



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2020 – 08:15 pm BST

PDB ID : 2WET
Title : Crystal structure of tryptophan 5-halogenase (PyrH) complex with FAD (tryptophan)
Authors : De Laurentis, W.; Zhu, X.; Naismith, J.H.
Deposited on : 2009-04-01
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

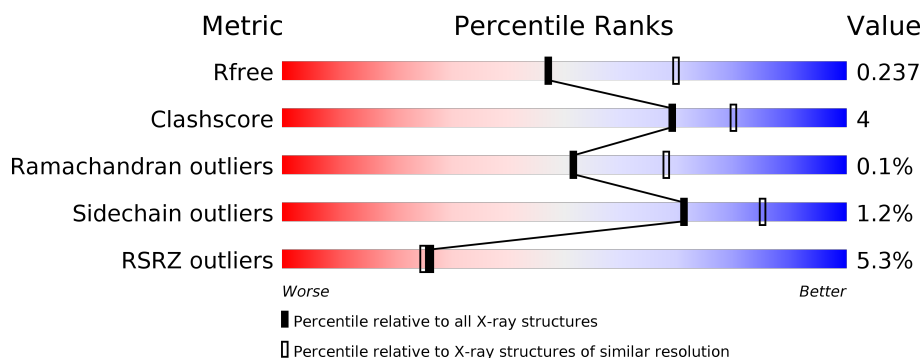
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	511	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 88%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 88% 9% </div> </div>
1	B	511	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 12%, green 85%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 85% 12% </div> </div>
1	C	511	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, orange 1%, yellow 1%, green 89%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 4% 89% 8% </div> </div>
1	D	511	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 15%, orange 1%, yellow 1%, green 90%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 15% 90% 6% </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17003 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.

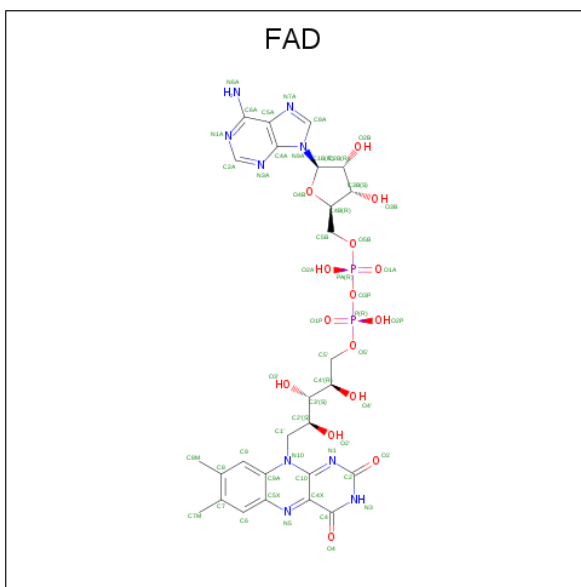
- Molecule 1 is a protein called TRYPTOPHAN 5-HALOGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	2	0
			4008	2547	708	734	19			
1	B	501	Total	C	N	O	S	0	3	0
			4052	2574	716	743	19			
1	C	494	Total	C	N	O	S	0	1	0
			3983	2533	701	730	19			
1	D	494	Total	C	N	O	S	0	0	0
			3974	2528	699	728	19			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

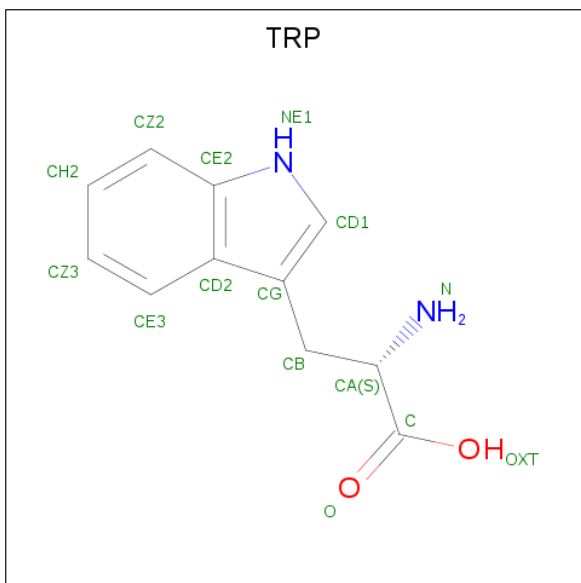
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Cl	0	0
			2	2		
2	A	2	Total	Cl	0	0
			2	2		
2	D	2	Total	Cl	0	0
			2	2		
2	C	2	Total	Cl	0	0
			2	2		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 4 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			15	11	2	2		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

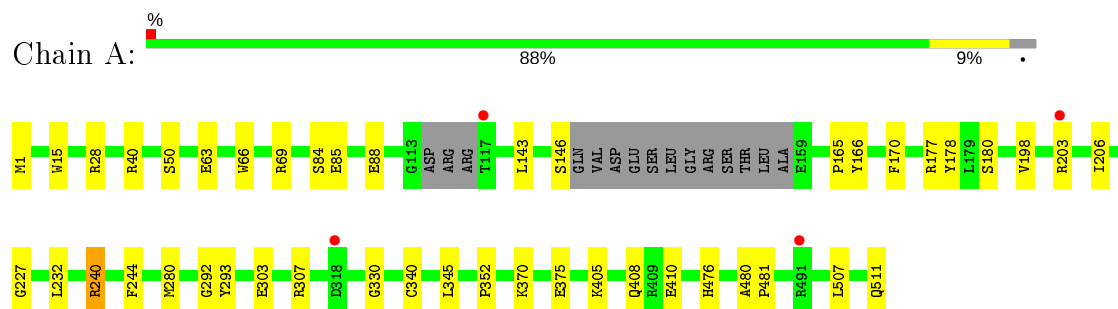
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	251	Total	O	0	0
			251	251		
6	B	207	Total	O	0	0
			207	207		
6	C	183	Total	O	0	0
			183	183		
6	D	105	Total	O	0	0
			105	105		

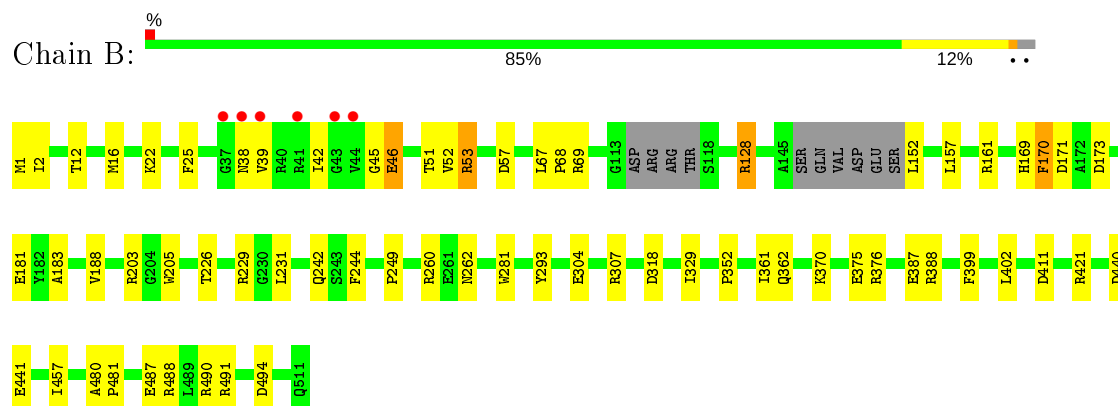
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

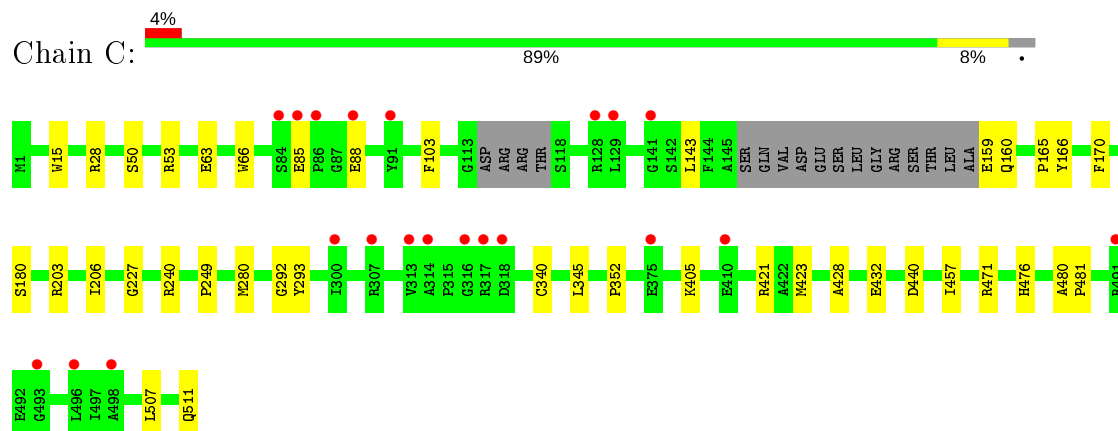
• Molecule 1: TRYPTOPHAN 5-HALOGENASE



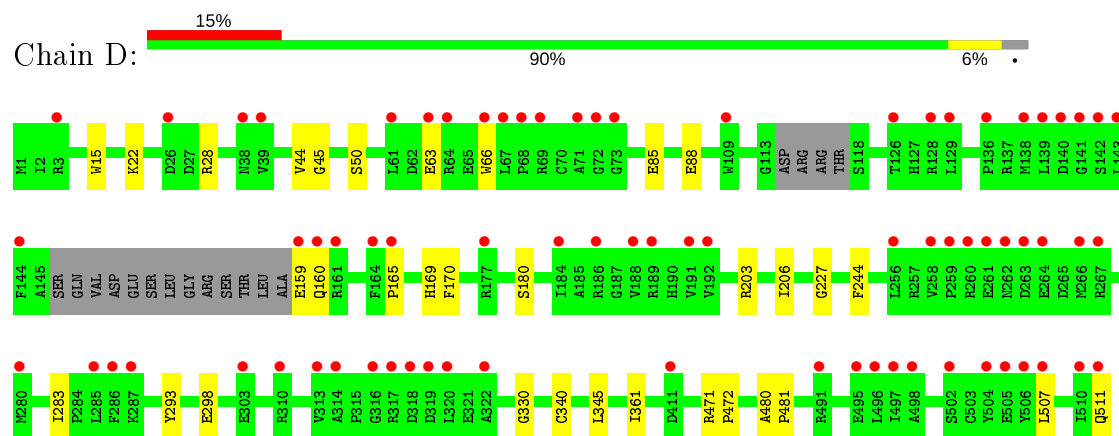
• Molecule 1: TRYPTOPHAN 5-HALOGENASE



• Molecule 1: TRYPTOPHAN 5-HALOGENASE



- Molecule 1: TRYPTOPHAN 5-HALOGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	137.53Å 137.53Å 307.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.06 – 2.40 48.07 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.3 (48.06-2.40) 98.3 (48.07-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.196 , 0.234 0.203 , 0.237	Depositor DCC
R_{free} test set	5684 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17003	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.69	1/4116 (0.0%)	0.73	3/5579 (0.1%)
1	B	0.66	0/4159	0.69	1/5636 (0.0%)
1	C	0.62	0/4090	0.66	2/5544 (0.0%)
1	D	0.54	0/4081	0.64	2/5532 (0.0%)
All	All	0.63	1/16446 (0.0%)	0.68	8/22291 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	303	GLU	CB-CG	-5.29	1.42	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	ARG	NE-CZ-NH2	-11.46	114.57	120.30
1	D	203	ARG	NE-CZ-NH1	-10.74	114.93	120.30
1	A	203	ARG	NE-CZ-NH1	10.35	125.47	120.30
1	C	203	ARG	NE-CZ-NH1	-8.63	115.98	120.30
1	D	203	ARG	NE-CZ-NH2	8.42	124.51	120.30
1	C	203	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	A	240	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	B	440	ASP	CB-CG-OD1	5.50	123.25	118.30

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	4008	0	3844	29	1
1	B	4052	0	3893	51	0
1	C	3983	0	3821	28	0
1	D	3974	0	3814	20	1
2	A	2	0	0	1	0
2	B	2	0	0	1	0
2	C	2	0	0	1	0
2	D	2	0	0	0	0
3	A	53	0	31	0	0
3	B	53	0	31	2	0
3	C	53	0	31	0	0
3	D	53	0	31	4	0
4	B	15	0	9	0	0
5	C	5	0	0	1	0
6	A	251	0	0	2	0
6	B	207	0	0	4	0
6	C	183	0	0	2	0
6	D	105	0	0	1	0
All	All	17003	0	15505	118	1

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 (118) 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:50:SER:HB2	1:C:165:PRO:HB2	1.81	0.62
1:B:51:THR:HB	1:B:157:LEU:HD23	1.81	0.62
1:D:85:GLU:HB2	1:D:88:GLU:HG3	1.84	0.60
1:B:361:ILE:HD11	3:B:1652:FAD:H5'1	1.83	0.59
1:A:410:GLU:HB3	1:B:262:ASN:HD21	1.66	0.59
1:C:85:GLU:HB2	1:C:88:GLU:HG3	1.84	0.59
1:A:307:ARG:HD3	1:B:490:ARG:NH2	2.17	0.59
1:B:2:ILE:O	1:B:2:ILE:HG13	2.03	0.58
1:B:57:ASP:OD2	1:B:152:LEU:HD12	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:H3	1:A:375:GLU:HB3	1.70	0.57
1:B:488:ARG:HG2	1:B:491:ARG:NH2	2.20	0.56
1:B:128[B]:ARG:HG3	1:B:128[B]:ARG:HH11	1.71	0.56
1:A:307:ARG:HD3	1:B:490:ARG:CZ	2.35	0.56
1:B:388:ARG:NH2	1:C:440:ASP:OD2	2.34	0.55
1:A:85:GLU:HB2	1:A:88:GLU:HG3	1.87	0.55
1:D:85:GLU:CB	1:D:88:GLU:HG3	2.36	0.55
1:C:85:GLU:CB	1:C:88:GLU:HG3	2.36	0.55
1:B:352:PRO:HA	2:B:700:CL:CL	2.44	0.55
1:A:206:ILE:HD12	1:A:340:CYS:HB2	1.89	0.54
1:A:1:MET:N	1:A:375:GLU:HB3	2.22	0.54
1:A:50:SER:HB2	1:A:165:PRO:HB2	1.89	0.54
1:D:50:SER:HB2	1:D:165:PRO:HB2	1.89	0.54
1:B:260:ARG:HD3	6:B:2077:HOH:O	2.06	0.54
1:B:488:ARG:HG2	1:B:491:ARG:HH22	1.73	0.53
1:A:480:ALA:HB3	1:A:481:PRO:HD3	1.89	0.53
1:B:128[B]:ARG:HG3	1:B:128[B]:ARG:NH1	2.22	0.53
1:B:457:ILE:HD11	6:B:2162:HOH:O	2.08	0.53
1:D:206:ILE:HD12	1:D:340:CYS:HB2	1.91	0.51
1:B:128[A]:ARG:NH2	1:B:494:ASP:OD1	2.42	0.51
1:C:457:ILE:HD11	6:C:2157:HOH:O	2.10	0.51
3:D:1513:FAD:H51A	6:D:2104:HOH:O	2.10	0.51
1:B:25:PHE:CD1	1:C:476:HIS:HB2	2.46	0.50
1:B:1:MET:N	1:B:375:GLU:OE2	2.37	0.50
1:B:25:PHE:CD1	1:C:476:HIS:CB	2.95	0.50
1:C:206:ILE:HD12	1:C:340:CYS:HB2	1.94	0.49
1:B:12:THR:HG22	1:B:16:MET:SD	2.52	0.49
1:A:85:GLU:CB	1:A:88:GLU:HG3	2.42	0.49
1:B:370:LYS:O	1:C:471:ARG:HD3	2.12	0.48
1:C:240:ARG:HD3	5:C:1514:SO4:O2	2.13	0.48
1:C:249:PRO:HG3	1:C:421:ARG:CZ	2.42	0.48
1:B:370:LYS:HE3	1:C:103:PHE:CE2	2.48	0.48
1:D:507:LEU:O	1:D:511:GLN:HG2	2.13	0.48
1:A:50:SER:HB3	1:A:165:PRO:O	2.13	0.48
1:B:318:ASP:OD1	1:B:318:ASP:N	2.42	0.48
1:B:411:ASP:OD1	1:B:411:ASP:N	2.45	0.48
1:B:229:ARG:HB2	6:B:2050:HOH:O	2.13	0.48
1:A:143:LEU:O	1:A:146:SER:HB3	2.14	0.47
1:B:53:ARG:HB3	1:B:53:ARG:HH11	1.79	0.47
1:B:67:LEU:HB3	1:B:68:PRO:HD3	1.96	0.47
1:A:84:SER:HB3	1:A:408:GLN:HB2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:ASP:OD1	1:B:173:ASP:HB2	2.14	0.47
1:B:128[B]:ARG:HH22	1:B:490:ARG:HG3	1.80	0.47
1:B:69:ARG:NH1	1:B:181:GLU:OE1	2.32	0.47
1:B:203:ARG:HG3	1:B:205:TRP:CD1	2.50	0.47
1:C:405:LYS:HE3	1:C:423:MET:HG2	1.97	0.47
1:D:45:GLY:HA2	3:D:1513:FAD:C4X	2.45	0.47
1:C:15:TRP:CE3	1:C:180:SER:HA	2.50	0.46
1:D:480:ALA:HB3	1:D:481:PRO:HD3	1.97	0.46
1:B:25:PHE:CG	1:C:476:HIS:HB3	2.50	0.46
1:A:198:VAL:HG21	1:A:232:LEU:HD22	1.98	0.46
1:A:476:HIS:NE2	6:A:2234:HOH:O	2.36	0.46
1:A:370:LYS:O	1:D:471:ARG:HD3	2.16	0.46
1:A:507:LEU:O	1:A:511:GLN:HG2	2.17	0.45
1:B:244:PHE:HB2	1:B:329:ILE:HG22	1.99	0.44
1:C:53:ARG:HD2	6:C:2015:HOH:O	2.15	0.44
1:C:63:GLU:HA	1:C:66:TRP:CD1	2.53	0.44
1:A:15:TRP:CE3	1:A:180:SER:HA	2.52	0.44
1:B:46:GLU:O	1:B:169:HIS:HA	2.18	0.44
1:D:44:VAL:HG21	3:D:1513:FAD:C7	2.47	0.44
1:A:227:GLY:HA2	1:A:345:LEU:HB2	1.99	0.44
1:A:280:MET:HA	1:A:292:GLY:O	2.17	0.44
1:B:46:GLU:HB3	1:B:170:PHE:O	2.16	0.44
1:C:507:LEU:O	1:C:511:GLN:HG2	2.18	0.44
1:C:428:ALA:O	1:C:432:GLU:HG3	2.17	0.44
1:B:441:GLU:CD	1:B:441:GLU:H	2.20	0.44
1:B:304:GLU:HG3	1:B:307:ARG:NH2	2.33	0.43
1:B:242:GLN:NE2	6:B:2052:HOH:O	2.39	0.43
1:D:15:TRP:CE3	1:D:180:SER:HA	2.54	0.43
1:D:361:ILE:HD11	3:D:1513:FAD:H5'1	2.00	0.43
1:B:480:ALA:HB3	1:B:481:PRO:HD3	2.01	0.43
1:B:226:THR:HG21	1:B:231:LEU:HB3	2.00	0.42
1:B:487:GLU:HA	1:B:487:GLU:OE2	2.19	0.42
1:B:25:PHE:CD1	1:C:476:HIS:HB3	2.54	0.42
1:A:244:PHE:CD2	1:A:330:GLY:HA2	2.55	0.42
1:C:480:ALA:HB3	1:C:481:PRO:HD3	2.01	0.42
1:D:159:GLU:HG3	1:D:160:GLN:H	1.84	0.42
1:B:51:THR:HB	1:B:157:LEU:CD2	2.49	0.42
1:D:471:ARG:HA	1:D:472:PRO:HD3	1.93	0.42
1:B:183:ALA:HB1	1:B:188:VAL:HG21	2.02	0.42
1:B:399:PHE:O	1:B:402:LEU:HB3	2.20	0.42
1:C:457:ILE:HD13	1:C:457:ILE:HG21	1.79	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:GLY:HA2	1:C:345:LEU:HB2	2.02	0.41
1:B:22:LYS:HA	1:B:22:LYS:HD3	1.81	0.41
1:B:52:VAL:HA	1:B:362:GLN:OE1	2.20	0.41
1:C:280:MET:HA	1:C:292:GLY:O	2.20	0.41
1:D:227:GLY:HA2	1:D:345:LEU:HB2	2.03	0.41
1:A:352:PRO:HA	2:A:700:CL:CL	2.57	0.41
1:A:40[A]:ARG:NH1	1:A:40[A]:ARG:HG3	2.35	0.41
1:B:249:PRO:HG3	1:B:421:ARG:CZ	2.51	0.41
1:D:50:SER:HB3	1:D:165:PRO:O	2.20	0.41
1:D:244:PHE:CD2	1:D:330:GLY:HA2	2.56	0.41
1:C:159:GLU:HG3	1:C:160:GLN:H	1.86	0.41
1:C:159:GLU:HG3	1:C:160:GLN:N	2.36	0.41
1:C:143:LEU:HD11	1:C:166:TYR:HE1	1.85	0.41
1:D:22:LYS:HA	1:D:22:LYS:HD3	1.95	0.41
1:A:405:LYS:HD3	1:A:405:LYS:HA	1.91	0.41
1:B:42:ILE:HA	1:B:42:ILE:HD12	1.95	0.41
3:B:1652:FAD:HO2'	3:B:1652:FAD:HO4'	1.69	0.40
1:A:63:GLU:HA	1:A:66:TRP:CD1	2.57	0.40
1:D:169:HIS:CD2	1:D:283:ILE:HG23	2.56	0.40
1:B:161:ARG:HD3	1:B:161:ARG:HA	1.82	0.40
1:A:177:ARG:HD3	6:A:2067:HOH:O	2.20	0.40
1:A:69:ARG:HG2	1:A:178:TYR:CE1	2.57	0.40
1:A:307:ARG:HD2	1:B:494:ASP:OD2	2.20	0.40
1:C:352:PRO:HA	2:C:700:CL:CL	2.59	0.40
1:D:471:ARG:HH11	1:D:471:ARG:HD3	1.78	0.40
1:A:143:LEU:HD11	1:A:166:TYR:HE1	1.86	0.40
1:D:63:GLU:HA	1:D:66:TRP:CD1	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ARG:NH2	1:D:298:GLU:O[7_555]	1.84	0.36

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	492/511 (96%)	474 (96%)	18 (4%)	0	100	100
1	B	498/511 (98%)	478 (96%)	18 (4%)	2 (0%)	34	48
1	C	489/511 (96%)	472 (96%)	17 (4%)	0	100	100
1	D	488/511 (96%)	472 (97%)	16 (3%)	0	100	100
All	All	1967/2044 (96%)	1896 (96%)	69 (4%)	2 (0%)	51	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	39	VAL
1	B	45	GLY

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	413/424 (97%)	410 (99%)	3 (1%)	84	92
1	B	417/424 (98%)	407 (98%)	10 (2%)	49	68
1	C	410/424 (97%)	407 (99%)	3 (1%)	84	92
1	D	409/424 (96%)	406 (99%)	3 (1%)	84	92
All	All	1649/1696 (97%)	1630 (99%)	19 (1%)	71	85

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	170	PHE
1	A	293	TYR
1	B	38	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	46	GLU
1	B	53	ARG
1	B	128[A]	ARG
1	B	128[B]	ARG
1	B	170	PHE
1	B	281	TRP
1	B	293	TYR
1	B	376	ARG
1	B	387	GLU
1	C	28	ARG
1	C	170	PHE
1	C	293	TYR
1	D	28	ARG
1	D	170	PHE
1	D	293	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	197	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 for Mogul analysis.

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
5	SO4	C	1514	-	4,4,4	0.42	0	6,6,6	0.66	0
3	FAD	C	1513	-	51,58,58	1.40	6 (11%)	60,89,89	1.71	9 (15%)
3	FAD	B	1652	-	51,58,58	1.49	8 (15%)	60,89,89	1.90	9 (15%)
3	FAD	A	1513	-	51,58,58	1.33	7 (13%)	60,89,89	1.76	9 (15%)
3	FAD	D	1513	-	51,58,58	1.52	7 (13%)	60,89,89	1.60	9 (15%)

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	C	1513	-	-	5/30/50/50	0/6/6/6
3	FAD	B	1652	-	-	6/30/50/50	0/6/6/6
3	FAD	A	1513	-	-	5/30/50/50	0/6/6/6
3	FAD	D	1513	-	-	5/30/50/50	0/6/6/6

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1513	FAD	C4X-N5	4.40	1.39	1.33
3	B	1652	FAD	C10-N1	4.38	1.38	1.33
3	C	1513	FAD	C10-N1	4.37	1.38	1.33
3	D	1513	FAD	C10-N1	4.32	1.38	1.33
3	A	1513	FAD	C4X-N5	4.08	1.39	1.33
3	B	1652	FAD	C2A-N3A	3.95	1.38	1.32
3	D	1513	FAD	C2A-N3A	3.87	1.38	1.32
3	C	1513	FAD	C2A-N3A	3.77	1.38	1.32
3	C	1513	FAD	C4-N3	3.70	1.39	1.33
3	B	1652	FAD	C4X-N5	3.65	1.38	1.33
3	C	1513	FAD	C4X-N5	3.64	1.38	1.33
3	D	1513	FAD	C1'-N10	3.63	1.52	1.48
3	B	1652	FAD	C1'-N10	3.55	1.51	1.48
3	A	1513	FAD	C10-N1	3.55	1.37	1.33
3	D	1513	FAD	C4-N3	3.54	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1513	FAD	C2A-N3A	3.48	1.37	1.32
3	B	1652	FAD	C4-N3	3.15	1.38	1.33
3	C	1513	FAD	C1'-N10	2.91	1.51	1.48
3	B	1652	FAD	C2A-N1A	2.66	1.38	1.33
3	A	1513	FAD	C4-N3	2.54	1.37	1.33
3	D	1513	FAD	C2A-N1A	2.50	1.38	1.33
3	D	1513	FAD	C5X-N5	2.46	1.39	1.35
3	B	1652	FAD	C5X-N5	2.39	1.39	1.35
3	C	1513	FAD	C2A-N1A	2.31	1.38	1.33
3	B	1652	FAD	C5'-C4'	2.29	1.55	1.51
3	A	1513	FAD	C2A-N1A	2.13	1.37	1.33
3	A	1513	FAD	C6-C5X	-2.11	1.38	1.41
3	A	1513	FAD	C1'-N10	2.09	1.50	1.48

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1652	FAD	C4-N3-C2	8.13	122.00	115.14
3	A	1513	FAD	C4-N3-C2	6.62	120.73	115.14
3	C	1513	FAD	C4-N3-C2	6.59	120.71	115.14
3	A	1513	FAD	N3A-C2A-N1A	-6.40	118.67	128.68
3	C	1513	FAD	N3A-C2A-N1A	-6.23	118.94	128.68
3	D	1513	FAD	C4-N3-C2	6.06	120.26	115.14
3	B	1652	FAD	N3A-C2A-N1A	-5.63	119.88	128.68
3	D	1513	FAD	N3A-C2A-N1A	-5.55	120.01	128.68
3	B	1652	FAD	C1'-N10-C9A	5.07	122.28	118.29
3	A	1513	FAD	C1'-N10-C9A	4.39	121.75	118.29
3	B	1652	FAD	C4X-N5-C5X	4.33	121.09	116.77
3	D	1513	FAD	C1'-N10-C9A	4.15	121.56	118.29
3	C	1513	FAD	C4X-N5-C5X	3.97	120.74	116.77
3	D	1513	FAD	C4X-N5-C5X	3.78	120.54	116.77
3	B	1652	FAD	C10-C4X-N5	-3.64	118.74	121.26
3	A	1513	FAD	C4X-N5-C5X	3.25	120.02	116.77
3	C	1513	FAD	C1'-N10-C9A	3.14	120.77	118.29
3	A	1513	FAD	C4-C4X-N5	3.12	122.16	118.60
3	B	1652	FAD	C4X-C4-N3	-2.98	119.36	123.43
3	B	1652	FAD	C4-C4X-N5	2.89	121.91	118.60
3	C	1513	FAD	C10-C4X-N5	-2.89	119.26	121.26
3	B	1652	FAD	C1'-N10-C10	-2.78	115.92	118.41
3	A	1513	FAD	C5X-C9A-N10	2.68	119.66	117.72
3	D	1513	FAD	C10-C4X-N5	-2.66	119.42	121.26
3	A	1513	FAD	C4-C4X-C10	-2.65	118.19	119.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1513	FAD	C4X-C4-N3	-2.65	119.81	123.43
3	C	1513	FAD	C4-C4X-N5	2.64	121.61	118.60
3	D	1513	FAD	C4X-C4-N3	-2.61	119.86	123.43
3	C	1513	FAD	O3B-C3B-C4B	-2.50	103.81	111.05
3	B	1652	FAD	O4B-C1B-C2B	-2.43	103.37	106.93
3	D	1513	FAD	C4-C4X-N5	2.39	121.33	118.60
3	A	1513	FAD	C10-C4X-N5	-2.34	119.64	121.26
3	D	1513	FAD	C5X-C9A-N10	2.25	119.34	117.72
3	A	1513	FAD	C4X-C4-N3	-2.22	120.39	123.43
3	C	1513	FAD	C5X-C9A-N10	2.18	119.29	117.72
3	D	1513	FAD	C4A-C5A-N7A	-2.14	107.17	109.40

There are no chirality outliers.

All (21) torsion outliers are listed below:

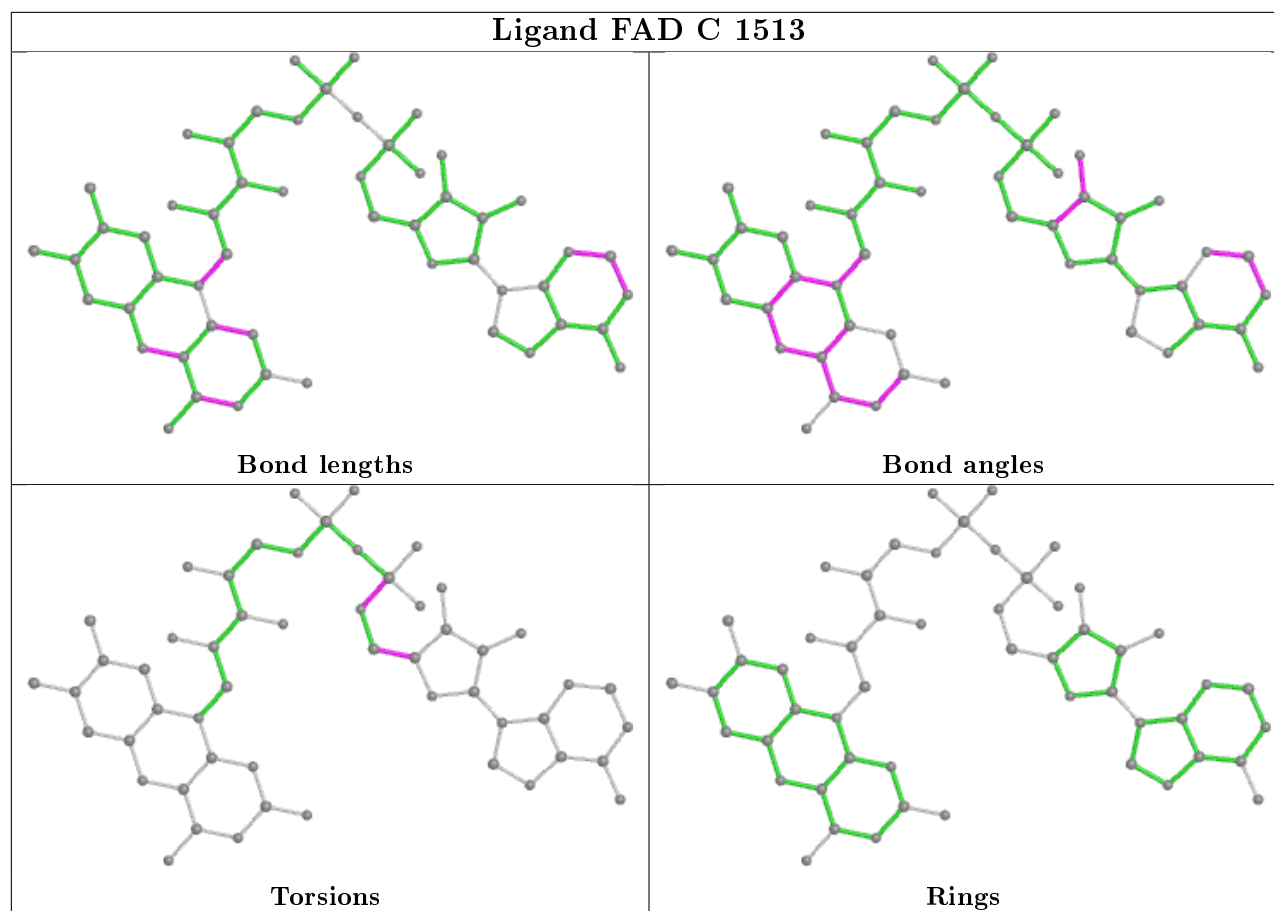
Mol	Chain	Res	Type	Atoms
3	B	1652	FAD	C5B-O5B-PA-O1A
3	C	1513	FAD	C5B-O5B-PA-O1A
3	B	1652	FAD	O4B-C4B-C5B-O5B
3	D	1513	FAD	O4B-C4B-C5B-O5B
3	B	1652	FAD	C3B-C4B-C5B-O5B
3	D	1513	FAD	C3B-C4B-C5B-O5B
3	D	1513	FAD	C5B-O5B-PA-O3P
3	C	1513	FAD	O4B-C4B-C5B-O5B
3	B	1652	FAD	C5B-O5B-PA-O2A
3	D	1513	FAD	C5B-O5B-PA-O1A
3	D	1513	FAD	C5B-O5B-PA-O2A
3	C	1513	FAD	C5B-O5B-PA-O2A
3	A	1513	FAD	C5B-O5B-PA-O2A
3	A	1513	FAD	O4B-C4B-C5B-O5B
3	C	1513	FAD	C3B-C4B-C5B-O5B
3	B	1652	FAD	C5B-O5B-PA-O3P
3	B	1652	FAD	C5'-O5'-P-O3P
3	C	1513	FAD	C5B-O5B-PA-O3P
3	A	1513	FAD	C5B-O5B-PA-O3P
3	A	1513	FAD	C5B-O5B-PA-O1A
3	A	1513	FAD	C3B-C4B-C5B-O5B

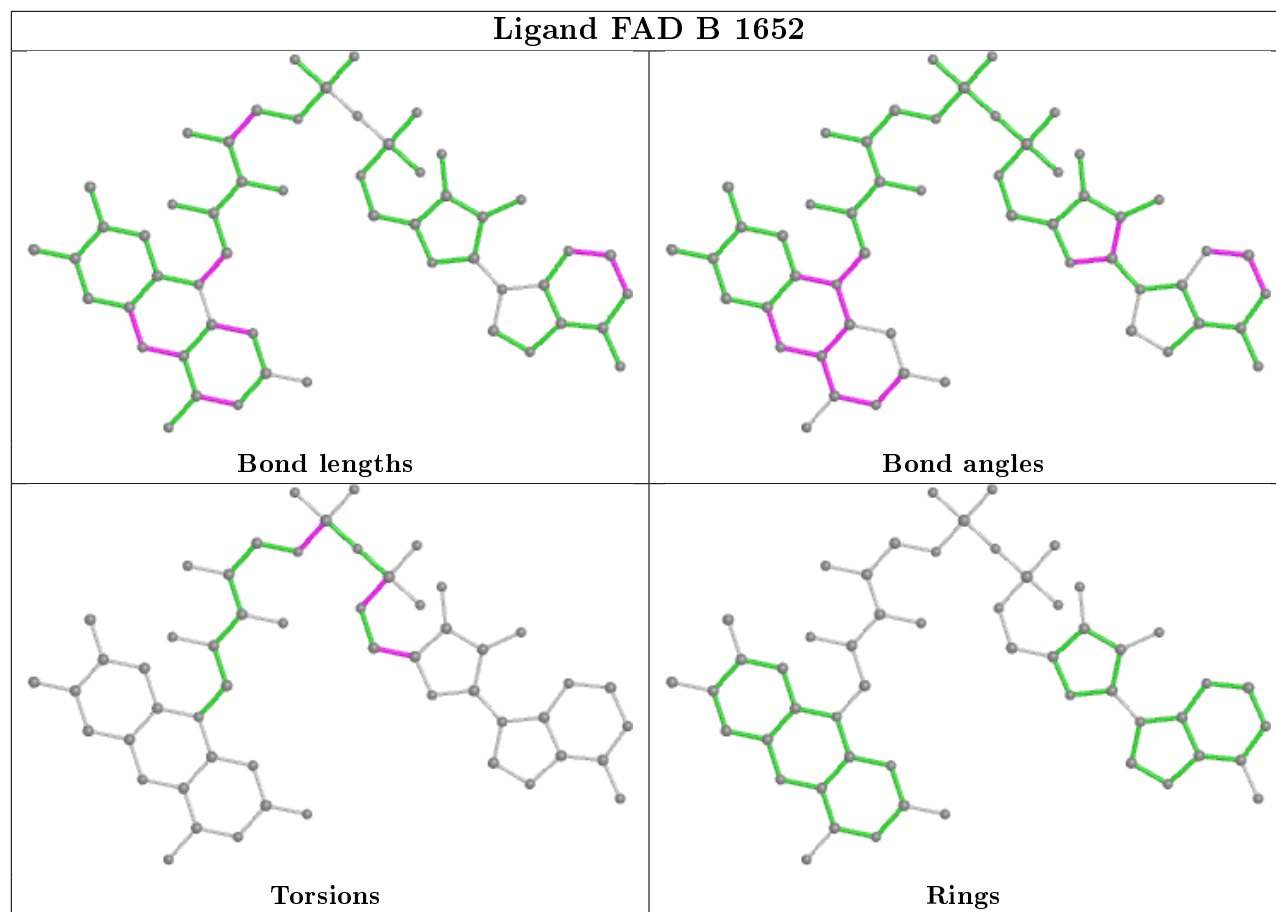
There are no ring outliers.

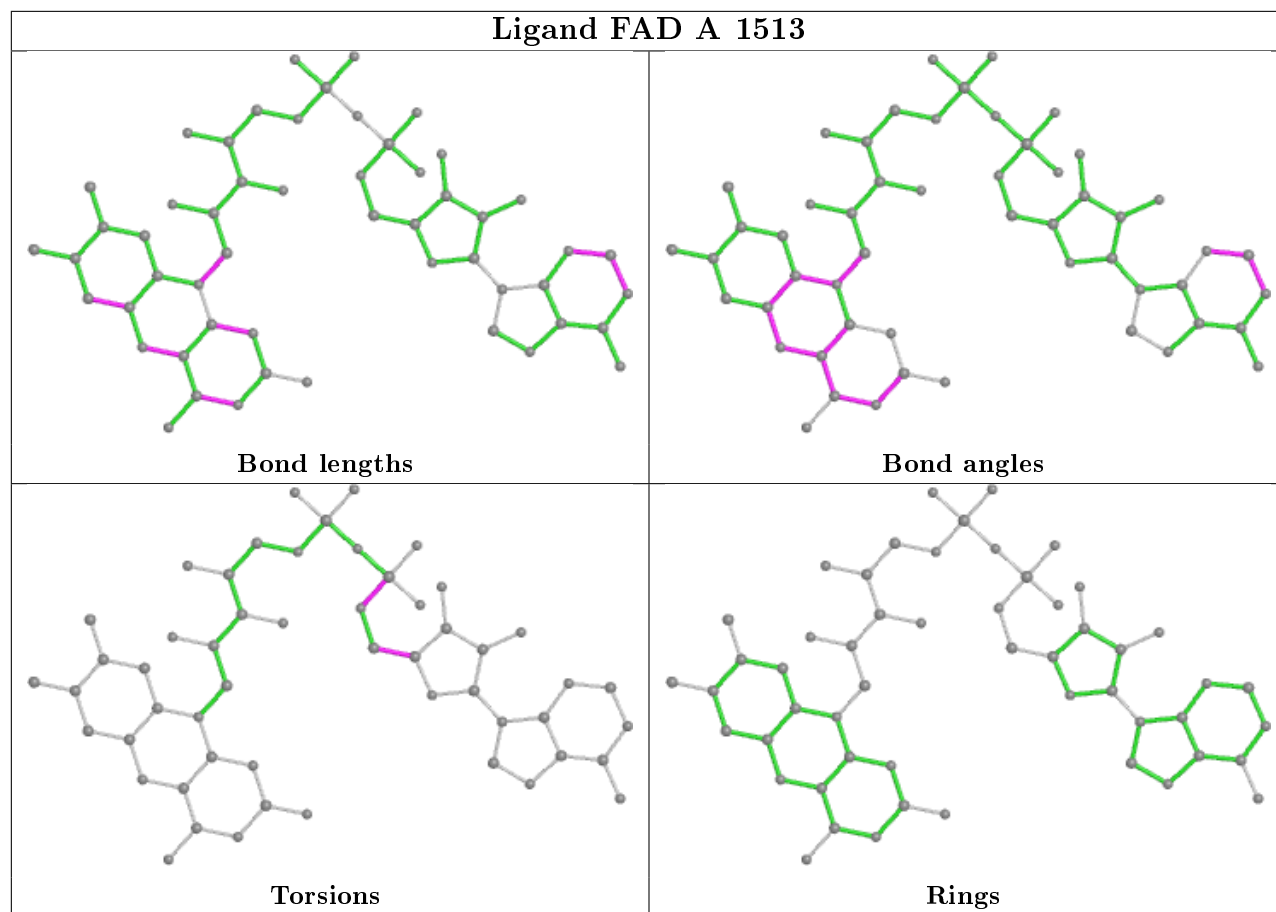
3 monomers are involved in 7 short contacts:

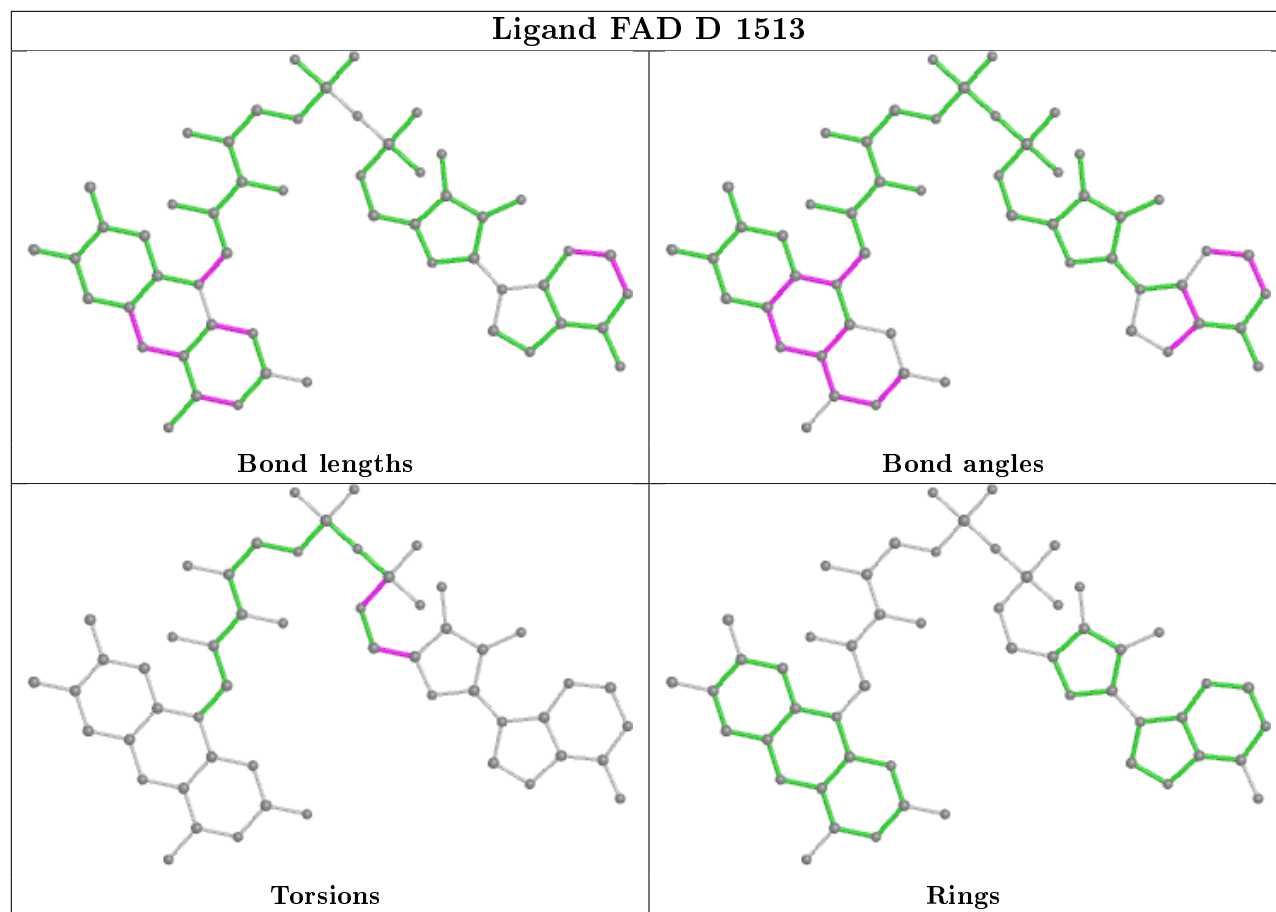
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1514	SO4	1	0
3	B	1652	FAD	2	0
3	D	1513	FAD	4	0

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, 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	496/511 (97%)	-0.03	4 (0%) 86 84	15, 19, 26, 32	0
1	B	501/511 (98%)	-0.01	6 (1%) 79 77	11, 20, 32, 53	0
1	C	494/511 (96%)	0.17	21 (4%) 35 33	15, 19, 25, 33	0
1	D	494/511 (96%)	0.68	75 (15%) 2 1	15, 19, 26, 32	0
All	All	1985/2044 (97%)	0.20	106 (5%) 26 25	11, 19, 28, 53	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	287	LYS	6.1
1	D	286	PHE	5.1
1	D	510	ILE	4.8
1	B	39	VAL	4.6
1	D	498	ALA	4.6
1	D	263	ASP	4.6
1	D	507	LEU	4.3
1	D	259	PRO	4.2
1	D	504	TYR	3.8
1	D	261	GLU	3.8
1	D	69	ARG	3.8
1	D	63	GLU	3.8
1	D	144	PHE	3.7
1	B	41	ARG	3.7
1	B	43	GLY	3.6
1	D	264	GLU	3.6
1	D	314	ALA	3.6
1	D	140	ASP	3.6
1	D	262	ASN	3.6
1	D	316	GLY	3.5
1	D	136	PRO	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	496	LEU	3.4
1	B	44	VAL	3.4
1	D	66	TRP	3.4
1	D	164	PHE	3.3
1	D	141	GLY	3.3
1	D	491	ARG	3.2
1	D	189	ARG	3.1
1	D	126	THR	3.1
1	D	61	LEU	3.1
1	D	73	GLY	3.0
1	D	318	ASP	2.9
1	C	493	GLY	2.9
1	B	37	GLY	2.9
1	D	258	VAL	2.9
1	D	322	ALA	2.9
1	D	186	ARG	2.9
1	B	38	ASN	2.9
1	D	184	ILE	2.9
1	D	139	LEU	2.8
1	C	316	GLY	2.8
1	D	285	LEU	2.8
1	D	411	ASP	2.8
1	D	64	ARG	2.8
1	D	138	MET	2.8
1	C	84	SER	2.7
1	D	188	VAL	2.7
1	C	85	GLU	2.7
1	D	3	ARG	2.7
1	A	491	ARG	2.7
1	D	165	PRO	2.7
1	D	128	ARG	2.7
1	C	141	GLY	2.7
1	A	117	THR	2.6
1	C	375	GLU	2.6
1	D	72	GLY	2.6
1	C	313	VAL	2.6
1	D	256	LEU	2.6
1	D	71	ALA	2.5
1	D	303	GLU	2.6
1	C	86	PRO	2.5
1	D	39	VAL	2.5
1	D	497	ILE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	300	ILE	2.5
1	D	310	ARG	2.5
1	D	129	LEU	2.5
1	D	260	ARG	2.5
1	C	88	GLU	2.5
1	D	159	GLU	2.5
1	C	318	ASP	2.5
1	D	511	GLN	2.5
1	C	91	TYR	2.4
1	D	506	TYR	2.4
1	D	496	LEU	2.4
1	C	317	ARG	2.4
1	A	203	ARG	2.4
1	C	491	ARG	2.4
1	D	67	LEU	2.4
1	D	505	GLU	2.4
1	D	280	MET	2.3
1	D	320	LEU	2.3
1	C	128	ARG	2.3
1	C	410	GLU	2.3
1	C	307	ARG	2.3
1	D	313	VAL	2.3
1	C	129	LEU	2.3
1	D	495	GLU	2.3
1	D	143	LEU	2.2
1	D	319	ASP	2.2
1	D	267	ARG	2.2
1	D	502	SER	2.1
1	D	177	ARG	2.1
1	C	314	ALA	2.1
1	C	498	ALA	2.1
1	D	317	ARG	2.1
1	D	160	GLN	2.1
1	D	192	VAL	2.1
1	A	318	ASP	2.1
1	D	142	SER	2.1
1	D	68	PRO	2.1
1	D	26	ASP	2.0
1	D	161	ARG	2.0
1	D	109	TRP	2.0
1	D	38	ASN	2.0
1	D	191	VAL	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	266	MET	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 carbohydrates in this entry.

6.4 Ligands [i](#)

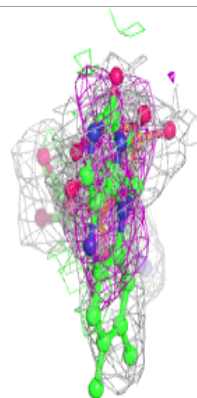
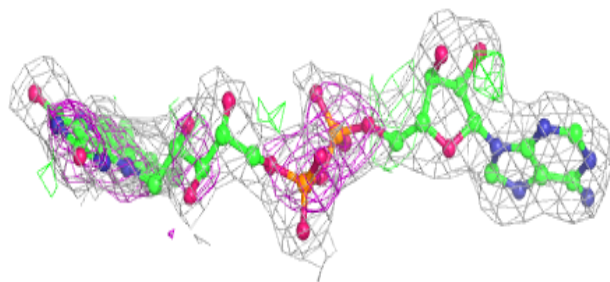
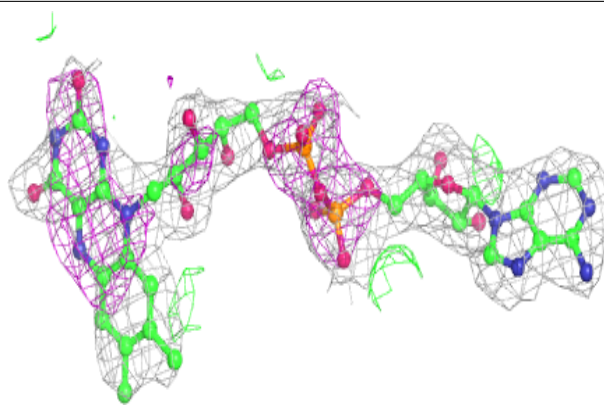
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	FAD	B	1652	53/53	0.92	0.17	16,23,27,27	0
3	FAD	D	1513	53/53	0.94	0.12	16,22,27,27	0
2	CL	B	700	1/1	0.94	0.15	50,50,50,50	0
4	TRP	B	650	15/15	0.94	0.17	41,44,47,47	0
5	SO4	C	1514	5/5	0.94	0.13	41,49,51,53	0
2	CL	D	1514	1/1	0.95	0.39	49,49,49,49	0
2	CL	D	700	1/1	0.96	0.10	39,39,39,39	0
3	FAD	C	1513	53/53	0.97	0.15	15,22,27,27	0
2	CL	A	1514	1/1	0.98	0.34	50,50,50,50	0
3	FAD	A	1513	53/53	0.98	0.18	15,21,27,27	0
2	CL	C	1515	1/1	0.99	0.30	41,41,41,41	0
2	CL	A	700	1/1	0.99	0.16	35,35,35,35	0
2	CL	B	1653	1/1	0.99	0.35	53,53,53,53	0
2	CL	C	700	1/1	0.99	0.10	37,37,37,37	0

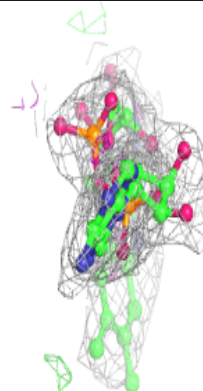
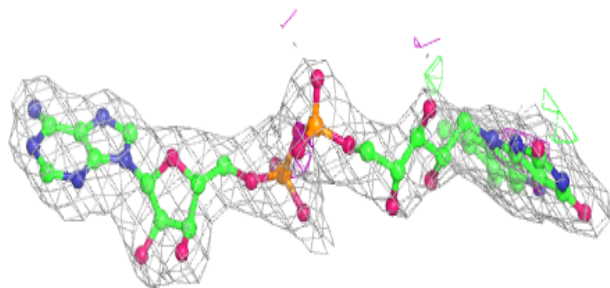
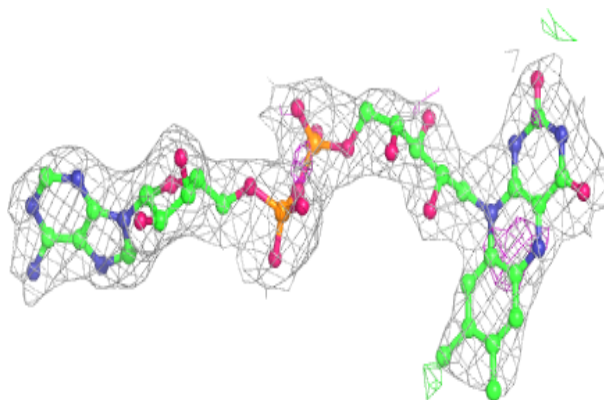
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD B 1652:

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

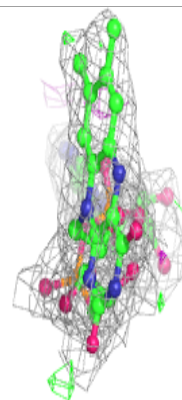
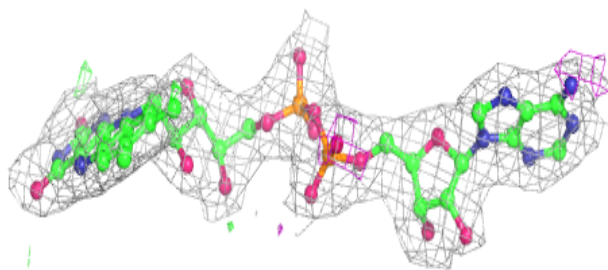
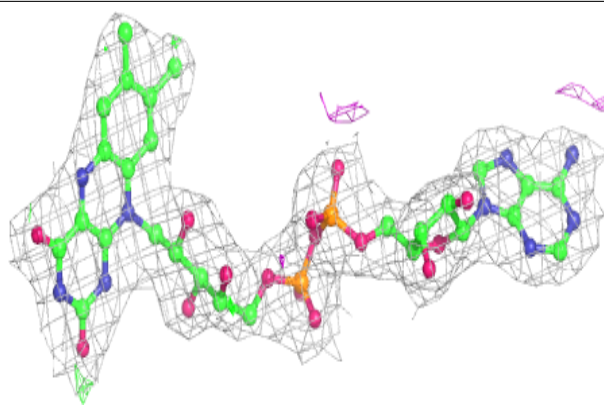
**Electron density around FAD D 1513:**

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

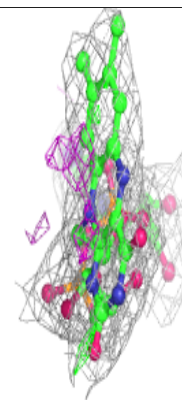
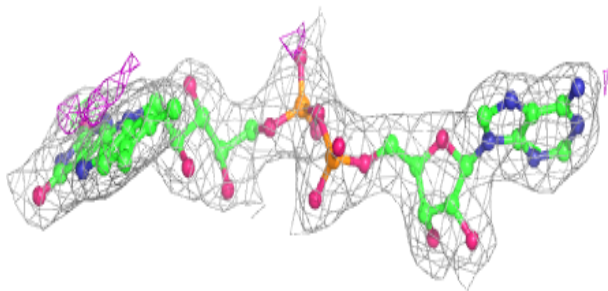
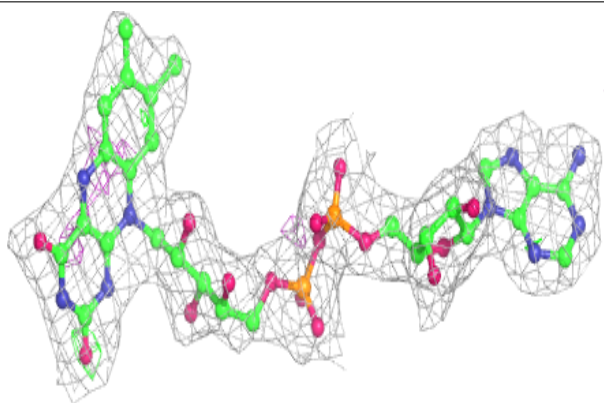


Electron density around FAD C 1513:

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

**Electron density around FAD A 1513:**

$2mF_o-DF_c$ (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.