



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 2, 2024 – 04:44 pm GMT

PDB ID : 5ADZ  
Title : Ether Lipid-Generating Enzyme AGPS in complex with inhibitor 1a  
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 : 2.20 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 : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

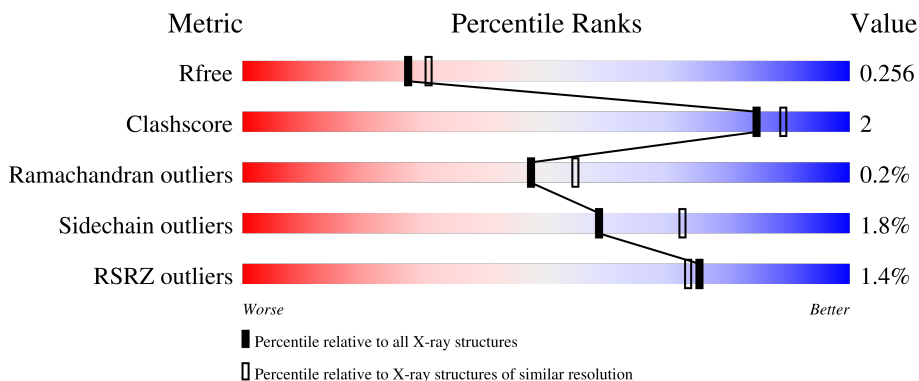
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	 2% 81% 5% 14%
1	B	658	 2% 76% 6% 18%
1	C	658	 75% 9% 15%
1	D	658	 78% 5% 16%

## 2 Entry composition [i](#)

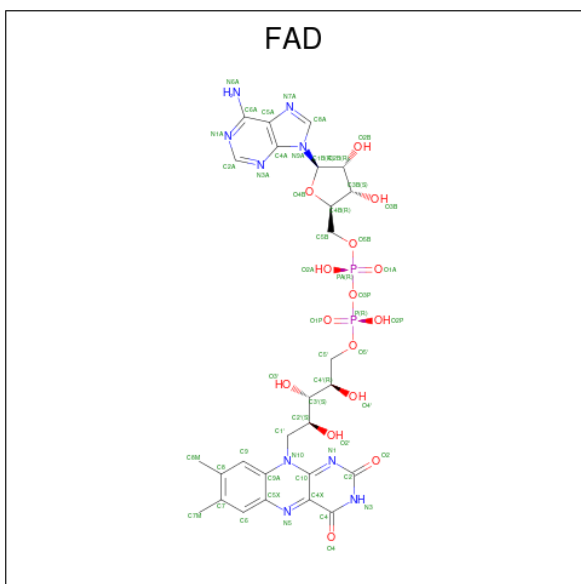
There are 4 unique types of molecules in this entry. The entry contains 18475 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	566	Total 4462	C 2842	N 775	O 821	S 24	0	1	0
1	B	542	Total 4266	C 2711	N 738	O 793	S 24	0	0	0
1	C	557	Total 4408	C 2795	N 766	O 823	S 24	0	1	0
1	D	552	Total 4358	C 2762	N 758	O 814	S 24	0	0	0

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



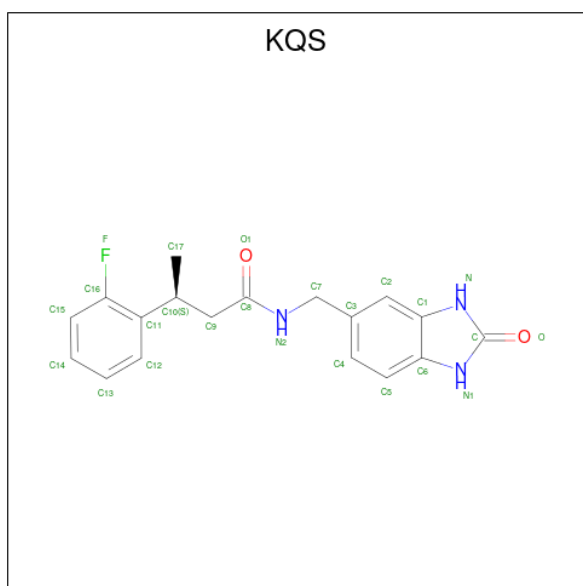
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is (3S)-3-(2-fluorophenyl)-N-((2-oxo-2,3-dihydro-1H-benzo[d]imidazol-5-yl)methyl)butanamide (three-letter code: KQS) (formula: C<sub>18</sub>H<sub>18</sub>FN<sub>3</sub>O<sub>2</sub>).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	189	Total	O	0	0
			189	189		
4	B	129	Total	O	0	0
			129	129		

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	C	217	Total 217	O 217	0	0
4	D	138	Total 138	O 138	0	0





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.06Å 99.61Å 107.97Å 90.57° 90.04° 94.76°	Depositor
Resolution (Å)	107.96 – 2.20 32.09 – 2.20	Depositor EDS
% Data completeness (in resolution range)	91.0 (107.96-2.20) 91.1 (32.09-2.20)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.8.0124	Depositor
R, $R_{free}$	0.195 , 0.253 0.200 , 0.256	Depositor DCC
$R_{free}$ test set	1260 reflections (1.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.8	Xtrriage
Anisotropy	0.090	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 39.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	18475	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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: FAD, KQS

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	0.71	0/4567	0.87	5/6173 (0.1%)
1	B	0.71	0/4363	0.84	7/5903 (0.1%)
1	C	0.74	0/4511	0.88	7/6099 (0.1%)
1	D	0.66	0/4456	0.86	8/6027 (0.1%)
All	All	0.71	0/17897	0.86	27/24202 (0.1%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	623	ARG	NE-CZ-NH2	-8.53	116.04	120.30
1	C	623	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	C	623	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	A	317	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	A	623	ARG	NE-CZ-NH1	7.33	123.96	120.30
1	D	623	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	C	536	ARG	NE-CZ-NH2	-6.65	116.98	120.30
1	C	406	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	A	317	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	C	536	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	D	317	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	B	474	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	D	342	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	B	536	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	117	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	D	353	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	D	422	ASP	CB-CG-OD1	5.91	123.62	118.30
1	D	353	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	D	547	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	B	331	ASP	CB-CG-OD1	-5.36	113.47	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	253	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	C	419	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	100	ASP	CB-CG-OD1	5.28	123.06	118.30
1	B	331	ASP	CB-CG-OD2	5.27	123.05	118.30
1	B	382	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	422	ASP	CB-CG-OD1	5.17	122.95	118.30
1	D	623	ARG	NE-CZ-NH2	-5.16	117.72	120.30

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	4462	0	4393	15	0
1	B	4266	0	4180	16	0
1	C	4408	0	4347	33	0
1	D	4358	0	4289	16	0
2	A	53	0	31	1	0
2	B	53	0	31	1	0
2	C	53	0	31	1	0
2	D	53	0	31	1	0
3	A	24	0	18	2	0
3	B	24	0	18	2	0
3	C	24	0	18	1	0
3	D	24	0	18	2	0
4	A	189	0	0	2	0
4	B	129	0	0	0	0
4	C	217	0	0	3	0
4	D	138	0	0	0	0
All	All	18475	0	17405	80	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 2.

All (80) 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:B:133:GLN:NE2	1:B:139:ASN:O	2.25	0.69
1:A:133:GLN:NE2	1:A:139:ASN:O	2.26	0.68
1:B:582:ALA:HB2	3:B:888:KQS:H15	1.79	0.65
1:C:178:GLU:O	1:C:182:ARG:HG3	1.95	0.65
1:C:635:GLY:HA2	1:C:638:MET:HE3	1.79	0.64
1:C:144:THR:HG21	1:C:519:LEU:O	1.98	0.64
1:A:94:ASN:HA	1:A:197:LEU:HD13	1.81	0.62
1:C:462:GLN:O	4:C:2156:HOH:O	2.16	0.62
1:C:195:PHE:CD2	1:C:592:LEU:HD11	2.38	0.59
1:D:192:HIS:HB3	1:D:243:TYR:OH	2.02	0.58
1:C:129:LYS:O	1:C:133:GLN:HG3	2.03	0.58
1:B:140:LEU:HD12	1:B:521:TYR:CD1	2.39	0.57
1:C:94:ASN:HA	1:C:197:LEU:HD13	1.86	0.56
2:A:999:FAD:HM72	3:A:888:KQS:C4	2.36	0.55
1:C:459:ASP:O	1:C:461:ASN:O	2.23	0.55
1:C:144:THR:HG22	1:C:520:GLU:HA	1.88	0.55
1:B:507:LEU:O	1:B:511:ILE:HD12	2.08	0.53
1:C:195:PHE:CG	1:C:592:LEU:HD11	2.43	0.52
1:C:277:HIS:HB3	4:C:2093:HOH:O	2.08	0.52
2:B:999:FAD:HM72	3:B:888:KQS:C4	2.40	0.52
1:A:230:LEU:HD13	1:A:256:ILE:HD11	1.91	0.51
2:C:999:FAD:HM72	3:C:888:KQS:C4	2.40	0.51
1:A:106:ASN:HD21	1:A:110:GLN:HE21	1.59	0.51
1:C:639:LEU:HD22	1:D:358:PRO:HG2	1.92	0.51
1:A:109:GLY:HA3	1:C:268:TRP:CE3	2.47	0.50
1:B:419:ARG:O	1:B:466:ALA:HA	2.10	0.50
1:C:138:ILE:HD11	1:C:523:ILE:HD11	1.92	0.50
1:C:119:PRO:HG2	1:C:506:LEU:HD22	1.92	0.50
1:C:419:ARG:HD2	1:C:505:TYR:CE1	2.46	0.50
1:C:619:VAL:HB	1:C:657:LEU:HD23	1.95	0.49
1:C:106:ASN:HB2	1:C:110:GLN:H	1.77	0.49
1:A:463:LEU:C	1:A:463:LEU:HD12	2.34	0.48
1:D:161:ASN:OD1	1:D:163:ASP:N	2.46	0.48
1:A:582:ALA:HB2	3:A:888:KQS:H15	1.95	0.48
1:C:150:LEU:CD2	1:C:180:ASP:HA	2.45	0.47
1:C:415:PRO:HB3	1:C:470:PHE:CD1	2.50	0.47
1:A:387:TYR:OH	1:A:389:LYS:HD3	2.15	0.47
1:D:421:MET:O	1:D:464:SER:HB2	2.15	0.46
1:C:314:ILE:HG23	1:C:365:MET:HG2	1.97	0.46
1:A:342:ARG:HD2	1:A:645:TYR:CZ	2.50	0.46
1:A:585:TYR:HB2	1:A:591:PRO:HB3	1.97	0.46
1:D:314:ILE:HG23	1:D:365:MET:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:638:MET:HE2	1:D:345:ILE:CD1	2.45	0.46
1:B:105:LEU:HD12	1:B:109:GLY:HA2	1.98	0.46
1:C:426:PHE:CD2	1:C:463:LEU:HD11	2.52	0.45
1:B:192:HIS:HB3	1:B:243:TYR:OH	2.17	0.45
1:C:388:GLN:NE2	1:C:471:GLU:OE1	2.50	0.45
1:B:340:THR:HB	1:B:646:VAL:HG13	1.99	0.45
1:C:230:LEU:CD1	1:C:256:ILE:HD11	2.47	0.45
1:B:114:THR:HG22	1:B:115:GLY:N	2.32	0.44
1:A:435:GLN:NE2	4:A:2137:HOH:O	2.50	0.44
1:C:137:GLY:HA3	1:C:559:PHE:CZ	2.52	0.44
1:C:638:MET:HE2	1:D:345:ILE:HD11	1.99	0.44
1:A:430:HIS:CD2	1:A:447:LEU:HD23	2.53	0.44
1:B:424:GLN:CB	1:B:564:THR:CG2	2.96	0.44
1:B:643:LYS:NZ	1:B:647:ASP:OD2	2.50	0.43
1:D:161:ASN:OD1	1:D:161:ASN:C	2.57	0.43
1:D:194:ILE:HA	1:D:197:LEU:HD12	1.99	0.43
4:C:2129:HOH:O	1:D:634:VAL:HG23	2.18	0.43
1:D:419:ARG:HD2	1:D:467:THR:OG1	2.19	0.43
1:B:547:ARG:NH1	1:B:605:GLU:OE1	2.46	0.43
1:D:127:THR:HG22	1:D:127:THR:O	2.19	0.43
1:C:175:TYR:HA	1:C:209:VAL:O	2.19	0.42
1:C:419:ARG:O	1:C:466:ALA:HA	2.19	0.42
1:B:140:LEU:HD12	1:B:521:TYR:CG	2.54	0.42
1:D:230:LEU:HD13	1:D:256:ILE:HD11	2.02	0.42
1:A:557:VAL:HA	1:A:588:ILE:HD11	2.01	0.42
1:D:260:THR:O	1:D:281:GLY:HA3	2.18	0.42
1:B:424:GLN:CB	1:B:564:THR:HG22	2.49	0.42
1:C:127:THR:HG23	1:C:431:ALA:O	2.20	0.42
1:A:419:ARG:O	1:A:466:ALA:HA	2.20	0.41
1:D:537:VAL:HG13	1:D:577:ILE:HD11	2.02	0.41
2:D:999:FAD:HM72	3:D:888:KQS:C4	2.50	0.41
1:B:138:ILE:HD13	1:B:521:TYR:HB3	2.03	0.41
1:C:426:PHE:CE2	1:C:463:LEU:HD11	2.55	0.41
1:C:192:HIS:HB3	1:C:243:TYR:OH	2.20	0.41
1:D:515:ARG:HA	3:D:888:KQS:H13	2.02	0.41
1:C:342:ARG:HD2	1:C:645:TYR:CZ	2.56	0.40
1:B:221:ILE:HG21	1:B:258:LEU:HD12	2.04	0.40
1:A:479:GLN:NE2	4:A:2143:HOH:O	2.54	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	563/658 (86%)	547 (97%)	14 (2%)	2 (0%)	34	37
1	B	536/658 (82%)	519 (97%)	16 (3%)	1 (0%)	47	55
1	C	554/658 (84%)	535 (97%)	18 (3%)	1 (0%)	47	55
1	D	548/658 (83%)	528 (96%)	20 (4%)	0	100	100
All	All	2201/2632 (84%)	2129 (97%)	68 (3%)	4 (0%)	47	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	ASP
1	A	198	ARG
1	C	106	ASN
1	B	458	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	477/545 (88%)	470 (98%)	7 (2%)	65	78
1	B	457/545 (84%)	448 (98%)	9 (2%)	55	69
1	C	478/545 (88%)	471 (98%)	7 (2%)	65	78
1	D	471/545 (86%)	461 (98%)	10 (2%)	53	67
All	All	1883/2180 (86%)	1850 (98%)	33 (2%)	59	72

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	ASP
1	A	140	LEU
1	A	263	MET
1	A	323	LYS
1	A	461	ASN
1	A	463	LEU
1	A	550	ARG
1	B	90	LEU
1	B	265	ARG
1	B	323	LYS
1	B	349	CYS
1	B	475	GLU
1	B	499	ASP
1	B	555	LYS
1	B	581	PHE
1	B	646	VAL
1	C	90	LEU
1	C	143	LYS
1	C	323	LYS
1	C	342	ARG
1	C	503	ARG
1	C	581	PHE
1	C	596	GLU
1	D	133	GLN
1	D	144	THR
1	D	161	ASN
1	D	323	LYS
1	D	419	ARG
1	D	500	ASN
1	D	576	CYS
1	D	596	GLU
1	D	625	GLN
1	D	630	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	177	GLN
1	A	189	HIS
1	A	430	HIS

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Mol	Chain	Res	Type
1	A	479	GLN
1	C	423	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FAD	C	999	-	53,58,58	1.55	6 (11%)	68,89,89	1.41	13 (19%)
2	FAD	B	999	-	53,58,58	1.40	4 (7%)	68,89,89	1.58	14 (20%)
2	FAD	D	999	-	53,58,58	1.30	6 (11%)	68,89,89	1.58	15 (22%)
3	KQS	A	888	-	26,26,26	1.79	5 (19%)	35,36,36	2.74	9 (25%)
2	FAD	A	999	-	53,58,58	1.37	3 (5%)	68,89,89	1.58	17 (25%)
3	KQS	D	888	-	26,26,26	1.86	3 (11%)	35,36,36	2.81	9 (25%)
3	KQS	C	888	-	26,26,26	1.61	3 (11%)	35,36,36	3.07	9 (25%)
3	KQS	B	888	-	26,26,26	1.78	3 (11%)	35,36,36	2.57	11 (31%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	C	999	-	-	3/30/50/50	0/6/6/6
2	FAD	B	999	-	-	3/30/50/50	0/6/6/6
2	FAD	D	999	-	-	3/30/50/50	0/6/6/6
3	KQS	A	888	-	-	0/13/13/13	0/3/3/3
2	FAD	A	999	-	-	5/30/50/50	0/6/6/6
3	KQS	D	888	-	-	0/13/13/13	0/3/3/3
3	KQS	C	888	-	-	0/13/13/13	0/3/3/3
3	KQS	B	888	-	-	0/13/13/13	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	888	KQS	C11-C16	7.05	1.51	1.38
3	B	888	KQS	C11-C16	6.65	1.50	1.38
2	B	999	FAD	C9A-C5X	5.88	1.51	1.41
2	C	999	FAD	C9A-C5X	5.71	1.50	1.41
3	A	888	KQS	C11-C16	5.67	1.48	1.38
2	A	999	FAD	C9A-C5X	5.50	1.50	1.41
3	C	888	KQS	C11-C16	5.32	1.48	1.38
2	D	999	FAD	C9A-C5X	4.41	1.48	1.41
2	D	999	FAD	C4-N3	-3.97	1.31	1.38
3	C	888	KQS	C1-C6	3.81	1.49	1.40
3	A	888	KQS	C1-C6	3.61	1.49	1.40
3	D	888	KQS	C1-C6	3.59	1.49	1.40
3	B	888	KQS	C1-C6	3.56	1.49	1.40
2	C	999	FAD	C4-N3	-3.38	1.32	1.38
2	C	999	FAD	O4B-C1B	3.32	1.45	1.41
2	C	999	FAD	C8-C7	3.22	1.48	1.40
3	A	888	KQS	O-C	3.12	1.29	1.23
2	A	999	FAD	C8-C7	3.09	1.48	1.40
2	B	999	FAD	C8-C7	3.04	1.48	1.40
2	B	999	FAD	O4-C4	2.85	1.29	1.23
3	A	888	KQS	C1-N	-2.85	1.33	1.38
3	C	888	KQS	C11-C10	-2.77	1.48	1.52
2	C	999	FAD	C5A-C4A	2.77	1.48	1.40
3	A	888	KQS	C11-C10	-2.74	1.48	1.52
2	D	999	FAD	C8-C7	2.56	1.47	1.40
2	A	999	FAD	C4X-N5	2.53	1.35	1.30
2	C	999	FAD	C4X-N5	2.53	1.35	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	888	KQS	O-C	2.52	1.28	1.23
2	B	999	FAD	C5X-N5	-2.46	1.34	1.39
3	D	888	KQS	C-N	-2.42	1.33	1.37
2	D	999	FAD	O4B-C1B	2.41	1.44	1.41
2	D	999	FAD	C5A-C4A	2.18	1.46	1.40
2	D	999	FAD	C2-N1	-2.14	1.31	1.36

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	888	KQS	N1-C-N	10.35	118.66	106.57
3	D	888	KQS	N1-C-N	9.63	117.82	106.57
3	A	888	KQS	N1-C-N	8.64	116.67	106.57
3	B	888	KQS	N1-C-N	8.38	116.36	106.57
3	C	888	KQS	C6-N1-C	-7.09	102.63	110.12
3	A	888	KQS	O-C-N	-7.08	118.68	126.72
3	C	888	KQS	O-C-N	-7.06	118.70	126.72
3	D	888	KQS	O-C-N	-6.69	119.12	126.72
3	A	888	KQS	C6-N1-C	-6.67	103.07	110.12
3	D	888	KQS	C6-N1-C	-6.57	103.19	110.12
3	C	888	KQS	C1-N-C	-6.57	103.19	110.12
3	D	888	KQS	C1-N-C	-6.02	103.77	110.12
3	B	888	KQS	C1-N-C	-5.64	104.17	110.12
3	B	888	KQS	O-C-N1	-4.86	121.20	126.72
3	A	888	KQS	C1-N-C	-4.83	105.02	110.12
3	B	888	KQS	C6-N1-C	-4.75	105.10	110.12
3	B	888	KQS	C15-C16-C11	-4.66	118.53	123.72
3	C	888	KQS	C15-C16-C11	-4.24	119.01	123.72
2	B	999	FAD	O2-C2-N1	-4.10	115.03	121.83
3	A	888	KQS	C9-C10-C11	-3.96	101.31	110.75
3	A	888	KQS	C15-C16-C11	-3.94	119.33	123.72
2	D	999	FAD	O2-C2-N1	-3.88	115.40	121.83
3	B	888	KQS	O-C-N	-3.77	122.44	126.72
2	B	999	FAD	N3A-C2A-N1A	-3.68	122.93	128.68
3	C	888	KQS	O-C-N1	-3.60	122.63	126.72
2	D	999	FAD	C5'-C4'-C3'	3.52	119.01	112.20
2	A	999	FAD	P-O3P-PA	-3.41	121.13	132.83
2	C	999	FAD	N3A-C2A-N1A	-3.37	123.40	128.68
3	D	888	KQS	O-C-N1	-3.23	123.05	126.72
3	B	888	KQS	C9-C8-N2	3.15	120.33	115.97
2	A	999	FAD	C5X-C9A-N10	3.14	121.19	117.95
2	A	999	FAD	C10-N1-C2	3.12	123.13	116.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	999	FAD	C4X-C10-N1	-3.10	117.54	124.73
3	D	888	KQS	C15-C16-C11	-3.09	120.28	123.72
2	A	999	FAD	O2-C2-N1	-3.08	116.72	121.83
2	B	999	FAD	C4A-C5A-N7A	-3.07	106.20	109.40
2	C	999	FAD	C1B-N9A-C4A	-3.04	121.29	126.64
2	B	999	FAD	C1'-N10-C9A	3.04	125.58	120.51
2	A	999	FAD	C9A-C5X-N5	-3.03	119.14	122.43
2	D	999	FAD	C4X-C10-N10	2.97	120.83	116.48
2	C	999	FAD	O2-C2-N1	-2.93	116.97	121.83
2	D	999	FAD	N3A-C2A-N1A	-2.93	124.10	128.68
3	C	888	KQS	C9-C10-C11	-2.92	103.78	110.75
2	D	999	FAD	C4-C4X-N5	2.90	122.36	118.23
2	D	999	FAD	O2A-PA-O1A	2.85	126.33	112.24
2	B	999	FAD	C9A-N10-C10	-2.77	116.45	120.77
2	B	999	FAD	C4X-C10-N10	2.77	120.53	116.48
2	A	999	FAD	C1B-N9A-C4A	-2.70	121.90	126.64
2	C	999	FAD	C2A-N1A-C6A	2.69	123.36	118.75
2	C	999	FAD	C4-C4X-N5	2.66	122.02	118.23
2	D	999	FAD	C4X-C4-N3	2.61	119.83	113.19
2	D	999	FAD	C4-N3-C2	-2.61	120.82	125.64
2	B	999	FAD	O3B-C3B-C4B	-2.60	103.53	111.05
2	A	999	FAD	C4-C4X-N5	2.59	121.91	118.23
3	B	888	KQS	F-C16-C11	2.58	122.41	118.23
2	B	999	FAD	O4B-C1B-C2B	-2.57	103.17	106.93
2	A	999	FAD	N3A-C2A-N1A	-2.56	124.68	128.68
2	B	999	FAD	O2A-PA-O1A	2.53	124.75	112.24
3	B	888	KQS	C2-C1-C6	-2.53	119.06	121.54
2	A	999	FAD	O4-C4-C4X	-2.50	119.97	126.60
2	C	999	FAD	O4-C4-C4X	-2.46	120.08	126.60
2	A	999	FAD	C4X-C10-N10	2.44	120.05	116.48
3	A	888	KQS	C5-C6-C1	-2.43	117.24	121.03
2	C	999	FAD	C4X-C10-N10	2.41	120.01	116.48
2	C	999	FAD	C4X-C10-N1	-2.39	119.17	124.73
2	B	999	FAD	C4-C4X-N5	2.39	121.63	118.23
2	D	999	FAD	C4X-C10-N1	-2.37	119.24	124.73
2	A	999	FAD	C9A-N10-C10	-2.36	117.09	120.77
2	D	999	FAD	C2A-N1A-C6A	2.34	122.77	118.75
2	B	999	FAD	C4X-C10-N1	-2.34	119.31	124.73
3	B	888	KQS	O1-C8-C9	-2.34	118.07	121.50
2	C	999	FAD	C4X-C4-N3	2.34	119.12	113.19
2	A	999	FAD	C4A-C5A-N7A	-2.33	106.97	109.40
3	D	888	KQS	C7-N2-C8	2.30	125.92	122.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	888	KQS	F-C16-C11	2.30	121.95	118.23
2	D	999	FAD	O4-C4-C4X	-2.27	120.57	126.60
2	D	999	FAD	C1'-N10-C9A	2.21	124.19	120.51
2	B	999	FAD	C5X-C9A-N10	2.20	120.23	117.95
2	B	999	FAD	O2P-P-O1P	2.20	123.10	112.24
3	C	888	KQS	C5-C6-C1	-2.19	117.61	121.03
2	A	999	FAD	O3'-C3'-C4'	2.15	114.00	108.81
2	D	999	FAD	C2B-C3B-C4B	2.15	106.81	102.64
2	D	999	FAD	C10-N1-C2	2.14	121.17	116.90
2	C	999	FAD	C5'-C4'-C3'	2.13	116.33	112.20
3	B	888	KQS	C14-C15-C16	2.13	121.95	118.46
3	A	888	KQS	C10-C9-C8	-2.13	110.07	113.03
2	A	999	FAD	C4X-C4-N3	2.13	118.59	113.19
3	C	888	KQS	C5-C6-N1	2.12	135.18	130.87
3	D	888	KQS	C9-C8-N2	2.10	118.87	115.97
2	A	999	FAD	C5X-N5-C4X	2.09	121.55	118.07
2	C	999	FAD	N6A-C6A-N1A	2.09	122.91	118.57
2	C	999	FAD	O2A-PA-O1A	2.08	122.52	112.24
2	C	999	FAD	O3'-C3'-C4'	2.05	113.77	108.81
2	A	999	FAD	O2A-PA-O1A	2.04	122.34	112.24
3	A	888	KQS	C5-C6-N1	2.04	135.02	130.87
2	D	999	FAD	C9A-N10-C10	-2.03	117.60	120.77
2	B	999	FAD	P-O3P-PA	-2.01	125.94	132.83

There are no chirality outliers.

All (14) torsion outliers are listed below:

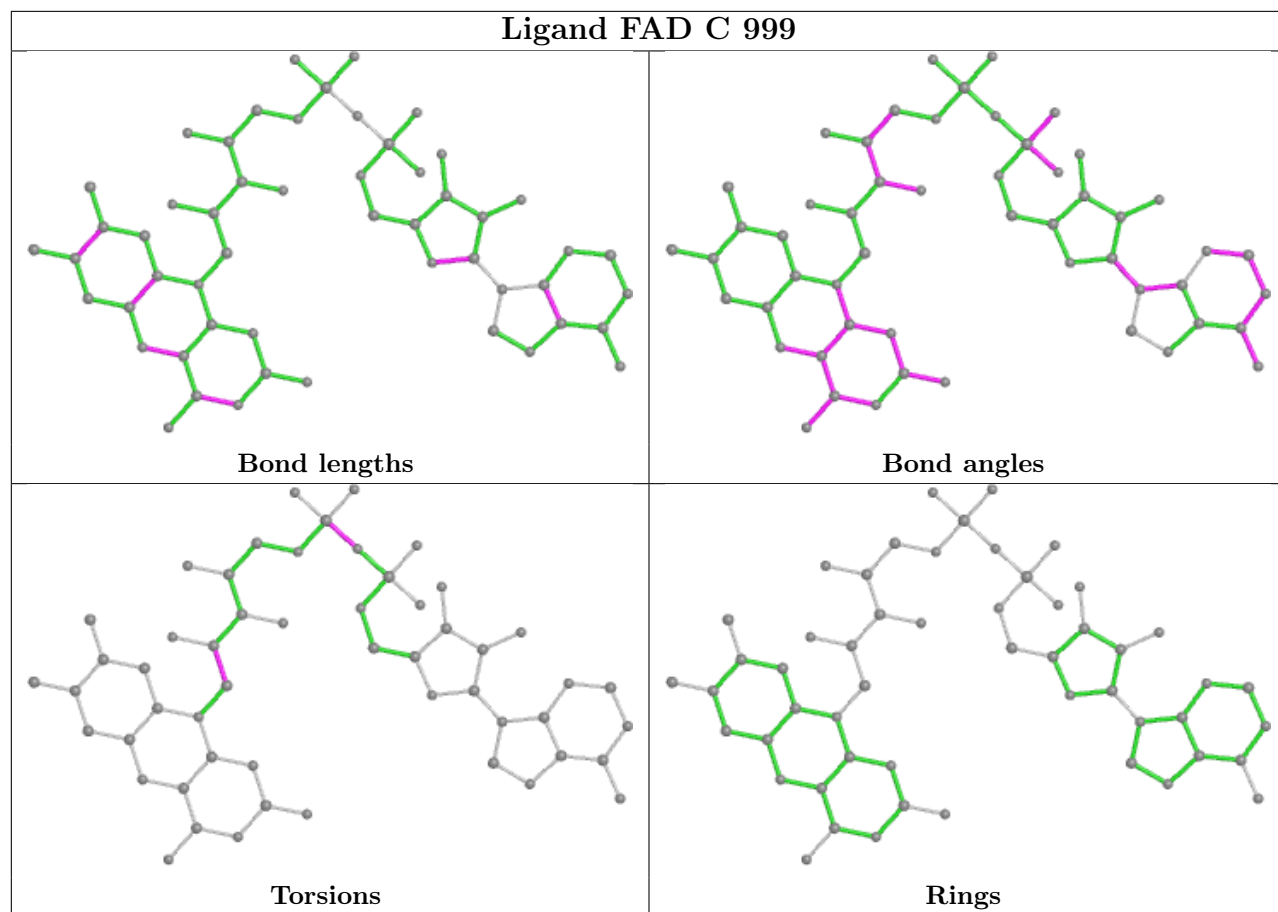
Mol	Chain	Res	Type	Atoms
2	A	999	FAD	N10-C1'-C2'-O2'
2	A	999	FAD	N10-C1'-C2'-C3'
2	B	999	FAD	N10-C1'-C2'-O2'
2	B	999	FAD	N10-C1'-C2'-C3'
2	C	999	FAD	N10-C1'-C2'-O2'
2	C	999	FAD	N10-C1'-C2'-C3'
2	D	999	FAD	N10-C1'-C2'-O2'
2	D	999	FAD	N10-C1'-C2'-C3'
2	A	999	FAD	PA-O3P-P-O1P
2	A	999	FAD	PA-O3P-P-O2P
2	B	999	FAD	PA-O3P-P-O1P
2	C	999	FAD	PA-O3P-P-O1P
2	D	999	FAD	PA-O3P-P-O1P
2	A	999	FAD	C3'-C4'-C5'-O5'

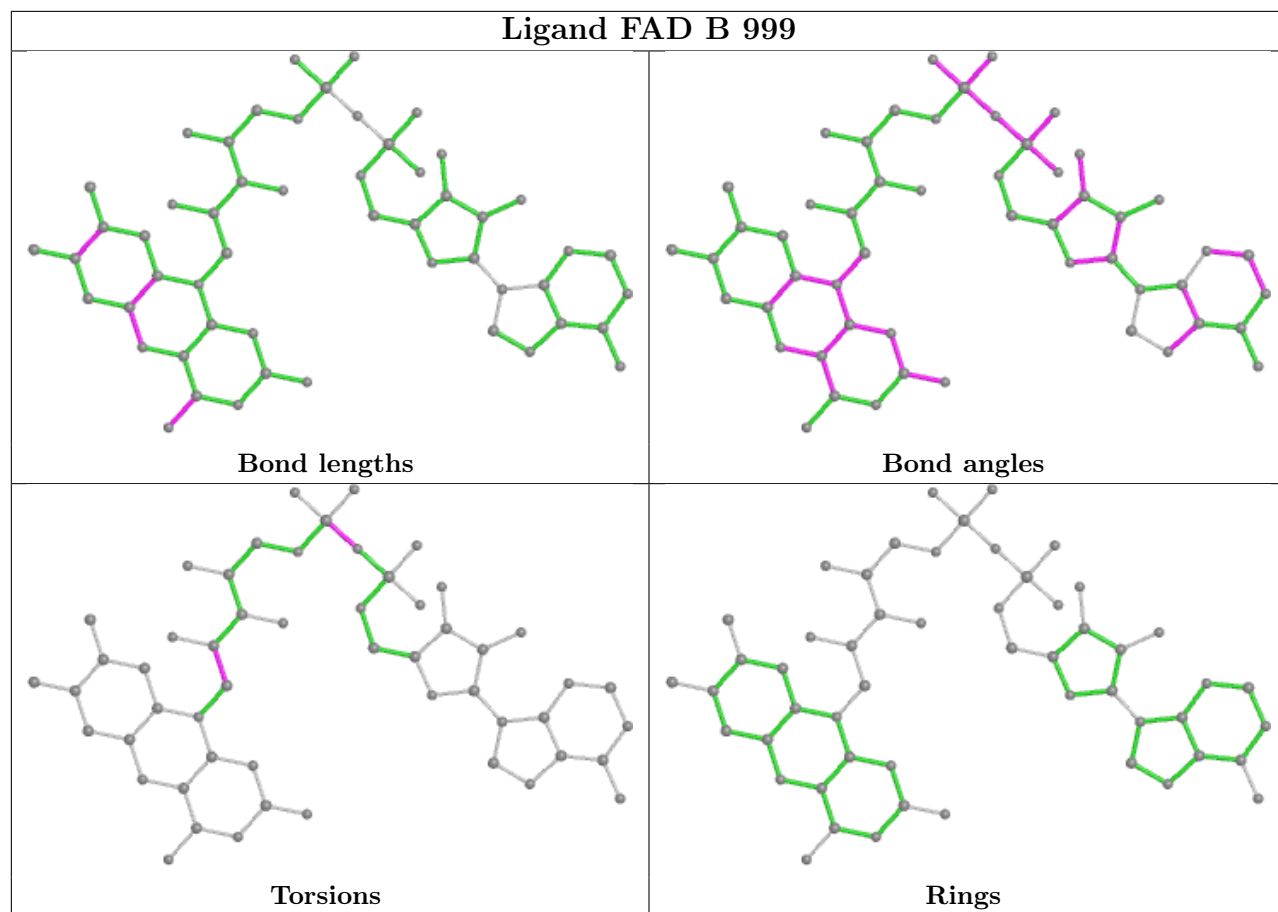
There are no ring outliers.

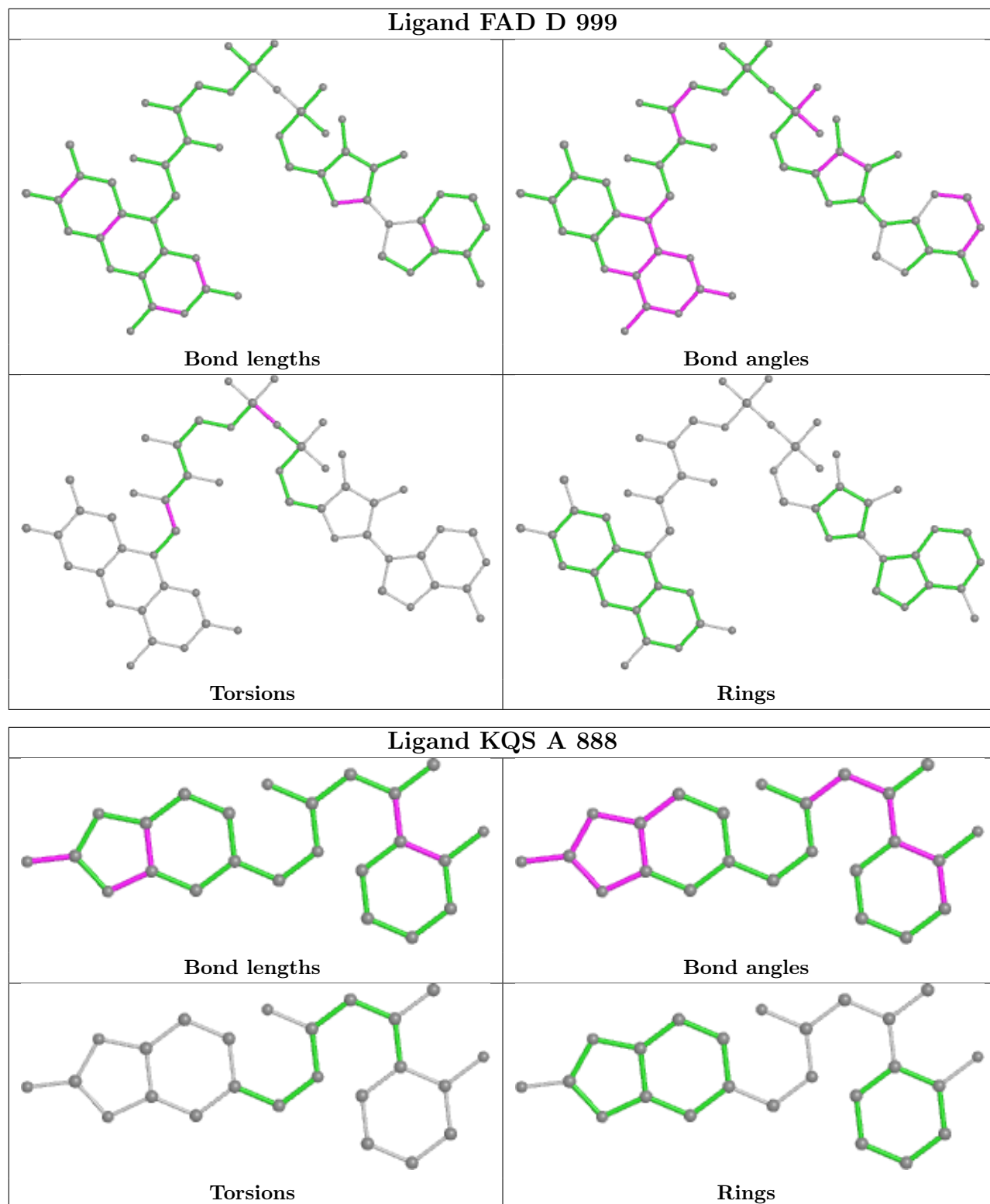
8 monomers are involved in 7 short contacts:

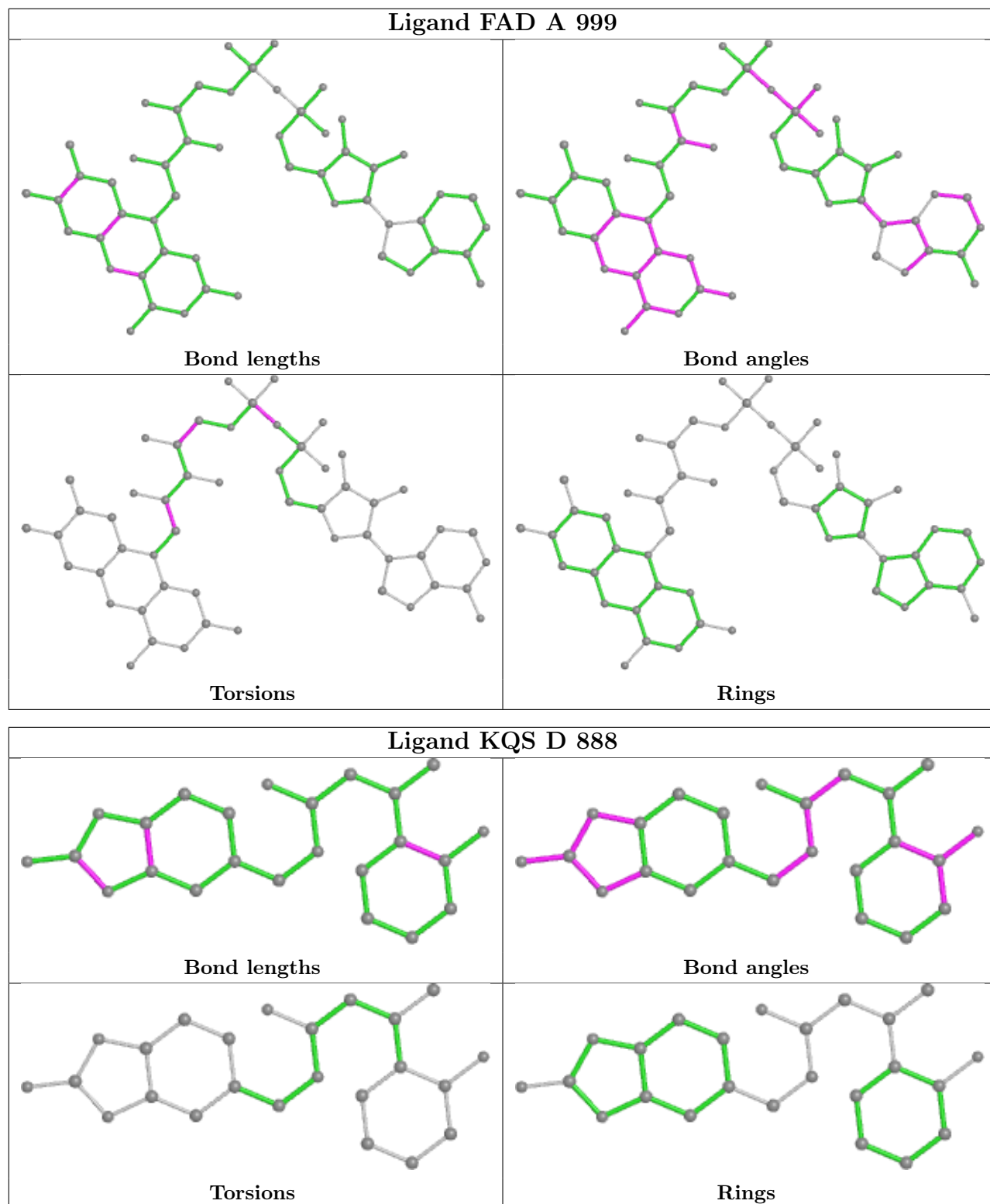
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	999	FAD	1	0
2	B	999	FAD	1	0
2	D	999	FAD	1	0
3	A	888	KQS	2	0
2	A	999	FAD	1	0
3	D	888	KQS	2	0
3	C	888	KQS	1	0
3	B	888	KQS	2	0

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.

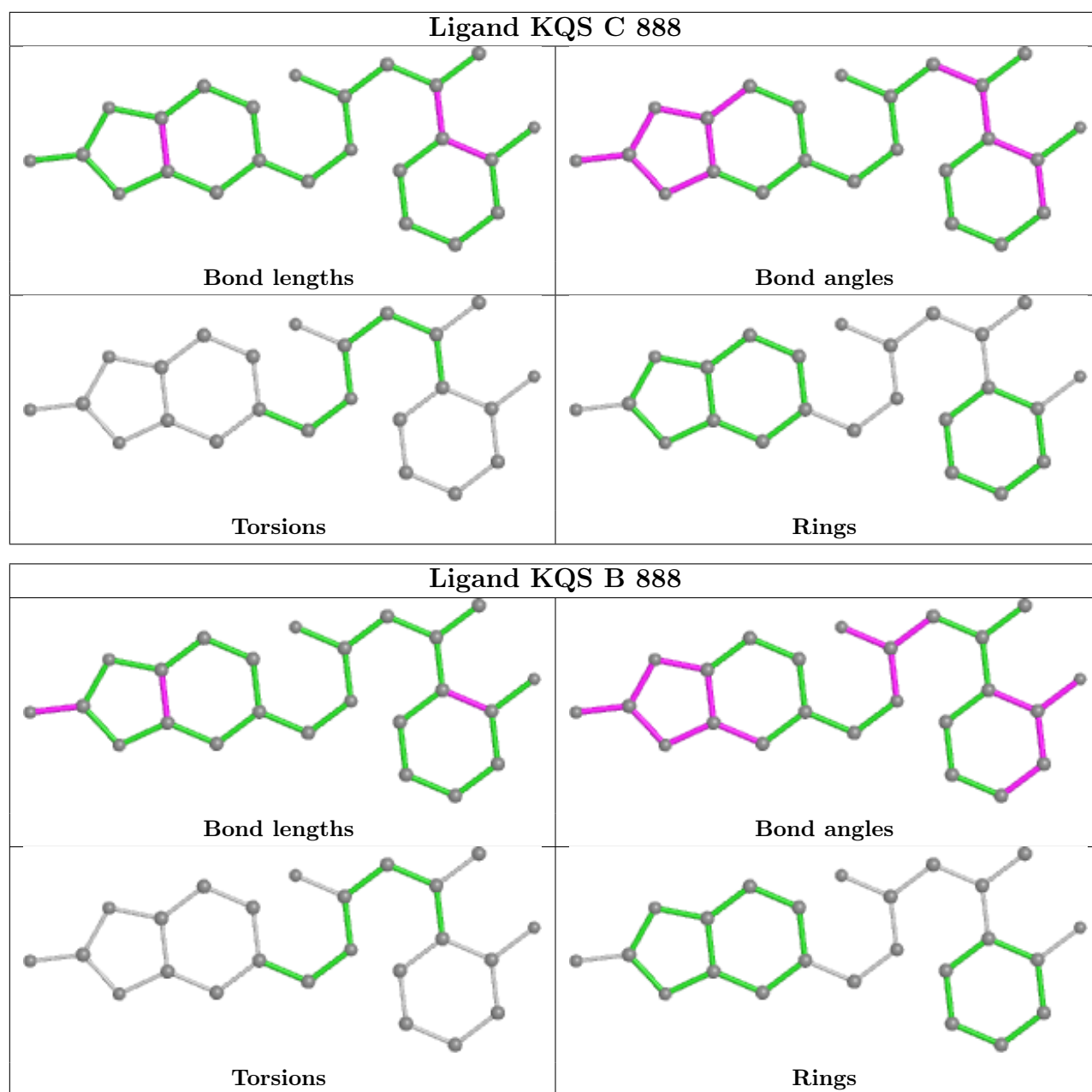












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [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, 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	566/658 (86%)	-0.28	15 (2%) 54 52	16, 31, 57, 89	0
1	B	542/658 (82%)	-0.27	11 (2%) 65 63	16, 33, 57, 84	0
1	C	557/658 (84%)	-0.40	3 (0%) 91 90	16, 29, 50, 77	1 (0%)
1	D	552/658 (83%)	-0.34	3 (0%) 91 90	19, 33, 59, 81	0
All	All	2217/2632 (84%)	-0.32	32 (1%) 75 73	16, 31, 57, 89	1 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	159	ILE	4.2
1	A	157	PRO	3.9
1	A	144	THR	3.7
1	B	81	GLY	3.5
1	B	460	PRO	3.5
1	B	458	PHE	3.4
1	B	159	ILE	3.2
1	D	558	GLN	2.9
1	B	499	ASP	2.9
1	D	559	PHE	2.8
1	B	199	GLU	2.7
1	B	434	PRO	2.7
1	A	589	SER	2.7
1	A	82	ILE	2.6
1	D	81	GLY	2.5
1	C	83	ILE	2.5
1	B	589	SER	2.5
1	A	81	GLY	2.4
1	A	445	ASP	2.4
1	A	453	THR	2.4
1	C	458	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	452	ILE	2.3
1	A	160	VAL	2.3
1	B	522	TYR	2.3
1	A	456	LYS	2.3
1	A	454	LYS	2.2
1	C	558	GLN	2.1
1	A	505	TYR	2.1
1	B	459	ASP	2.0
1	B	197	LEU	2.0
1	A	556	GLY	2.0
1	A	89	GLU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

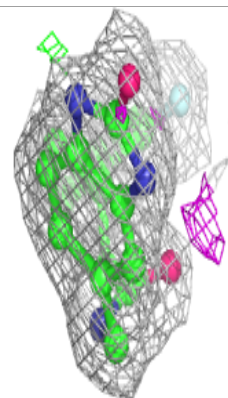
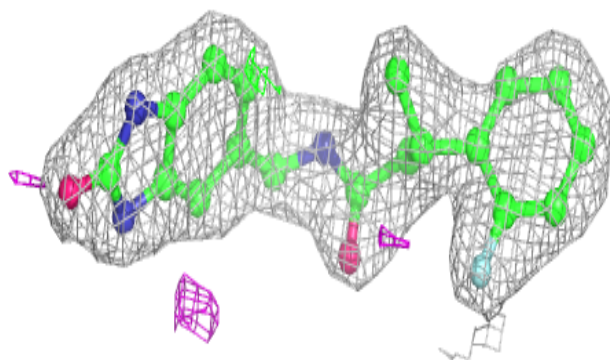
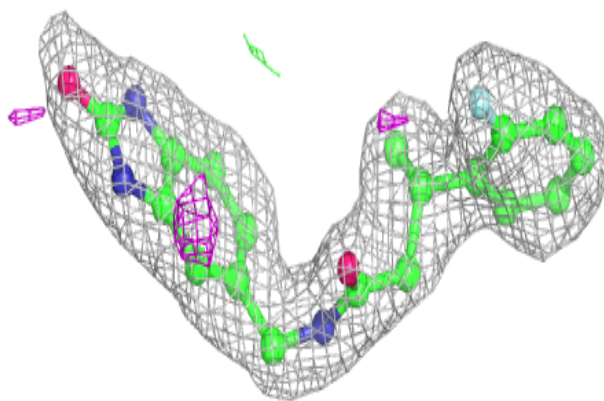
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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
3	KQS	D	888	24/24	0.94	0.15	26,34,48,54	0
3	KQS	B	888	24/24	0.95	0.13	29,33,39,41	0
3	KQS	C	888	24/24	0.96	0.14	20,23,33,38	0
3	KQS	A	888	24/24	0.96	0.13	25,29,39,41	0
2	FAD	D	999	53/53	0.97	0.14	17,20,23,24	0
2	FAD	C	999	53/53	0.98	0.14	14,16,18,20	0
2	FAD	A	999	53/53	0.98	0.15	14,19,23,26	0
2	FAD	B	999	53/53	0.98	0.15	15,18,23,24	0

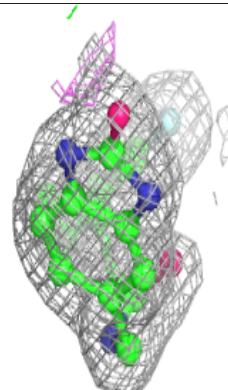
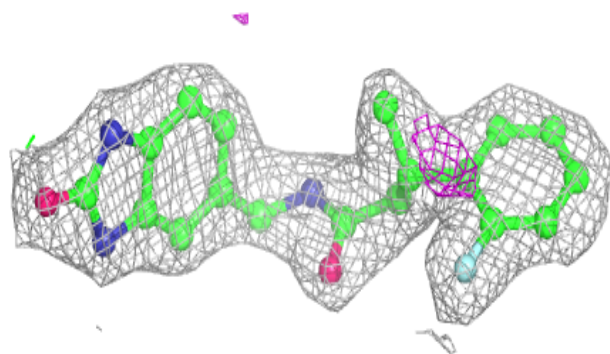
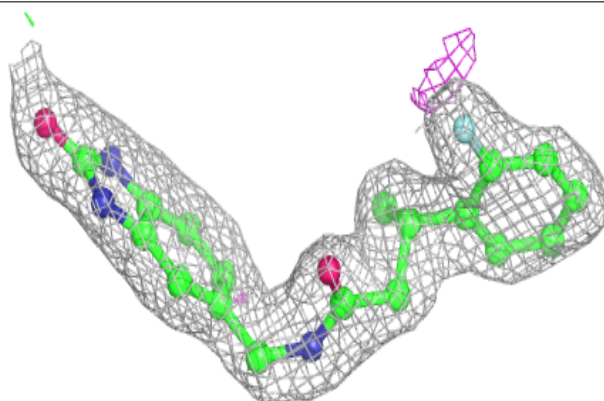
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around KQS 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)

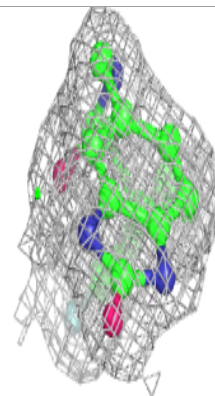
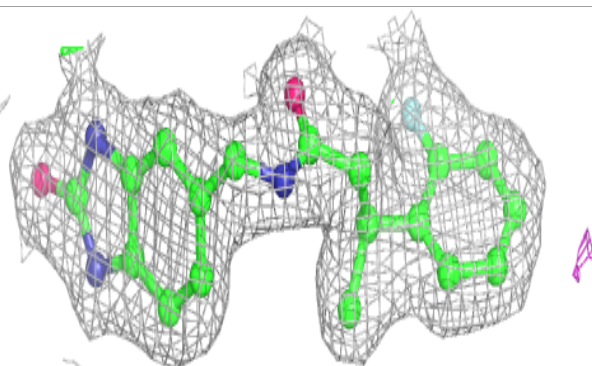
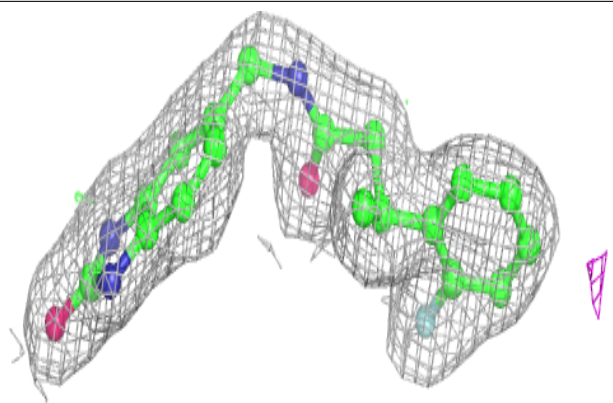
**Electron density around KQS B 888:**

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

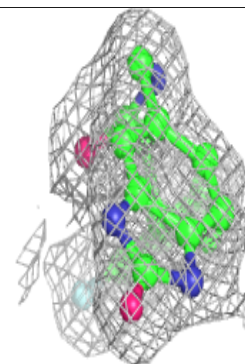
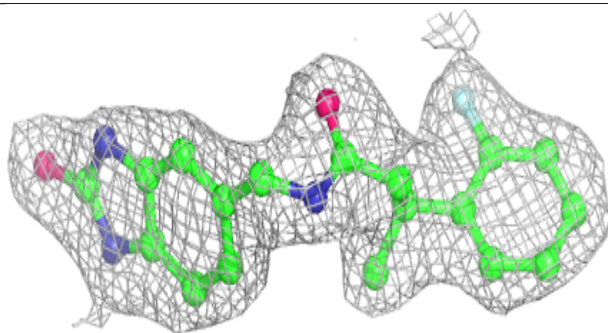
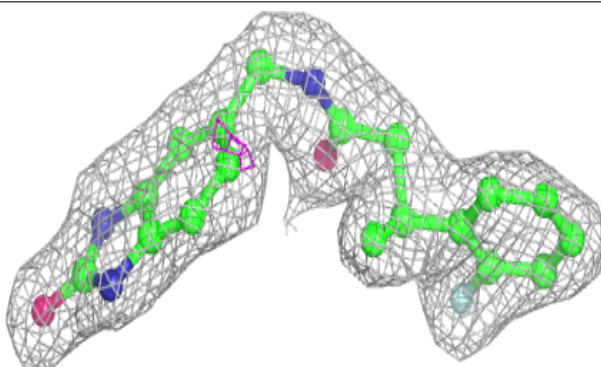


**Electron density around KQS C 888:**

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

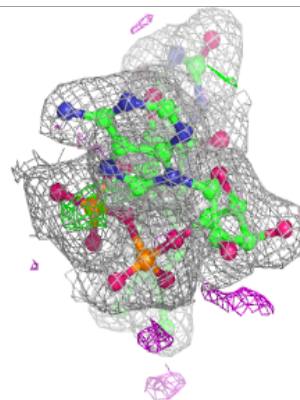
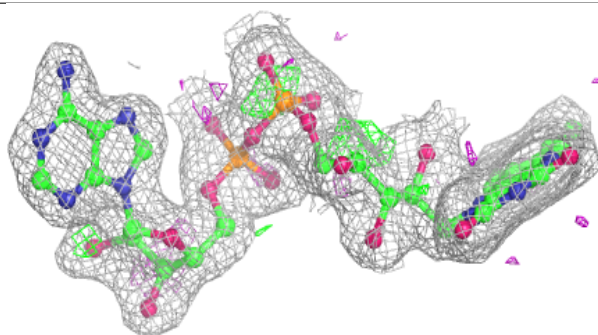
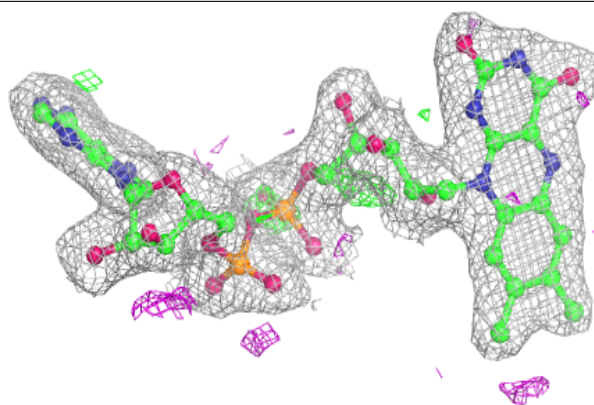
**Electron density around KQS A 888:**

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

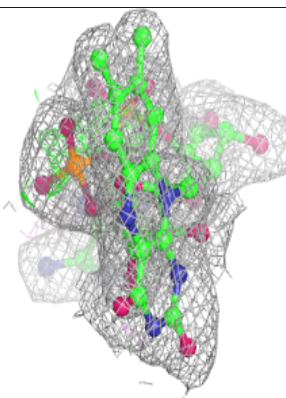
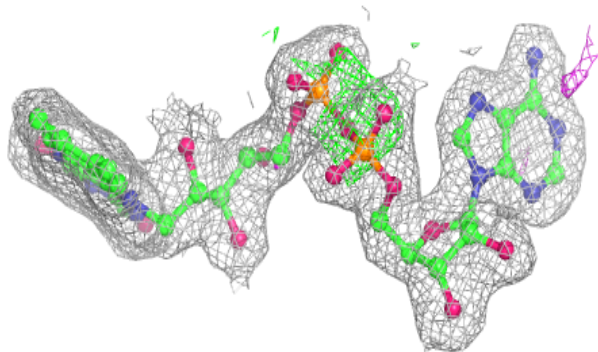
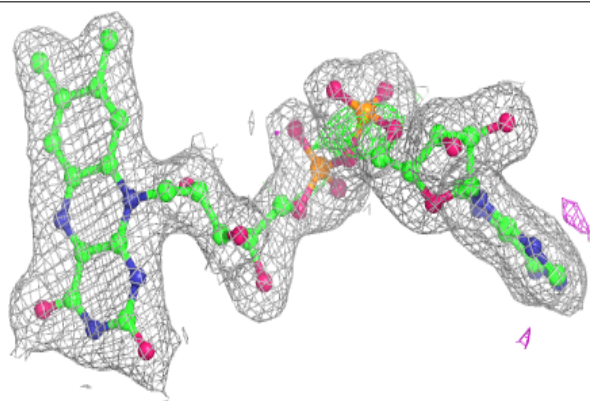


**Electron density around FAD D 999:**

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

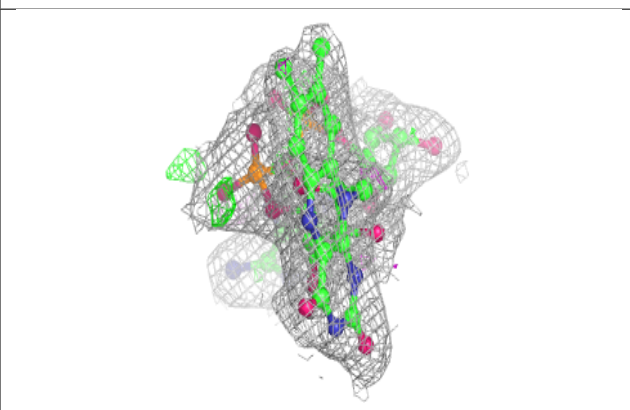
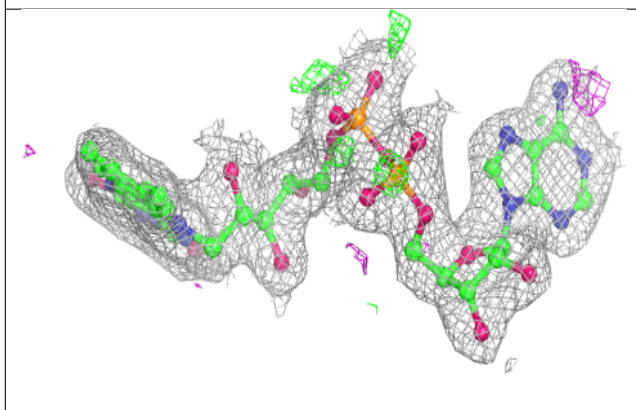
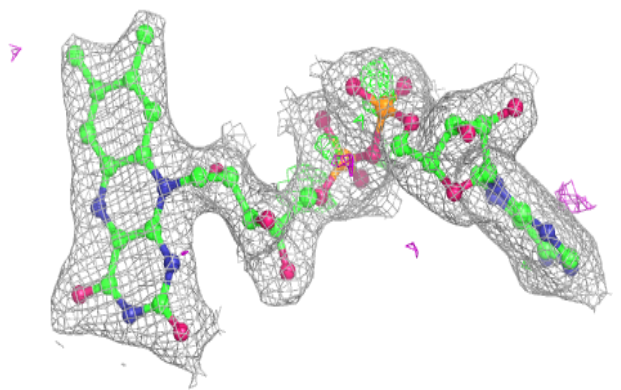
**Electron density around FAD C 999:**

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

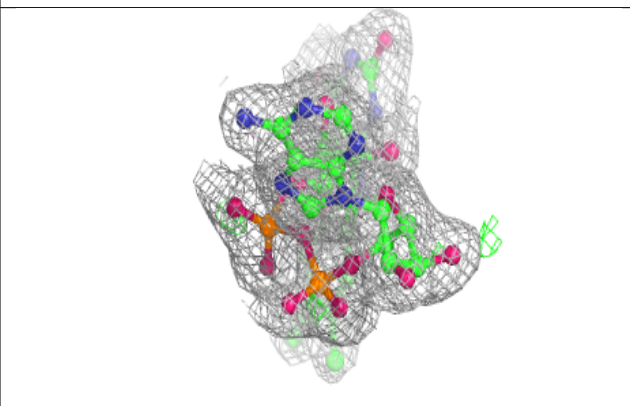
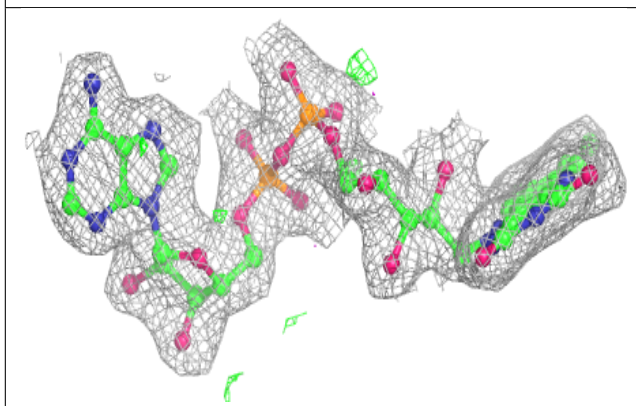
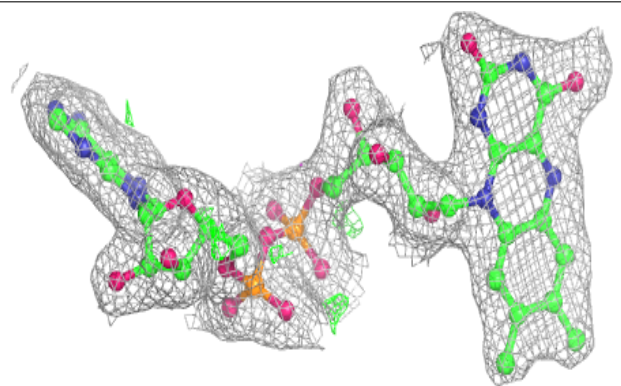


**Electron density around FAD A 999:**

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

**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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.