



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:55 PM UTC

PDB ID : 5AE3 / pdb_00005ae3
Title : Ether Lipid-Generating Enzyme AGPS in complex with antimycin A
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 : 2.18 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (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

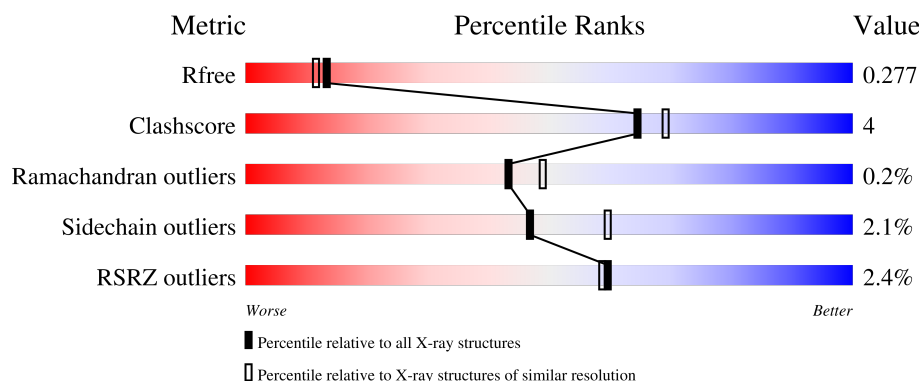
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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

Mol	Chain	Length	Quality of chain
1	A	658	2% 72% 9% 18%
1	B	658	3% 71% 10% 18%
1	C	658	2% 76% 8% 16%
1	D	658	2% 74% 9% 17%

2 Entry composition [i](#)

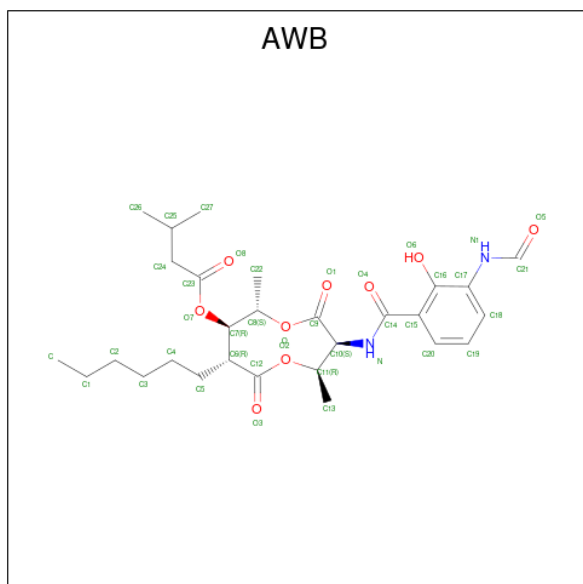
There are 5 unique types of molecules in this entry. The entry contains 18106 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	539	Total	C	N	O	S	0	0	0
			4252	2697	740	791	24			
1	B	539	Total	C	N	O	S	0	0	0
			4241	2696	734	787	24			
1	C	551	Total	C	N	O	S	0	2	0
			4333	2746	747	815	25			
1	D	547	Total	C	N	O	S	0	1	0
			4308	2729	752	803	24			

- Molecule 2 is [(2R,3S,6S,7R,8R)-3-[(3-formamido-2-oxidanyl-phenyl)carbonylamino]-8-hexyl-2,6-dimethyl-4,9-bis(oxidanylidene)-1,5-dioxonan-7-yl] 3-methylbutanoate (CCD ID: AWB) (formula: C₂₈H₄₀N₂O₉).



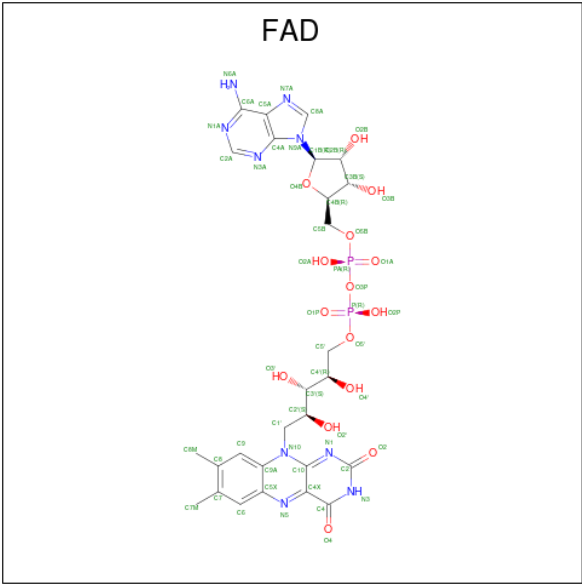
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			39	28	2	9		

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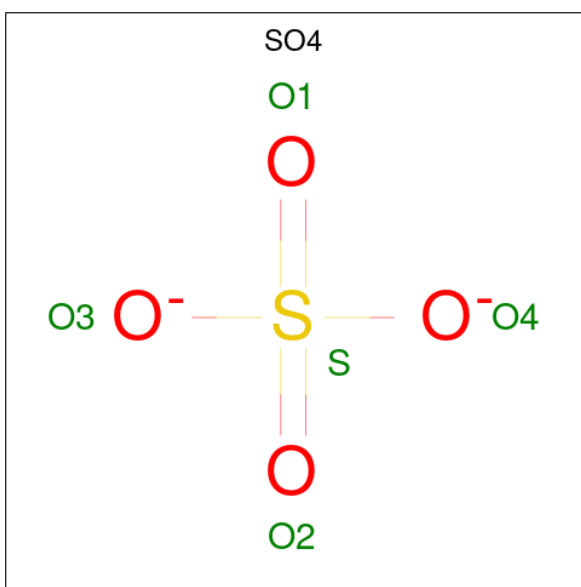
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			39	28	2	9		
2	C	1	Total	C	N	O	0	0
			39	28	2	9		
2	D	1	Total	C	N	O	0	0
			39	28	2	9		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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		

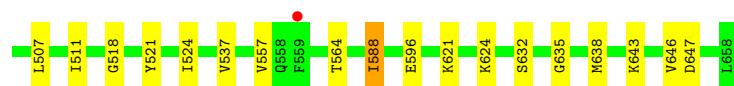
- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



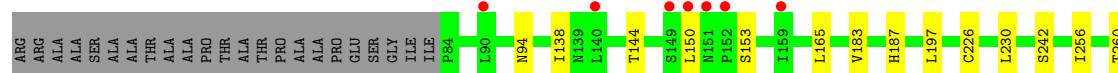
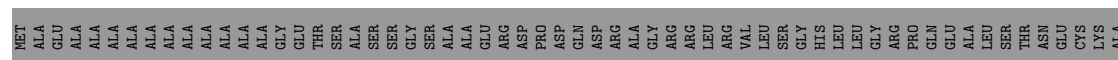
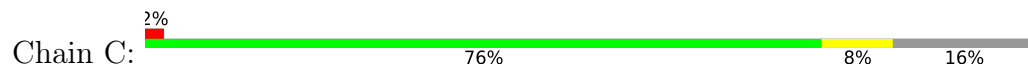
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

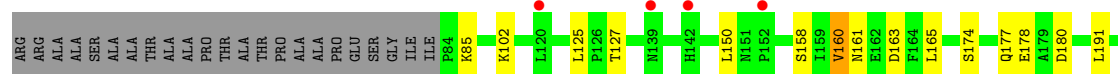
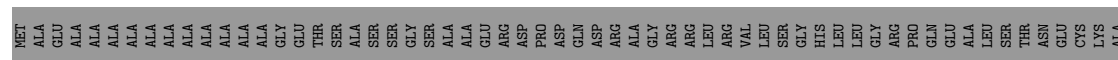
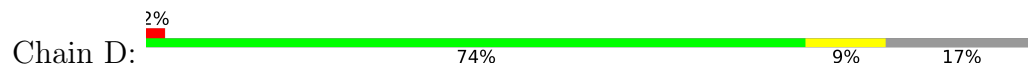
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	162	Total	O	0	0
			162	162		
5	B	119	Total	O	0	0
			119	119		
5	C	174	Total	O	0	0
			174	174		
5	D	134	Total	O	0	0
			134	134		



- Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE, PEROXISOMAL



- Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE, PEROXISOMAL



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.16Å 98.85Å 107.72Å 90.80° 90.50° 94.79°	Depositor
Resolution (Å)	107.71 – 2.18 107.71 – 2.18	Depositor EDS
% Data completeness (in resolution range)	94.2 (107.71-2.18) 94.2 (107.71-2.18)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, R_{free}	0.191 , 0.259 (Not available) , 0.277	Depositor DCC
R_{free} test set	1333 reflections (1.08%)	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18106	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	3/4347 (0.1%)	1.07	10/5876 (0.2%)
1	B	1.08	3/4337 (0.1%)	1.09	4/5867 (0.1%)
1	C	1.13	3/4436 (0.1%)	1.10	8/6002 (0.1%)
1	D	1.09	3/4407 (0.1%)	1.08	8/5959 (0.1%)
All	All	1.10	12/17527 (0.1%)	1.09	30/23704 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	333	VAL	C-O	-7.33	1.16	1.24
1	B	233	ILE	CA-C	7.26	1.59	1.53
1	C	325	ILE	C-O	-6.28	1.16	1.23
1	A	560	PRO	CA-C	6.27	1.57	1.52
1	C	379	ILE	C-O	-6.00	1.18	1.24
1	D	320	GLY	CA-C	-5.95	1.46	1.52
1	B	323	LYS	CA-CB	5.95	1.62	1.53
1	C	379	ILE	N-CA	-5.67	1.39	1.46
1	D	568	THR	N-CA	5.52	1.53	1.45
1	A	278	VAL	C-O	-5.28	1.18	1.23
1	D	264	ASN	CA-C	-5.25	1.46	1.53
1	B	301	GLU	CA-C	-5.08	1.46	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	414	ALA	CA-C-N	-7.36	113.15	120.21
1	C	414	ALA	C-N-CA	-7.36	113.15	120.21
1	A	156	PRO	N-CA-C	6.88	119.09	110.70
1	D	325	ILE	CB-CA-C	-6.43	103.83	111.94
1	D	524	ILE	N-CA-CB	6.14	118.00	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	631	ILE	N-CA-C	5.94	118.86	113.10
1	C	345	ILE	CB-CA-C	-5.93	103.55	110.91
1	A	342	ARG	N-CA-C	5.89	120.31	113.18
1	A	574	GLY	N-CA-C	5.82	118.01	110.45
1	C	406	ARG	CA-CB-CG	5.80	125.70	114.10
1	D	511	ILE	CB-CA-C	-5.77	104.35	112.14
1	C	486	ASP	N-CA-C	5.57	117.03	111.07
1	B	332	LEU	N-CA-C	5.49	119.15	112.23
1	B	261	SER	N-CA-C	5.43	117.96	111.71
1	C	406	ARG	CG-CD-NE	5.37	123.81	112.00
1	D	125	LEU	CA-C-N	5.31	125.37	119.32
1	D	125	LEU	C-N-CA	5.31	125.37	119.32
1	C	153	SER	N-CA-C	5.30	117.05	111.28
1	B	232	ILE	N-CA-C	5.22	115.37	107.80
1	A	616	HIS	N-CA-C	5.21	120.56	114.62
1	A	155	THR	CA-C-N	5.16	125.69	120.38
1	A	155	THR	C-N-CA	5.16	125.69	120.38
1	A	529	GLU	N-CA-C	5.14	116.80	109.14
1	D	160	VAL	N-CA-C	5.14	115.31	108.27
1	D	566	ARG	N-CA-CB	-5.13	101.84	111.13
1	A	117	ARG	N-CA-C	5.12	118.68	112.23
1	A	256	ILE	CB-CA-C	-5.11	104.57	110.91
1	A	615	HIS	N-CA-C	5.09	116.63	111.14
1	D	354	MET	CG-SD-CE	-5.06	89.76	100.90
1	B	537	VAL	N-CA-C	5.06	115.28	110.42

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	4252	0	4163	36	0
1	B	4241	0	4157	45	0
1	C	4333	0	4242	24	0
1	D	4308	0	4238	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	39	0	40	8	0
2	B	39	0	40	5	0
2	C	39	0	39	4	0
2	D	39	0	39	4	0
3	A	53	0	31	0	0
3	B	53	0	31	1	0
3	C	53	0	31	0	0
3	D	53	0	31	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	D	5	0	0	0	0
5	A	162	0	0	1	0
5	B	119	0	0	2	0
5	C	174	0	0	1	0
5	D	134	0	0	4	0
All	All	18106	0	17082	135	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 (135) 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:D:191:LEU:HD21	1:D:524:ILE:HG22	1.61	0.79
1:A:635:GLY:HA2	1:A:638:MET:HE3	1.65	0.78
1:D:210:LEU:HD13	1:D:256:ILE:HG23	1.67	0.75
1:C:388:GLN:NE2	1:C:471:GLU:OE1	2.23	0.70
1:B:635:GLY:HA2	1:B:638:MET:HE3	1.73	0.69
1:A:140:LEU:O	1:A:142:HIS:N	2.26	0.69
1:C:635:GLY:HA2	1:C:638:MET:HE3	1.76	0.66
1:D:518:GLY:HA3	2:D:800:AWB:H27	1.77	0.65
1:B:298:THR:HG21	1:B:379:ILE:HD12	1.80	0.63
1:B:314:ILE:HG23	1:B:365:MET:HG2	1.80	0.63
1:A:421:MET:HE1	2:A:800:AWB:C21	2.31	0.61
1:A:421:MET:HE2	1:A:566:ARG:CZ	2.32	0.60
1:B:230:LEU:HD13	1:B:256:ILE:HD11	1.83	0.59
1:C:634:VAL:HG12	1:C:638:MET:HE2	1.85	0.58
1:A:635:GLY:HA2	1:A:638:MET:CE	2.34	0.58
1:D:551:GLU:O	1:D:555:LYS:HD3	2.04	0.58
1:B:421:MET:HG3	1:B:425:GLN:NE2	2.19	0.57
1:C:150:LEU:HD11	1:C:183:VAL:HB	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:425:GLN:O	2:C:800:AWB:H20	2.05	0.56
1:D:518:GLY:HA3	2:D:800:AWB:C27	2.34	0.56
1:B:192:HIS:HB3	1:B:243:TYR:OH	2.05	0.56
1:D:507:LEU:HB2	2:D:800:AWB:C21	2.36	0.56
1:D:411:GLN:CD	5:D:2098:HOH:O	2.49	0.56
1:B:635:GLY:HA2	1:B:638:MET:CE	2.35	0.55
1:B:421:MET:HG3	1:B:425:GLN:HE21	1.72	0.55
1:A:428:PHE:CZ	2:A:800:AWB:H22B	2.42	0.55
1:A:518:GLY:HA2	2:A:800:AWB:H27A	1.89	0.54
1:B:133:GLN:NE2	1:B:139:ASN:O	2.32	0.54
1:B:511:ILE:HG22	2:B:800:AWB:HA	1.89	0.54
1:D:209:VAL:C	1:D:210:LEU:HD12	2.33	0.54
1:D:411:GLN:CG	5:D:2098:HOH:O	2.56	0.54
1:B:425:GLN:O	2:B:800:AWB:H20	2.08	0.53
1:D:635:GLY:HA2	1:D:638:MET:HE2	1.89	0.53
1:B:421:MET:HE1	1:B:467:THR:HG23	1.91	0.52
1:C:314:ILE:HG23	1:C:365:MET:HG2	1.91	0.52
1:B:129:LYS:HG3	1:B:140:LEU:HD23	1.92	0.52
1:B:423:ASN:ND2	1:B:461:ASN:C	2.68	0.52
1:B:419:ARG:NH1	2:B:800:AWB:O5	2.42	0.52
1:D:127:THR:HG21	1:D:431:ALA:HB1	1.92	0.52
1:A:201:MET:SD	1:A:202:PHE:N	2.83	0.51
1:C:187:HIS:CE1	1:C:197:LEU:HD11	2.46	0.51
1:A:333:VAL:HG11	1:A:336:MET:HE2	1.93	0.51
1:C:523:ILE:HG21	2:C:800:AWB:H26A	1.92	0.51
1:D:230:LEU:HD13	1:D:256:ILE:HD11	1.93	0.51
1:D:161:ASN:OD1	1:D:163:ASP:N	2.44	0.50
1:D:85:LYS:HZ1	1:D:174:SER:CB	2.24	0.50
1:D:624:LYS:HE3	1:D:655:ARG:O	2.12	0.50
1:D:191:LEU:HD13	1:D:191:LEU:C	2.36	0.50
1:A:475:GLU:O	1:A:479:GLN:HG3	2.11	0.49
1:A:518:GLY:CA	2:A:800:AWB:H27A	2.42	0.49
1:B:94:ASN:HA	1:B:197:LEU:HD13	1.93	0.49
1:A:511:ILE:HD12	2:A:800:AWB:H13B	1.94	0.49
1:C:613:LEU:HD11	1:C:623:ARG:HB3	1.95	0.49
1:B:557:VAL:HG22	1:B:588:ILE:HD11	1.95	0.48
1:B:140:LEU:CD1	1:B:521:TYR:CZ	2.97	0.48
1:A:342:ARG:HD2	1:A:645:TYR:CZ	2.49	0.48
1:A:419:ARG:CB	1:A:421:MET:HE3	2.44	0.48
1:B:422:ASP:OD1	1:B:422:ASP:C	2.56	0.48
1:A:314:ILE:HG23	1:A:365:MET:HG2	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:VAL:HG22	1:A:485:TYR:CE1	2.49	0.47
1:A:419:ARG:HB3	1:A:421:MET:HE3	1.95	0.47
2:A:800:AWB:C12	2:A:800:AWB:O	2.62	0.47
1:B:139:ASN:O	1:B:140:LEU:CB	2.62	0.47
1:A:425:GLN:O	2:A:800:AWB:H20	2.14	0.47
1:B:340:THR:HB	1:B:646:VAL:HG13	1.96	0.47
1:C:323:LYS:HG3	1:C:328:ASN:CG	2.40	0.47
1:C:226:CYS:HA	1:C:651:ILE:HD11	1.97	0.46
1:B:239:THR:OG1	3:B:999:FAD:O1P	2.30	0.46
1:B:507:LEU:HB3	1:B:511:ILE:HD11	1.96	0.46
1:B:504:GLY:HA3	2:B:800:AWB:C21	2.46	0.46
1:C:422:ASP:OD1	1:C:422:ASP:C	2.58	0.46
1:B:187:HIS:CE1	1:B:197:LEU:HD11	2.51	0.46
1:A:616:HIS:HA	1:B:355:SER:HB2	1.98	0.46
2:D:800:AWB:O	2:D:800:AWB:C12	2.63	0.46
1:B:323:LYS:HG2	1:B:324:ASN:N	2.31	0.45
1:D:503:ARG:HA	1:D:506:LEU:HD12	1.98	0.45
1:A:588:ILE:HG21	1:A:591:PRO:HA	1.97	0.45
1:A:424:GLN:NE2	1:A:562:LEU:HD12	2.32	0.45
5:C:2093:HOH:O	1:D:634:VAL:HG23	2.15	0.45
1:B:474:ARG:O	1:B:478:LEU:HG	2.17	0.45
1:D:158:SER:OG	1:D:177:GLN:HG2	2.16	0.45
1:A:419:ARG:O	1:A:466:ALA:HA	2.17	0.45
1:B:425:GLN:HG3	1:B:564:THR:OG1	2.16	0.45
1:D:314:ILE:HG23	1:D:365:MET:HG2	1.98	0.45
1:A:426:PHE:CD2	1:A:463:LEU:HD12	2.51	0.45
1:C:138:ILE:HG23	1:C:584:ASN:ND2	2.32	0.45
1:C:260:THR:O	1:C:281:GLY:HA3	2.17	0.45
1:B:92:LYS:NZ	5:B:2007:HOH:O	2.51	0.44
1:B:225:ALA:HA	1:B:230:LEU:HD12	2.00	0.44
2:C:800:AWB:O	2:C:800:AWB:C12	2.65	0.44
1:D:635:GLY:HA2	1:D:638:MET:CE	2.48	0.44
1:B:518:GLY:CA	2:B:800:AWB:H27A	2.47	0.44
1:B:333:VAL:HG11	1:B:336:MET:HE2	2.01	0.43
1:C:507:LEU:HB2	2:C:800:AWB:H21	2.01	0.43
1:A:230:LEU:HD13	1:A:256:ILE:HD11	2.00	0.43
1:D:127:THR:HG22	1:D:127:THR:O	2.18	0.43
1:A:160:VAL:HG11	1:A:165:LEU:HD13	2.01	0.43
1:A:585:TYR:HB2	1:A:591:PRO:HB3	2.01	0.43
1:C:459:ASP:C	1:C:459:ASP:OD1	2.60	0.43
1:A:346:GLU:O	1:B:632:SER:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:GLU:OE2	1:A:289:ARG:NE	2.43	0.43
1:B:643:LYS:HD2	1:B:647:ASP:HB3	2.00	0.43
1:C:419:ARG:NH2	1:C:504:GLY:O	2.48	0.43
1:B:621:LYS:HA	1:B:624:LYS:HD3	2.01	0.42
1:D:411:GLN:HG2	5:D:2098:HOH:O	2.19	0.42
1:A:632:SER:HB3	1:B:346:GLU:O	2.19	0.42
1:B:267:LEU:HD12	1:B:277:HIS:CD2	2.54	0.42
1:B:112:GLU:OE1	5:B:2014:HOH:O	2.21	0.42
1:B:286:GLU:OE2	1:B:289:ARG:NH2	2.50	0.42
1:B:395:PHE:O	1:B:463:LEU:HD22	2.18	0.42
1:A:511:ILE:CD1	2:A:800:AWB:H13B	2.50	0.42
1:C:600:ALA:O	1:C:604:GLU:HG2	2.19	0.42
1:A:136:PHE:CD2	1:A:523:ILE:HD13	2.55	0.42
1:B:643:LYS:NZ	1:B:647:ASP:OD2	2.51	0.42
1:C:242:SER:O	1:C:620:GLY:HA3	2.19	0.42
1:D:394:ALA:O	1:D:493:GLY:HA2	2.20	0.42
1:A:535:ASP:HB3	1:B:272:ASN:HB3	2.02	0.41
1:D:422:ASP:C	1:D:422:ASP:OD1	2.62	0.41
1:A:129:LYS:HG3	1:A:140:LEU:HD22	2.02	0.41
1:A:167:GLU:OE2	1:A:228:TYR:OH	2.31	0.41
1:C:524:ILE:O	1:C:582:ALA:HA	2.21	0.41
1:C:305:LEU:HD12	1:C:306:GLU:N	2.35	0.41
1:D:258:LEU:C	1:D:258:LEU:HD23	2.46	0.41
1:A:426:PHE:CG	1:A:463:LEU:HD12	2.56	0.41
1:A:174:SER:HB3	5:A:2003:HOH:O	2.20	0.41
1:B:423:ASN:HD22	1:B:462:GLN:C	2.29	0.41
1:D:160:VAL:HG11	1:D:165:LEU:HD13	2.03	0.41
1:D:340:THR:HB	1:D:341:PRO:HD2	2.03	0.41
1:C:230:LEU:CD1	1:C:256:ILE:HD11	2.51	0.41
1:D:266:ILE:HD12	1:D:290:GLN:HB3	2.01	0.41
1:D:399:GLU:H	1:D:399:GLU:CD	2.29	0.40
1:C:638:MET:HE1	1:D:345:ILE:CD1	2.51	0.40
1:D:102:LYS:NZ	5:D:2014:HOH:O	2.54	0.40
1:B:187:HIS:NE2	1:B:197:LEU:HD11	2.36	0.40
1:C:94:ASN:HA	1:C:197:LEU:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	531/658 (81%)	512 (96%)	16 (3%)	3 (1%)	21	20
1	B	533/658 (81%)	515 (97%)	18 (3%)	0	100	100
1	C	549/658 (83%)	528 (96%)	21 (4%)	0	100	100
1	D	544/658 (83%)	530 (97%)	13 (2%)	1 (0%)	43	49
All	All	2157/2632 (82%)	2085 (97%)	68 (3%)	4 (0%)	43	49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	ASP
1	A	142	HIS
1	D	657	LEU
1	A	156	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	456/545 (84%)	444 (97%)	12 (3%)	40	51
1	B	454/545 (83%)	444 (98%)	10 (2%)	45	58
1	C	467/545 (86%)	459 (98%)	8 (2%)	53	66
1	D	463/545 (85%)	454 (98%)	9 (2%)	50	63
All	All	1840/2180 (84%)	1801 (98%)	39 (2%)	47	59

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	90	LEU
1	A	119	PRO
1	A	138	ILE
1	A	140	LEU
1	A	142	HIS
1	A	197	LEU
1	A	286	GLU
1	A	465	VAL
1	A	510	VAL
1	A	526	GLU
1	A	646	VAL
1	B	90	LEU
1	B	105	LEU
1	B	140	LEU
1	B	174	SER
1	B	323	LYS
1	B	406	ARG
1	B	500	ASN
1	B	524	ILE
1	B	588	ILE
1	B	596	GLU
1	C	144	THR
1	C	165	LEU
1	C	294	SER
1	C	323	LYS
1	C	406	ARG
1	C	480	HIS
1	C	536	ARG
1	C	568	THR
1	D	150	LEU
1	D	178	GLU
1	D	180	ASP
1	D	196	LEU
1	D	294	SER
1	D	384	THR
1	D	463	LEU
1	D	510	VAL
1	D	524	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	A	617	HIS
1	B	400	GLN
1	B	411	GLN
1	B	423	ASN
1	C	172	ASN
1	C	462	GLN
1	C	480	HIS
1	D	133	GLN
1	D	192	HIS
1	D	277	HIS

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

11 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	A	999	-	58,58,58	2.06	12 (20%)	85,89,89	1.70	21 (24%)
4	SO4	A	1659	-	4,4,4	0.54	0	6,6,6	0.63	0
2	AWB	D	800	-	40,40,40	1.84	9 (22%)	34,54,54	2.11	11 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FAD	C	999	-	58,58,58	1.56	9 (15%)	85,89,89	1.83	20 (23%)
3	FAD	B	999	-	58,58,58	1.78	12 (20%)	85,89,89	1.74	22 (25%)
3	FAD	D	999	-	58,58,58	1.72	15 (25%)	85,89,89	1.71	26 (30%)
2	AWB	A	800	-	40,40,40	1.97	7 (17%)	34,54,54	1.87	8 (23%)
4	SO4	D	1659	-	4,4,4	0.50	0	6,6,6	0.70	0
2	AWB	C	800	-	40,40,40	1.87	7 (17%)	34,54,54	1.52	4 (11%)
4	SO4	B	1659	-	4,4,4	0.61	0	6,6,6	0.62	0
2	AWB	B	800	-	40,40,40	1.84	7 (17%)	34,54,54	2.20	10 (29%)

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	A	999	-	-	2/34/50/50	0/6/6/6
2	AWB	D	800	-	-	7/38/53/53	0/1/2/2
3	FAD	C	999	-	-	2/34/50/50	0/6/6/6
3	FAD	B	999	-	-	2/34/50/50	0/6/6/6
3	FAD	D	999	-	-	2/34/50/50	0/6/6/6
2	AWB	A	800	-	-	9/38/53/53	0/1/2/2
2	AWB	C	800	-	-	14/38/53/53	0/1/2/2
2	AWB	B	800	-	-	10/38/53/53	0/1/2/2

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	FAD	C9A-C5X	8.01	1.54	1.41
3	A	999	FAD	P-O3P	6.11	1.66	1.59
2	C	800	AWB	O2-C12	6.05	1.48	1.34
2	A	800	AWB	C17-C16	6.04	1.49	1.40
3	D	999	FAD	C9A-C5X	5.65	1.50	1.41
3	B	999	FAD	C9A-C5X	5.57	1.50	1.41
2	A	800	AWB	C15-C16	5.24	1.50	1.41
2	B	800	AWB	O-C8	-5.14	1.38	1.46
3	C	999	FAD	C9A-C5X	5.14	1.49	1.41
3	A	999	FAD	PA-O3P	4.85	1.64	1.59
3	B	999	FAD	C5A-C4A	4.76	1.47	1.39
2	D	800	AWB	O2-C12	4.75	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	800	AWB	C17-C16	4.74	1.47	1.40
3	A	999	FAD	C8-C7	4.56	1.51	1.40
3	C	999	FAD	C4-N3	-4.49	1.30	1.38
2	A	800	AWB	O2-C12	4.42	1.44	1.34
2	D	800	AWB	O7-C23	4.41	1.46	1.34
3	D	999	FAD	C4-N3	-4.29	1.30	1.38
2	A	800	AWB	O-C9	4.25	1.44	1.34
2	B	800	AWB	O7-C23	4.23	1.46	1.34
3	D	999	FAD	C5A-C4A	4.21	1.46	1.39
2	B	800	AWB	O2-C12	4.17	1.43	1.34
2	B	800	AWB	O-C9	4.12	1.43	1.34
2	B	800	AWB	C17-C16	4.12	1.46	1.40
2	A	800	AWB	O7-C23	4.08	1.45	1.34
2	C	800	AWB	O-C9	4.04	1.43	1.34
2	C	800	AWB	C15-C16	4.03	1.48	1.41
2	C	800	AWB	O7-C23	3.99	1.45	1.34
3	A	999	FAD	C5A-C4A	3.91	1.46	1.39
2	B	800	AWB	C17-N1	-3.85	1.35	1.41
3	B	999	FAD	C4-N3	-3.73	1.31	1.38
2	D	800	AWB	C15-C16	3.62	1.47	1.41
2	C	800	AWB	C17-N1	-3.54	1.36	1.41
2	C	800	AWB	C17-C16	3.53	1.45	1.40
3	C	999	FAD	C5X-N5	-3.52	1.33	1.39
3	B	999	FAD	C8-C7	3.47	1.49	1.40
2	D	800	AWB	O-C9	3.35	1.42	1.34
3	B	999	FAD	C5X-N5	-3.33	1.33	1.39
3	D	999	FAD	C8-C7	3.30	1.48	1.40
2	C	800	AWB	O-C8	-3.14	1.41	1.46
3	C	999	FAD	C8-C7	3.05	1.48	1.40
2	D	800	AWB	O-C8	-3.03	1.41	1.46
2	B	800	AWB	C15-C16	3.01	1.46	1.41
3	B	999	FAD	O4-C4	2.98	1.29	1.23
3	B	999	FAD	C4A-N9A	-2.95	1.31	1.37
3	D	999	FAD	O4-C4	2.94	1.29	1.23
3	A	999	FAD	C4X-C10	2.88	1.52	1.44
2	D	800	AWB	O2-C11	-2.82	1.42	1.46
3	A	999	FAD	C4A-N9A	-2.81	1.31	1.37
3	D	999	FAD	C4A-N9A	-2.71	1.32	1.37
3	B	999	FAD	C2-N3	-2.68	1.33	1.39
2	D	800	AWB	C17-N1	-2.67	1.37	1.41
2	D	800	AWB	O7-C7	-2.65	1.40	1.44
2	A	800	AWB	O-C8	-2.63	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	999	FAD	C4A-N9A	-2.54	1.32	1.37
3	A	999	FAD	C5A-N7A	-2.50	1.34	1.39
3	B	999	FAD	C5A-N7A	-2.49	1.34	1.39
3	B	999	FAD	C2A-N1A	2.46	1.38	1.33
3	D	999	FAD	C4X-N5	2.45	1.36	1.30
3	D	999	FAD	C10-N10	2.44	1.42	1.37
2	A	800	AWB	C18-C17	2.44	1.43	1.39
3	D	999	FAD	O2-C2	2.43	1.29	1.24
3	D	999	FAD	C5X-N5	-2.36	1.35	1.39
3	C	999	FAD	O4B-C4B	-2.32	1.39	1.45
3	B	999	FAD	C5A-C6A	2.30	1.47	1.41
3	C	999	FAD	C5A-C4A	2.29	1.43	1.39
3	A	999	FAD	C8A-N7A	2.26	1.36	1.31
3	A	999	FAD	O4-C4	2.24	1.27	1.23
3	A	999	FAD	C10-N10	2.22	1.42	1.37
3	D	999	FAD	C2-N1	-2.17	1.31	1.36
3	B	999	FAD	C1'-C2'	2.17	1.55	1.52
3	A	999	FAD	C4-N3	-2.14	1.34	1.38
3	D	999	FAD	C6-C5X	2.09	1.43	1.40
3	D	999	FAD	C2-N3	-2.08	1.34	1.39
3	C	999	FAD	C9-C8	-2.06	1.36	1.39
3	C	999	FAD	C5A-N7A	-2.05	1.35	1.39
3	D	999	FAD	C1'-C2'	2.05	1.55	1.52
3	D	999	FAD	PA-O3P	2.04	1.61	1.59

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	AWB	O7-C23-C24	5.92	122.05	111.43
2	A	800	AWB	O7-C23-C24	5.64	121.54	111.43
2	D	800	AWB	C7-O7-C23	-5.31	108.95	117.59
2	B	800	AWB	C17-N1-C21	-4.83	117.20	126.87
3	C	999	FAD	N3A-C2A-N1A	-4.74	121.41	128.58
3	A	999	FAD	C5A-C4A-N3A	-4.70	120.25	126.72
3	C	999	FAD	C5A-C4A-N3A	-4.66	120.30	126.72
3	B	999	FAD	N3A-C2A-N1A	-4.62	121.60	128.58
2	B	800	AWB	C7-O7-C23	-4.33	110.55	117.59
2	D	800	AWB	C18-C17-C16	-4.30	116.97	119.75
2	C	800	AWB	O5-C21-N1	-4.28	119.85	125.72
3	C	999	FAD	N3A-C4A-N9A	4.27	134.42	127.17
2	D	800	AWB	O5-C21-N1	-4.20	119.95	125.72
3	B	999	FAD	C5A-C4A-N3A	-4.17	120.98	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	999	FAD	C4A-N9A-C8A	4.15	110.09	105.74
3	C	999	FAD	C2A-N3A-C4A	4.08	121.78	111.83
2	A	800	AWB	C18-C17-C16	-3.99	117.17	119.75
3	B	999	FAD	C4-C4X-N5	3.97	123.70	118.21
3	A	999	FAD	O4B-C1B-N9A	-3.94	100.53	108.09
3	C	999	FAD	C4-C4X-N5	3.89	123.58	118.21
3	A	999	FAD	N3A-C4A-N9A	3.73	133.51	127.17
3	D	999	FAD	C4A-N9A-C8A	3.73	109.65	105.74
3	A	999	FAD	N3A-C2A-N1A	-3.63	123.09	128.58
2	B	800	AWB	O5-C21-N1	-3.62	120.75	125.72
2	C	800	AWB	C18-C17-C16	-3.55	117.46	119.75
2	D	800	AWB	O7-C23-C24	3.48	117.67	111.43
2	A	800	AWB	C7-O7-C23	-3.47	111.94	117.59
3	D	999	FAD	C5A-C4A-N3A	-3.44	121.98	126.72
3	B	999	FAD	C2A-N1A-C6A	3.44	124.38	118.73
3	A	999	FAD	C2A-N3A-C4A	3.40	120.14	111.83
2	B	800	AWB	O2-C12-O3	-3.39	119.90	124.10
2	D	800	AWB	C25-C24-C23	-3.39	101.30	114.42
3	B	999	FAD	C4X-C10-N10	3.38	121.32	116.48
3	D	999	FAD	C5'-C4'-C3'	3.38	118.59	112.22
2	C	800	AWB	C18-C17-N1	-3.35	117.47	122.54
3	B	999	FAD	C2A-N3A-C4A	3.34	119.99	111.83
3	A	999	FAD	C5X-C9A-N10	3.31	120.96	117.97
3	B	999	FAD	C10-N1-C2	3.31	124.00	116.85
3	D	999	FAD	C4X-C10-N10	3.28	121.17	116.48
3	D	999	FAD	O4B-C1B-N9A	-3.27	101.81	108.09
3	D	999	FAD	C4-C4X-N5	3.25	122.70	118.21
2	D	800	AWB	O8-C23-C24	-3.25	117.11	124.65
3	B	999	FAD	N3A-C4A-N9A	3.23	132.66	127.17
3	A	999	FAD	O3'-C3'-C4'	3.22	116.26	108.93
3	B	999	FAD	C4A-C5A-N7A	-3.18	106.95	110.58
3	D	999	FAD	N3A-C4A-N9A	3.16	132.54	127.17
3	B	999	FAD	C4X-C10-N1	-3.11	116.97	124.59
2	C	800	AWB	O7-C23-C24	3.10	116.98	111.43
3	A	999	FAD	O3P-P-O1P	-3.04	101.55	110.70
2	D	800	AWB	C18-C17-N1	-3.01	117.97	122.54
2	A	800	AWB	O2-C12-O3	-2.97	120.42	124.10
3	D	999	FAD	C10-N1-C2	2.95	123.25	116.85
3	C	999	FAD	O3B-C3B-C2B	-2.95	102.38	111.82
3	D	999	FAD	O2P-P-O1P	2.93	126.05	112.44
3	A	999	FAD	C5'-C4'-C3'	2.92	117.72	112.22
3	C	999	FAD	C2B-C3B-C4B	2.91	108.22	102.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	FAD	O2A-PA-O1A	2.85	125.69	112.44
3	B	999	FAD	C2B-C1B-N9A	2.82	120.32	113.30
3	C	999	FAD	N9A-C8A-N7A	-2.81	109.96	113.94
3	B	999	FAD	C9A-N10-C10	-2.78	116.51	120.75
3	C	999	FAD	O2A-PA-O1A	2.74	125.19	112.44
2	B	800	AWB	O-C9-C10	2.71	114.54	110.28
3	D	999	FAD	O2-C2-N1	-2.71	117.31	121.80
2	B	800	AWB	O8-C23-C24	-2.68	118.43	124.65
3	D	999	FAD	C4A-C5A-N7A	-2.66	107.54	110.58
3	D	999	FAD	C5X-C9A-N10	2.66	120.37	117.97
3	B	999	FAD	O2P-P-O1P	2.65	124.79	112.44
3	D	999	FAD	C2A-N3A-C4A	2.65	118.31	111.83
3	D	999	FAD	C9A-N10-C10	-2.65	116.71	120.75
3	C	999	FAD	O4B-C1B-N9A	-2.65	103.01	108.09
3	A	999	FAD	O2P-P-O1P	2.61	124.60	112.44
2	D	800	AWB	O-C9-O1	-2.60	120.87	124.10
2	A	800	AWB	O8-C23-C24	-2.60	118.61	124.65
3	A	999	FAD	C4A-N9A-C8A	2.60	108.46	105.74
3	D	999	FAD	C6A-C5A-N7A	2.59	137.08	132.09
3	D	999	FAD	N9A-C8A-N7A	-2.58	110.28	113.94
3	D	999	FAD	C4X-C10-N1	-2.57	118.28	124.59
3	C	999	FAD	C4X-C4-N3	2.56	119.77	113.25
3	A	999	FAD	C2A-N1A-C6A	2.54	122.91	118.73
3	B	999	FAD	C6A-C5A-N7A	2.54	136.99	132.09
3	A	999	FAD	C4A-C5A-N7A	-2.52	107.70	110.58
2	D	800	AWB	C27-C25-C24	-2.52	101.37	111.16
3	B	999	FAD	C3B-C2B-C1B	2.47	106.13	101.46
3	A	999	FAD	C9A-C5X-N5	-2.46	119.84	122.45
2	B	800	AWB	O4-C14-C15	-2.45	116.54	121.03
3	C	999	FAD	C10-N1-C2	2.43	122.12	116.85
3	B	999	FAD	C10-C4X-N5	-2.43	119.84	124.81
3	C	999	FAD	C6A-C5A-N7A	2.42	136.76	132.09
2	D	800	AWB	O-C9-C10	2.41	114.08	110.28
3	D	999	FAD	C9A-C5X-N5	-2.41	119.90	122.45
2	B	800	AWB	C10-N-C14	2.40	126.36	121.53
3	A	999	FAD	C4X-C10-N1	-2.39	118.72	124.59
3	B	999	FAD	C5X-N5-C4X	2.39	121.95	118.09
3	D	999	FAD	O2A-PA-O3P	2.37	113.68	107.27
2	B	800	AWB	O-C9-O1	-2.37	121.16	124.10
3	D	999	FAD	N3A-C2A-N1A	-2.36	125.00	128.58
3	C	999	FAD	O2'-C2'-C3'	-2.34	103.78	109.25
3	B	999	FAD	O2-C2-N1	-2.33	117.93	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	FAD	C9A-N10-C10	-2.32	117.21	120.75
3	D	999	FAD	O2-C2-N3	2.31	123.01	118.58
3	A	999	FAD	C4X-C10-N10	2.28	119.74	116.48
3	C	999	FAD	O4-C4-N3	-2.27	115.84	120.11
3	C	999	FAD	O2'-C2'-C1'	2.27	119.52	110.20
2	D	800	AWB	C27-C25-C26	2.26	120.62	110.53
3	D	999	FAD	C5A-N7A-C8A	2.23	106.96	103.45
3	C	999	FAD	C4X-C10-N1	-2.22	119.14	124.59
2	A	800	AWB	O-C9-O1	-2.18	121.39	124.10
3	B	999	FAD	O4B-C1B-C2B	-2.18	101.95	106.62
2	A	800	AWB	C17-N1-C21	-2.17	122.52	126.87
3	D	999	FAD	O3P-P-O1P	-2.16	104.19	110.70
3	C	999	FAD	C5'-C4'-C3'	2.14	116.26	112.22
3	D	999	FAD	C10-C4X-N5	-2.14	120.44	124.81
3	C	999	FAD	C4X-C10-N10	2.12	119.51	116.48
3	A	999	FAD	C7M-C7-C6	2.11	123.29	119.57
3	A	999	FAD	C6A-C5A-N7A	2.11	136.15	132.09
2	A	800	AWB	C19-C18-C17	2.10	122.96	118.69
3	B	999	FAD	C4B-O4B-C1B	2.08	114.07	109.47
3	B	999	FAD	C5X-C9A-N10	2.08	119.85	117.97
3	D	999	FAD	O2A-PA-O1A	2.05	121.96	112.44
3	D	999	FAD	C4A-N9A-C1B	-2.03	121.88	126.63
3	A	999	FAD	C7M-C7-C8	-2.02	116.64	120.76
3	B	999	FAD	C4A-N9A-C8A	2.00	107.84	105.74

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	800	AWB	C10-C11-O2-C12
2	A	800	AWB	C23-C24-C25-C26
2	A	800	AWB	C23-C24-C25-C27
2	B	800	AWB	C16-C17-N1-C21
2	B	800	AWB	O5-C21-N1-C17
2	B	800	AWB	C10-C11-O2-C12
2	B	800	AWB	C23-C24-C25-C26
2	C	800	AWB	C16-C17-N1-C21
2	C	800	AWB	O5-C21-N1-C17
2	C	800	AWB	C23-C24-C25-C27
3	A	999	FAD	N10-C1'-C2'-O2'
3	A	999	FAD	N10-C1'-C2'-C3'
3	B	999	FAD	N10-C1'-C2'-O2'

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Mol	Chain	Res	Type	Atoms
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'
2	C	800	AWB	C18-C17-N1-C21
2	D	800	AWB	C18-C17-N1-C21
2	D	800	AWB	C24-C23-O7-C7
2	D	800	AWB	O8-C23-O7-C7
2	C	800	AWB	C3-C4-C5-C6
2	B	800	AWB	C3-C4-C5-C6
2	B	800	AWB	C23-C24-C25-C27
2	C	800	AWB	C23-C24-C25-C26
2	C	800	AWB	C24-C23-O7-C7
2	D	800	AWB	C2-C3-C4-C5
2	A	800	AWB	C1-C2-C3-C4
2	C	800	AWB	C1-C2-C3-C4
2	D	800	AWB	C-C1-C2-C3
2	A	800	AWB	C2-C3-C4-C5
2	C	800	AWB	O8-C23-O7-C7
2	B	800	AWB	C2-C3-C4-C5
2	A	800	AWB	C-C1-C2-C3
2	D	800	AWB	C16-C17-N1-C21
2	A	800	AWB	O8-C23-C24-C25
2	A	800	AWB	O7-C23-C24-C25
2	A	800	AWB	C3-C4-C5-C6
2	C	800	AWB	O8-C23-C24-C25
2	C	800	AWB	O7-C23-C24-C25
2	C	800	AWB	C4-C5-C6-C12
2	B	800	AWB	O7-C23-C24-C25
2	B	800	AWB	O8-C23-C24-C25
2	B	800	AWB	O8-C23-O7-C7
2	C	800	AWB	C10-C11-O2-C12
2	D	800	AWB	C10-C11-O2-C12
2	C	800	AWB	C-C1-C2-C3

There are no ring outliers.

5 monomers are involved in 22 short contacts:

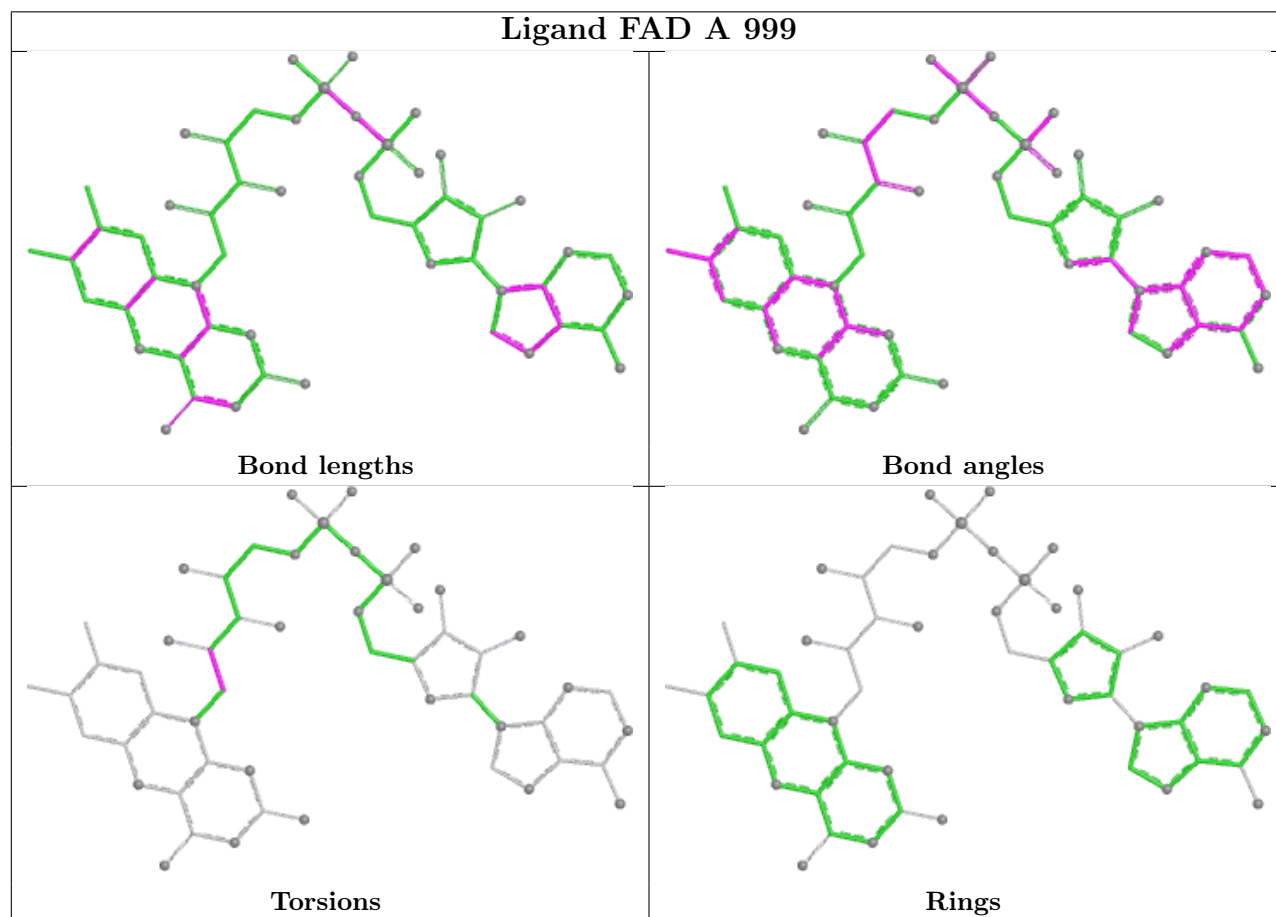
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	800	AWB	4	0
3	B	999	FAD	1	0

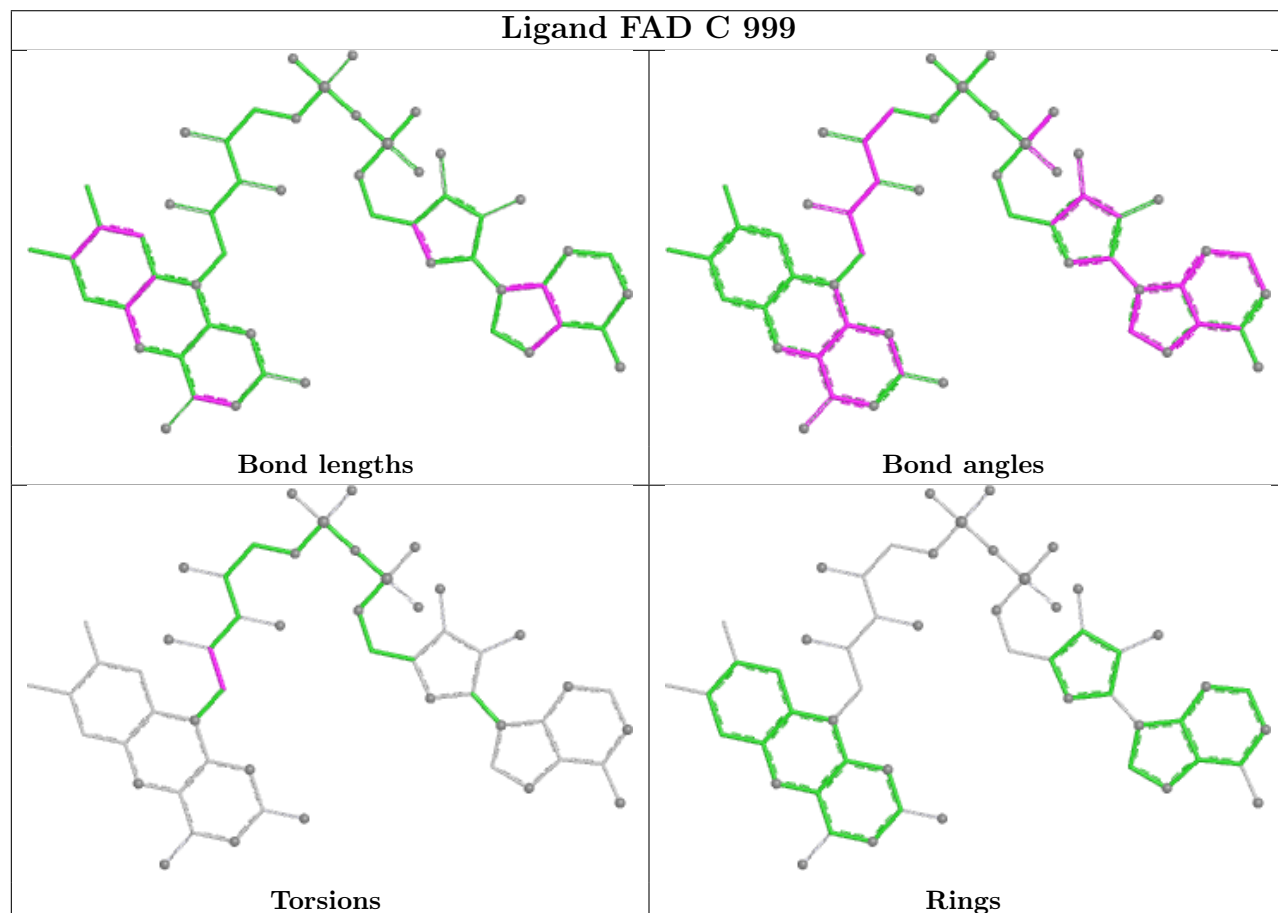
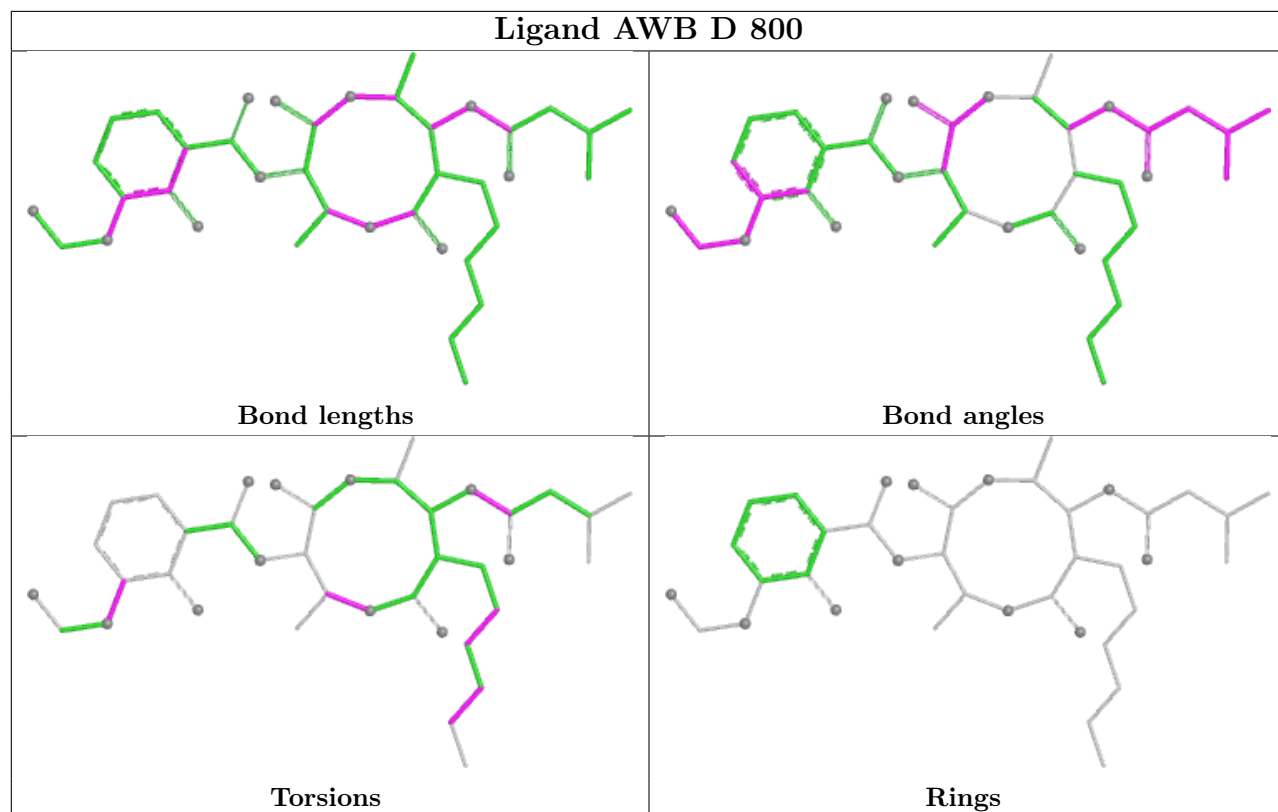
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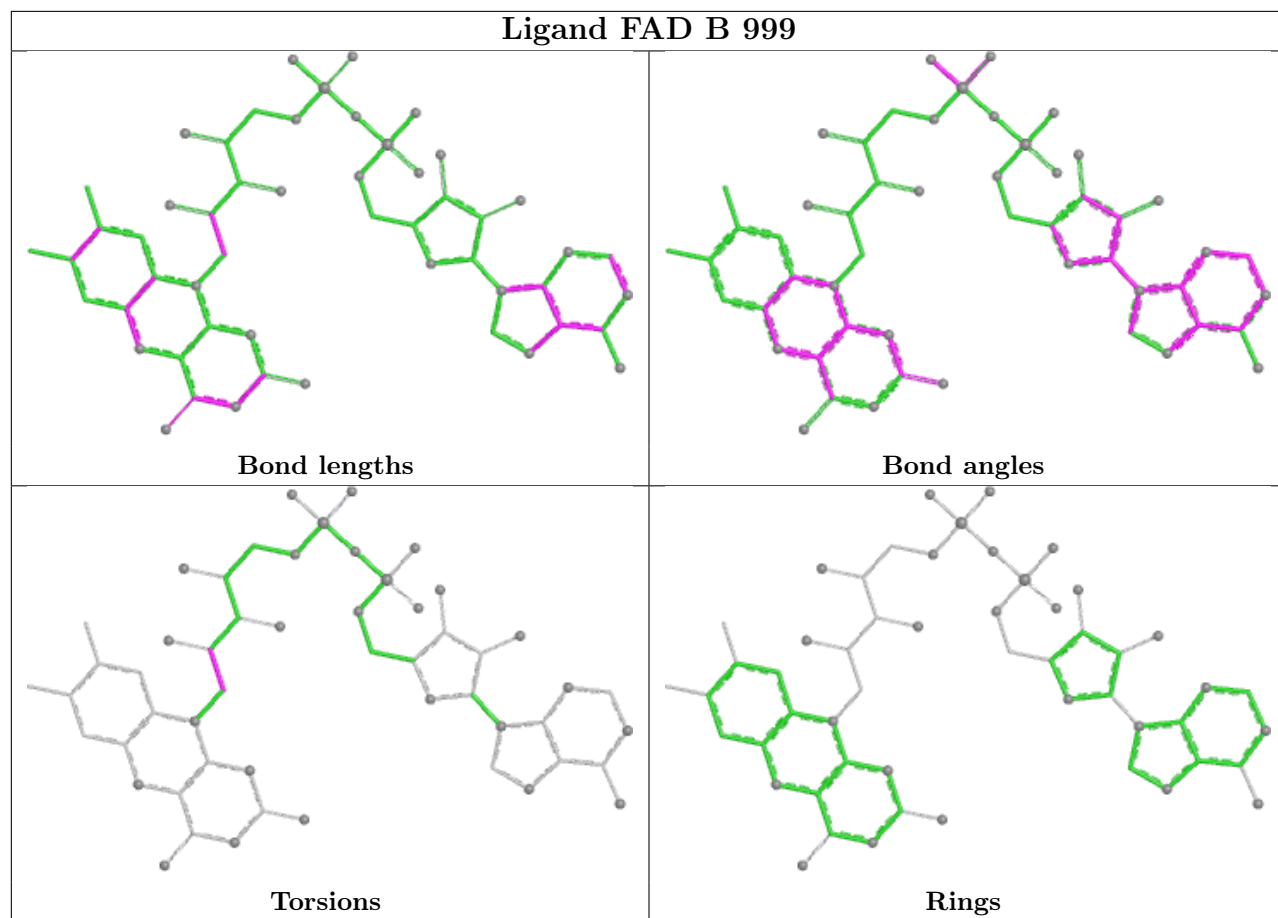
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	AWB	8	0
2	C	800	AWB	4	0
2	B	800	AWB	5	0

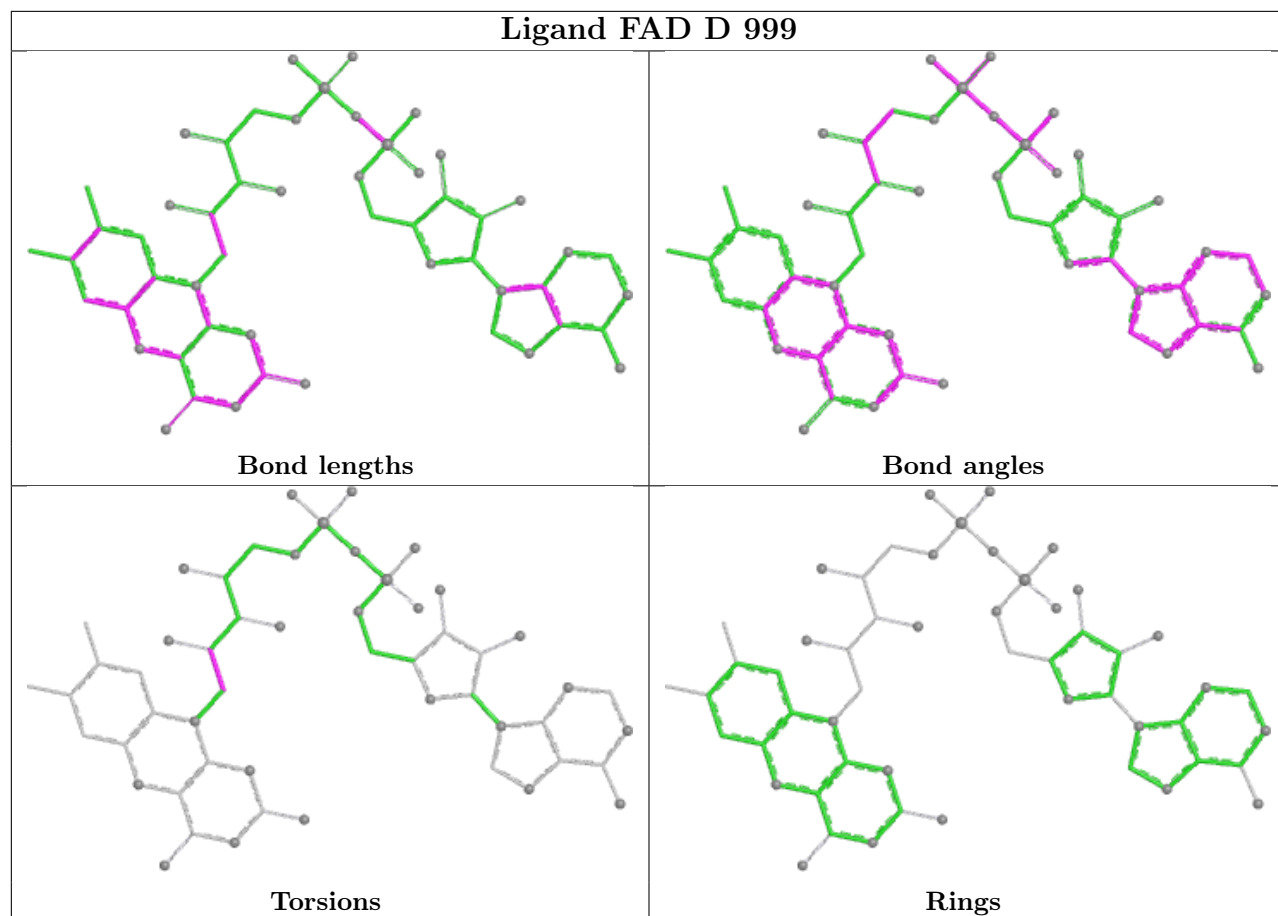
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



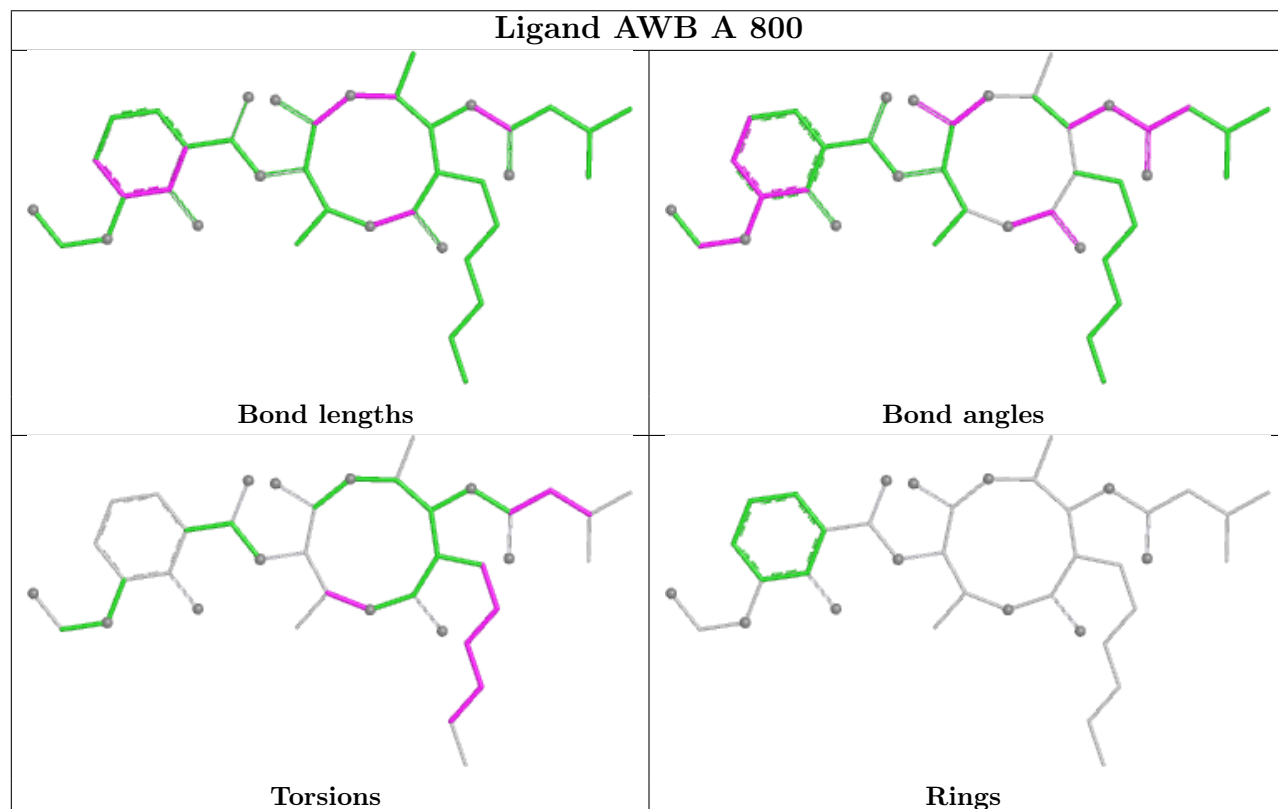


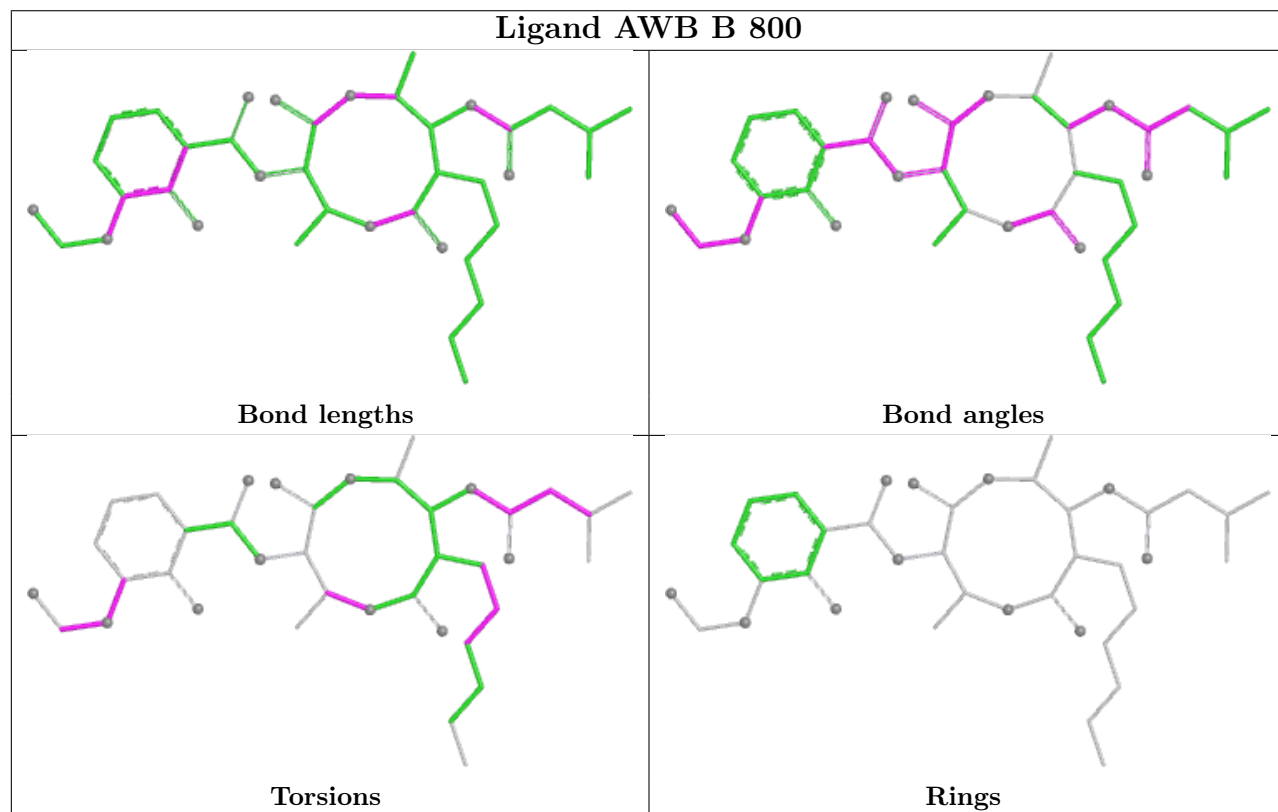
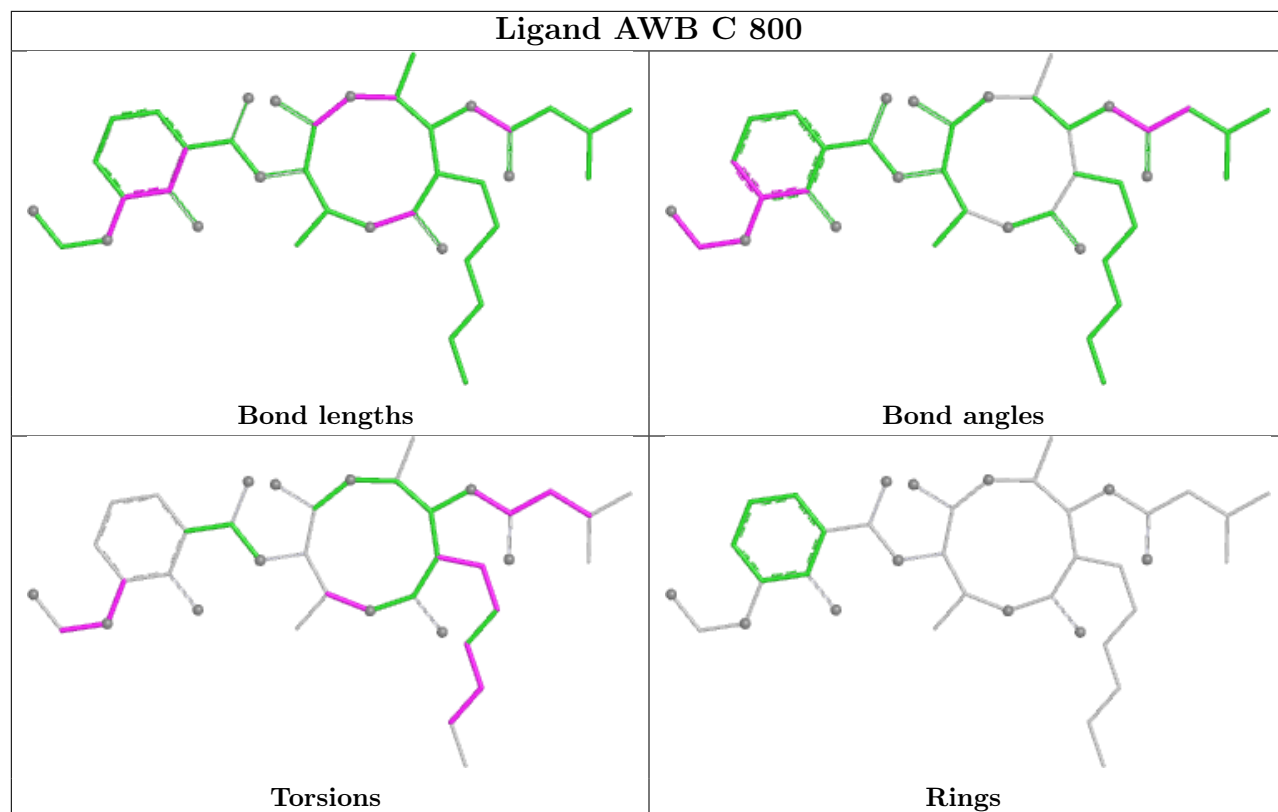


Ligand FAD D 999



Ligand AWB A 800





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	539/658 (81%)	0.18	15 (2%) 55 54	18, 35, 64, 81	0
1	B	539/658 (81%)	0.28	17 (3%) 50 49	18, 38, 66, 81	0
1	C	551/658 (83%)	0.08	10 (1%) 67 67	14, 33, 60, 78	2 (0%)
1	D	547/658 (83%)	0.19	10 (1%) 67 67	12, 35, 61, 79	1 (0%)
All	All	2176/2632 (82%)	0.18	52 (2%) 59 59	12, 35, 63, 81	3 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	431	ALA	4.6
1	C	159	ILE	4.2
1	C	150	LEU	4.0
1	A	559	PHE	3.7
1	B	140	LEU	3.6
1	B	457	GLY	3.5
1	D	460	PRO	3.4
1	B	83	ILE	3.4
1	A	141	ASP	3.3
1	B	431	ALA	3.3
1	A	159	ILE	3.1
1	D	142	HIS	3.1
1	C	152	PRO	3.0
1	B	138	ILE	3.0
1	A	84	PRO	2.9
1	A	202	PHE	2.8
1	B	501	GLY	2.8
1	A	249	ALA	2.8
1	C	457	GLY	2.7
1	B	559	PHE	2.7
1	A	457	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	139	ASN	2.6
1	C	432	LEU	2.6
1	D	559	PHE	2.5
1	B	432	LEU	2.5
1	A	142	HIS	2.5
1	B	458	PHE	2.5
1	A	458	PHE	2.4
1	B	478	LEU	2.4
1	D	120	LEU	2.4
1	D	152	PRO	2.3
1	A	139	ASN	2.2
1	C	140	LEU	2.2
1	C	494	LEU	2.2
1	B	202	PHE	2.2
1	D	496	ALA	2.2
1	B	159	ILE	2.1
1	A	143	LYS	2.1
1	A	195	PHE	2.1
1	D	524	ILE	2.1
1	B	155	THR	2.1
1	C	149	SER	2.1
1	C	151	ASN	2.1
1	B	157	PRO	2.1
1	C	90	LEU	2.0
1	B	460	PRO	2.0
1	D	202	PHE	2.0
1	B	161	ASN	2.0
1	A	432	LEU	2.0
1	A	506	LEU	2.0
1	A	250	ASP	2.0
1	B	135	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

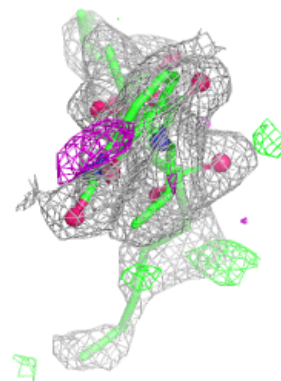
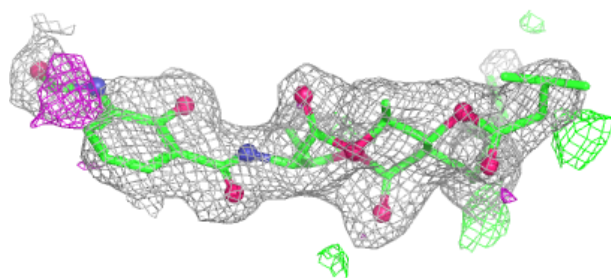
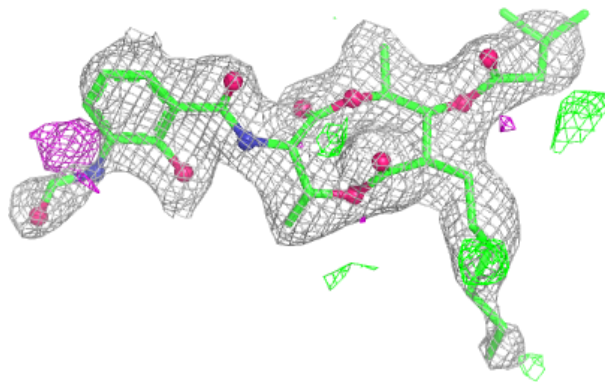
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	AWB	A	800	39/39	0.87	0.14	32,44,63,67	0
2	AWB	B	800	39/39	0.88	0.13	39,46,71,74	0
4	SO4	B	1659	5/5	0.88	0.16	49,60,66,69	0
2	AWB	D	800	39/39	0.91	0.12	32,43,61,63	0
4	SO4	D	1659	5/5	0.92	0.14	57,59,61,73	0
2	AWB	C	800	39/39	0.94	0.09	28,38,55,59	0
4	SO4	A	1659	5/5	0.96	0.12	47,49,61,65	0
3	FAD	A	999	53/53	0.98	0.04	15,19,24,25	0
3	FAD	B	999	53/53	0.98	0.05	19,21,23,26	0
3	FAD	D	999	53/53	0.98	0.06	15,19,23,24	0
3	FAD	C	999	53/53	0.99	0.04	15,18,20,21	0

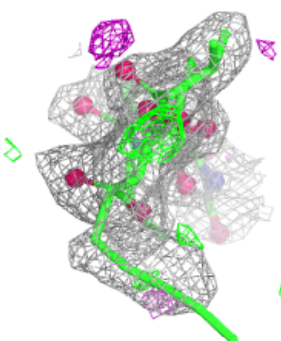
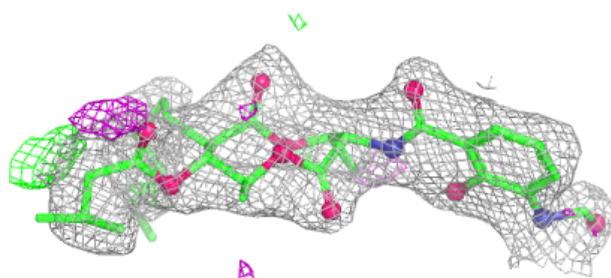
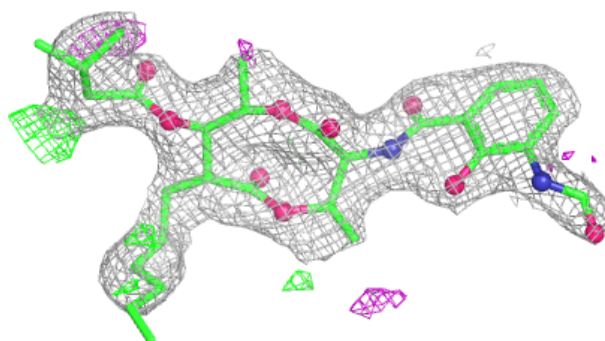
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AWB A 800:

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

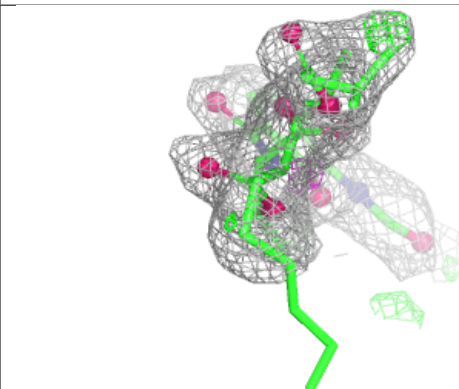
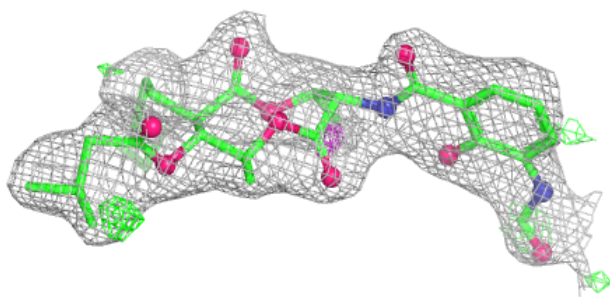
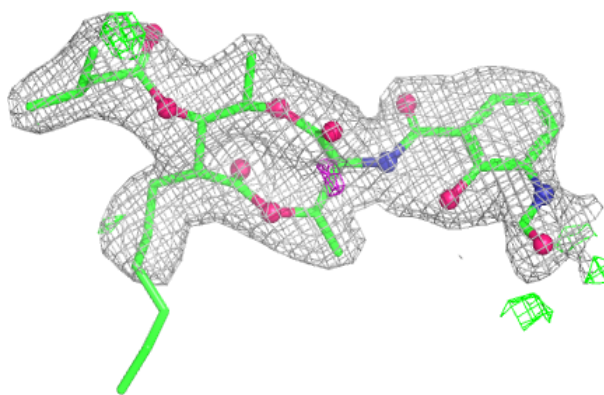
**Electron density around AWB B 800:**

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

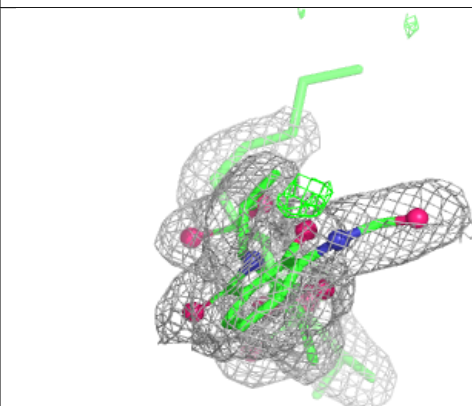
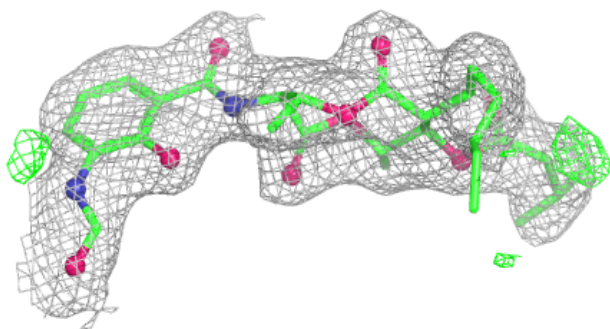
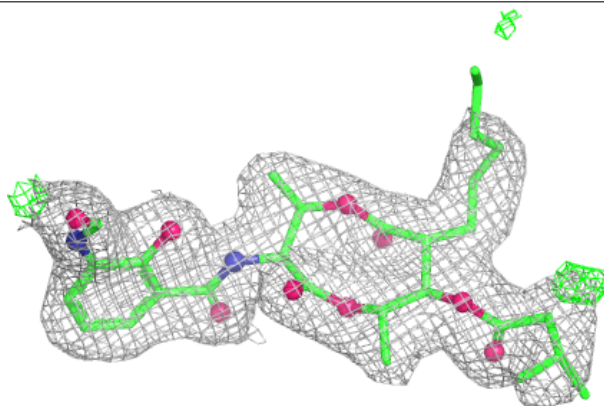


Electron density around AWB D 800:

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

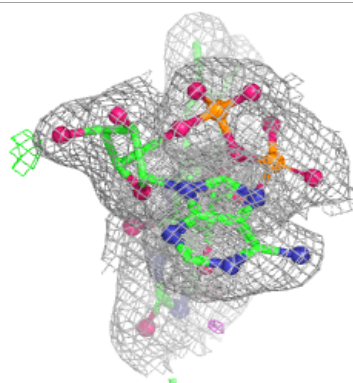
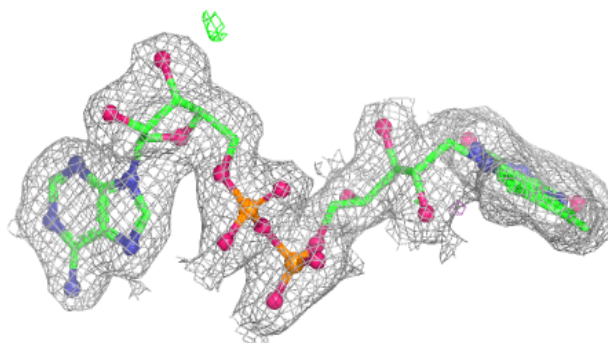
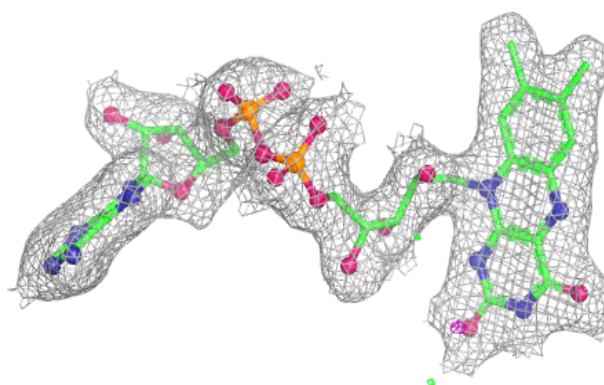
**Electron density around AWB C 800:**

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

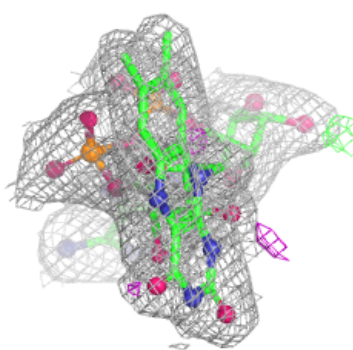
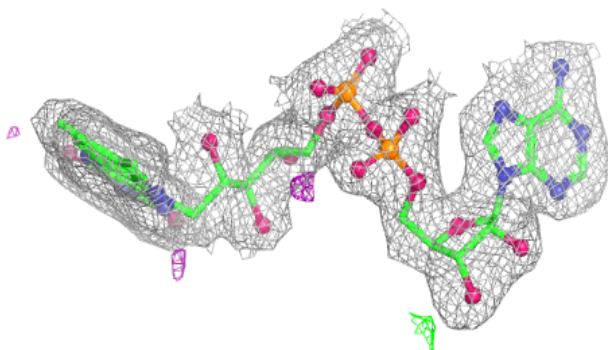
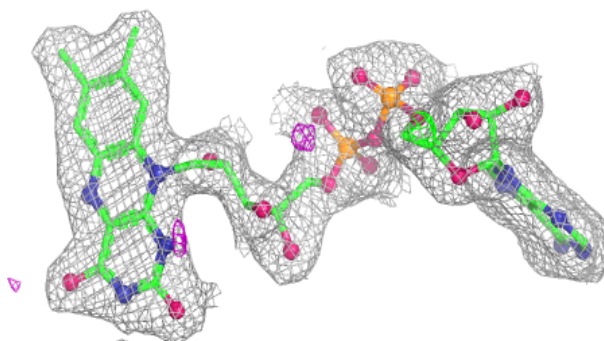


Electron density around FAD A 999:

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

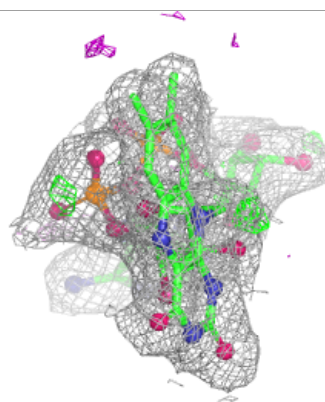
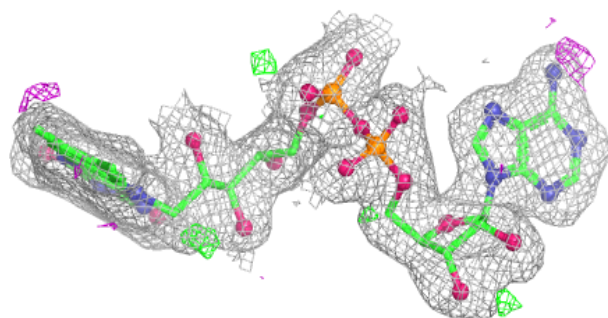
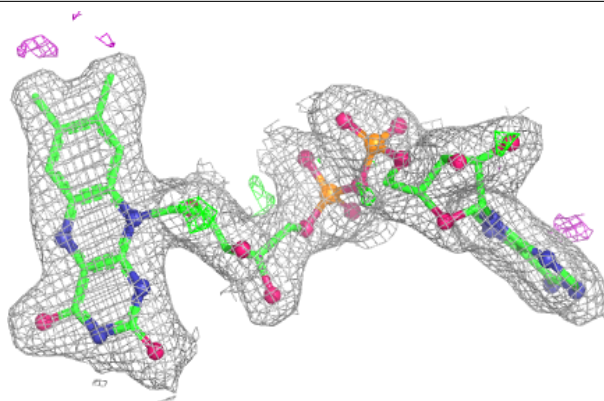
**Electron density around FAD B 999:**

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

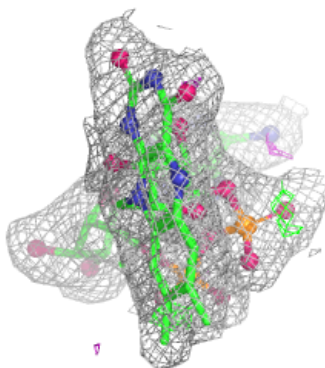
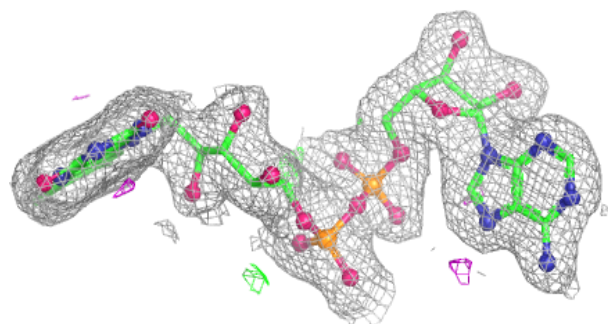
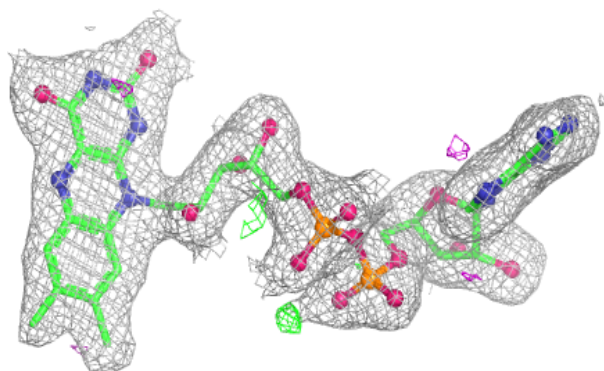


Electron density around FAD D 999:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.