



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 03:58 PM BST

PDB ID : 5AE2
Title : Ether Lipid-Generating Enzyme AGPS in complex with inhibitor 1e
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 : 2.00 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 : 2.13.1
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) : 2.13.1

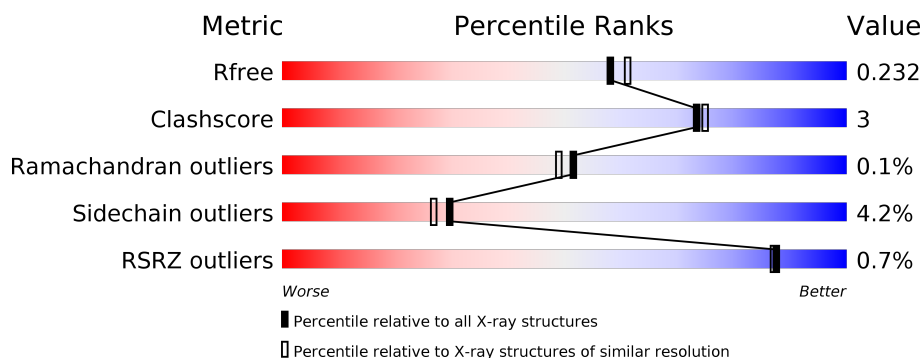
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 on 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	658	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; text-align: center;">%</div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 11%, yellow 11%, yellow 15%, grey 15%);"></div> <div style="position: absolute; bottom: -10px; left: 0; width: 100%; text-align: center;">73% 11% • 15%</div> </div> </div>
1	B	658	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; text-align: center;">%</div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 9%, yellow 9%, yellow 18%, grey 18%);"></div> <div style="position: absolute; bottom: -10px; left: 0; width: 100%; text-align: center;">72% 9% • 18%</div> </div> </div>
1	C	658	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, green 0%, green 75%, yellow 75%, yellow 8%, grey 8%, grey 15%);"></div> <div style="position: absolute; bottom: -10px; left: 0; width: 100%; text-align: center;">75% 8% • 15%</div> </div> </div>
1	D	658	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, green 0%, green 74%, yellow 74%, yellow 9%, grey 9%, grey 16%);"></div> <div style="position: absolute; bottom: -10px; left: 0; width: 100%; text-align: center;">74% 9% • 16%</div> </div> </div>

2 Entry composition [i](#)

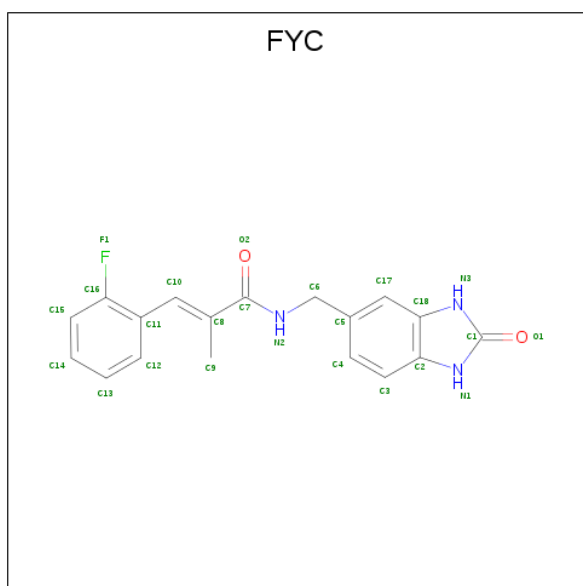
There are 5 unique types of molecules in this entry. The entry contains 18801 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	561	Total	C	N	O	S	0	0	0
			4431	2813	769	825	24			
1	B	542	Total	C	N	O	S	0	0	0
			4292	2727	745	796	24			
1	C	557	Total	C	N	O	S	0	1	0
			4402	2789	766	823	24			
1	D	550	Total	C	N	O	S	0	1	0
			4355	2761	757	812	25			

- Molecule 2 is 3-(2-fluorophenyl)-2-methyl-N-((2-oxo-2,3-dihydro-1H-benzo[d]imidazol-5-yl)methyl)acrylamide (three-letter code: FYC) (formula: C₁₈H₁₆FN₃O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			24	18	1	3	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	F	N	O	0	0
			24	18	1	3	2		
2	C	1	Total	C	F	N	O	0	0
			24	18	1	3	2		
2	D	1	Total	C	F	N	O	0	0
			24	18	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		

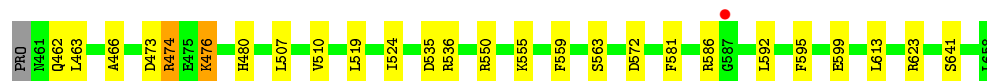
- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	282	Total	O	0	0
			282	282		
5	B	223	Total	O	0	0
			223	223		
5	C	268	Total	O	0	0
			268	268		
5	D	220	Total	O	0	0
			220	220		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.53Å 98.57Å 107.07Å 90.57° 90.14° 95.67°	Depositor
Resolution (Å)	107.06 – 2.00 72.69 – 2.00	Depositor EDS
% Data completeness (in resolution range)	85.3 (107.06-2.00) 85.3 (72.69-2.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, R_{free}	0.175 , 0.229 0.183 , 0.232	Depositor DCC
R_{free} test set	1516 reflections (1.07%)	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18801	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FYC, SO4, 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	0.84	2/4530 (0.0%)	0.99	17/6123 (0.3%)
1	B	0.85	1/4389 (0.0%)	0.98	17/5932 (0.3%)
1	C	0.84	0/4504	1.00	23/6090 (0.4%)
1	D	0.84	1/4455 (0.0%)	0.98	14/6022 (0.2%)
All	All	0.84	4/17878 (0.0%)	0.99	71/24167 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	516	ASP	CB-CG	8.27	1.69	1.51
1	D	641	SER	CB-OG	6.17	1.50	1.42
1	B	603	ARG	CD-NE	-5.96	1.36	1.46
1	A	626	TRP	CE3-CZ3	5.48	1.47	1.38

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	623	ARG	NE-CZ-NH2	-17.53	111.53	120.30
1	D	623	ARG	NE-CZ-NH2	-16.11	112.25	120.30
1	A	623	ARG	NE-CZ-NH2	-13.31	113.65	120.30
1	C	623	ARG	NE-CZ-NH1	12.33	126.46	120.30
1	A	623	ARG	NE-CZ-NH1	10.92	125.76	120.30
1	D	623	ARG	NE-CZ-NH1	10.78	125.69	120.30
1	D	317	ARG	NE-CZ-NH2	-10.58	115.01	120.30
1	B	603	ARG	NE-CZ-NH2	-9.49	115.55	120.30
1	B	603	ARG	NE-CZ-NH1	9.24	124.92	120.30
1	A	603	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	B	317	ARG	NE-CZ-NH2	-8.43	116.08	120.30
1	B	515	ARG	NE-CZ-NH2	-7.61	116.50	120.30
1	C	100	ASP	CB-CG-OD1	7.43	124.99	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	342	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	C	638	MET	CG-SD-CE	-7.24	88.62	100.20
1	D	100	ASP	CB-CG-OD1	7.22	124.80	118.30
1	A	603	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	C	536	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	C	463	LEU	CA-CB-CG	7.11	131.64	115.30
1	B	515	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	A	463	LEU	CA-CB-CG	6.99	131.38	115.30
1	B	382	ARG	NE-CZ-NH1	6.73	123.66	120.30
1	A	100	ASP	CB-CG-OD1	6.72	124.35	118.30
1	C	536	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	B	100	ASP	CB-CG-OD1	6.62	124.26	118.30
1	C	265	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	B	536	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	A	406	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	D	474	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	C	547	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	B	265	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	B	331	ASP	CB-CG-OD1	-6.28	112.65	118.30
1	C	623	ARG	CG-CD-NE	-6.25	98.68	111.80
1	A	535	ASP	CB-CG-OD1	6.24	123.92	118.30
1	A	572	ASP	CB-CG-OD1	6.22	123.90	118.30
1	C	265	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	B	542	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	C	515	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	D	412	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	B	331	ASP	CB-CG-OD2	5.85	123.56	118.30
1	D	623	ARG	CG-CD-NE	-5.81	99.59	111.80
1	A	317	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	B	270	ASP	CB-CG-OD1	5.77	123.49	118.30
1	C	106	ASN	CB-CA-C	-5.73	98.93	110.40
1	C	542	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	B	535	ASP	CB-CG-OD1	5.53	123.28	118.30
1	B	536	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	C	91	MET	CG-SD-CE	-5.52	91.37	100.20
1	B	359	ASP	CB-CG-OD1	5.51	123.26	118.30
1	D	419	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	C	185	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	D	463	LEU	CA-CB-CG	5.46	127.87	115.30
1	A	303	ASP	CB-CG-OD1	5.44	123.20	118.30
1	D	550	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	C	198	ARG	NE-CZ-NH2	-5.37	117.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	613	LEU	CB-CG-CD2	5.28	119.97	111.00
1	A	331	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	542	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	A	303	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	C	382	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	C	515	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	D	207	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	204	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	C	359	ASP	CB-CG-OD2	-5.13	113.69	118.30
1	D	303	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	246	MET	CG-SD-CE	5.12	108.39	100.20
1	B	572	ASP	CB-CG-OD1	5.09	122.88	118.30
1	D	204	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	C	542	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	A	547	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	C	365	MET	CG-SD-CE	-5.02	92.17	100.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4431	0	4360	39	0
1	B	4292	0	4234	30	0
1	C	4402	0	4340	28	0
1	D	4355	0	4300	19	0
2	A	24	0	16	4	0
2	B	24	0	16	5	0
2	C	24	0	16	1	0
2	D	24	0	16	2	0
3	A	53	0	31	1	0
3	B	53	0	31	2	0
3	C	53	0	31	1	0
3	D	53	0	31	2	0
4	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	A	282	0	0	3	0
5	B	223	0	0	2	0
5	C	268	0	0	6	0
5	D	220	0	0	1	0
All	All	18801	0	17422	115	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 (115) 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:516:ASP:OD2	5:C:2012:HOH:O	1.87	0.92
2:B:888:FYC:H62C	3:B:999:FAD:HM72	1.53	0.88
1:C:419:ARG:HD3	5:C:2197:HOH:O	1.80	0.79
2:D:888:FYC:H62C	3:D:999:FAD:HM72	1.66	0.78
1:B:192:HIS:HB3	1:B:243:TYR:OH	1.83	0.77
1:C:625:GLN:OE1	5:C:2247:HOH:O	2.06	0.73
1:C:106:ASN:HB2	1:C:110:GLN:O	1.89	0.71
1:A:192:HIS:HB3	1:A:243:TYR:OH	1.92	0.69
1:B:425:GLN:HG3	1:B:564:THR:OG1	1.95	0.67
2:A:888:FYC:H62C	3:A:999:FAD:HM72	1.78	0.66
2:C:888:FYC:H62C	3:C:999:FAD:HM72	1.81	0.62
1:B:298:THR:HG23	1:B:300:HIS:H	1.64	0.62
1:C:423:ASN:HD21	1:C:427:GLN:HE21	1.49	0.61
1:A:539:ASP:OD1	1:A:542:ARG:NH2	2.34	0.61
1:D:473:ASP:HB2	1:D:476:LYS:HD3	1.82	0.61
1:A:394:ALA:HB1	1:A:463:LEU:CD2	2.31	0.60
1:B:635:GLY:HA2	1:B:638:MET:HE3	1.82	0.60
1:C:314:ILE:HG23	1:C:365:MET:HG2	1.84	0.60
1:B:613:LEU:HD22	1:B:623:ARG:HD2	1.83	0.60
1:C:634:VAL:HG12	1:C:638:MET:HE2	1.83	0.60
1:A:215:HIS:HE1	5:A:2078:HOH:O	1.86	0.58
1:A:133:GLN:NE2	1:A:139:ASN:O	2.35	0.58
1:A:439:ILE:HG23	1:D:535:ASP:HA	1.84	0.58
1:A:215:HIS:HD2	1:A:375:THR:OG1	1.87	0.57
1:A:430:HIS:CD2	1:A:447:LEU:HD13	2.40	0.56
2:B:888:FYC:C6	3:B:999:FAD:HM72	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:ARG:HD3	5:B:2098:HOH:O	2.04	0.56
1:A:143:LYS:NZ	5:A:2045:HOH:O	2.32	0.55
1:C:127:THR:O	1:C:127:THR:HG22	2.06	0.55
1:A:442:SER:O	1:A:443:PHE:CB	2.54	0.55
1:A:426:PHE:CD2	1:A:463:LEU:HD12	2.43	0.54
1:C:419:ARG:CD	5:C:2197:HOH:O	2.50	0.54
1:B:526:GLU:HB3	1:B:595:PHE:HZ	1.74	0.53
1:D:171:THR:O	1:D:172:ASN:HB3	2.08	0.53
1:B:340:THR:HB	1:B:646:VAL:HG13	1.90	0.53
1:B:298:THR:CG2	1:B:300:HIS:H	2.22	0.52
1:A:106:ASN:ND2	1:A:110:GLN:H	2.08	0.52
1:A:439:ILE:CG2	1:D:535:ASP:HA	2.40	0.52
1:A:187:HIS:HD2	1:A:188:GLY:O	1.92	0.52
1:B:127:THR:HG22	5:B:2035:HOH:O	2.09	0.52
1:D:106:ASN:HB2	1:D:110:GLN:O	2.10	0.52
1:B:419:ARG:O	1:B:466:ALA:HA	2.09	0.51
1:B:192:HIS:HB3	1:B:243:TYR:HH	1.71	0.51
1:B:94:ASN:HA	1:B:197:LEU:HD13	1.91	0.51
1:A:582:ALA:HB2	2:A:888:FYC:H15	1.93	0.50
1:A:415:PRO:HB3	1:A:470:PHE:CE2	2.47	0.50
1:A:106:ASN:C	1:A:106:ASN:HD22	2.15	0.50
1:B:140:LEU:HA	1:B:521:TYR:CE1	2.45	0.50
1:D:151:ASN:HB3	1:D:154:ASP:OD2	2.12	0.50
1:A:515:ARG:HA	2:A:888:FYC:H13	1.94	0.49
1:D:314:ILE:HG23	1:D:365:MET:HG2	1.93	0.49
1:C:382:ARG:HD3	1:D:412:ARG:CZ	2.44	0.48
1:B:582:ALA:HB2	2:B:888:FYC:H15	1.96	0.48
1:C:265:ARG:HD3	1:C:279:GLU:OE1	2.13	0.48
1:C:226:CYS:SG	1:C:651:ILE:CD1	3.02	0.48
1:B:552:CYS:SG	1:B:561:PRO:HG3	2.54	0.47
1:C:230:LEU:HD22	1:C:254:THR:HB	1.96	0.47
2:D:888:FYC:C6	3:D:999:FAD:HM72	2.39	0.47
1:A:189:HIS:HD2	5:A:2228:HOH:O	1.98	0.47
1:A:335:HIS:HE1	1:A:346:GLU:OE2	1.98	0.47
1:B:133:GLN:NE2	1:B:139:ASN:O	2.47	0.46
1:B:415:PRO:HB3	1:B:470:PHE:CD2	2.50	0.46
1:C:536:ARG:HD2	5:C:2220:HOH:O	2.16	0.46
1:C:215:HIS:CE1	1:C:337:LYS:HD3	2.51	0.46
1:C:412:ARG:CZ	1:D:382:ARG:HD3	2.45	0.46
1:D:423:ASN:ND2	1:D:427:GLN:OE1	2.49	0.45
1:A:94:ASN:HA	1:A:197:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:619:VAL:HB	1:A:657:LEU:HD23	1.97	0.45
1:A:109:GLY:HA3	1:C:268:TRP:CE3	2.51	0.45
1:D:171:THR:O	1:D:172:ASN:CB	2.64	0.45
1:D:421:MET:HB3	1:D:425:GLN:HB2	1.98	0.45
1:D:83:ILE:HG23	1:D:91:MET:HE1	1.98	0.45
1:C:138:ILE:CG2	1:C:584:ASN:ND2	2.80	0.45
1:A:430:HIS:CG	1:A:447:LEU:HD13	2.52	0.45
1:C:529:GLU:C	1:C:529:GLU:OE1	2.55	0.44
1:A:439:ILE:HG13	1:C:272:ASN:ND2	2.32	0.44
1:C:568:THR:HG21	5:C:2229:HOH:O	2.15	0.44
1:D:572:ASP:HB2	5:D:2191:HOH:O	2.17	0.44
1:B:540:LEU:C	1:B:540:LEU:HD23	2.38	0.44
1:C:419:ARG:O	1:C:466:ALA:HA	2.18	0.44
1:A:187:HIS:CE1	1:A:197:LEU:HD11	2.54	0.43
1:A:585:TYR:HB2	1:A:591:PRO:HB3	1.99	0.43
1:A:427:GLN:HG2	1:A:447:LEU:HD21	2.01	0.43
1:C:619:VAL:HB	1:C:657:LEU:HD23	2.00	0.43
1:B:525:GLY:HA3	2:B:888:FYC:C15	2.49	0.43
1:D:191:LEU:HD12	1:D:595:PHE:CD2	2.53	0.43
1:A:119:PRO:HG2	1:A:506:LEU:HD22	1.99	0.43
1:B:397:ASN:HA	1:B:462:GLN:O	2.19	0.43
1:B:167:GLU:HA	1:B:170:LYS:HD3	1.99	0.43
1:A:386:GLU:HG2	1:A:473:ASP:HA	2.00	0.43
1:A:372:GLY:HA2	1:A:652:PHE:CZ	2.54	0.43
1:B:515:ARG:HG2	2:B:888:FYC:C12	2.49	0.43
1:C:490:LYS:N	1:C:490:LYS:HD2	2.34	0.43
1:A:394:ALA:HB1	1:A:463:LEU:HD21	2.00	0.42
1:B:179:ALA:O	1:B:183:VAL:HG23	2.19	0.42
1:C:138:ILE:HG23	1:C:584:ASN:ND2	2.35	0.42
1:D:519:LEU:CD2	1:D:524:ILE:HG22	2.50	0.42
1:A:310:VAL:HA	1:A:313:TRP:CE3	2.55	0.42
1:D:419:ARG:O	1:D:466:ALA:HA	2.19	0.42
1:B:394:ALA:O	1:B:493:GLY:HA2	2.20	0.42
1:A:345:ILE:HD13	1:B:638:MET:CE	2.49	0.41
1:B:526:GLU:CB	1:B:595:PHE:HZ	2.32	0.41
1:C:389:LYS:HE2	1:C:481:GLU:OE1	2.19	0.41
1:C:458:PHE:CE1	1:C:494:LEU:HD11	2.55	0.41
1:A:268:TRP:CZ2	1:A:277:HIS:HB2	2.56	0.41
1:A:557:VAL:HA	1:A:588:ILE:HD11	2.02	0.41
1:B:128:PHE:CD1	1:B:432:LEU:HD11	2.56	0.41
1:A:268:TRP:CE2	1:A:277:HIS:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:ASN:OD1	1:D:163:ASP:N	2.54	0.41
1:D:260:THR:O	1:D:281:GLY:HA3	2.20	0.41
1:B:100:ASP:O	1:B:114:THR:HG22	2.20	0.41
1:A:138:ILE:HD13	1:A:521:TYR:HB3	2.04	0.40
1:A:525:GLY:HA3	2:A:888:FYC:H15	2.03	0.40
1:B:421:MET:CE	1:B:467:THR:HG23	2.51	0.40
1:C:127:THR:O	1:C:127:THR:CG2	2.70	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	30
1	B	536/658 (82%)	526 (98%)	10 (2%)	0	100	100
1	C	554/658 (84%)	540 (98%)	13 (2%)	1 (0%)	47	44
1	D	547/658 (83%)	535 (98%)	12 (2%)	0	100	100
All	All	2192/2632 (83%)	2144 (98%)	45 (2%)	3 (0%)	51	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	ASP
1	C	106	ASN
1	A	443	PHE

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	478/545 (88%)	462 (97%)	16 (3%)	38	37
1	B	463/545 (85%)	442 (96%)	21 (4%)	27	24
1	C	477/545 (88%)	459 (96%)	18 (4%)	33	31
1	D	472/545 (87%)	448 (95%)	24 (5%)	24	19
All	All	1890/2180 (87%)	1811 (96%)	79 (4%)	30	27

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	A	140	LEU
1	A	195	PHE
1	A	323	LYS
1	A	406	ARG
1	A	445	ASP
1	A	463	LEU
1	A	476	LYS
1	A	516	ASP
1	A	553	LYS
1	A	559	PHE
1	A	563	SER
1	A	589	SER
1	A	596	GLU
1	A	599	GLU
1	A	603	ARG
1	B	105	LEU
1	B	114	THR
1	B	116	LYS
1	B	120	LEU
1	B	138	ILE
1	B	140	LEU
1	B	191	LEU
1	B	197	LEU
1	B	263	MET
1	B	292	LYS
1	B	298	THR
1	B	323	LYS

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Mol	Chain	Res	Type
1	B	476	LYS
1	B	482	LYS
1	B	500	ASN
1	B	507	LEU
1	B	515	ARG
1	B	526	GLU
1	B	568	THR
1	B	613	LEU
1	B	646	VAL
1	C	86	LYS
1	C	90	LEU
1	C	140	LEU
1	C	141	ASP
1	C	142	HIS
1	C	144	THR
1	C	199	GLU
1	C	224	LEU
1	C	323	LYS
1	C	406	ARG
1	C	421	MET
1	C	432	LEU
1	C	461	ASN
1	C	463	LEU
1	C	479	GLN
1	C	490	LYS
1	C	529	GLU
1	C	613	LEU
1	D	107	LYS
1	D	127	THR
1	D	141	ASP
1	D	142	HIS
1	D	150	LEU
1	D	199	GLU
1	D	224	LEU
1	D	323	LYS
1	D	406	ARG
1	D	462	GLN
1	D	474	ARG
1	D	476	LYS
1	D	480	HIS
1	D	507	LEU
1	D	510	VAL

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Mol	Chain	Res	Type
1	D	536	ARG
1	D	555	LYS
1	D	559	PHE
1	D	563	SER
1	D	581	PHE
1	D	586	ARG
1	D	592	LEU
1	D	599	GLU
1	D	613	LEU

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

Mol	Chain	Res	Type
1	A	106	ASN
1	A	187	HIS
1	A	189	HIS
1	A	215	HIS
1	A	262	GLN
1	A	324	ASN
1	A	328	ASN
1	A	335	HIS
1	A	362	HIS
1	A	430	HIS
1	B	423	ASN
1	B	558	GLN
1	C	142	HIS
1	C	423	ASN
1	D	285	GLN
1	D	423	ASN
1	D	424	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [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	$\# Z > 2$
3	FAD	D	999	-	51,58,58	1.88	3 (5%)	60,89,89	2.50	15 (25%)
4	SO4	A	1659	-	4,4,4	0.54	0	6,6,6	0.54	0
3	FAD	B	999	-	51,58,58	1.77	13 (25%)	60,89,89	2.72	17 (28%)
2	FYC	D	888	-	23,26,26	0.98	0	28,36,36	2.38	13 (46%)
4	SO4	C	1659	-	4,4,4	0.43	0	6,6,6	0.64	0
2	FYC	B	888	-	23,26,26	1.23	4 (17%)	28,36,36	2.82	13 (46%)
2	FYC	A	888	-	23,26,26	1.20	3 (13%)	28,36,36	2.82	12 (42%)
2	FYC	C	888	-	23,26,26	0.99	1 (4%)	28,36,36	2.34	10 (35%)
4	SO4	B	1659	-	4,4,4	0.61	0	6,6,6	0.89	0
4	SO4	D	1659	-	4,4,4	0.41	0	6,6,6	0.51	0
3	FAD	A	999	-	51,58,58	1.86	5 (9%)	60,89,89	2.52	14 (23%)
3	FAD	C	999	-	51,58,58	1.83	10 (19%)	60,89,89	2.31	15 (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
3	FAD	D	999	-	-	2/30/50/50	0/6/6/6
3	FAD	B	999	-	-	2/30/50/50	0/6/6/6
2	FYC	D	888	-	-	6/13/13/13	0/3/3/3
2	FYC	B	888	-	-	4/13/13/13	0/3/3/3
2	FYC	A	888	-	-	6/13/13/13	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FYC	C	888	-	-	6/13/13/13	0/3/3/3
3	FAD	A	999	-	-	2/30/50/50	0/6/6/6
3	FAD	C	999	-	-	2/30/50/50	0/6/6/6

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	999	FAD	C4X-C10	10.38	1.49	1.38
3	A	999	FAD	C4X-C10	10.13	1.48	1.38
3	C	999	FAD	C4X-C10	7.57	1.46	1.38
3	B	999	FAD	C4X-C10	6.04	1.44	1.38
3	C	999	FAD	C1'-N10	-4.69	1.43	1.48
3	B	999	FAD	C9A-N10	4.26	1.44	1.38
3	D	999	FAD	C4-C4X	4.21	1.48	1.41
3	A	999	FAD	C9A-C5X	3.87	1.50	1.42
3	C	999	FAD	C9A-C5X	3.86	1.50	1.42
3	C	999	FAD	C4-C4X	3.68	1.47	1.41
3	B	999	FAD	C2-N1	-3.64	1.31	1.38
3	B	999	FAD	C2'-C3'	3.38	1.59	1.53
3	D	999	FAD	C9A-C5X	3.37	1.49	1.42
3	B	999	FAD	C4-C4X	3.17	1.46	1.41
3	C	999	FAD	C8-C7	3.11	1.48	1.40
3	A	999	FAD	C8-C7	2.86	1.48	1.40
2	B	888	FYC	C11-C10	-2.78	1.42	1.46
3	B	999	FAD	C9A-C5X	2.64	1.47	1.42
3	C	999	FAD	C2-N3	-2.60	1.33	1.38
3	B	999	FAD	C1'-N10	-2.50	1.45	1.48
3	B	999	FAD	C8-C7	2.46	1.47	1.40
3	A	999	FAD	C1'-N10	2.45	1.50	1.48
2	A	888	FYC	C7-N2	2.40	1.37	1.33
2	B	888	FYC	C17-C18	-2.36	1.38	1.41
2	C	888	FYC	C17-C18	-2.35	1.38	1.41
3	B	999	FAD	C5A-C4A	2.29	1.47	1.40
2	A	888	FYC	C3-C4	2.27	1.41	1.36
3	C	999	FAD	C9A-N10	2.27	1.41	1.38
2	B	888	FYC	C7-N2	2.27	1.37	1.33
3	C	999	FAD	C2-N1	-2.25	1.33	1.38
3	C	999	FAD	C5A-C4A	2.22	1.46	1.40
2	A	888	FYC	C17-C18	-2.18	1.38	1.41
3	B	999	FAD	C2B-C1B	-2.11	1.50	1.53
3	A	999	FAD	C4X-N5	2.09	1.36	1.33
3	B	999	FAD	C10-N1	2.08	1.35	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	999	FAD	C10-N1	2.08	1.35	1.33
3	B	999	FAD	C2A-N3A	2.05	1.35	1.32
2	B	888	FYC	C3-C4	2.04	1.40	1.36
3	B	999	FAD	C5A-N7A	-2.04	1.32	1.39

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	999	FAD	C4-N3-C2	12.13	125.39	115.14
3	A	999	FAD	C4-N3-C2	11.47	124.82	115.14
3	D	999	FAD	C4-N3-C2	10.16	123.72	115.14
3	C	999	FAD	C4-N3-C2	8.65	122.45	115.14
3	C	999	FAD	C4-C4X-C10	-8.03	114.64	119.95
3	D	999	FAD	C4-C4X-C10	-7.79	114.80	119.95
2	A	888	FYC	C5-C17-C18	-7.08	114.86	121.08
3	D	999	FAD	C1'-N10-C9A	6.99	123.80	118.29
2	D	888	FYC	C6-N2-C7	-6.92	112.81	122.08
3	A	999	FAD	C4-C4X-C10	-6.77	115.47	119.95
3	A	999	FAD	C1'-N10-C9A	6.51	123.42	118.29
3	B	999	FAD	C4X-N5-C5X	6.46	123.23	116.77
3	B	999	FAD	C1'-N10-C9A	6.40	123.33	118.29
3	B	999	FAD	C4-C4X-C10	-6.39	115.72	119.95
2	A	888	FYC	C4-C3-C2	-6.29	112.92	120.84
3	C	999	FAD	C1'-N10-C9A	5.58	122.69	118.29
2	B	888	FYC	C12-C11-C16	5.46	122.26	115.98
2	C	888	FYC	C9-C8-C10	5.30	133.69	125.11
2	B	888	FYC	C10-C8-C7	-5.11	105.52	121.13
3	B	999	FAD	C4X-C4-N3	-5.03	116.56	123.43
3	C	999	FAD	C4X-N5-C5X	4.98	121.75	116.77
2	B	888	FYC	C6-N2-C7	-4.91	115.50	122.08
2	B	888	FYC	C15-C16-C11	-4.83	117.29	123.94
2	B	888	FYC	C6-C5-C17	-4.70	113.10	121.51
3	A	999	FAD	C5X-C9A-N10	4.60	121.05	117.72
3	D	999	FAD	C5X-C9A-N10	4.55	121.01	117.72
2	A	888	FYC	C6-N2-C7	-4.52	116.02	122.08
3	C	999	FAD	C4-C4X-N5	4.37	123.59	118.60
3	A	999	FAD	C4X-N5-C5X	4.35	121.12	116.77
2	C	888	FYC	C6-N2-C7	-4.34	116.27	122.08
2	C	888	FYC	C10-C8-C7	-4.23	108.21	121.13
2	C	888	FYC	C5-C17-C18	-4.19	117.40	121.08
3	A	999	FAD	C4X-C4-N3	-4.16	117.75	123.43
2	B	888	FYC	C5-C17-C18	-4.14	117.44	121.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	888	FYC	C10-C8-C7	-3.97	109.02	121.13
2	C	888	FYC	C6-C5-C17	-3.96	114.42	121.51
2	A	888	FYC	C12-C11-C16	3.96	120.53	115.98
2	A	888	FYC	F1-C16-C11	3.86	123.50	118.10
2	D	888	FYC	C9-C8-C10	3.84	131.33	125.11
2	D	888	FYC	C5-C17-C18	-3.78	117.76	121.08
3	D	999	FAD	O2A-PA-O1A	3.76	130.83	112.24
3	B	999	FAD	N3A-C2A-N1A	-3.73	122.86	128.68
2	D	888	FYC	C1-N1-C2	3.67	111.05	103.78
3	D	999	FAD	C4X-C4-N3	-3.65	118.44	123.43
3	A	999	FAD	C6-C5X-N5	3.62	123.04	119.05
2	B	888	FYC	F1-C16-C11	3.61	123.16	118.10
3	B	999	FAD	C2A-N1A-C6A	3.57	124.86	118.75
2	D	888	FYC	C10-C8-C7	-3.57	110.25	121.13
3	D	999	FAD	C9A-N10-C10	-3.55	117.27	121.91
3	B	999	FAD	C5X-C9A-N10	3.51	120.26	117.72
2	A	888	FYC	C9-C8-C7	3.50	124.12	115.28
2	B	888	FYC	C9-C8-C7	3.48	124.08	115.28
2	C	888	FYC	C1-N1-C2	3.33	110.38	103.78
2	D	888	FYC	C4-C3-C2	-3.33	116.65	120.84
3	D	999	FAD	C4-C4X-N5	3.31	122.38	118.60
3	A	999	FAD	C4-C4X-N5	3.29	122.36	118.60
2	B	888	FYC	C9-C8-C10	3.27	130.41	125.11
2	A	888	FYC	C6-C5-C17	-3.25	115.69	121.51
2	A	888	FYC	C1-N1-C2	3.25	110.22	103.78
3	C	999	FAD	C4X-C4-N3	-3.20	119.05	123.43
3	B	999	FAD	C1B-N9A-C4A	-3.19	121.04	126.64
3	C	999	FAD	O2'-C2'-C1'	3.11	117.07	109.59
3	B	999	FAD	C9A-C5X-N5	-3.09	117.53	122.36
2	B	888	FYC	C4-C3-C2	-3.06	116.99	120.84
3	B	999	FAD	C4-C4X-N5	3.03	122.06	118.60
2	B	888	FYC	C1-N1-C2	3.02	109.77	103.78
3	D	999	FAD	C1B-N9A-C4A	-2.99	121.39	126.64
2	C	888	FYC	C4-C3-C2	-2.92	117.16	120.84
3	A	999	FAD	C1B-N9A-C4A	-2.91	121.54	126.64
2	D	888	FYC	C6-C5-C17	-2.90	116.31	121.51
3	C	999	FAD	O2A-PA-O1A	2.88	126.47	112.24
3	B	999	FAD	C6-C5X-N5	2.86	122.20	119.05
3	B	999	FAD	N6A-C6A-N1A	2.85	124.48	118.57
2	C	888	FYC	C12-C11-C16	2.83	119.24	115.98
3	B	999	FAD	C9A-N10-C10	-2.83	118.20	121.91
3	A	999	FAD	C9A-C5X-N5	-2.79	118.00	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	999	FAD	C4A-C5A-N7A	-2.74	106.54	109.40
3	C	999	FAD	C6-C5X-N5	2.72	122.04	119.05
2	B	888	FYC	C12-C11-C10	-2.70	116.76	122.48
3	C	999	FAD	C1B-N9A-C4A	-2.69	121.91	126.64
3	D	999	FAD	O5B-PA-O1A	-2.62	98.82	109.07
3	A	999	FAD	C5'-C4'-C3'	2.55	117.12	112.20
2	A	888	FYC	C12-C11-C10	-2.51	117.16	122.48
2	A	888	FYC	C15-C16-C11	-2.48	120.53	123.94
2	C	888	FYC	C1-N3-C18	2.47	108.67	103.78
3	C	999	FAD	C5'-C4'-C3'	2.46	116.95	112.20
2	D	888	FYC	C12-C11-C10	-2.43	117.34	122.48
3	A	999	FAD	O2A-PA-O1A	2.41	124.13	112.24
3	D	999	FAD	C5'-C4'-C3'	2.38	116.80	112.20
3	B	999	FAD	O3B-C3B-C4B	-2.37	104.19	111.05
2	B	888	FYC	C6-C5-C4	2.37	125.83	120.91
2	D	888	FYC	C12-C11-C16	2.32	118.64	115.98
3	A	999	FAD	N3A-C2A-N1A	-2.31	125.06	128.68
3	C	999	FAD	C5X-C9A-N10	2.27	119.36	117.72
2	D	888	FYC	F1-C16-C11	2.26	121.26	118.10
3	C	999	FAD	C9A-N10-C10	-2.26	118.95	121.91
3	B	999	FAD	O2P-P-O1P	2.20	123.13	112.24
2	C	888	FYC	C15-C16-C11	-2.19	120.93	123.94
2	D	888	FYC	C16-C11-C10	2.18	123.94	120.12
3	D	999	FAD	O3B-C3B-C4B	-2.18	104.75	111.05
3	C	999	FAD	C4A-C5A-N7A	-2.16	107.15	109.40
3	A	999	FAD	C4X-C10-N10	-2.12	118.12	120.30
3	D	999	FAD	C4X-N5-C5X	2.09	118.86	116.77
3	B	999	FAD	C5A-C6A-N1A	-2.09	115.60	120.35
2	D	888	FYC	C1-N3-C18	2.08	107.90	103.78
2	A	888	FYC	C13-C12-C11	-2.08	117.86	121.00
2	D	888	FYC	C15-C16-C11	-2.05	121.11	123.94
3	D	999	FAD	O4B-C1B-C2B	-2.01	103.99	106.93
3	C	999	FAD	C9A-C5X-N5	-2.01	119.22	122.36

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	999	FAD	N10-C1'-C2'-O2'
3	D	999	FAD	N10-C1'-C2'-C3'
3	B	999	FAD	N10-C1'-C2'-O2'
3	B	999	FAD	N10-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
2	D	888	FYC	C8-C10-C11-C16
2	B	888	FYC	C8-C10-C11-C16
2	A	888	FYC	C8-C10-C11-C16
2	C	888	FYC	C8-C10-C11-C16
3	A	999	FAD	N10-C1'-C2'-O2'
3	A	999	FAD	N10-C1'-C2'-C3'
3	C	999	FAD	N10-C1'-C2'-O2'
3	C	999	FAD	N10-C1'-C2'-C3'
2	C	888	FYC	C8-C10-C11-C12
2	D	888	FYC	C8-C10-C11-C12
2	A	888	FYC	C8-C10-C11-C12
2	D	888	FYC	O2-C7-C8-C9
2	A	888	FYC	O2-C7-C8-C9
2	D	888	FYC	N2-C7-C8-C10
2	A	888	FYC	N2-C7-C8-C10
2	B	888	FYC	C8-C10-C11-C12
2	D	888	FYC	N2-C7-C8-C9
2	A	888	FYC	N2-C7-C8-C9
2	C	888	FYC	N2-C7-C8-C9
2	D	888	FYC	O2-C7-C8-C10
2	C	888	FYC	O2-C7-C8-C10
2	C	888	FYC	O2-C7-C8-C9
2	A	888	FYC	O2-C7-C8-C10
2	B	888	FYC	N2-C7-C8-C10
2	B	888	FYC	O2-C7-C8-C10
2	C	888	FYC	N2-C7-C8-C10

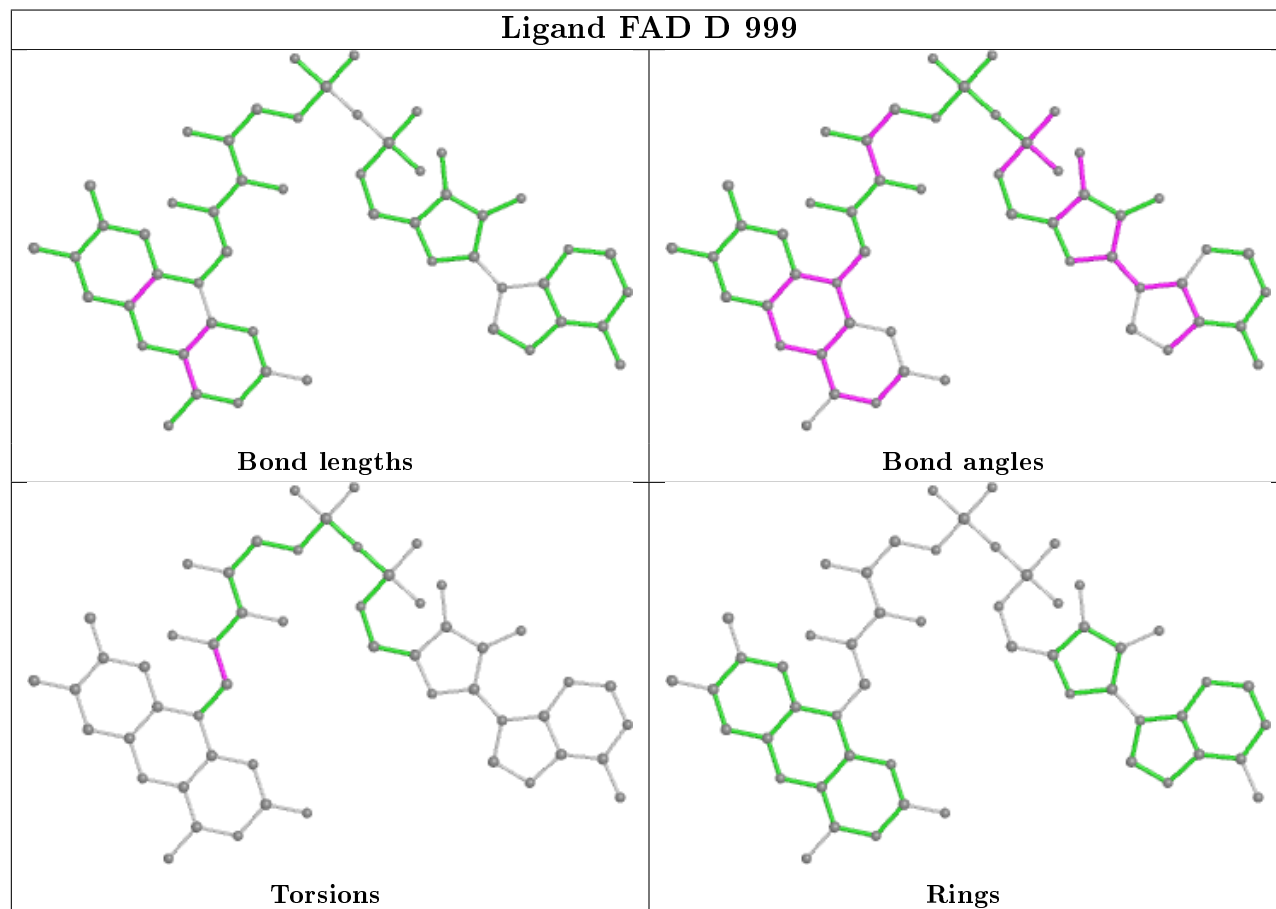
There are no ring outliers.

8 monomers are involved in 12 short contacts:

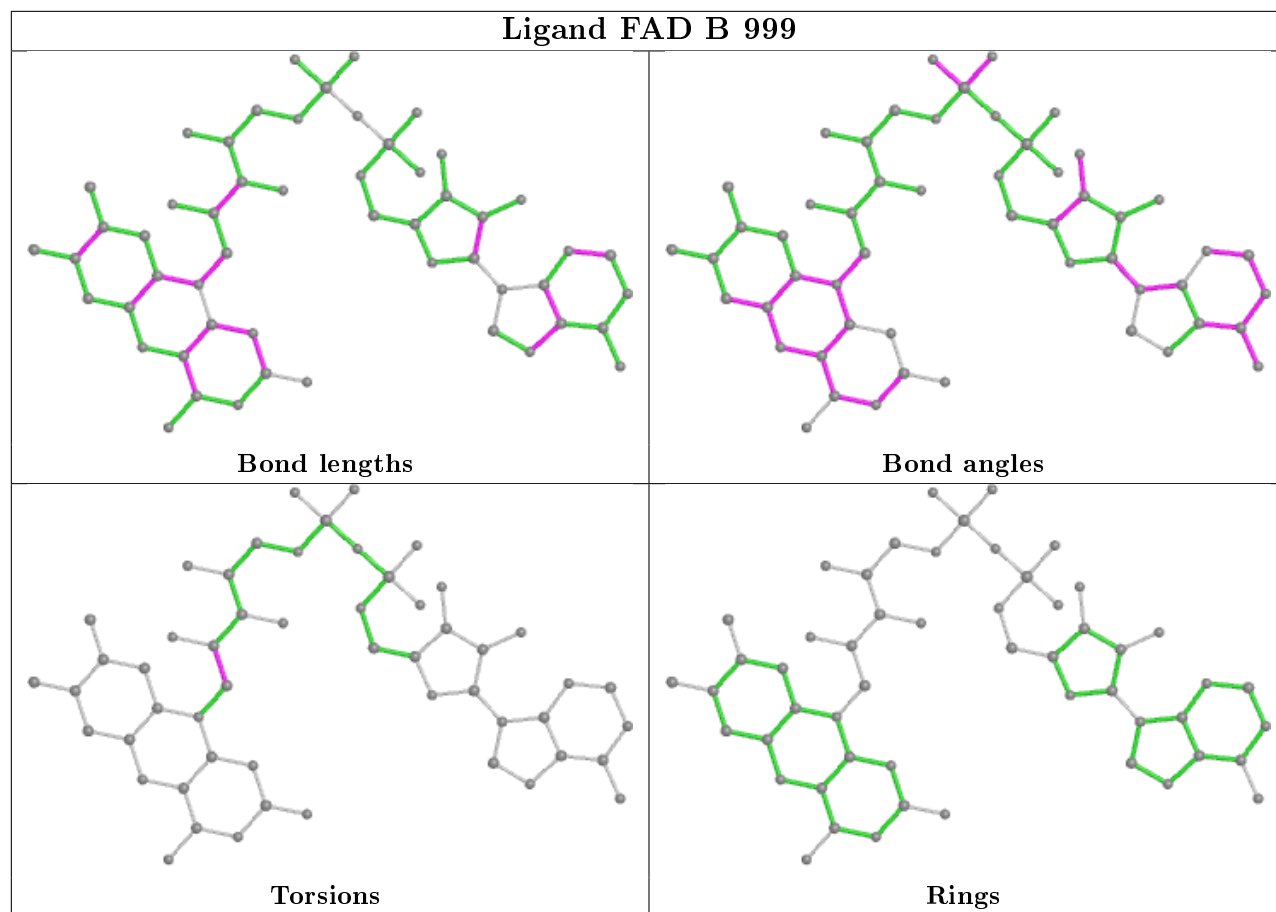
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	999	FAD	2	0
3	B	999	FAD	2	0
2	D	888	FYC	2	0
2	B	888	FYC	5	0
2	A	888	FYC	4	0
2	C	888	FYC	1	0
3	A	999	FAD	1	0
3	C	999	FAD	1	0

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

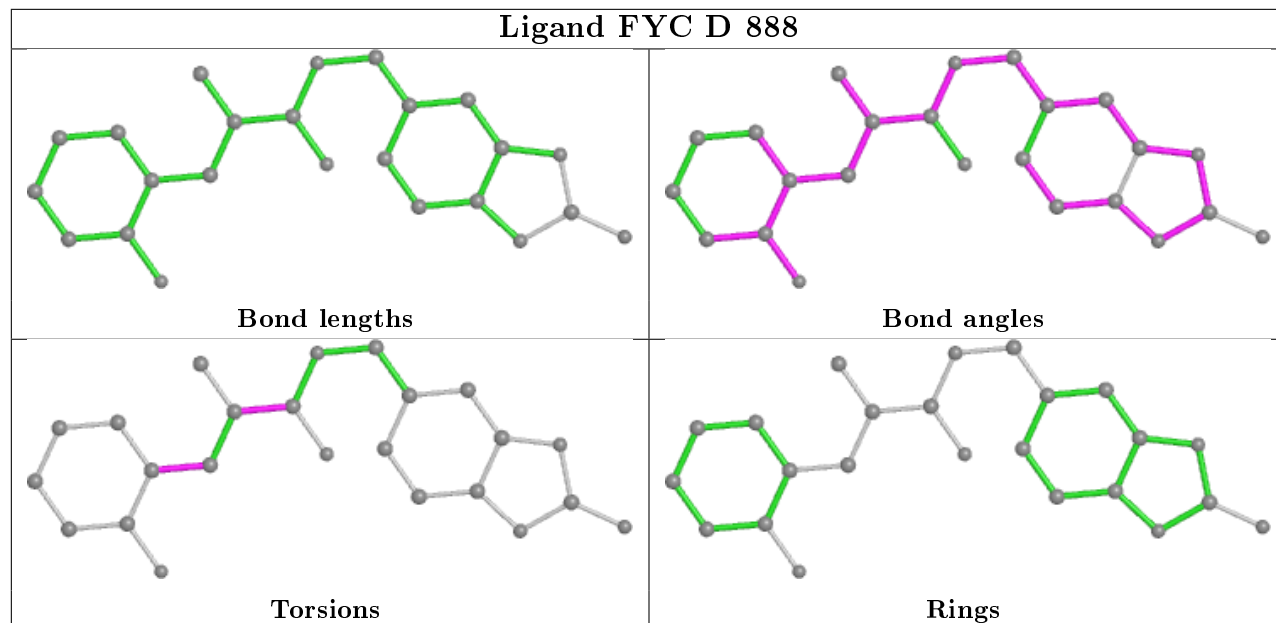
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.



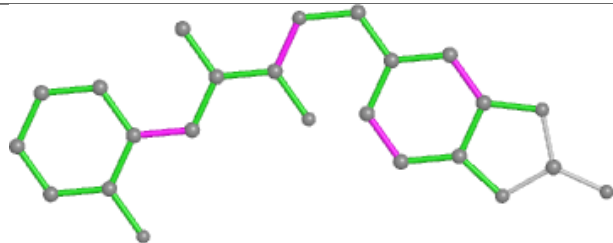
Ligand FAD B 999



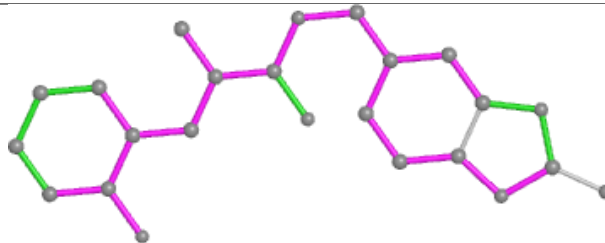
Ligand FYC D 888



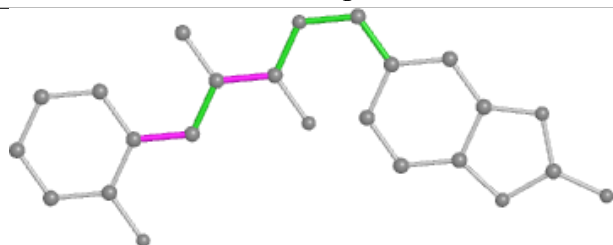
Ligand FYC B 888



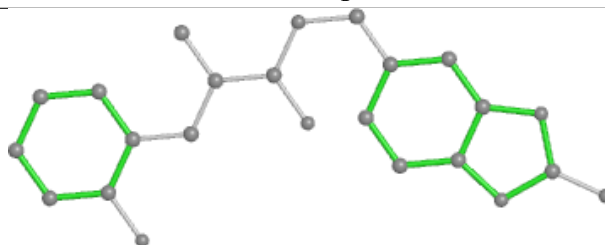
Bond lengths



Bond angles

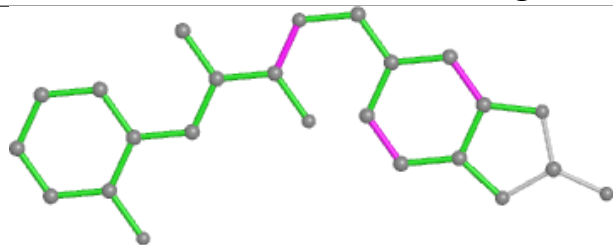


Torsions

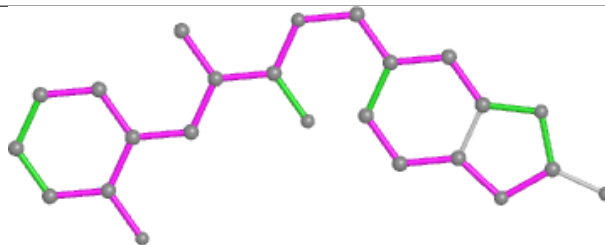


Rings

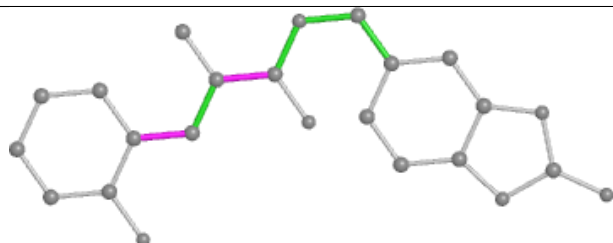
Ligand FYC A 888



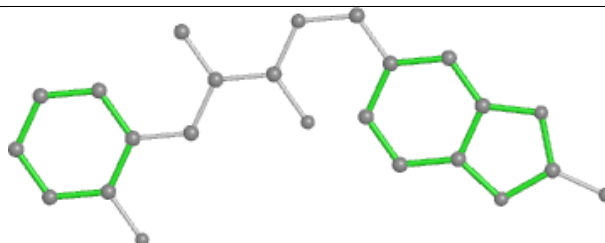
Bond lengths



Bond angles

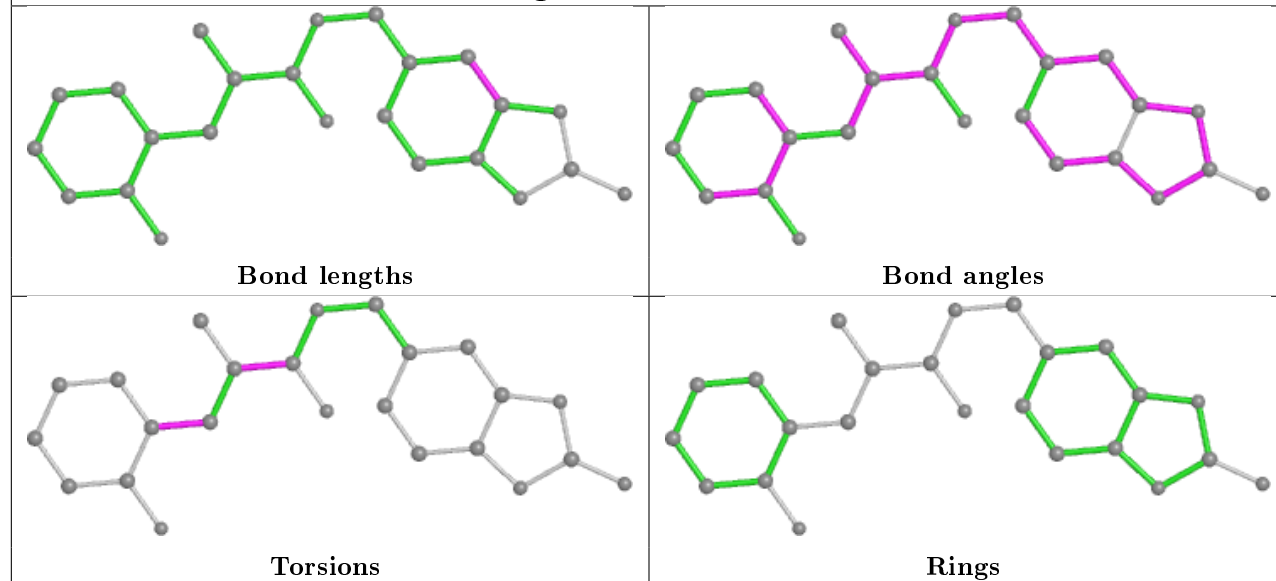


Torsions

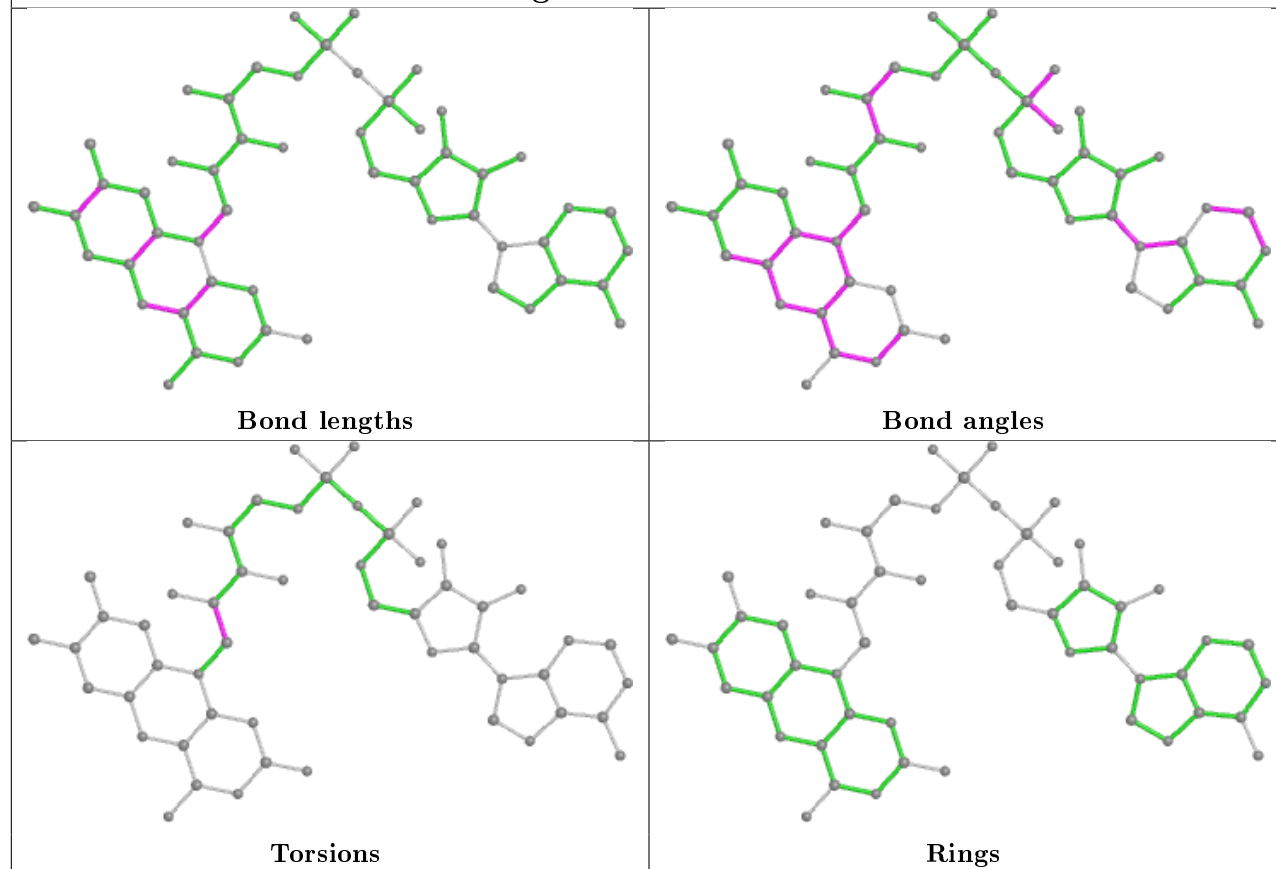


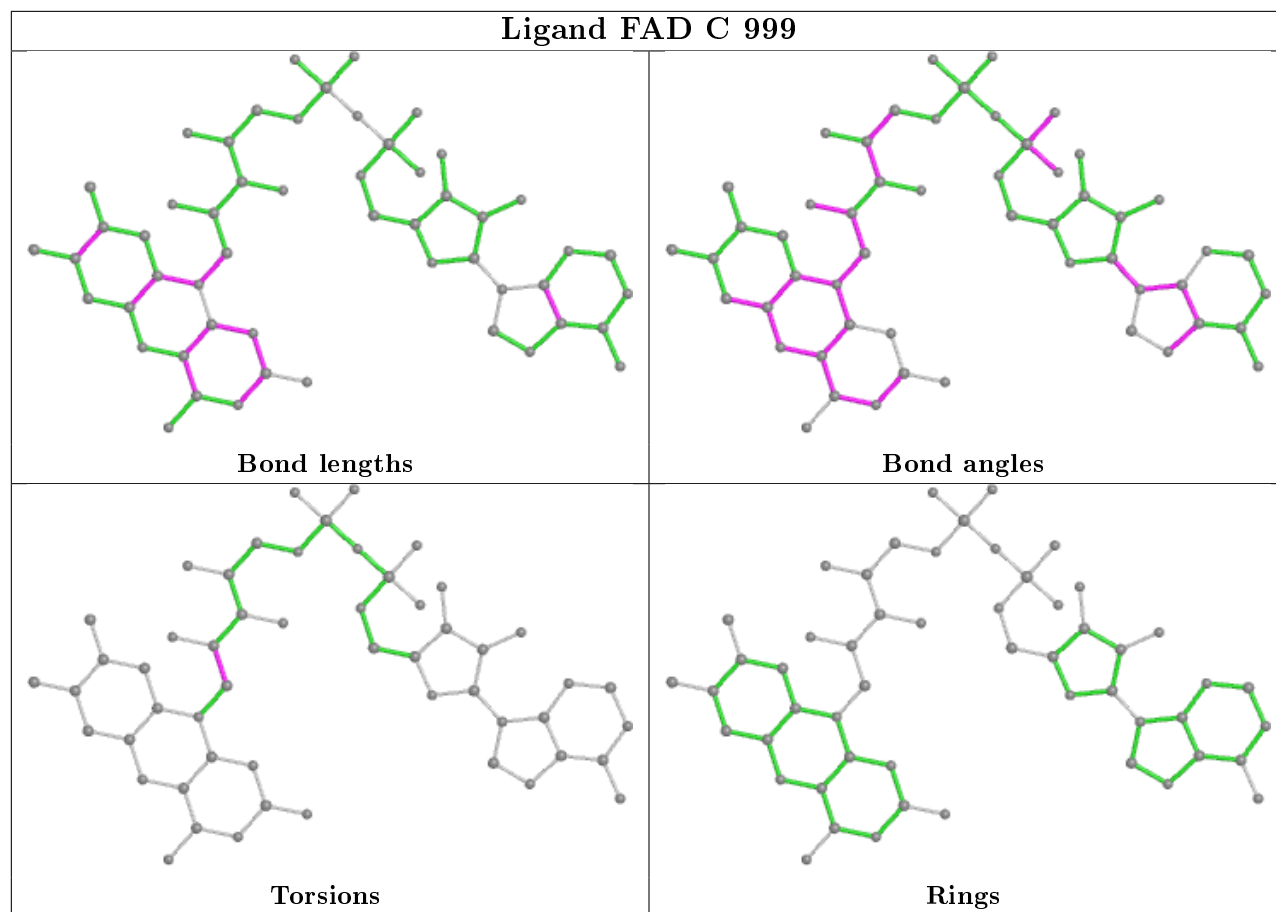
Rings

Ligand FYC C 888



Ligand FAD A 999





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	561/658 (85%)	-0.36	5 (0%) 84 83	11, 24, 54, 90	0
1	B	542/658 (82%)	-0.34	7 (1%) 77 76	12, 24, 49, 96	0
1	C	557/658 (84%)	-0.37	2 (0%) 92 92	10, 24, 46, 81	1 (0%)
1	D	550/658 (83%)	-0.35	1 (0%) 95 94	13, 25, 49, 75	0
All	All	2210/2632 (83%)	-0.35	15 (0%) 87 87	10, 24, 49, 96	1 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	458	PHE	5.4
1	A	144	THR	4.8
1	A	81	GLY	4.0
1	B	459	ASP	3.9
1	C	435	GLN	3.6
1	B	457	GLY	3.2
1	B	460	PRO	3.1
1	A	82	ILE	2.6
1	D	587	GLY	2.6
1	C	432	LEU	2.3
1	A	589	SER	2.3
1	B	140	LEU	2.2
1	A	435	GLN	2.1
1	B	157	PRO	2.1
1	B	81	GLY	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

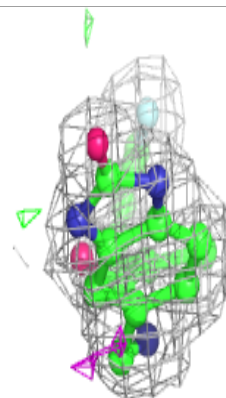
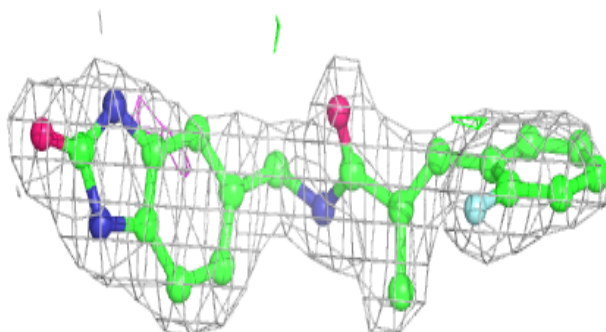
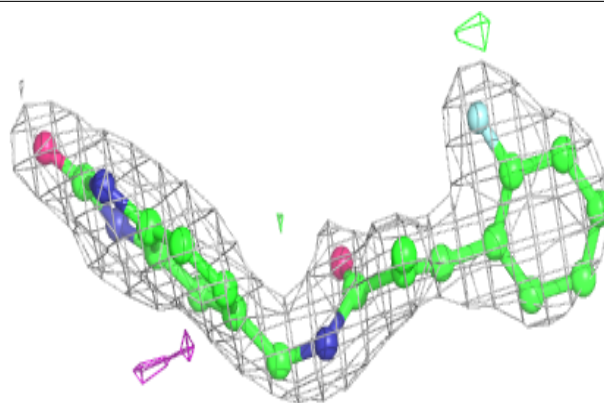
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FYC	D	888	24/24	0.91	0.19	32,43,57,58	0
2	FYC	B	888	24/24	0.91	0.17	32,47,57,62	0
2	FYC	C	888	24/24	0.91	0.16	27,36,52,57	0
4	SO4	B	1659	5/5	0.91	0.20	50,53,57,58	0
2	FYC	A	888	24/24	0.94	0.15	25,37,63,66	0
4	SO4	D	1659	5/5	0.96	0.18	38,46,48,48	0
4	SO4	C	1659	5/5	0.97	0.15	40,43,49,56	0
4	SO4	A	1659	5/5	0.97	0.12	36,39,41,44	0
3	FAD	B	999	53/53	0.99	0.09	11,13,16,18	0
3	FAD	D	999	53/53	0.99	0.09	10,12,14,15	0
3	FAD	A	999	53/53	0.99	0.09	11,13,17,20	0
3	FAD	C	999	53/53	0.99	0.10	9,10,13,13	0

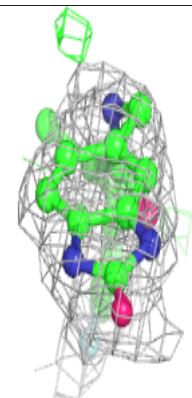
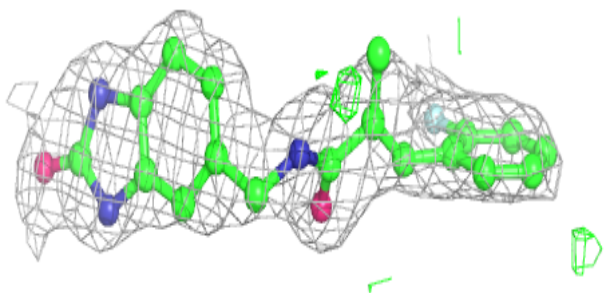
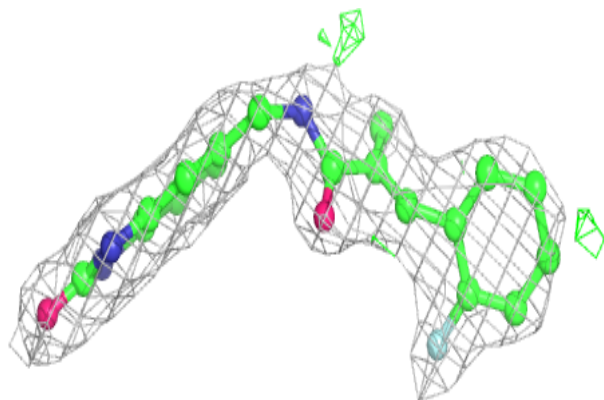
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FYC 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)

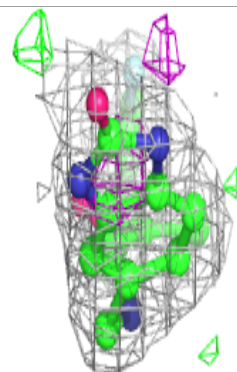
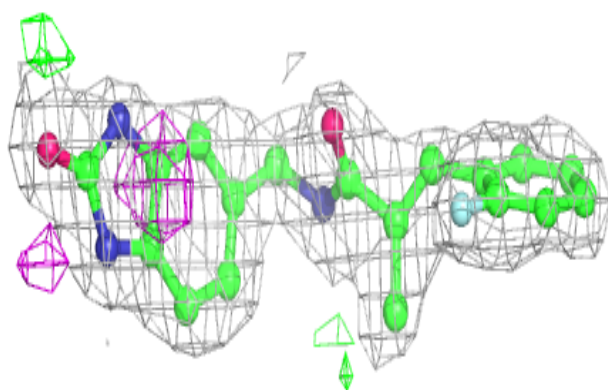
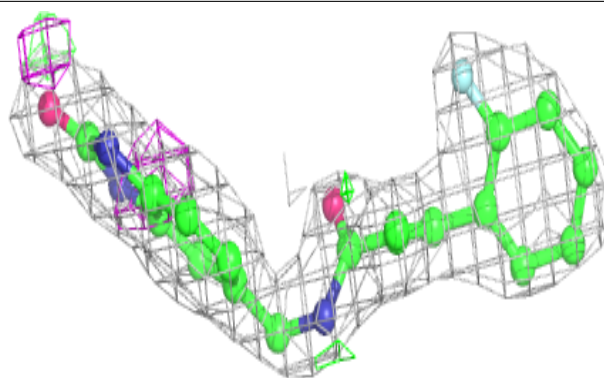
**Electron density around FYC B 888:**

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

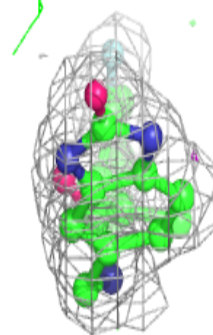
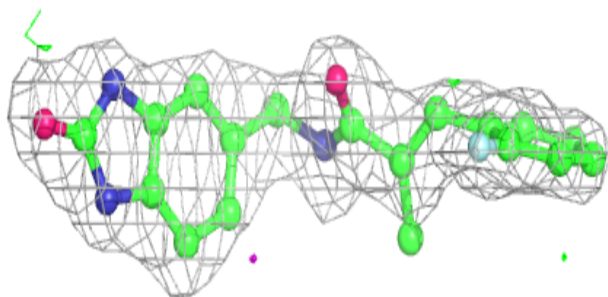
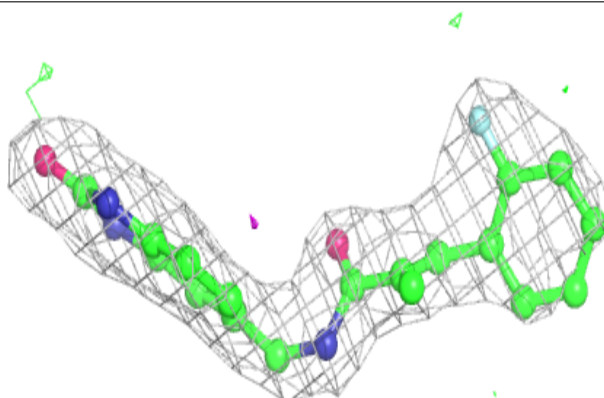


Electron density around FYC C 888:

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

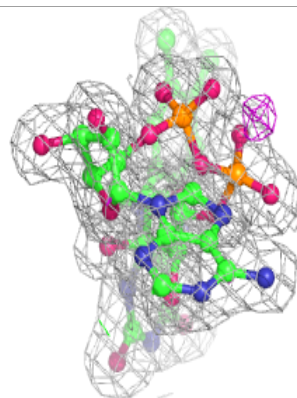
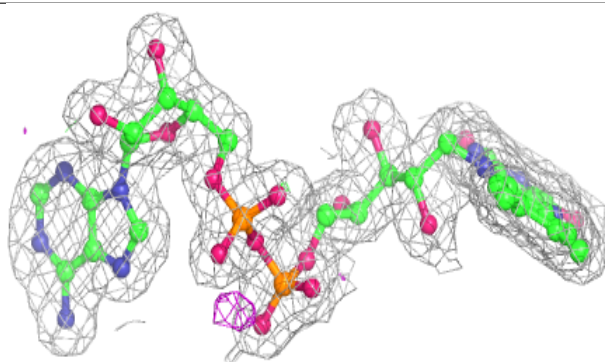
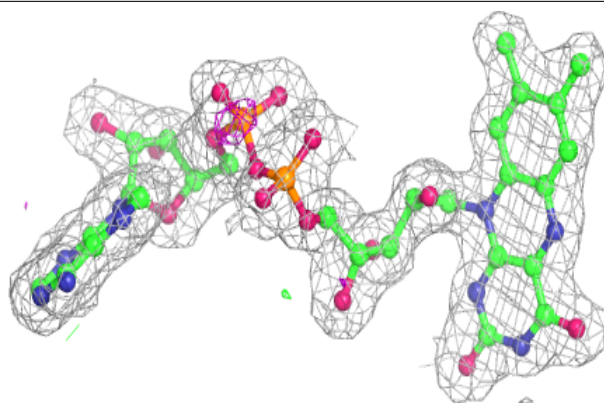
**Electron density around FYC A 888:**

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

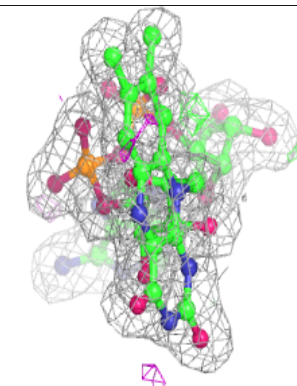
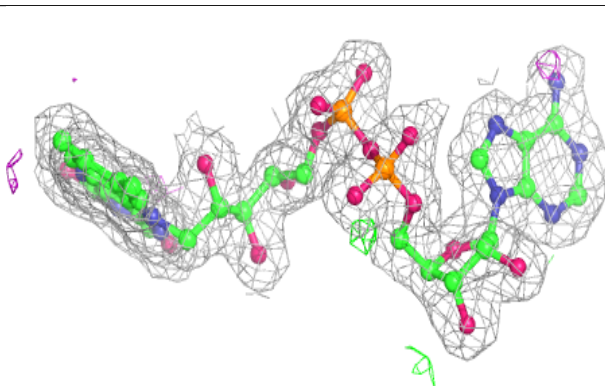
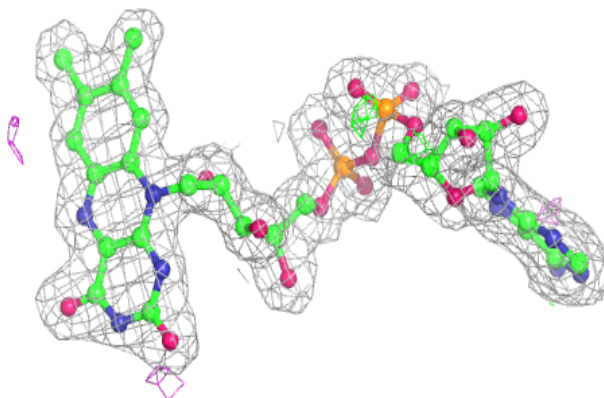


Electron density around FAD B 999:

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

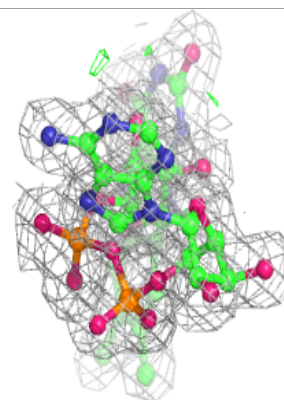
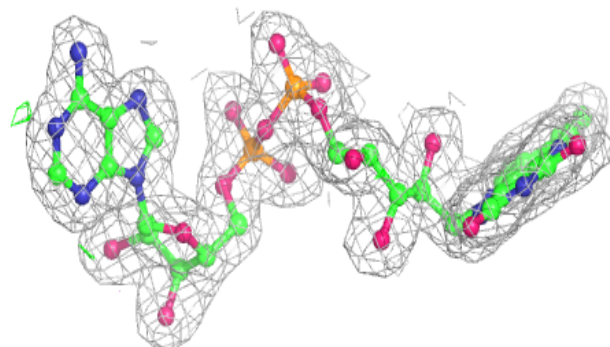
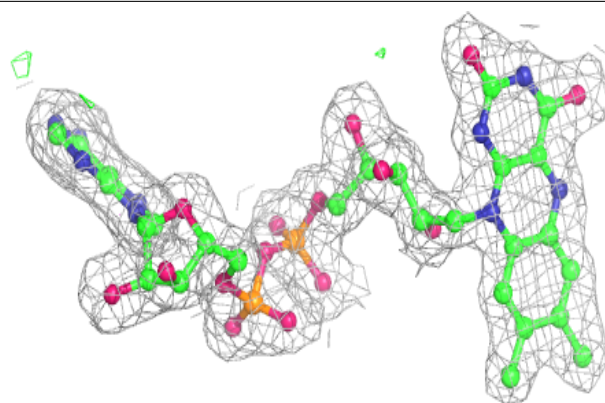
**Electron density around FAD D 999:**

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

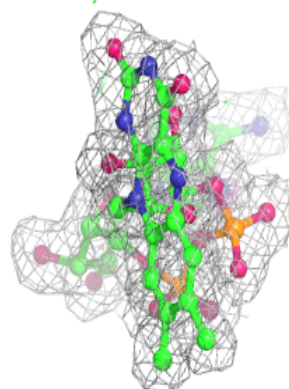
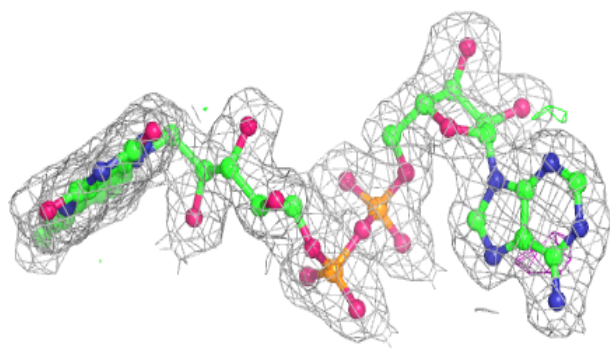
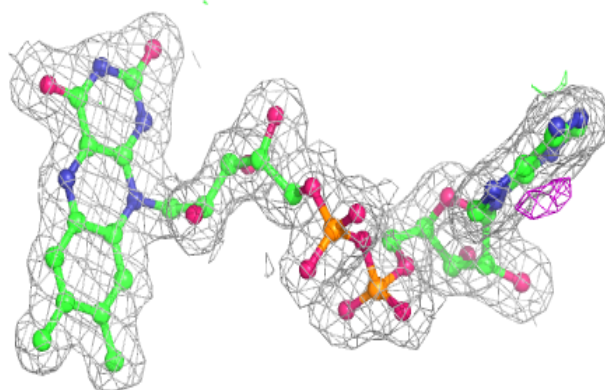


Electron density around FAD A 999:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.