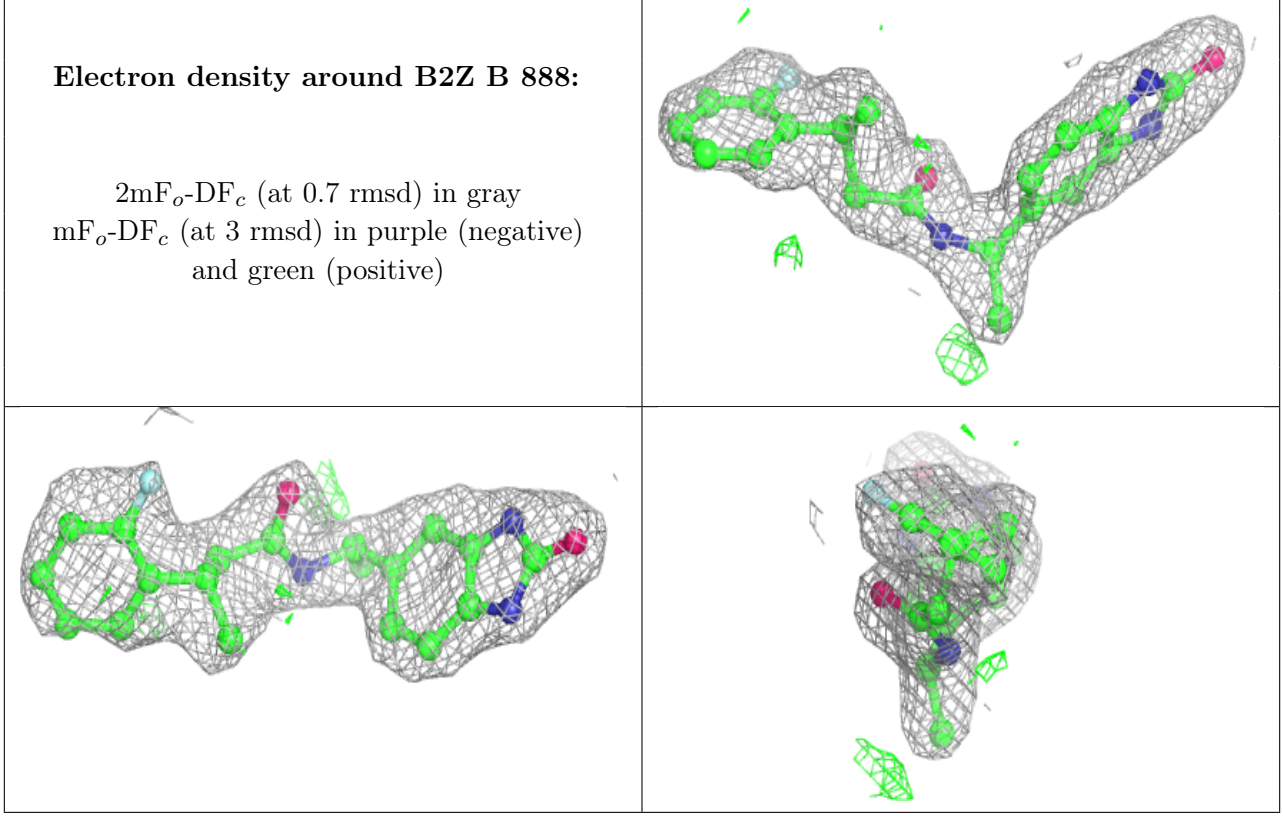
Electron density around B2Z D 888:

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



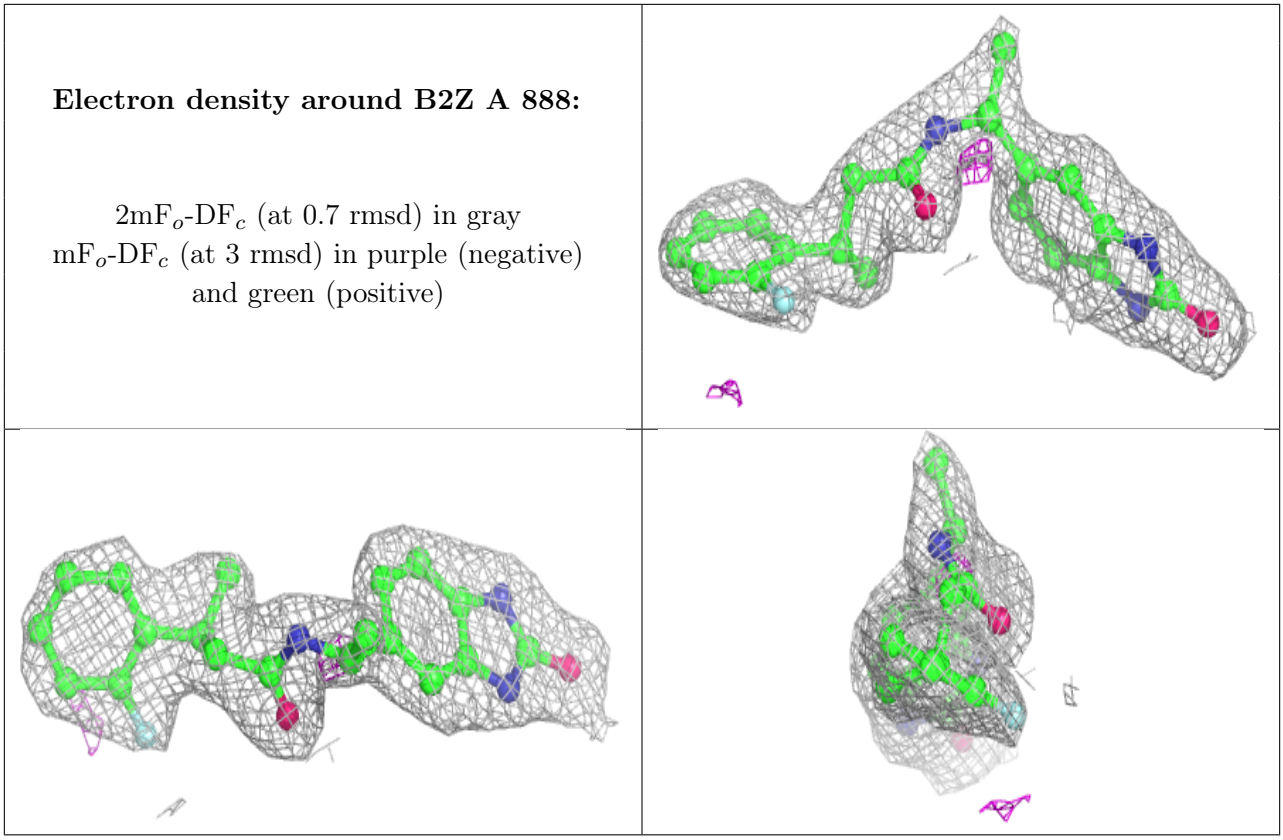
Electron density around B2Z B 888:

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



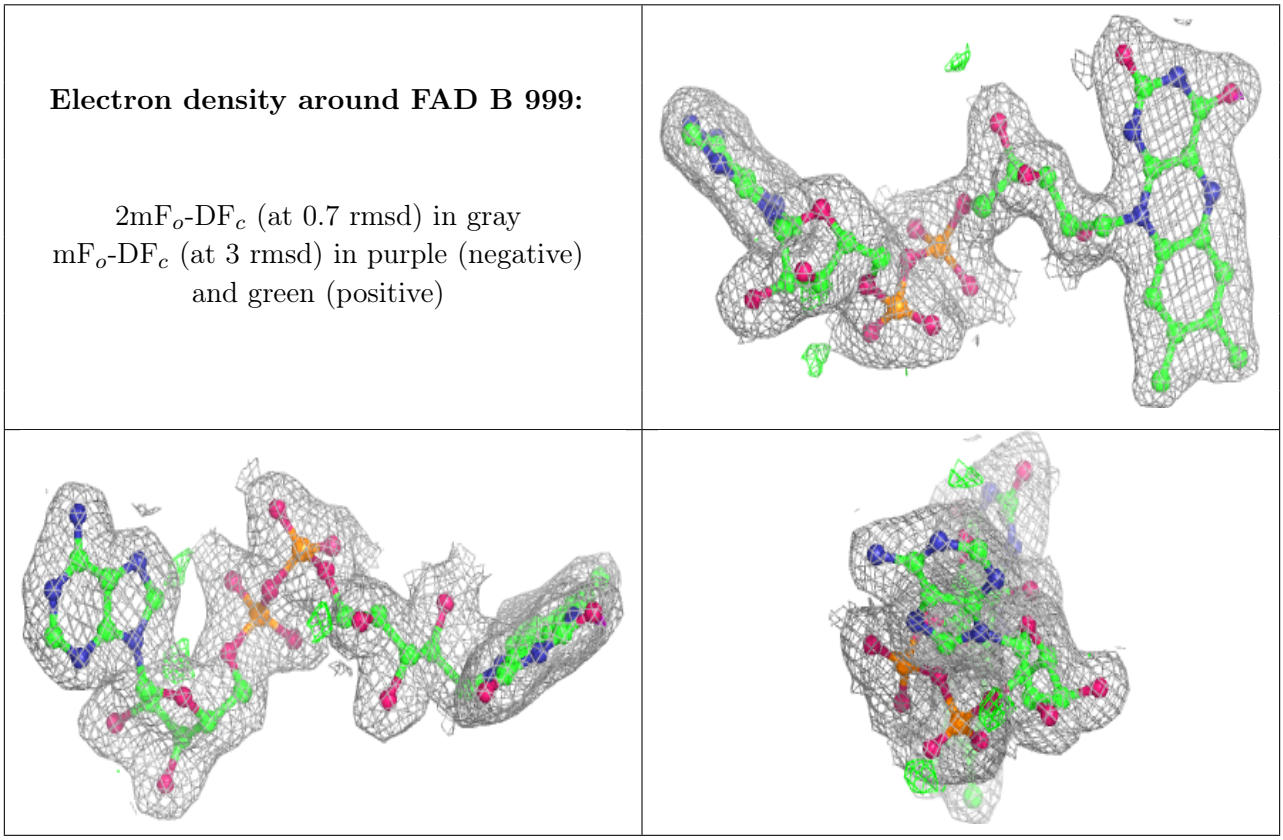
Electron density around B2Z A 888:

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



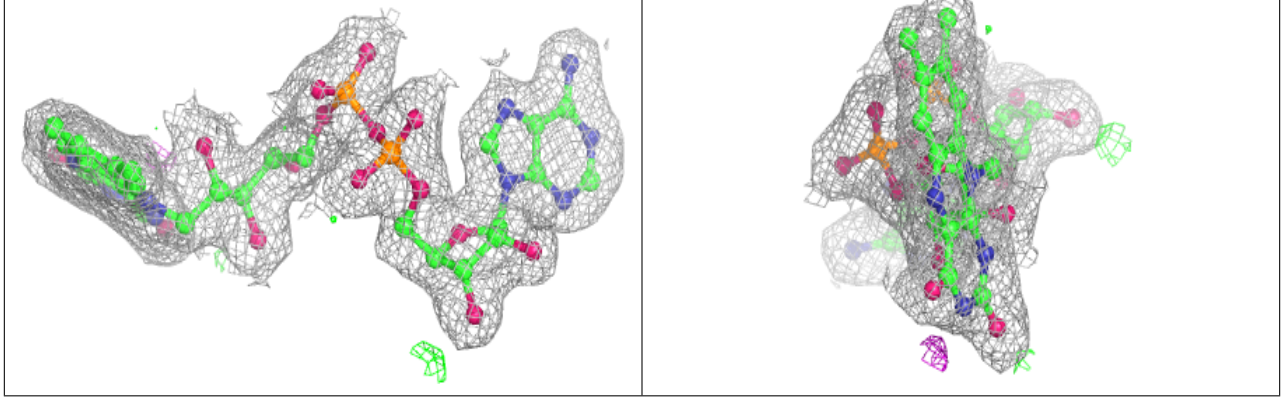
Electron density around FAD B 999:

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



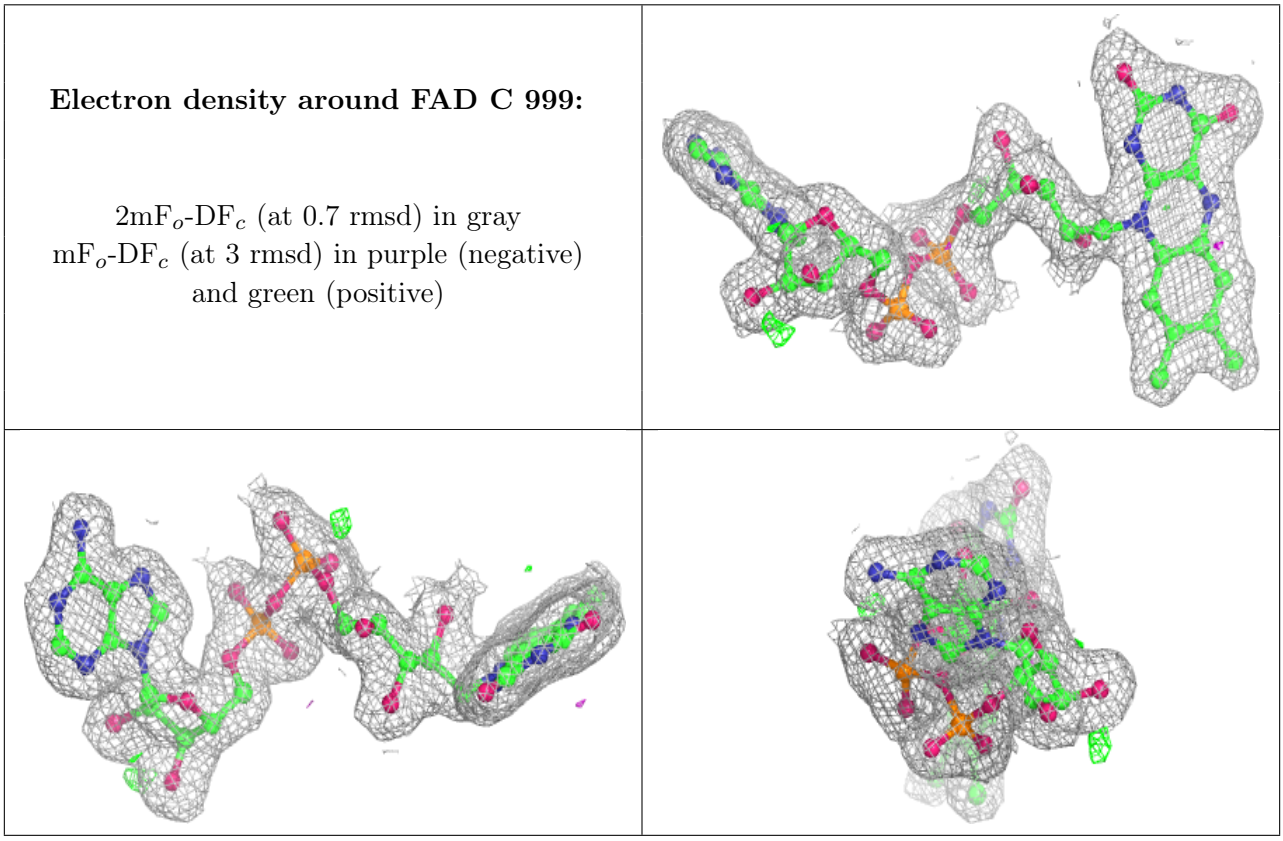
Electron density around FAD D 999:

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



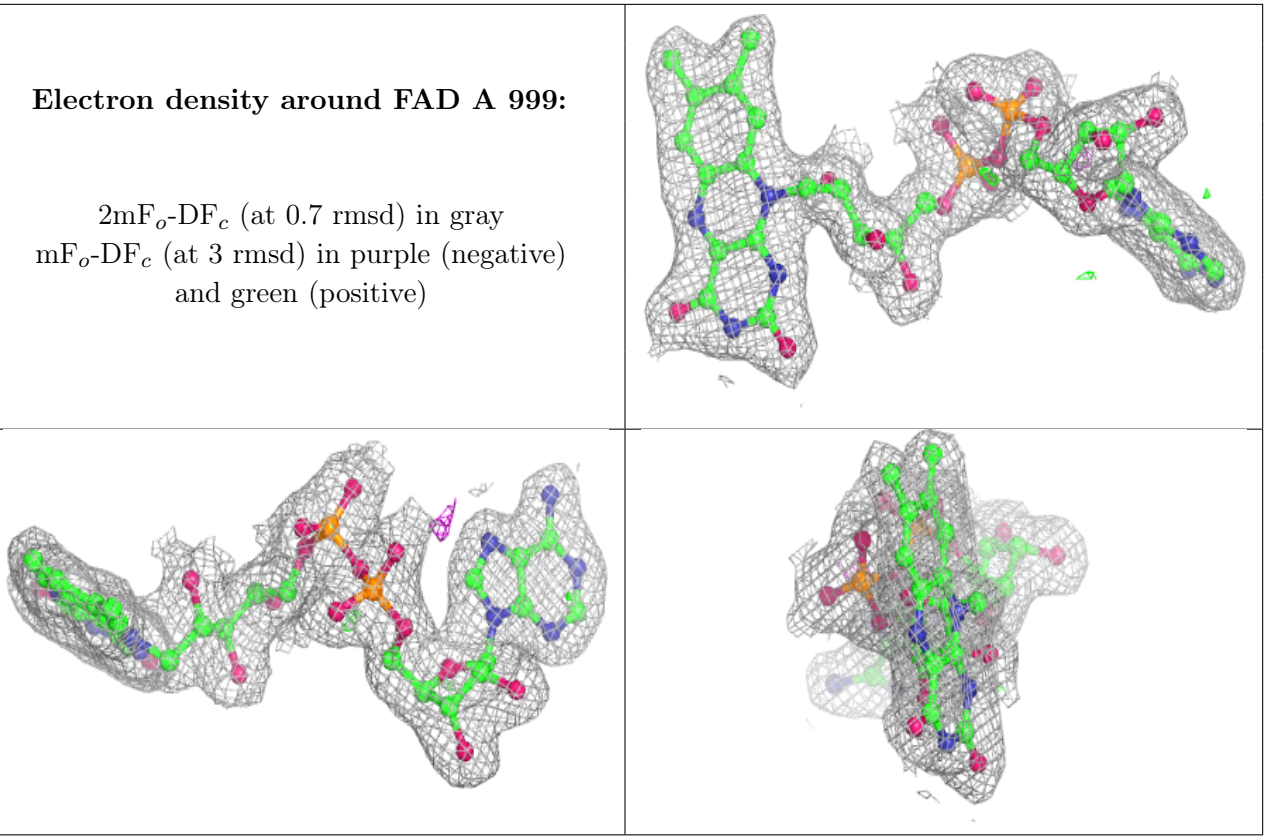
Electron density around FAD C 999:

$2mF_o$-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 999:

$2mF_o$-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.