



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:32 PM UTC

PDB ID : 5AE2 / pdb\_00005ae2  
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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

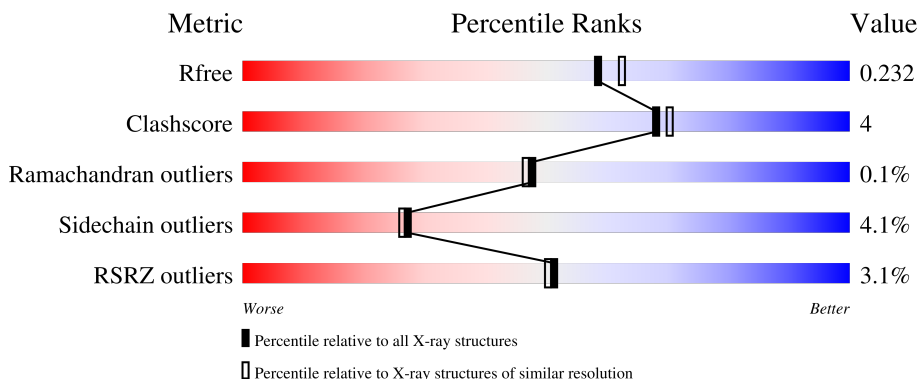
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	 3% 75% 10% 15%
1	B	658	 2% 72% 9% 18%
1	C	658	 2% 74% 10% 15%
1	D	658	 3% 74% 10% 16%

## 2 Entry composition [i](#)

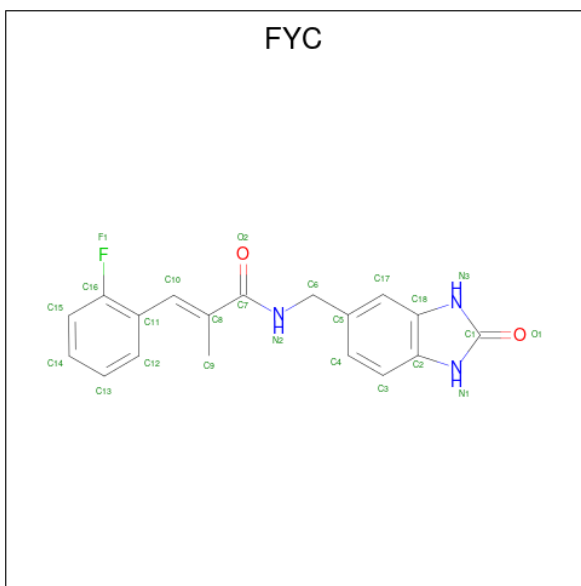
There are 5 unique types of molecules in this entry. The entry contains 18801 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 2 is 3-(2-fluorophenyl)-2-methyl-N-((2-oxo-2,3-dihydro-1H-benzo[d]imidazol-5-yl)methyl)acrylamide (CCD ID: FYC) (formula:  $C_{18}H_{16}FN_3O_2$ ).



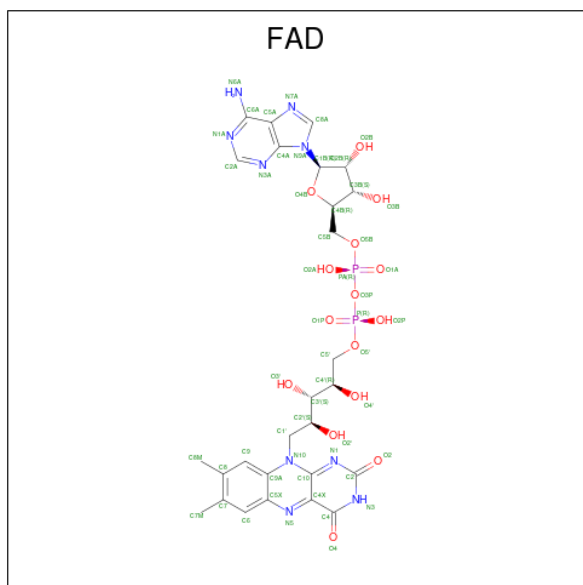
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
2	A	1	Total 24	C 18	F 1	N 3	O 2	0	0

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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 (CCD ID: 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 (CCD ID: 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	282	Total O 282 282	0	0
5	B	223	Total O 223 223	0	0
5	C	268	Total O 268 268	0	0
5	D	220	Total O 220 220	0	0





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.53Å 98.57Å 107.07Å 90.57° 90.14° 95.67°	Depositor
Resolution (Å)	107.06 – 2.00 107.06 – 2.00	Depositor EDS
% Data completeness (in resolution range)	85.3 (107.06-2.00) 85.3 (107.06-2.00)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 2.00Å)	Xtrriage
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 <sup>2</sup> )	22.0	Xtrriage
Anisotropy	0.019	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 40.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	18801	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

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

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	1.10	4/4530 (0.1%)	1.12	4/6123 (0.1%)
1	B	1.11	4/4389 (0.1%)	1.12	7/5932 (0.1%)
1	C	1.11	1/4504 (0.0%)	1.10	11/6090 (0.2%)
1	D	1.11	3/4455 (0.1%)	1.09	4/6022 (0.1%)
All	All	1.11	12/17878 (0.1%)	1.11	26/24167 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	603	ARG	CD-NE	-7.10	1.36	1.46
1	A	516	ASP	CB-CG	6.83	1.69	1.52
1	B	414	ALA	CA-C	6.17	1.59	1.53
1	C	623	ARG	CD-NE	-5.87	1.38	1.46
1	D	623	ARG	CD-NE	-5.67	1.38	1.46
1	B	105	LEU	CA-C	-5.48	1.46	1.52
1	B	363	PHE	C-O	-5.30	1.17	1.24
1	D	205	ILE	C-O	-5.19	1.20	1.24
1	A	567	VAL	CA-CB	-5.13	1.48	1.53
1	A	602	ALA	C-O	-5.12	1.18	1.24
1	D	214	CYS	CA-C	-5.10	1.46	1.52
1	A	333	VAL	C-O	-5.06	1.18	1.24

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	623	ARG	NE-CZ-NH2	-8.52	111.53	119.20
1	D	623	ARG	NE-CZ-NH2	-7.73	112.25	119.20
1	B	195	PHE	N-CA-C	6.82	118.36	111.07
1	B	160	VAL	N-CA-C	6.20	117.02	107.78
1	A	623	ARG	NE-CZ-NH2	-6.17	113.65	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	623	ARG	CG-CD-NE	-6.05	98.68	112.00
1	A	516	ASP	N-CA-C	-5.81	104.85	111.07
1	C	106	ASN	CB-CA-C	-5.77	98.93	110.42
1	D	180	ASP	CB-CA-C	-5.68	101.72	110.81
1	B	114	THR	N-CA-CB	-5.68	102.14	110.26
1	D	623	ARG	CG-CD-NE	-5.64	99.59	112.00
1	B	117	ARG	N-CA-C	5.63	117.50	111.36
1	D	508	THR	N-CA-C	5.62	117.40	111.28
1	C	638	MET	CG-SD-CE	-5.58	88.62	100.90
1	C	142	HIS	N-CA-CB	5.51	118.22	109.51
1	C	554	GLU	N-CA-C	5.44	117.96	111.71
1	C	537	VAL	N-CA-C	5.34	115.55	110.42
1	B	89	GLU	CB-CA-C	-5.30	101.67	110.68
1	B	134	ASN	N-CA-C	5.21	116.65	111.07
1	A	198	ARG	N-CA-C	5.21	116.96	111.28
1	C	505	TYR	N-CA-C	5.19	116.94	111.28
1	C	349	CYS	N-CA-C	5.16	117.25	109.41
1	C	505	TYR	CA-CB-CG	-5.14	104.66	113.90
1	B	500	ASN	N-CA-C	5.13	116.56	111.07
1	C	139	ASN	N-CA-C	5.10	121.21	114.12
1	A	141	ASP	N-CA-C	-5.08	99.98	110.80

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	4431	0	4360	42	0
1	B	4292	0	4234	31	0
1	C	4402	0	4340	36	0
1	D	4355	0	4300	23	0
2	A	24	0	16	4	0
2	B	24	0	16	5	0
2	C	24	0	16	0	0
2	D	24	0	16	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	53	0	31	1	0
3	B	53	0	31	2	0
3	C	53	0	31	0	0
3	D	53	0	31	1	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	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	127	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 4.

All (127) 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
1:C:419:ARG:HD3	5:C:2197:HOH:O	1.80	0.79
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:C:421:MET:HE2	1:C:465:VAL:HB	1.73	0.70
1:C:634:VAL:HG12	1:C:638:MET:HE2	1.72	0.69
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:B:888:FYC:H62C	3:B:999:FAD:HM71	1.77	0.66
1:B:83:ILE:HG23	1:B:91:MET:HE1	1.80	0.64
1:B:635:GLY:HA2	1:B:638:MET:HE3	1.80	0.64
1:B:298:THR:HG23	1:B:300:HIS:H	1.64	0.62
2:D:888:FYC:H62C	3:D:999:FAD:HM71	1.81	0.62
1:C:83:ILE:HG23	1:C:91:MET:HE1	1.82	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:D:83:ILE:HG23	1:D:91:MET:HE1	1.83	0.61
1:A:394:ALA:HB1	1:A:463:LEU:CD2	2.31	0.60
1:C:314:ILE:HG23	1:C:365:MET:HG2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:613:LEU:HD22	1:B:623:ARG:HD2	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:C:635:GLY:HA2	1:C:638:MET:HE3	1.86	0.57
1:A:215:HIS:HD2	1:A:375:THR:OG1	1.87	0.57
1:A:345:ILE:HD13	1:B:638:MET:HE1	1.87	0.57
1:A:430:HIS:CD2	1:A:447:LEU:HD13	2.40	0.56
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:A:442:SER:O	1:A:443:PHE:CB	2.54	0.55
1:A:106:ASN:HD22	1:A:106:ASN:C	2.15	0.55
1:A:83:ILE:HG23	1:A:91:MET:HE1	1.89	0.54
1:C:421:MET:HE1	1:C:426:PHE:HA	1.89	0.54
1:A:426:PHE:CD2	1:A:463:LEU:HD12	2.43	0.54
1:C:127:THR:HG22	1:C:127:THR:O	2.06	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:B:340:THR:HB	1:B:646:VAL:HG13	1.90	0.53
1:D:171:THR:O	1:D:172:ASN:HB3	2.08	0.52
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:94:ASN:HA	1:B:197:LEU:HD13	1.91	0.51
1:C:421:MET:HE1	1:C:426:PHE:CA	2.41	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: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:529:GLU:OE1	1:C:529:GLU:C	2.55	0.49
1:C:382:ARG:HD3	1:D:412:ARG:CZ	2.44	0.48
1:B:540:LEU:C	1:B:540:LEU:HD23	2.38	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:421:MET:HE1	1:C:426:PHE:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:421:MET:HE2	1:D:465:VAL:HB	1.98	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
1:A:109:GLY:HA3	1:C:268:TRP:CE3	2.51	0.45
1:A:619:VAL:HB	1:A:657:LEU:HD23	1.97	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:A:463:LEU:C	1:A:463:LEU:HD13	2.42	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: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:C:459:ASP:OD1	1:C:459:ASP:C	2.61	0.44
1:D:572:ASP:HB2	5:D:2191:HOH:O	2.17	0.44
2:A:888:FYC:H62C	3:A:999:FAD:HM71	2.00	0.44
1:C:419:ARG:O	1:C:466:ALA:HA	2.18	0.44
1:C:638:MET:HE1	1:D:345:ILE:CD1	2.48	0.43
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:372:GLY:HA2	1:A:652:PHE:CZ	2.54	0.43
1:A:386:GLU:HG2	1:A:473:ASP:HA	2.00	0.43
1:B:515:ARG:HG2	2:B:888:FYC:C12	2.49	0.43
1:C:490:LYS:HD2	1:C:490:LYS:N	2.34	0.43
2:B:888:FYC:H62C	3:B:999:FAD:C7M	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:D:102:LYS:C	1:D:113:LEU:HD12	2.47	0.40
1:D:323:LYS:C	1:D:323:LYS:HD2	2.47	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%)	30 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	536/658 (82%)	526 (98%)	10 (2%)	0	100	100
1	C	554/658 (84%)	540 (98%)	13 (2%)	1 (0%)	43	42
1	D	547/658 (83%)	535 (98%)	12 (2%)	0	100	100
All	All	2192/2632 (83%)	2144 (98%)	45 (2%)	3 (0%)	48	46

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%)	467 (98%)	11 (2%)	44	49
1	B	463/545 (85%)	442 (96%)	21 (4%)	24	23
1	C	477/545 (88%)	457 (96%)	20 (4%)	26	25
1	D	472/545 (87%)	447 (95%)	25 (5%)	20	18
All	All	1890/2180 (87%)	1813 (96%)	77 (4%)	27	26

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	A	140	LEU
1	A	463	LEU
1	A	476	LYS
1	A	516	ASP
1	A	553	LYS
1	A	559	PHE
1	A	563	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	589	SER
1	A	596	GLU
1	A	599	GLU
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	162	GLU
1	B	191	LEU
1	B	197	LEU
1	B	298	THR
1	B	432	LEU
1	B	476	LYS
1	B	482	LYS
1	B	500	ASN
1	B	507	LEU
1	B	510	VAL
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	120	LEU
1	C	140	LEU
1	C	141	ASP
1	C	142	HIS
1	C	144	THR
1	C	150	LEU
1	C	199	GLU
1	C	224	LEU
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	510	VAL
1	C	553	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	613	LEU
1	C	628	LYS
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	360	ILE
1	D	462	GLN
1	D	463	LEU
1	D	474	ARG
1	D	480	HIS
1	D	482	LYS
1	D	507	LEU
1	D	510	VAL
1	D	536	ARG
1	D	553	LYS
1	D	555	LYS
1	D	563	SER
1	D	581	PHE
1	D	586	ARG
1	D	588	ILE
1	D	592	LEU
1	D	599	GLU
1	D	613	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	106	ASN
1	A	172	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	424	GLN
1	A	430	HIS

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Mol	Chain	Res	Type
1	A	479	GLN
1	B	177	GLN
1	B	192	HIS
1	B	388	GLN
1	C	142	HIS
1	C	272	ASN
1	C	423	ASN
1	D	350	GLN
1	D	423	ASN
1	D	625	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 oligosaccharides 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	FYC	B	888	-	26,26,26	1.03	2 (7%)	35,36,36	2.46	13 (37%)
3	FAD	D	999	-	58,58,58	1.47	8 (13%)	85,89,89	1.66	22 (25%)
4	SO4	C	1659	-	4,4,4	0.50	0	6,6,6	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FYC	D	888	-	26,26,26	0.76	1 (3%)	35,36,36	2.05	12 (34%)
4	SO4	D	1659	-	4,4,4	0.49	0	6,6,6	0.48	0
4	SO4	A	1659	-	4,4,4	0.61	0	6,6,6	0.50	0
3	FAD	C	999	-	58,58,58	1.70	11 (18%)	85,89,89	1.57	17 (20%)
3	FAD	B	999	-	58,58,58	1.68	10 (17%)	85,89,89	1.72	19 (22%)
2	FYC	A	888	-	26,26,26	0.97	1 (3%)	35,36,36	2.22	15 (42%)
4	SO4	B	1659	-	4,4,4	0.68	0	6,6,6	0.81	0
3	FAD	A	999	-	58,58,58	1.57	10 (17%)	85,89,89	1.55	14 (16%)
2	FYC	C	888	-	26,26,26	0.79	0	35,36,36	1.90	6 (17%)

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	FYC	B	888	-	-	6/13/13/13	0/3/3/3
3	FAD	D	999	-	-	3/34/50/50	0/6/6/6
2	FYC	D	888	-	-	6/13/13/13	0/3/3/3
3	FAD	C	999	-	-	2/34/50/50	0/6/6/6
3	FAD	B	999	-	-	2/34/50/50	0/6/6/6
2	FYC	A	888	-	-	6/13/13/13	0/3/3/3
3	FAD	A	999	-	-	2/34/50/50	0/6/6/6
2	FYC	C	888	-	-	6/13/13/13	0/3/3/3

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	FAD	C9A-C5X	5.69	1.50	1.41
3	C	999	FAD	C9A-C5X	5.67	1.50	1.41
3	D	999	FAD	C9A-C5X	5.06	1.49	1.41
3	B	999	FAD	C5A-C4A	4.43	1.47	1.39
3	B	999	FAD	C4-N3	-4.37	1.30	1.38
3	C	999	FAD	C5A-C4A	4.33	1.46	1.39
3	C	999	FAD	PA-O3P	4.24	1.64	1.59
3	B	999	FAD	C9A-C5X	4.15	1.47	1.41
3	A	999	FAD	P-O3P	4.08	1.63	1.59
3	B	999	FAD	C5A-N7A	-3.69	1.32	1.39
3	B	999	FAD	C2'-C3'	3.67	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	999	FAD	PA-O3P	3.54	1.63	1.59
3	D	999	FAD	C5A-C4A	3.50	1.45	1.39
3	A	999	FAD	PA-O3P	3.47	1.63	1.59
3	C	999	FAD	C8-C7	3.21	1.48	1.40
3	B	999	FAD	C5X-N5	-3.20	1.33	1.39
3	D	999	FAD	C4A-N9A	-3.19	1.31	1.37
3	B	999	FAD	C4A-N9A	-2.96	1.31	1.37
3	A	999	FAD	C8-C7	2.94	1.48	1.40
3	C	999	FAD	C4A-N9A	-2.90	1.31	1.37
3	C	999	FAD	C1'-C2'	2.88	1.56	1.52
3	A	999	FAD	C5A-C4A	2.87	1.44	1.39
3	C	999	FAD	P-O3P	2.71	1.62	1.59
3	C	999	FAD	C2-N3	-2.71	1.33	1.39
2	B	888	FYC	C11-C10	-2.69	1.42	1.46
3	A	999	FAD	C4X-N5	2.58	1.36	1.30
3	C	999	FAD	C5X-N5	-2.56	1.34	1.39
3	B	999	FAD	C8-C7	2.53	1.47	1.40
3	B	999	FAD	C2-N1	-2.50	1.31	1.36
3	A	999	FAD	C5A-C6A	2.47	1.47	1.41
3	D	999	FAD	C4X-N5	2.43	1.36	1.30
2	A	888	FYC	C7-N2	2.43	1.37	1.33
3	B	999	FAD	O4-C4	2.40	1.28	1.23
3	D	999	FAD	C4-N3	-2.38	1.34	1.38
3	C	999	FAD	C4-N3	-2.36	1.34	1.38
2	B	888	FYC	C7-N2	2.30	1.37	1.33
3	A	999	FAD	C8A-N9A	-2.15	1.33	1.37
3	A	999	FAD	C8A-N7A	2.12	1.35	1.31
3	D	999	FAD	C8A-N9A	-2.09	1.34	1.37
3	C	999	FAD	C4X-N5	2.07	1.35	1.30
2	D	888	FYC	C7-N2	2.02	1.37	1.33
3	A	999	FAD	C4A-N3A	2.02	1.38	1.34
3	D	999	FAD	C5X-N5	-2.01	1.35	1.39

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	888	FYC	C6-N2-C7	-6.48	112.81	122.07
2	C	888	FYC	C9-C8-C10	5.82	133.69	125.14
2	B	888	FYC	C12-C11-C16	5.42	122.26	115.99
2	B	888	FYC	C10-C8-C7	-5.25	105.52	120.85
2	B	888	FYC	C15-C16-C11	-5.05	117.29	123.88
3	B	999	FAD	C9A-C5X-N5	-4.65	117.53	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	888	FYC	C6-N2-C7	-4.59	115.50	122.07
2	C	888	FYC	C10-C8-C7	-4.32	108.21	120.85
3	D	999	FAD	C4A-N9A-C8A	4.32	110.28	105.74
2	A	888	FYC	C6-N2-C7	-4.23	116.02	122.07
3	C	999	FAD	C4A-N9A-C8A	4.22	110.17	105.74
2	D	888	FYC	C9-C8-C10	4.22	131.33	125.14
3	A	999	FAD	C9A-C5X-N5	-4.20	118.00	122.45
3	B	999	FAD	C4A-N9A-C8A	4.15	110.10	105.74
2	C	888	FYC	C6-N2-C7	-4.06	116.27	122.07
2	A	888	FYC	F1-C16-C11	4.05	123.50	118.11
2	A	888	FYC	C10-C8-C7	-4.05	109.02	120.85
3	A	999	FAD	C5A-C4A-N3A	-4.01	121.20	126.72
3	D	999	FAD	O2A-PA-O1A	3.95	130.83	112.44
2	A	888	FYC	C12-C11-C16	3.92	120.53	115.99
3	A	999	FAD	C4A-N9A-C8A	3.91	109.85	105.74
3	C	999	FAD	C4-C4X-N5	3.90	123.59	118.21
3	B	999	FAD	O2-C2-N1	-3.88	115.36	121.80
3	A	999	FAD	N3A-C4A-N9A	3.85	133.71	127.17
2	B	888	FYC	F1-C16-C11	3.79	123.16	118.11
3	B	999	FAD	N3A-C2A-N1A	-3.78	122.86	128.58
3	B	999	FAD	C2A-N1A-C6A	3.73	124.86	118.73
2	D	888	FYC	C10-C8-C7	-3.63	110.25	120.85
2	A	888	FYC	C9-C8-C7	3.63	124.12	115.22
2	B	888	FYC	C9-C8-C7	3.61	124.08	115.22
2	B	888	FYC	C9-C8-C10	3.59	130.41	125.14
3	D	999	FAD	C4A-C5A-N7A	-3.53	106.54	110.58
2	B	888	FYC	C6-C5-C17	-3.53	113.10	120.63
3	B	999	FAD	N3A-C4A-N9A	3.52	133.15	127.17
3	D	999	FAD	C5A-C4A-N3A	-3.51	121.89	126.72
2	A	888	FYC	C4-C3-C2	-3.45	112.92	119.57
2	A	888	FYC	C18-C17-C5	-3.43	114.86	120.60
3	A	999	FAD	C5X-C9A-N10	3.41	121.05	117.97
3	D	999	FAD	C5X-C9A-N10	3.37	121.01	117.97
3	B	999	FAD	C5X-N5-C4X	3.18	123.23	118.09
2	A	888	FYC	C18-N3-C1	-3.11	106.64	110.03
3	B	999	FAD	C5A-C4A-N3A	-3.07	122.48	126.72
3	C	999	FAD	C9A-C5X-N5	-3.04	119.22	122.45
2	D	888	FYC	O1-C1-N3	3.04	130.14	126.68
3	D	999	FAD	C4-C4X-N5	3.02	122.38	118.21
3	C	999	FAD	O2A-PA-O1A	3.01	126.47	112.44
3	A	999	FAD	C4-C4X-N5	3.00	122.36	118.21
3	C	999	FAD	C4A-C5A-N7A	-3.00	107.15	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	888	FYC	C6-C5-C17	-2.91	114.42	120.63
3	D	999	FAD	N9A-C8A-N7A	-2.85	109.89	113.94
3	C	999	FAD	C6A-C5A-N7A	2.83	137.54	132.09
3	D	999	FAD	N3A-C4A-N9A	2.83	131.98	127.17
2	C	888	FYC	C12-C11-C16	2.80	119.24	115.99
3	B	999	FAD	C4-C4X-N5	2.79	122.06	118.21
3	A	999	FAD	C6-C5X-N5	2.77	123.04	118.44
3	B	999	FAD	N9A-C8A-N7A	-2.75	110.03	113.94
2	D	888	FYC	O1-C1-N1	-2.75	123.54	126.68
3	B	999	FAD	N6A-C6A-N1A	2.74	124.48	118.38
2	B	888	FYC	C12-C11-C10	-2.64	116.76	122.49
3	A	999	FAD	O2P-P-O3P	2.60	114.31	107.27
3	A	999	FAD	C5'-C4'-C3'	2.60	117.12	112.22
2	B	888	FYC	O1-C1-N1	-2.60	123.72	126.68
3	C	999	FAD	O2-C2-N1	-2.58	117.52	121.80
2	A	888	FYC	C15-C16-C11	-2.57	120.53	123.88
2	B	888	FYC	C18-N3-C1	-2.57	107.23	110.03
3	D	999	FAD	O5B-PA-O1A	-2.55	98.82	108.94
3	B	999	FAD	C5X-C9A-N10	2.53	120.26	117.97
3	C	999	FAD	O4B-C1B-N9A	-2.53	103.24	108.09
3	A	999	FAD	O2A-PA-O1A	2.51	124.13	112.44
3	C	999	FAD	C5'-C4'-C3'	2.51	116.95	112.22
3	C	999	FAD	N9A-C8A-N7A	-2.50	110.39	113.94
2	A	888	FYC	C3-C2-C18	2.47	124.64	121.11
2	A	888	FYC	C12-C11-C10	-2.46	117.16	122.49
3	A	999	FAD	O4-C4-C4X	-2.45	120.05	126.53
3	D	999	FAD	C5'-C4'-C3'	2.43	116.80	112.22
3	A	999	FAD	C2A-N3A-C4A	2.40	117.70	111.83
3	C	999	FAD	C5A-C4A-N3A	-2.40	123.41	126.72
2	B	888	FYC	C6-C5-C4	2.40	125.83	120.94
3	B	999	FAD	O3B-C3B-C4B	-2.40	104.19	111.08
3	B	999	FAD	C4A-N9A-C1B	-2.39	121.04	126.63
2	D	888	FYC	C12-C11-C10	-2.38	117.34	122.49
2	B	888	FYC	C2-C18-N3	2.38	109.44	106.42
3	D	999	FAD	C6A-C5A-N7A	2.37	136.66	132.09
2	D	888	FYC	F1-C16-C11	2.37	121.26	118.11
2	D	888	FYC	C16-C11-C10	2.35	123.94	119.92
3	D	999	FAD	C5A-N7A-C8A	2.34	107.13	103.45
2	A	888	FYC	C4-C5-C17	2.34	121.78	118.55
3	D	999	FAD	C4'-C3'-C2'	2.33	117.45	113.57
3	A	999	FAD	N3A-C2A-N1A	-2.33	125.06	128.58
2	A	888	FYC	C6-C5-C17	-2.31	115.69	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	999	FAD	O2P-P-O1P	2.30	123.13	112.44
2	D	888	FYC	C12-C11-C16	2.29	118.64	115.99
3	D	999	FAD	C9A-N10-C10	-2.29	117.27	120.75
3	C	999	FAD	C4X-C4-N3	2.28	119.05	113.25
3	B	999	FAD	C6-C5X-N5	2.27	122.20	118.44
3	C	999	FAD	C5X-N5-C4X	2.26	121.75	118.09
2	C	888	FYC	C15-C16-C11	-2.26	120.93	123.88
3	D	999	FAD	C4A-N9A-C1B	-2.24	121.39	126.63
2	D	888	FYC	C2-C18-N3	2.23	109.25	106.42
3	B	999	FAD	C4'-C3'-C2'	2.21	117.25	113.57
3	D	999	FAD	O3B-C3B-C4B	-2.21	104.75	111.08
3	B	999	FAD	C5A-N7A-C8A	2.19	106.89	103.45
3	A	999	FAD	C4A-N9A-C1B	-2.18	121.54	126.63
3	B	999	FAD	O2-C2-N3	2.17	122.75	118.58
3	C	999	FAD	C6-C5X-N5	2.17	122.04	118.44
3	D	999	FAD	C2A-N3A-C4A	2.16	117.10	111.83
3	D	999	FAD	O4B-C1B-N9A	-2.15	103.96	108.09
3	D	999	FAD	C4X-C10-N10	2.12	119.52	116.48
2	D	888	FYC	C15-C16-C11	-2.12	121.11	123.88
3	C	999	FAD	C2B-C1B-N9A	2.08	118.48	113.30
2	A	888	FYC	C2-C18-N3	2.08	109.06	106.42
3	D	999	FAD	C9A-C9-C8	2.07	123.39	119.22
3	C	999	FAD	O4-C4-C4X	-2.06	121.09	126.53
3	D	999	FAD	C10-N1-C2	2.05	121.29	116.85
2	A	888	FYC	C13-C12-C11	-2.04	117.86	120.95
3	D	999	FAD	C4X-C4-N3	2.04	118.44	113.25
2	D	888	FYC	C6-C5-C17	-2.02	116.31	120.63
3	C	999	FAD	C4A-N9A-C1B	-2.02	121.91	126.63

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	888	FYC	C8-C10-C11-C16
2	B	888	FYC	C8-C10-C11-C16
2	C	888	FYC	C8-C10-C11-C16
2	D	888	FYC	C8-C10-C11-C16
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'

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Mol	Chain	Res	Type	Atoms
3	C	999	FAD	N10-C1'-C2'-C3'
3	D	999	FAD	N10-C1'-C2'-O2'
3	D	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	O2-C7-C8-C9
2	D	888	FYC	O2-C7-C8-C9
2	A	888	FYC	C8-C10-C11-C12
2	A	888	FYC	N2-C7-C8-C10
2	D	888	FYC	N2-C7-C8-C10
2	B	888	FYC	C8-C10-C11-C12
2	A	888	FYC	N2-C7-C8-C9
2	C	888	FYC	N2-C7-C8-C9
2	D	888	FYC	N2-C7-C8-C9
2	C	888	FYC	O2-C7-C8-C10
2	D	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
2	B	888	FYC	N2-C7-C8-C9
2	B	888	FYC	O2-C7-C8-C9
3	D	999	FAD	PA-O3P-P-O2P

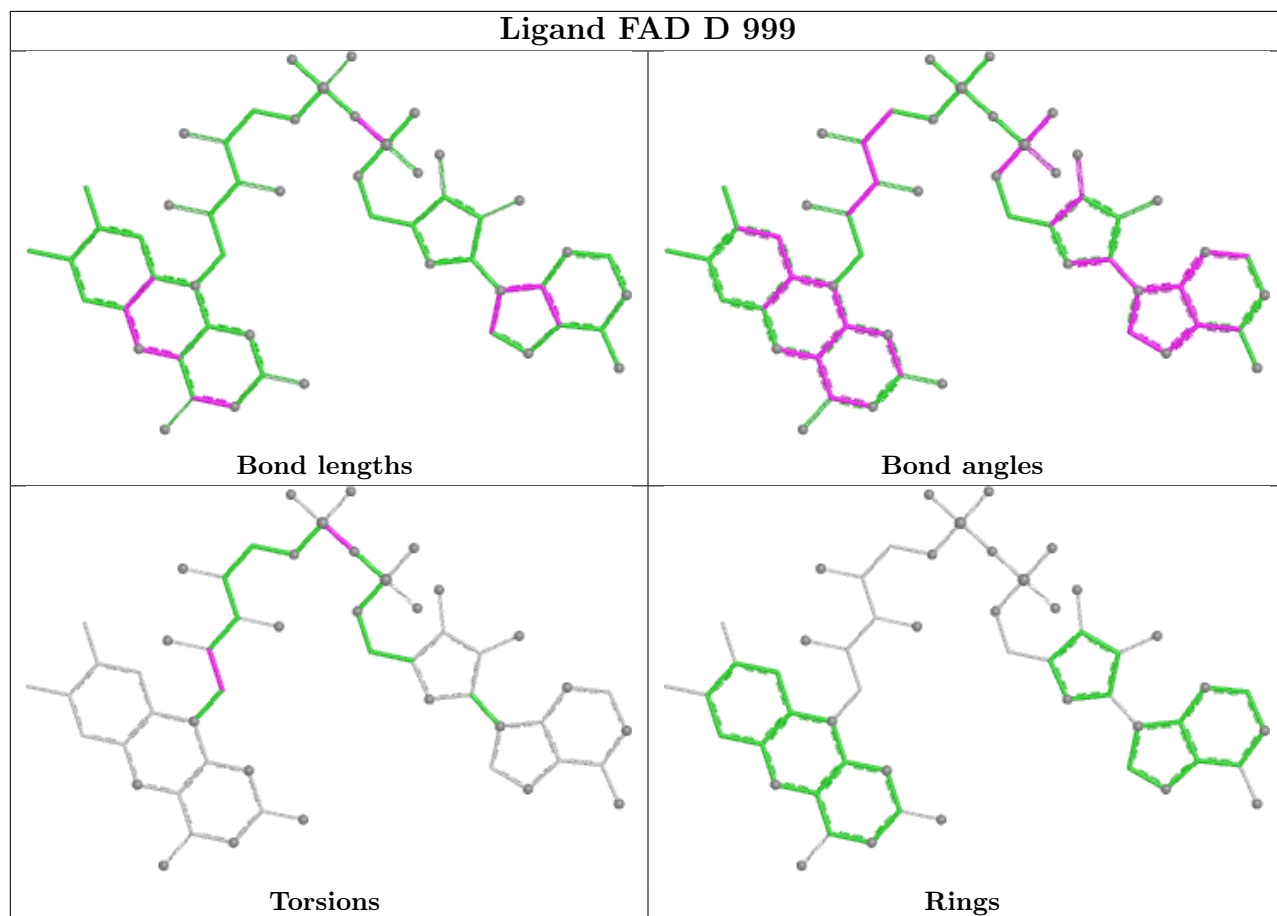
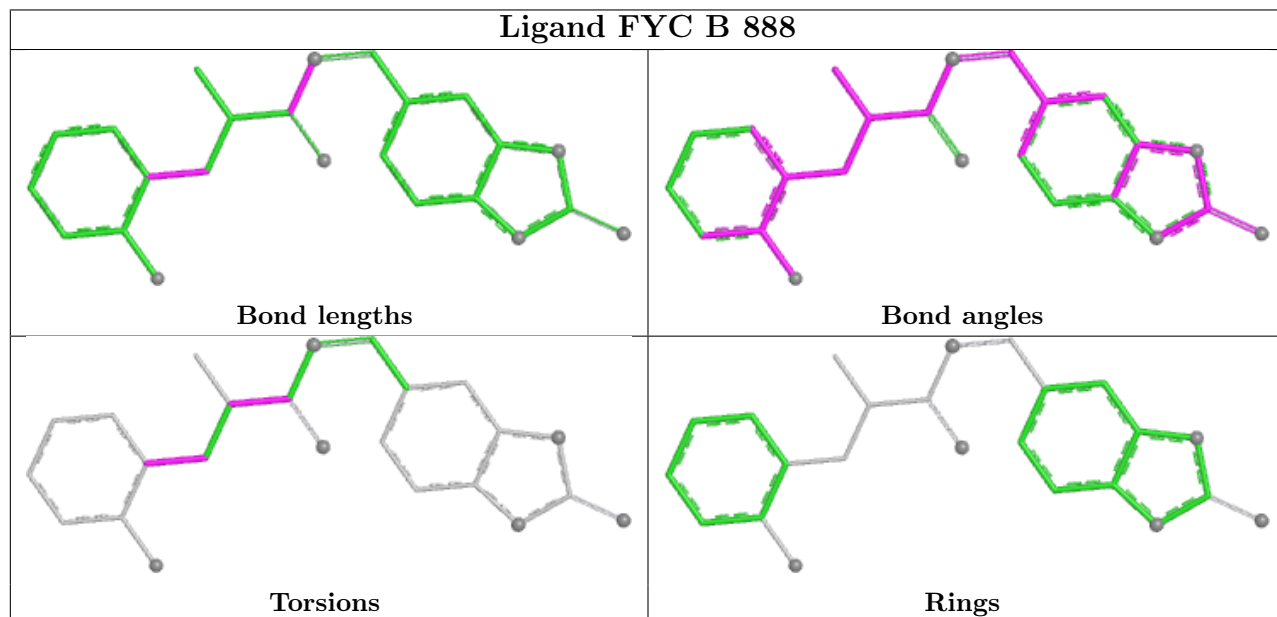
There are no ring outliers.

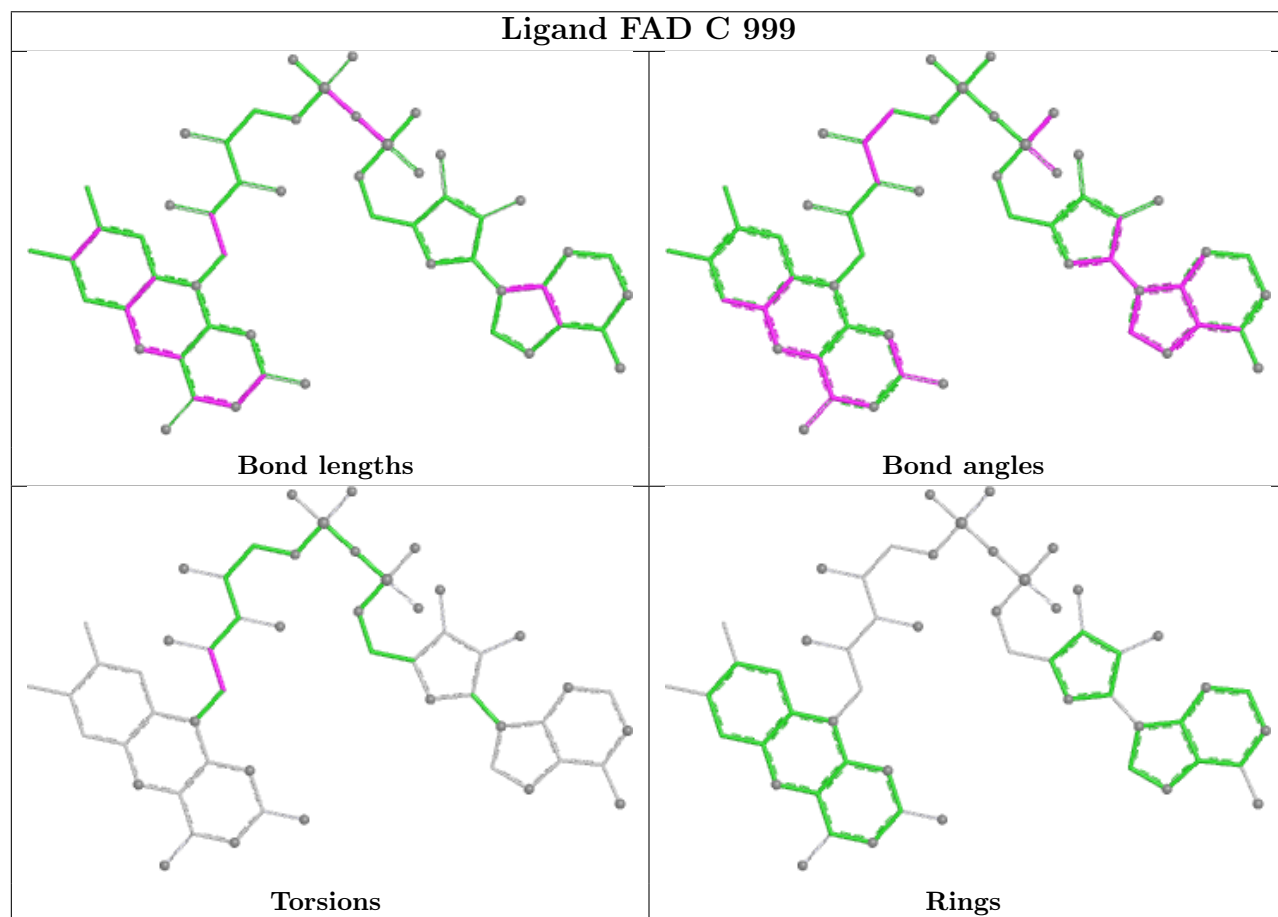
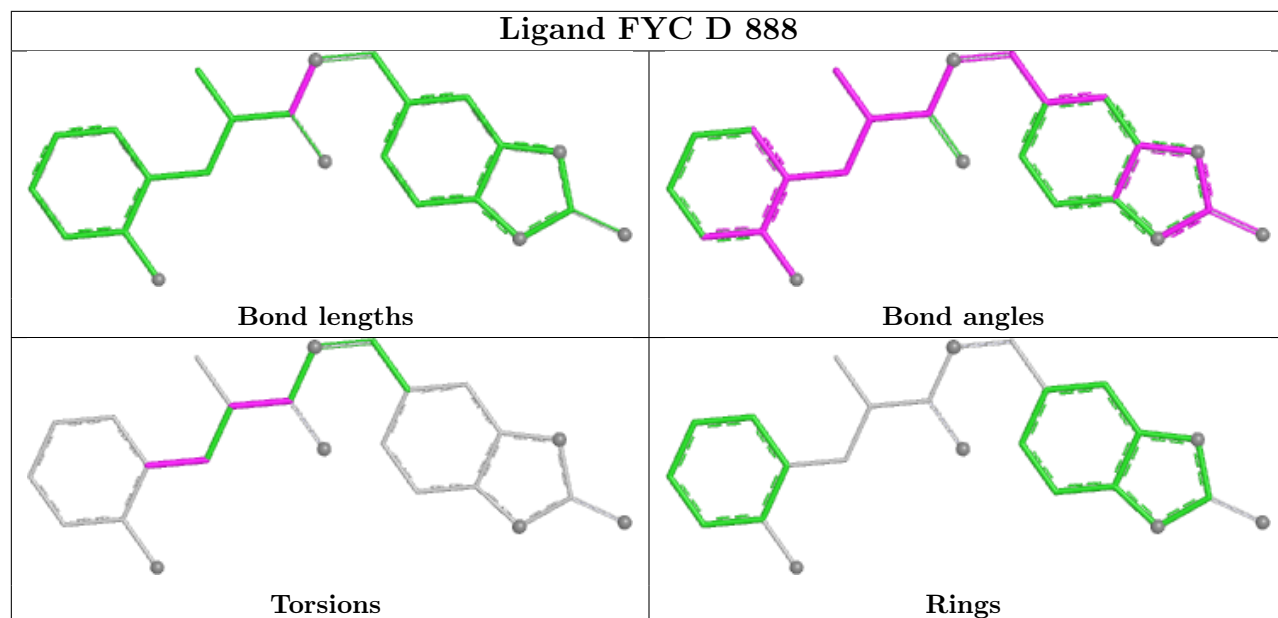
6 monomers are involved in 10 short contacts:

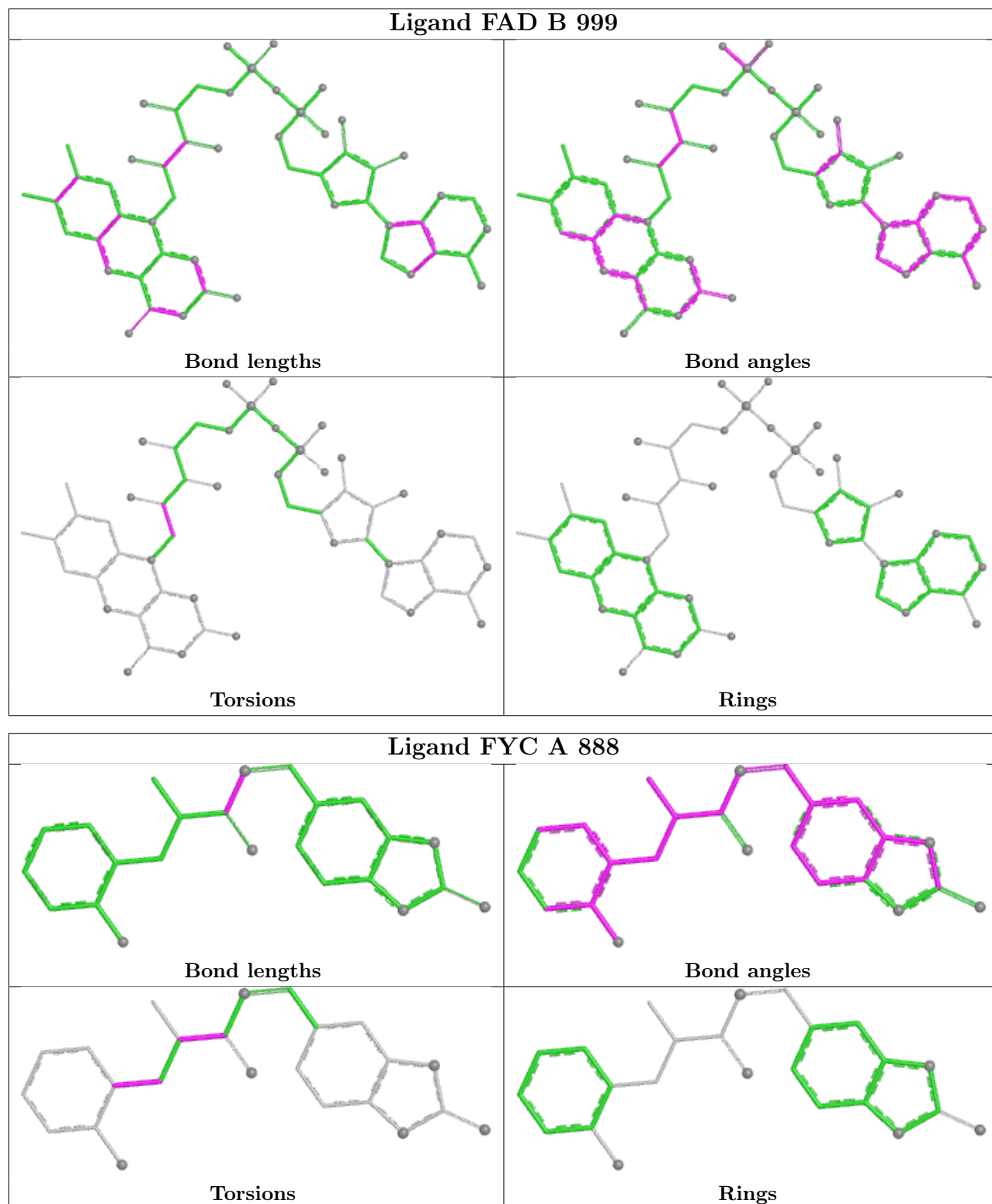
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	888	FYC	5	0
3	D	999	FAD	1	0
2	D	888	FYC	1	0
3	B	999	FAD	2	0
2	A	888	FYC	4	0
3	A	999	FAD	1	0

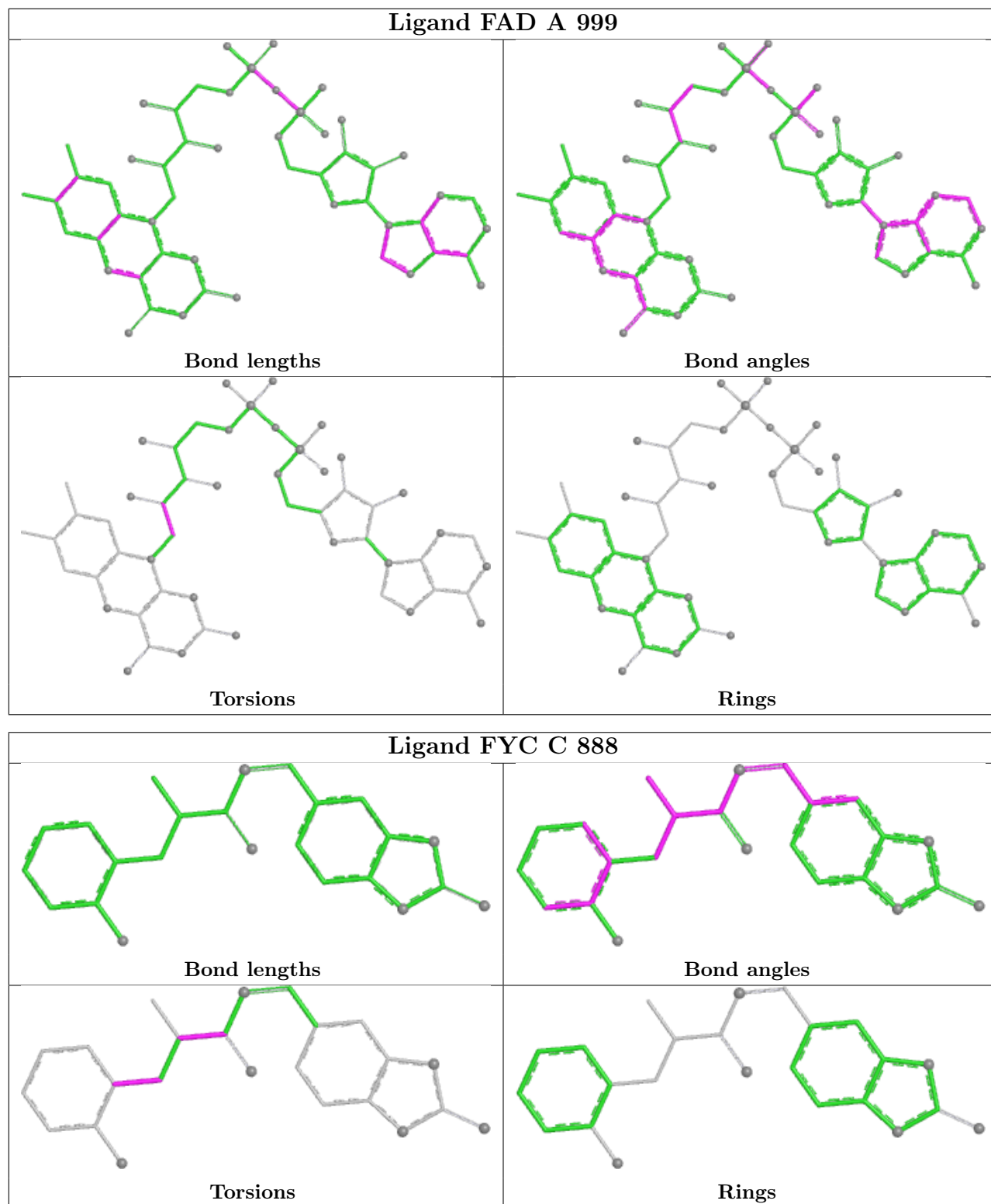
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	561/658 (85%)	-0.05	22 (3%) 43 42	11, 24, 54, 90	0
1	B	542/658 (82%)	-0.06	16 (2%) 52 51	12, 24, 49, 96	0
1	C	557/658 (84%)	-0.09	14 (2%) 58 58	10, 24, 46, 81	2 (0%)
1	D	550/658 (83%)	0.00	17 (3%) 51 50	13, 25, 49, 75	1 (0%)
All	All	2210/2632 (83%)	-0.05	69 (3%) 51 50	10, 24, 49, 96	3 (0%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	457	GLY	5.4
1	B	459	ASP	4.8
1	A	443	PHE	4.3
1	B	458	PHE	4.3
1	A	144	THR	4.2
1	D	559	PHE	3.7
1	B	460	PRO	3.6
1	C	434	PRO	3.5
1	B	157	PRO	3.3
1	C	432	LEU	3.2
1	C	457	GLY	3.2
1	A	82	ILE	3.1
1	A	156	PRO	3.0
1	A	559	PHE	3.0
1	B	159	ILE	3.0
1	B	434	PRO	3.0
1	D	587	GLY	2.9
1	A	435	GLN	2.9
1	B	428	PHE	2.8
1	C	81	GLY	2.7
1	C	505	TYR	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	83	ILE	2.7
1	D	461	ASN	2.7
1	A	195	PHE	2.7
1	A	196	LEU	2.7
1	A	81	GLY	2.7
1	A	141	ASP	2.6
1	A	436	VAL	2.5
1	C	503	ARG	2.5
1	D	165	LEU	2.5
1	C	142	HIS	2.4
1	C	106	ASN	2.4
1	D	106	ASN	2.4
1	C	559	PHE	2.4
1	C	150	LEU	2.3
1	D	411	GLN	2.3
1	A	159	ILE	2.3
1	B	156	PRO	2.3
1	B	81	GLY	2.3
1	D	137	GLY	2.3
1	A	450	PHE	2.3
1	B	155	THR	2.3
1	C	435	GLN	2.3
1	A	140	LEU	2.3
1	A	142	HIS	2.2
1	D	138	ILE	2.2
1	A	434	PRO	2.2
1	A	586	ARG	2.2
1	D	122	GLY	2.2
1	D	351	GLY	2.2
1	B	140	LEU	2.2
1	D	120	LEU	2.2
1	A	505	TYR	2.2
1	A	589	SER	2.2
1	B	195	PHE	2.1
1	D	350	GLN	2.1
1	D	586	ARG	2.1
1	D	141	ASP	2.1
1	A	157	PRO	2.1
1	D	430	HIS	2.1
1	C	587	GLY	2.1
1	C	588	ILE	2.1
1	B	426	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	589	SER	2.1
1	B	199	GLU	2.0
1	C	349	CYS	2.0
1	A	201	MET	2.0
1	D	139	ASN	2.0
1	D	105	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

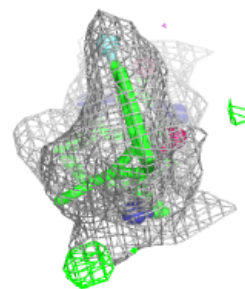
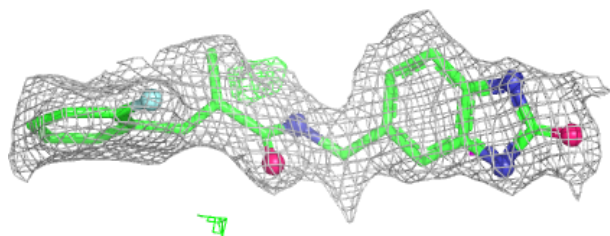
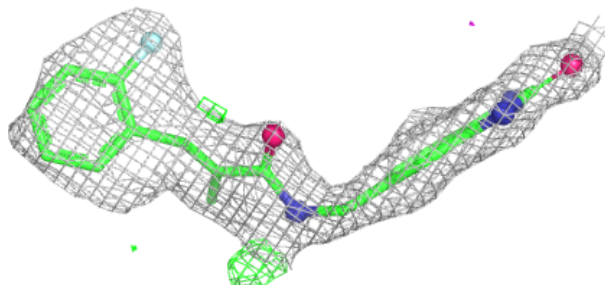
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	FYC	B	888	24/24	0.88	0.13	32,47,57,62	0
4	SO4	B	1659	5/5	0.88	0.13	50,53,57,58	0
2	FYC	C	888	24/24	0.90	0.12	27,36,52,57	0
2	FYC	D	888	24/24	0.91	0.12	32,43,57,58	0
2	FYC	A	888	24/24	0.91	0.12	25,37,63,66	0
4	SO4	A	1659	5/5	0.92	0.14	36,39,41,44	0
4	SO4	C	1659	5/5	0.93	0.15	40,43,49,56	0
4	SO4	D	1659	5/5	0.94	0.16	38,46,48,48	0
3	FAD	A	999	53/53	0.99	0.03	11,13,17,20	0
3	FAD	B	999	53/53	0.99	0.04	11,13,16,18	0
3	FAD	C	999	53/53	0.99	0.04	9,10,13,13	0
3	FAD	D	999	53/53	0.99	0.04	10,12,14,15	0

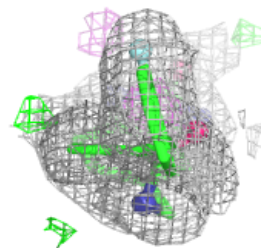
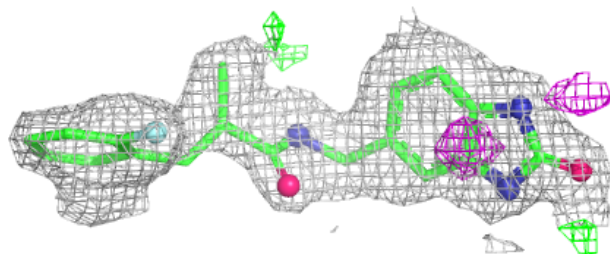
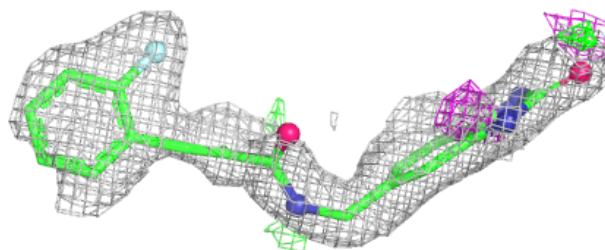
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around FYC 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)

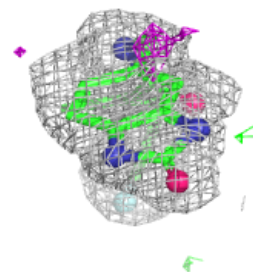
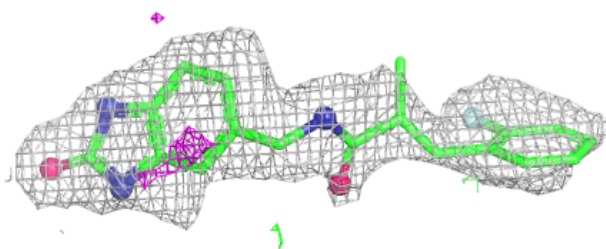
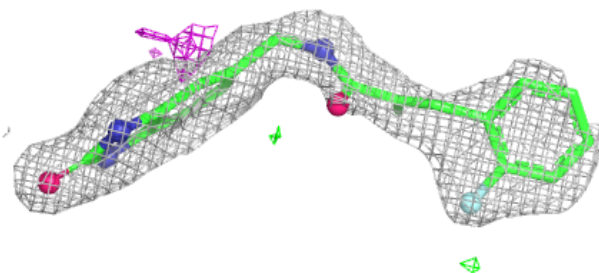
**Electron density around FYC C 888:**

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

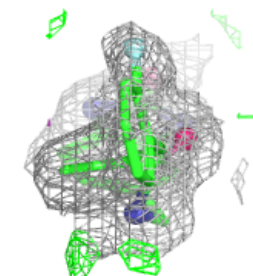
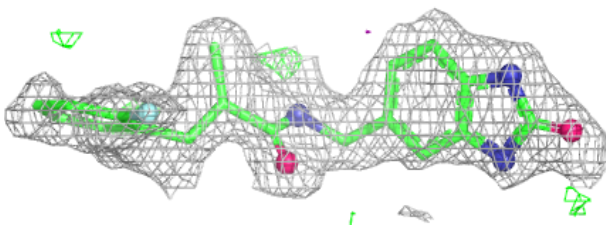


**Electron density around FYC D 888:**

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

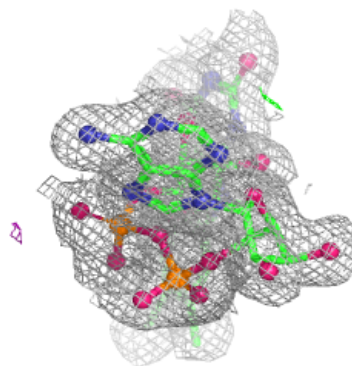
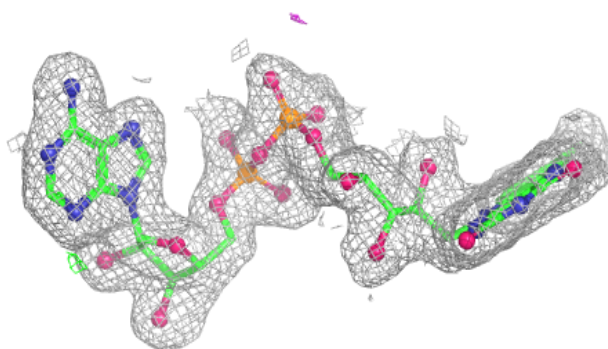
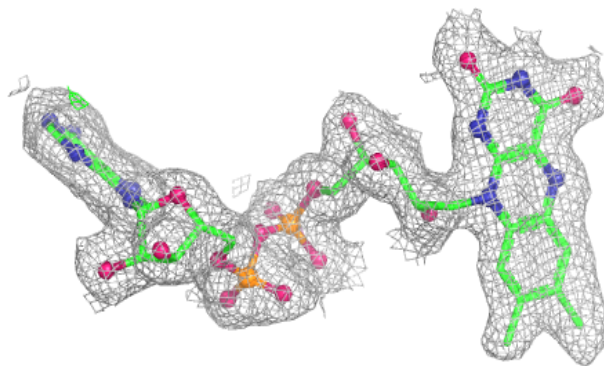
**Electron density around FYC A 888:**

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

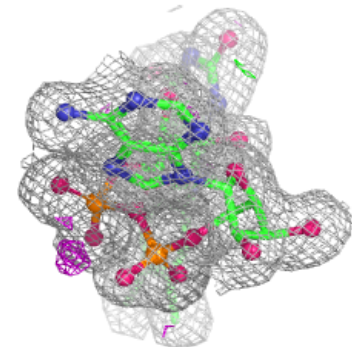
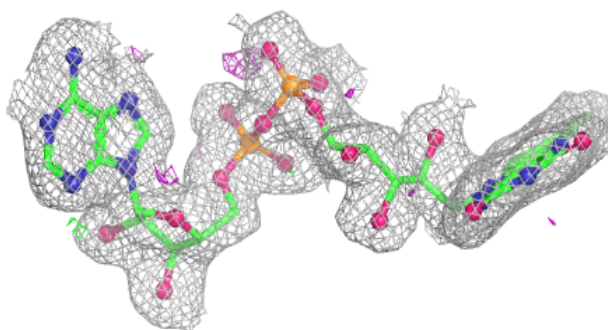
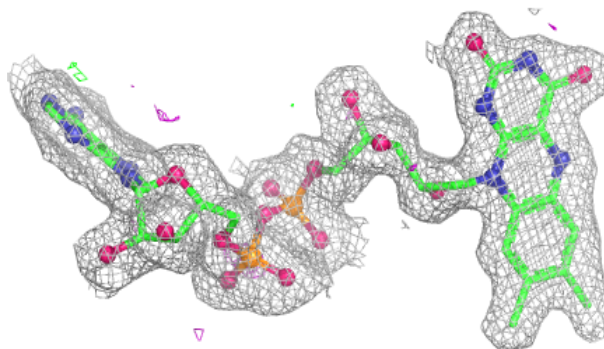


**Electron density around FAD A 999:**

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

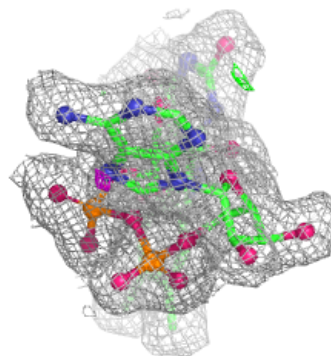
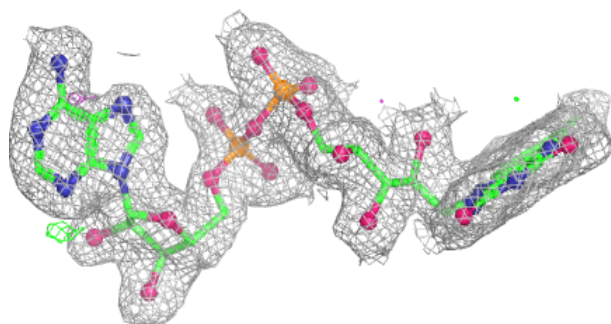
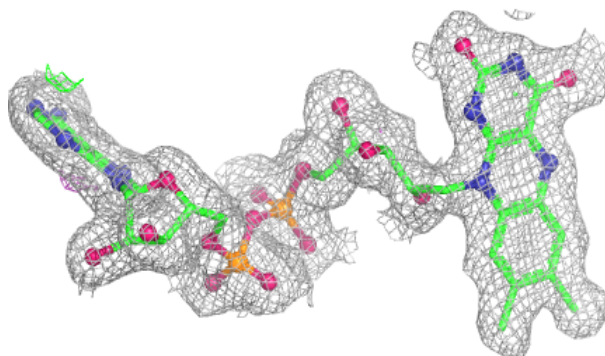
**Electron density around FAD B 999:**

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

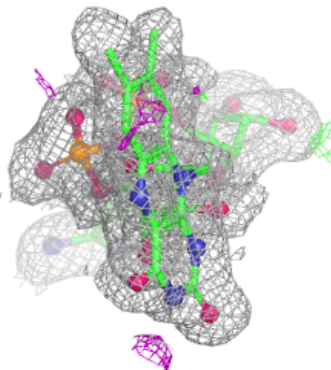
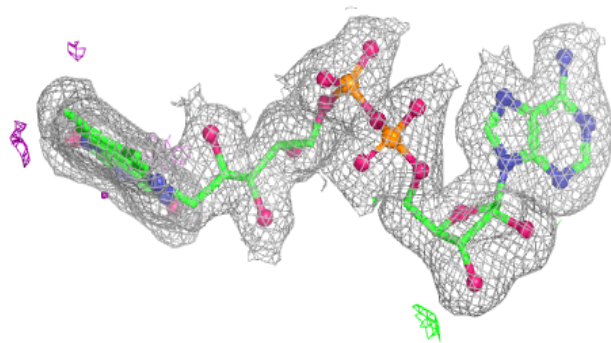
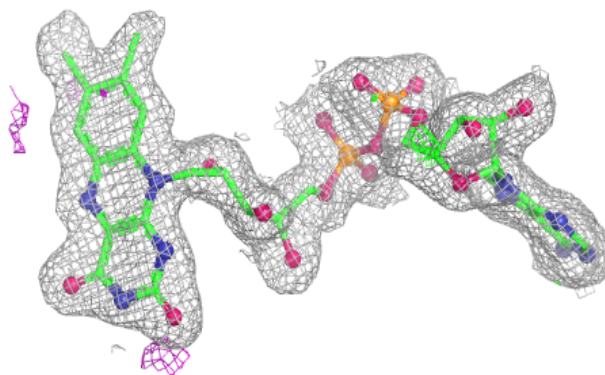


**Electron density around FAD C 999:**

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

**Electron density around FAD 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.