



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 15, 2022 – 02:13 PM JST

PDB ID : 7VWP
Title : Structure of the flavin-dependent monooxygenase FlsO1 from the biosynthesis of fluostatinsin
Authors : Zhang, Y.; Yang, C.; Zhang, L.; Zhang, C.
Deposited on : 2021-11-11
Resolution : 2.30 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.30
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)	:	2.30

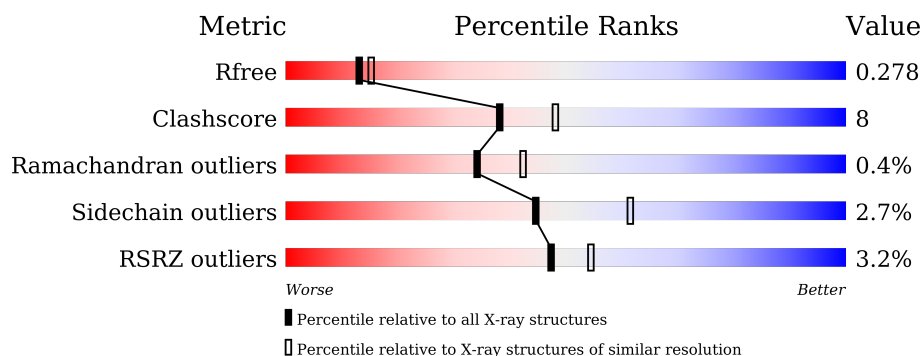
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	497	<div> <div>4%</div> <div>79%</div> <div>17%</div> <div>..</div> </div>
1	B	497	<div> <div>3%</div> <div>83%</div> <div>15%</div> <div>..</div> </div>
1	C	497	<div> <div>4%</div> <div>76%</div> <div>18%</div> <div>5%</div> </div>
1	D	497	<div> <div>2%</div> <div>85%</div> <div>11%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	B	505	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15743 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.

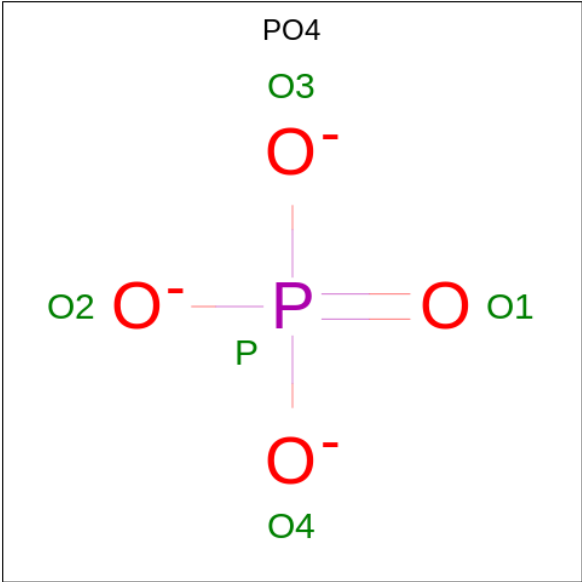
- Molecule 1 is a protein called FlsO1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	484	Total	C	N	O	S	0	1	0
			3648	2298	662	675	13			
1	A	480	Total	C	N	O	S	0	0	0
			3594	2266	649	666	13			
1	B	491	Total	C	N	O	S	0	1	0
			3689	2317	669	690	13			
1	C	471	Total	C	N	O	S	0	1	0
			3514	2213	638	650	13			

There are 8 discrepancies between the modelled and reference sequences:

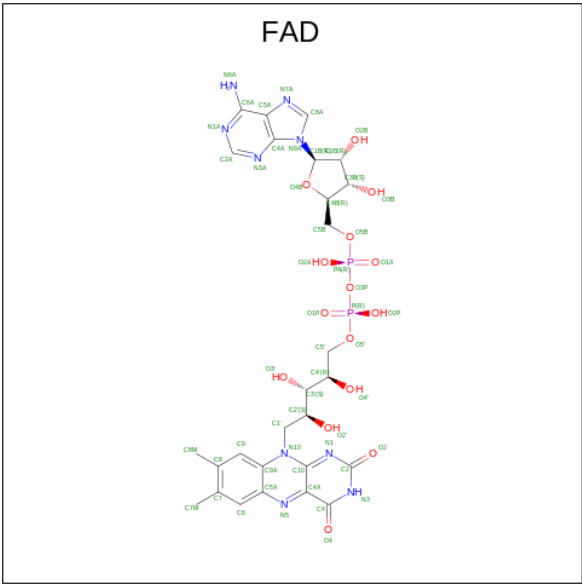
Chain	Residue	Modelled	Actual	Comment	Reference
D	108	ALA	GLN	engineered mutation	UNP A0A0P0I576
D	109	ALA	ARG	engineered mutation	UNP A0A0P0I576
A	108	ALA	GLN	engineered mutation	UNP A0A0P0I576
A	109	ALA	ARG	engineered mutation	UNP A0A0P0I576
B	108	ALA	GLN	engineered mutation	UNP A0A0P0I576
B	109	ALA	ARG	engineered mutation	UNP A0A0P0I576
C	108	ALA	GLN	engineered mutation	UNP A0A0P0I576
C	109	ALA	ARG	engineered mutation	UNP A0A0P0I576

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



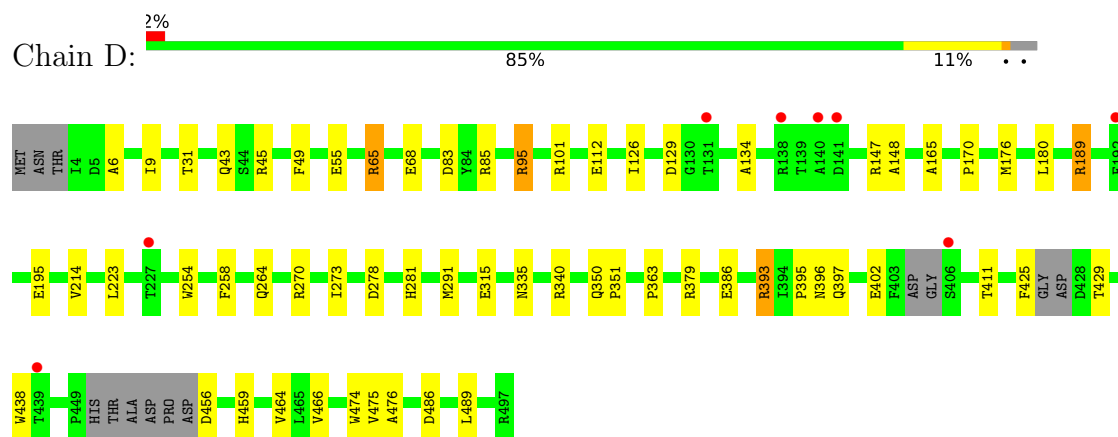
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	173	Total	O	0	0
			173	173		

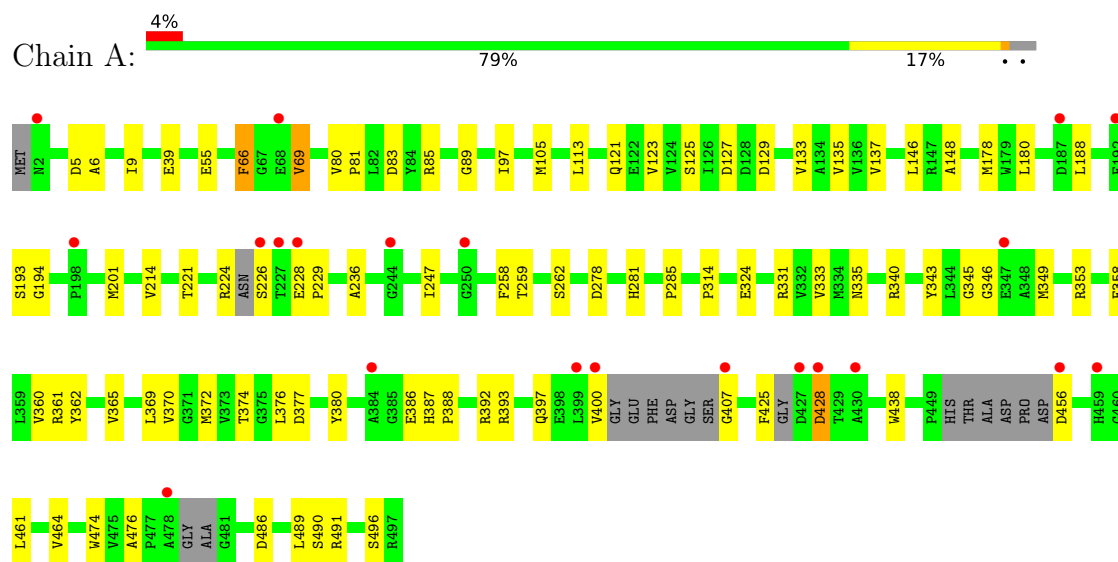
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

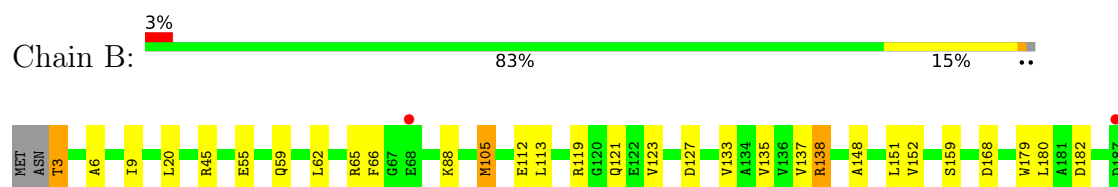
• Molecule 1: FlsO1

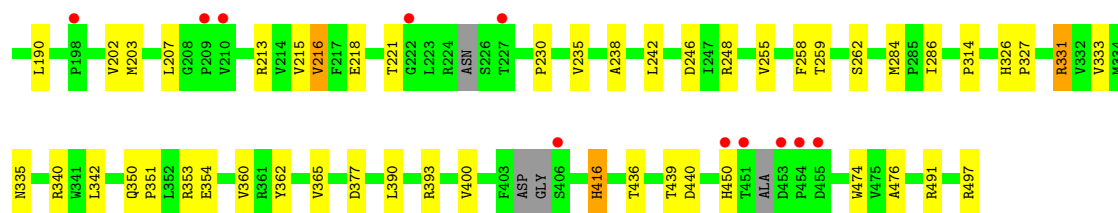


• Molecule 1: FlsO1

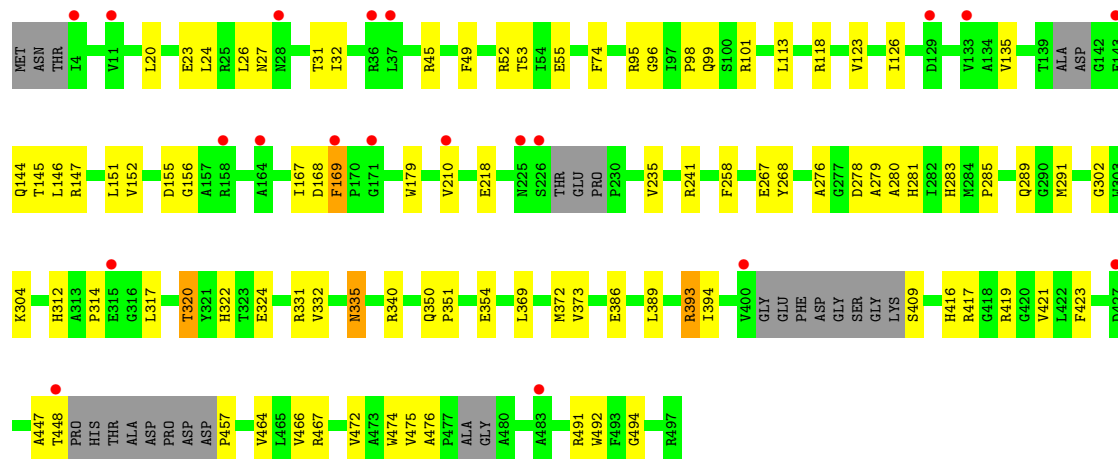
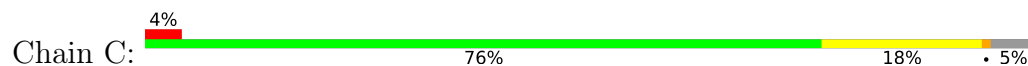


• Molecule 1: FlsO1





● Molecule 1: FlsO1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	76.54Å 84.64Å 102.80Å 91.31° 107.86° 115.39°	Depositor
Resolution (Å)	13.18 – 2.30 13.18 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.5 (13.18-2.30) 99.0 (13.18-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.8.0267, PHENIX 1.19.2-4158	Depositor
R, R_{free}	0.211 , 0.271 0.222 , 0.278	Depositor DCC
R_{free} test set	4704 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15743	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, FAD, NA

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	0/3667	0.85	0/4977
1	B	0.71	0/3766	0.87	3/5113 (0.1%)
1	C	0.69	0/3583	0.82	2/4860 (0.0%)
1	D	0.71	0/3725	0.87	4/5055 (0.1%)
All	All	0.70	0/14741	0.85	9/20005 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	393	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	B	331	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	C	393	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	B	331	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	D	65	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	B	138	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	D	189	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	D	65	ARG	CG-CD-NE	-5.18	100.93	111.80
1	C	169	PHE	CB-CA-C	5.08	120.56	110.40

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	3594	0	3522	54	0
1	B	3689	0	3605	59	0
1	C	3514	0	3433	64	0
1	D	3648	0	3580	42	0
2	A	20	0	0	3	0
2	B	35	0	0	3	0
2	C	5	0	0	0	0
2	D	10	0	0	0	0
3	A	53	0	31	1	0
3	B	53	0	31	2	0
3	C	53	0	31	2	0
3	D	53	0	31	2	0
4	B	1	0	0	0	0
5	A	244	0	0	8	0
5	B	297	0	0	5	0
5	C	173	0	0	11	0
5	D	301	0	0	10	0
All	All	15743	0	14264	220	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 8.

All (220) 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:A:224:ARG:C	1:A:226:SER:N	2.14	1.00
1:C:317:LEU:O	1:C:320:THR:HG22	1.70	0.91
1:C:335:ASN:HB2	1:C:372:MET:HE2	1.56	0.86
1:B:440:ASP:OD2	1:B:497:ARG:HD2	1.82	0.80
1:B:62:LEU:HD22	1:B:105:MET:HE1	1.64	0.79
1:A:369:LEU:HD23	1:A:372:MET:HE2	1.67	0.77
1:C:335:ASN:HB2	1:C:372:MET:CE	2.14	0.77
3:C:502:FAD:O1A	5:C:601:HOH:O	2.03	0.76
1:A:358:GLU:O	1:A:361:ARG:HG2	1.87	0.75
1:D:134:ALA:HB2	1:D:147:ARG:HH11	1.52	0.74
1:D:68:GLU:O	5:D:601:HOH:O	2.05	0.73
1:A:331:ARG:NH2	1:A:377:ASP:OD2	2.22	0.72
1:D:395:PRO:O	1:D:411:THR:HG21	1.90	0.71
1:B:3:THR:N	5:B:602:HOH:O	2.24	0.70
1:C:276:ALA:O	5:C:602:HOH:O	2.09	0.70
1:D:223:LEU:N	5:D:602:HOH:O	2.25	0.69
1:C:304:LYS:HZ3	1:C:320:THR:HG23	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ASP:OD2	1:B:248:ARG:NH1	2.27	0.68
1:B:331:ARG:NH2	1:B:377:ASP:OD2	2.26	0.68
1:C:52:ARG:NH1	1:C:393:ARG:HG3	2.09	0.66
1:C:55:GLU:OE1	1:C:393:ARG:HD2	1.94	0.66
1:A:39:GLU:OE1	5:A:601:HOH:O	2.14	0.65
1:C:145:THR:C	1:C:146:LEU:HD12	2.19	0.63
1:D:456:ASP:N	5:D:608:HOH:O	2.33	0.61
1:C:168:ASP:HB3	5:C:615:HOH:O	2.01	0.61
1:A:259:THR:N	2:A:501:PO4:O2	2.33	0.61
1:A:113:LEU:HD22	2:A:503:PO4:O2	2.01	0.60
1:B:123:VAL:HG13	1:B:135:VAL:HG13	1.82	0.60
1:D:165:ALA:O	1:D:270:ARG:NH1	2.34	0.60
1:B:190:LEU:HD12	1:B:190:LEU:H	1.65	0.60
1:C:32:ILE:HD12	1:C:118:ARG:HE	1.67	0.59
1:A:89:GLY:N	5:A:607:HOH:O	2.34	0.59
1:B:284:MET:HE2	1:B:286:ILE:HD11	1.85	0.59
1:A:83:ASP:OD1	1:A:85:ARG:HD3	2.03	0.59
1:C:23:GLU:O	1:C:27:ASN:ND2	2.37	0.58
1:B:62:LEU:HD22	1:B:105:MET:CE	2.33	0.58
1:B:113:LEU:HD22	2:B:504:PO4:O1	2.04	0.58
1:B:121:GLN:HB3	1:B:137:VAL:HG11	1.84	0.58
1:B:416:HIS:HE1	5:B:643:HOH:O	1.87	0.58
1:B:360:VAL:HA	1:B:365:VAL:HG22	1.86	0.58
1:D:397:GLN:H	1:D:411:THR:HG22	1.70	0.57
1:A:123:VAL:HG13	1:A:135:VAL:HG13	1.86	0.57
1:D:396:ASN:HA	1:D:411:THR:CG2	2.34	0.57
1:B:203:MET:HB2	1:B:215:VAL:HB	1.87	0.57
1:B:474:TRP:CH2	1:B:476:ALA:HB2	2.39	0.57
1:D:396:ASN:HA	1:D:411:THR:HG22	1.86	0.57
1:C:24:LEU:CB	1:C:31:THR:HG21	2.34	0.56
1:A:387:HIS:NE2	1:A:461:LEU:HD11	2.21	0.56
1:A:194:GLY:HA3	1:A:201:MET:HE2	1.88	0.56
2:A:504:PO4:O3	5:A:602:HOH:O	2.18	0.55
1:C:350:GLN:NE2	5:C:604:HOH:O	2.31	0.55
1:B:55:GLU:O	1:B:59:GLN:HG3	2.07	0.55
1:C:155:ASP:HB2	3:C:502:FAD:C8A	2.38	0.54
1:D:438:TRP:CE3	1:D:489:LEU:HD13	2.42	0.54
1:D:134:ALA:HB2	1:D:147:ARG:NH1	2.21	0.54
1:A:362:TYR:HB2	1:A:365:VAL:HG13	1.89	0.54
1:D:49:PHE:HB3	1:D:291:MET:HE3	1.89	0.54
1:B:284:MET:CE	1:B:286:ILE:HD11	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:ASP:O	1:A:490:SER:OG	2.22	0.53
1:B:259:THR:O	2:B:505:PO4:O1	2.26	0.53
1:D:65:ARG:NH2	1:D:112:GLU:OE1	2.36	0.53
1:B:497:ARG:NH1	5:B:613:HOH:O	2.42	0.53
1:B:119:ARG:HD2	5:B:735:HOH:O	2.08	0.52
1:A:345:GLY:HA3	1:A:349:MET:HG3	1.92	0.52
1:D:129:ASP:OD2	1:D:147:ARG:NH2	2.43	0.52
1:C:314:PRO:HG2	1:C:491:ARG:O	2.09	0.52
1:C:466:VAL:HG12	1:C:467:ARG:O	2.10	0.51
1:C:32:ILE:CD1	1:C:118:ARG:HE	2.23	0.51
1:A:376:LEU:HD22	1:A:393:ARG:HH11	1.75	0.51
1:A:194:GLY:CA	1:A:201:MET:HE2	2.41	0.51
1:C:314:PRO:HD2	1:C:317:LEU:HD22	1.93	0.50
1:D:258:PHE:HD2	3:D:503:FAD:HM73	1.77	0.50
1:D:315:GLU:N	5:D:606:HOH:O	2.31	0.50
1:C:304:LYS:NZ	1:C:320:THR:HG23	2.25	0.50
1:B:179:TRP:HB2	1:B:216:VAL:HG12	1.94	0.50
1:D:386:GLU:HB3	5:D:651:HOH:O	2.11	0.50
1:C:167:ILE:HA	5:C:736:HOH:O	2.11	0.50
1:C:283:HIS:CE1	1:C:332:VAL:HG12	2.47	0.49
1:C:278:ASP:HA	1:C:281:HIS:O	2.12	0.49
1:C:24:LEU:HB3	1:C:31:THR:HG21	1.94	0.49
1:D:49:PHE:HB3	1:D:291:MET:CE	2.41	0.49
1:B:350:GLN:O	1:B:354[B]:GLU:HG2	2.13	0.49
1:C:268:TYR:CZ	1:C:280:ALA:HB1	2.48	0.49
1:B:180:LEU:HD11	1:B:213:ARG:HD3	1.95	0.49
1:B:216:VAL:HG22	1:B:242:LEU:CD1	2.42	0.49
1:C:416:HIS:O	5:C:603:HOH:O	2.19	0.49
1:A:407:GLY:N	5:A:616:HOH:O	2.46	0.49
1:B:179:TRP:HB3	1:B:235:VAL:HG22	1.95	0.49
1:B:218:GLU:HB2	1:B:221:THR:HG22	1.95	0.49
1:D:425:PHE:C	5:D:667:HOH:O	2.51	0.48
1:A:5:ASP:OD2	1:A:146:LEU:HA	2.13	0.48
1:A:456:ASP:N	5:A:615:HOH:O	2.45	0.48
1:D:464:VAL:HG22	1:D:475:VAL:HG12	1.96	0.48
1:B:238:ALA:O	1:B:242:LEU:HD12	2.13	0.48
1:C:354:GLU:OE2	5:C:604:HOH:O	2.20	0.48
1:C:369:LEU:O	1:C:373:VAL:HG23	2.13	0.48
1:B:350:GLN:N	1:B:351:PRO:CD	2.77	0.48
1:A:346:GLY:O	1:A:353:ARG:NH2	2.44	0.48
1:A:474:TRP:CH2	1:A:476:ALA:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:PHE:O	5:C:605:HOH:O	2.20	0.48
1:A:324:GLU:HB3	1:A:380:TYR:CE1	2.49	0.47
1:C:49:PHE:HB3	1:C:291:MET:CE	2.45	0.47
1:D:45:ARG:HG2	3:D:503:FAD:C8	2.44	0.47
1:C:20:LEU:CD2	1:C:152:VAL:HG11	2.44	0.47
1:C:55:GLU:OE1	1:C:393:ARG:CD	2.60	0.47
1:D:55:GLU:OE1	1:D:393:ARG:HD2	2.14	0.47
1:D:315:GLU:HA	5:D:605:HOH:O	2.13	0.47
1:C:96:GLY:O	1:C:98:PRO:HD3	2.15	0.47
1:C:457:PRO:HA	5:C:749:HOH:O	2.13	0.47
1:B:20:LEU:CD2	1:B:152:VAL:HG11	2.44	0.47
1:B:133:VAL:HG21	1:B:151:LEU:HB2	1.97	0.47
1:B:123:VAL:HG22	1:B:135:VAL:CG1	2.45	0.47
1:D:95:ARG:NH1	1:B:127:ASP:HB2	2.30	0.46
1:A:66:PHE:CE2	1:A:105:MET:CE	2.98	0.46
1:A:127:ASP:OD1	1:C:95:ARG:HD3	2.15	0.46
1:D:189:ARG:HD2	1:B:168:ASP:HA	1.98	0.46
1:A:258:PHE:CD2	1:A:285:PRO:HD2	2.50	0.46
1:C:26:LEU:HD13	1:C:417:ARG:O	2.16	0.46
1:D:474:TRP:CH2	1:D:476:ALA:HB2	2.50	0.46
1:A:194:GLY:HA3	1:A:201:MET:CE	2.45	0.46
1:A:180:LEU:HA	1:A:214:VAL:O	2.15	0.45
1:B:66:PHE:CZ	1:B:105:MET:HG2	2.51	0.45
1:B:182:ASP:CG	1:B:207:LEU:HD11	2.37	0.45
1:B:314:PRO:HG2	1:B:491:ARG:O	2.16	0.45
1:D:126:ILE:HD12	1:D:273:ILE:HD13	1.99	0.45
1:A:55:GLU:OE1	1:A:393:ARG:HD2	2.16	0.45
1:A:188:LEU:HD11	1:A:247:ILE:HG21	1.96	0.45
1:B:218:GLU:CB	1:B:221:THR:HG22	2.46	0.45
1:C:45:ARG:HB2	1:C:99:GLN:OE1	2.15	0.45
1:D:180:LEU:HA	1:D:214:VAL:O	2.16	0.45
1:A:388:PRO:O	1:A:392:ARG:HD2	2.17	0.45
1:B:6:ALA:O	1:B:148:ALA:HA	2.17	0.45
1:B:342:LEU:O	1:B:353:ARG:NH1	2.41	0.45
1:C:179:TRP:HB3	1:C:235:VAL:HG22	1.98	0.45
1:D:9:ILE:HG13	1:D:148:ALA:HB2	1.98	0.45
1:A:69:VAL:O	1:A:69:VAL:CG1	2.65	0.45
1:A:370:VAL:O	1:A:374:THR:HG23	2.17	0.45
1:C:126:ILE:HD12	1:C:151:LEU:HD23	1.99	0.45
1:A:278:ASP:HA	1:A:281:HIS:O	2.17	0.45
1:D:393:ARG:NH2	5:D:627:HOH:O	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:GLU:HA	1:C:322:HIS:CE1	2.51	0.44
1:D:6:ALA:O	1:D:148:ALA:HA	2.17	0.44
1:A:360:VAL:HA	1:A:365:VAL:HG22	2.00	0.44
1:C:394:ILE:HD12	1:C:466:VAL:HG21	1.99	0.44
1:C:464:VAL:HG22	1:C:475:VAL:HG12	1.99	0.44
1:D:83:ASP:OD2	1:D:85:ARG:NH2	2.40	0.44
1:A:228:GLU:HG3	1:A:229:PRO:HD2	1.98	0.44
1:B:258:PHE:HB2	2:B:505:PO4:O1	2.18	0.44
1:D:278:ASP:HA	1:D:281:HIS:O	2.17	0.43
1:A:221:THR:HG21	5:A:794:HOH:O	2.17	0.43
1:C:49:PHE:HB2	1:C:53:THR:HG21	2.00	0.43
1:B:230:PRO:O	1:B:255:VAL:HG11	2.18	0.43
1:B:262:SER:HB3	1:B:333:VAL:HG13	1.99	0.43
1:D:189:ARG:NH2	1:D:195:GLU:OE1	2.49	0.43
1:A:393:ARG:NH2	5:A:628:HOH:O	2.51	0.43
1:C:210:VAL:HG22	1:C:210:VAL:O	2.18	0.43
1:C:335:ASN:OD1	1:C:335:ASN:C	2.57	0.43
1:C:218:GLU:OE2	1:C:241:ARG:NE	2.49	0.43
1:C:289:GLN:HE22	1:C:335:ASN:ND2	2.16	0.43
1:C:320:THR:O	1:C:324:GLU:HB2	2.17	0.43
1:D:189:ARG:HD3	5:D:794:HOH:O	2.18	0.43
1:D:379:ARG:NH2	5:D:614:HOH:O	2.38	0.43
1:C:283:HIS:CE1	1:C:332:VAL:CG1	3.02	0.43
1:B:216:VAL:CG2	1:B:242:LEU:CD1	2.97	0.43
1:C:123:VAL:HG22	1:C:135:VAL:CG1	2.48	0.43
1:D:43:GLN:HG2	1:D:254:TRP:CG	2.53	0.43
1:A:129:ASP:OD1	1:A:129:ASP:C	2.57	0.43
1:B:203:MET:CB	1:B:215:VAL:HB	2.48	0.43
1:B:350:GLN:N	1:B:351:PRO:HD2	2.34	0.43
1:A:69:VAL:O	1:A:69:VAL:HG13	2.19	0.43
1:D:350:GLN:N	1:D:351:PRO:CD	2.82	0.42
1:A:314:PRO:CG	1:A:491:ARG:O	2.67	0.42
1:A:386:GLU:N	1:A:386:GLU:OE1	2.52	0.42
1:A:6:ALA:O	1:A:148:ALA:HA	2.20	0.42
1:B:218:GLU:HG3	1:B:242:LEU:HD11	2.00	0.42
1:A:262:SER:HB3	1:A:333:VAL:HG13	2.00	0.42
1:C:421:VAL:HG11	1:C:423:PHE:CZ	2.55	0.42
1:A:55:GLU:OE2	1:A:393:ARG:NH1	2.53	0.42
1:C:258:PHE:CD1	1:C:285:PRO:HD2	2.55	0.42
1:C:474:TRP:CZ2	1:C:476:ALA:HB2	2.54	0.42
1:A:69:VAL:HG23	1:A:97:ILE:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:505:FAD:H9	3:A:505:FAD:HI1	1.82	0.42
1:C:167:ILE:HD13	1:C:267:GLU:HB2	2.02	0.42
1:D:180:LEU:C	1:D:180:LEU:HD12	2.40	0.42
1:B:436:THR:O	1:B:439:THR:HG23	2.20	0.42
1:C:350:GLN:N	1:C:351:PRO:CD	2.82	0.42
1:B:9:ILE:HG13	1:B:148:ALA:HB2	2.02	0.42
1:B:45:ARG:HG2	3:B:509:FAD:C8	2.49	0.42
1:D:456:ASP:C	1:D:456:ASP:OD1	2.57	0.42
1:C:24:LEU:HB2	1:C:31:THR:HG21	2.00	0.42
1:C:167:ILE:HD13	1:C:267:GLU:O	2.20	0.42
1:C:389:LEU:HG	1:C:472:VAL:HG21	2.02	0.42
1:B:65:ARG:NH2	1:B:112:GLU:OE1	2.53	0.41
1:C:156:GLY:O	1:C:279:ALA:HA	2.20	0.41
1:B:123:VAL:HG22	1:B:135:VAL:HG11	2.02	0.41
1:C:147:ARG:NH1	5:C:633:HOH:O	2.53	0.41
1:D:189:ARG:HH22	1:D:195:GLU:CD	2.23	0.41
1:B:326:HIS:HB3	1:B:327:PRO:HD3	2.02	0.41
1:B:400:VAL:HG21	1:B:450:HIS:CE1	2.56	0.41
1:C:26:LEU:HD23	1:C:113:LEU:HD13	2.03	0.41
1:C:331:ARG:O	1:C:335:ASN:HB3	2.20	0.41
1:A:438:TRP:CE3	1:A:489:LEU:HD13	2.55	0.41
1:B:88:LYS:HD2	1:B:88:LYS:HA	1.93	0.41
1:C:419:ARG:HD2	5:C:676:HOH:O	2.20	0.41
3:B:509:FAD:H9	3:B:509:FAD:HI1	1.85	0.41
1:D:170:PRO:HD2	1:D:264:GLN:O	2.20	0.41
1:A:425:PHE:CE2	1:A:464:VAL:HG23	2.56	0.41
1:B:203:MET:HE3	1:B:215:VAL:HG11	2.03	0.41
1:B:362:TYR:HB2	1:B:365:VAL:HG13	2.03	0.41
1:C:320:THR:HG21	1:C:492:TRP:HZ3	1.85	0.41
1:A:376:LEU:HD22	1:A:393:ARG:NH1	2.36	0.41
1:A:9:ILE:HG13	1:A:148:ALA:HB2	2.02	0.40
1:A:80:VAL:HA	1:A:81:PRO:HD2	1.93	0.40
1:A:236:ALA:HA	1:A:247:ILE:HD11	2.03	0.40
1:A:361:ARG:NH1	5:A:634:HOH:O	2.53	0.40
1:C:312:HIS:O	1:C:494:GLY:HA3	2.21	0.40
1:A:121:GLN:OE1	1:A:137:VAL:HG11	2.22	0.40
1:B:138:ARG:HH11	1:B:138:ARG:HG2	1.85	0.40
1:B:218:GLU:CD	5:B:634:HOH:O	2.59	0.40
1:B:390:LEU:HD12	1:B:390:LEU:HA	1.82	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	468/497 (94%)	453 (97%)	14 (3%)	1 (0%)	47	58
1	B	484/497 (97%)	470 (97%)	13 (3%)	1 (0%)	47	58
1	C	460/497 (93%)	426 (93%)	31 (7%)	3 (1%)	22	26
1	D	477/497 (96%)	457 (96%)	18 (4%)	2 (0%)	34	42
All	All	1889/1988 (95%)	1806 (96%)	76 (4%)	7 (0%)	34	42

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	159	SER
1	D	459	HIS
1	C	144	GLN
1	C	447	ALA
1	D	402	GLU
1	A	428	ASP
1	C	302	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	357/377 (95%)	344 (96%)	13 (4%)	35	49
1	B	368/377 (98%)	360 (98%)	8 (2%)	52	69
1	C	345/377 (92%)	337 (98%)	8 (2%)	50	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	364/377 (97%)	354 (97%)	10 (3%)	44 61
All	All	1434/1508 (95%)	1395 (97%)	39 (3%)	44 61

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

Mol	Chain	Res	Type
1	D	31	THR
1	D	95	ARG
1	D	101	ARG
1	D	176	MET
1	D	335	ASN
1	D	340	ARG
1	D	363	PRO
1	D	429	THR
1	D	466	VAL
1	D	486	ASP
1	A	66	PHE
1	A	69	VAL
1	A	125	SER
1	A	133	VAL
1	A	178	MET
1	A	193	SER
1	A	335	ASN
1	A	340	ARG
1	A	343	TYR
1	A	397	GLN
1	A	400	VAL
1	A	428	ASP
1	A	496	SER
1	B	3	THR
1	B	105	MET
1	B	202	VAL
1	B	216	VAL
1	B	335	ASN
1	B	340	ARG
1	B	393	ARG
1	B	416	HIS
1	C	101	ARG
1	C	169	PHE
1	C	320	THR
1	C	335	ASN
1	C	340	ARG

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Mol	Chain	Res	Type
1	C	386	GLU
1	C	409	SER
1	C	448	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	397	GLN
1	B	397	GLN
1	B	416	HIS
1	B	450	HIS
1	C	283	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 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	$\# Z > 2$
2	PO4	B	505	-	4,4,4	0.51	0	6,6,6	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	B	507	-	4,4,4	0.78	0	6,6,6	0.55	0
2	PO4	B	504	-	4,4,4	0.57	0	6,6,6	0.51	0
2	PO4	D	501	-	4,4,4	0.64	0	6,6,6	0.44	0
2	PO4	B	506	-	4,4,4	1.05	0	6,6,6	0.37	0
3	FAD	B	509	-	53,58,58	0.67	0	68,89,89	0.82	1 (1%)
2	PO4	C	501	-	4,4,4	0.70	0	6,6,6	0.37	0
2	PO4	B	502	-	4,4,4	0.62	0	6,6,6	0.53	0
3	FAD	A	505	-	53,58,58	0.64	0	68,89,89	0.91	6 (8%)
3	FAD	C	502	-	53,58,58	0.67	0	68,89,89	0.76	2 (2%)
2	PO4	A	503	-	4,4,4	0.87	0	6,6,6	0.30	0
2	PO4	A	504	-	4,4,4	0.59	0	6,6,6	0.45	0
2	PO4	A	502	-	4,4,4	0.85	0	6,6,6	0.54	0
3	FAD	D	503	-	53,58,58	0.70	0	68,89,89	0.80	0
2	PO4	B	503	-	4,4,4	1.51	1 (25%)	6,6,6	0.58	0
2	PO4	B	501	-	4,4,4	0.74	0	6,6,6	0.52	0
2	PO4	D	502	-	4,4,4	0.98	0	6,6,6	0.49	0
2	PO4	A	501	-	4,4,4	0.85	0	6,6,6	0.50	0

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	502	-	-	1/30/50/50	0/6/6/6
3	FAD	A	505	-	-	1/30/50/50	0/6/6/6
3	FAD	B	509	-	-	2/30/50/50	0/6/6/6
3	FAD	D	503	-	-	1/30/50/50	0/6/6/6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	503	PO4	P-O1	2.69	1.57	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	505	FAD	O2A-PA-O1A	2.33	123.76	112.24
3	A	505	FAD	C4'-C3'-C2'	2.28	118.10	113.36
3	B	509	FAD	O2P-P-O1P	2.25	123.37	112.24
3	C	502	FAD	C5A-C6A-N6A	2.24	123.76	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	FAD	P-O3P-PA	-2.24	125.15	132.83
3	A	505	FAD	C5A-C6A-N6A	2.19	123.67	120.35
3	A	505	FAD	O4-C4-C4X	-2.16	120.88	126.60
3	A	505	FAD	C4X-C4-N3	2.11	118.55	113.19
3	A	505	FAD	O2P-P-O1P	2.10	122.61	112.24

There are no chirality outliers.

All (5) torsion outliers are listed below:

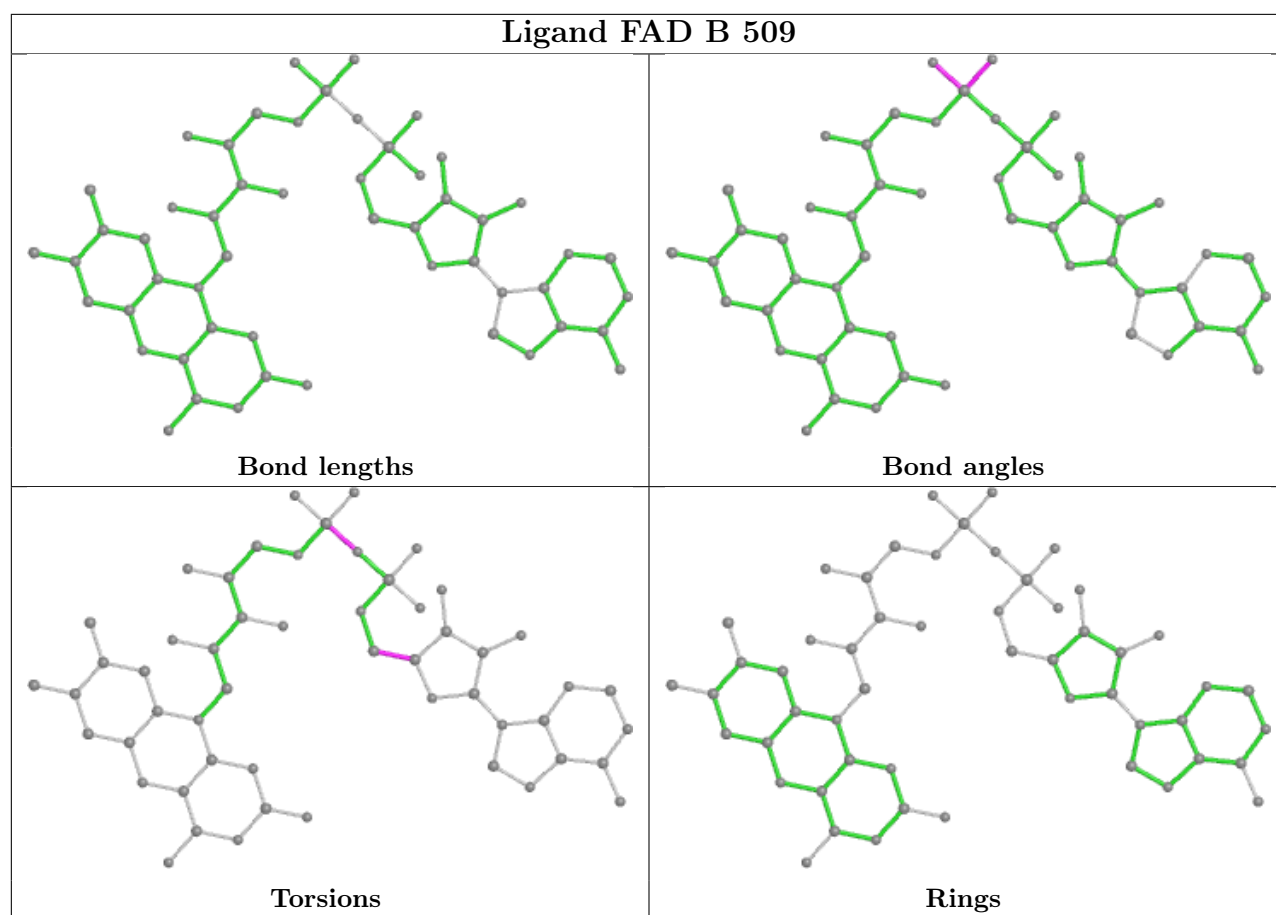
Mol	Chain	Res	Type	Atoms
3	B	509	FAD	PA-O3P-P-O5'
3	A	505	FAD	O4B-C4B-C5B-O5B
3	D	503	FAD	O4B-C4B-C5B-O5B
3	C	502	FAD	O4B-C4B-C5B-O5B
3	B	509	FAD	O4B-C4B-C5B-O5B

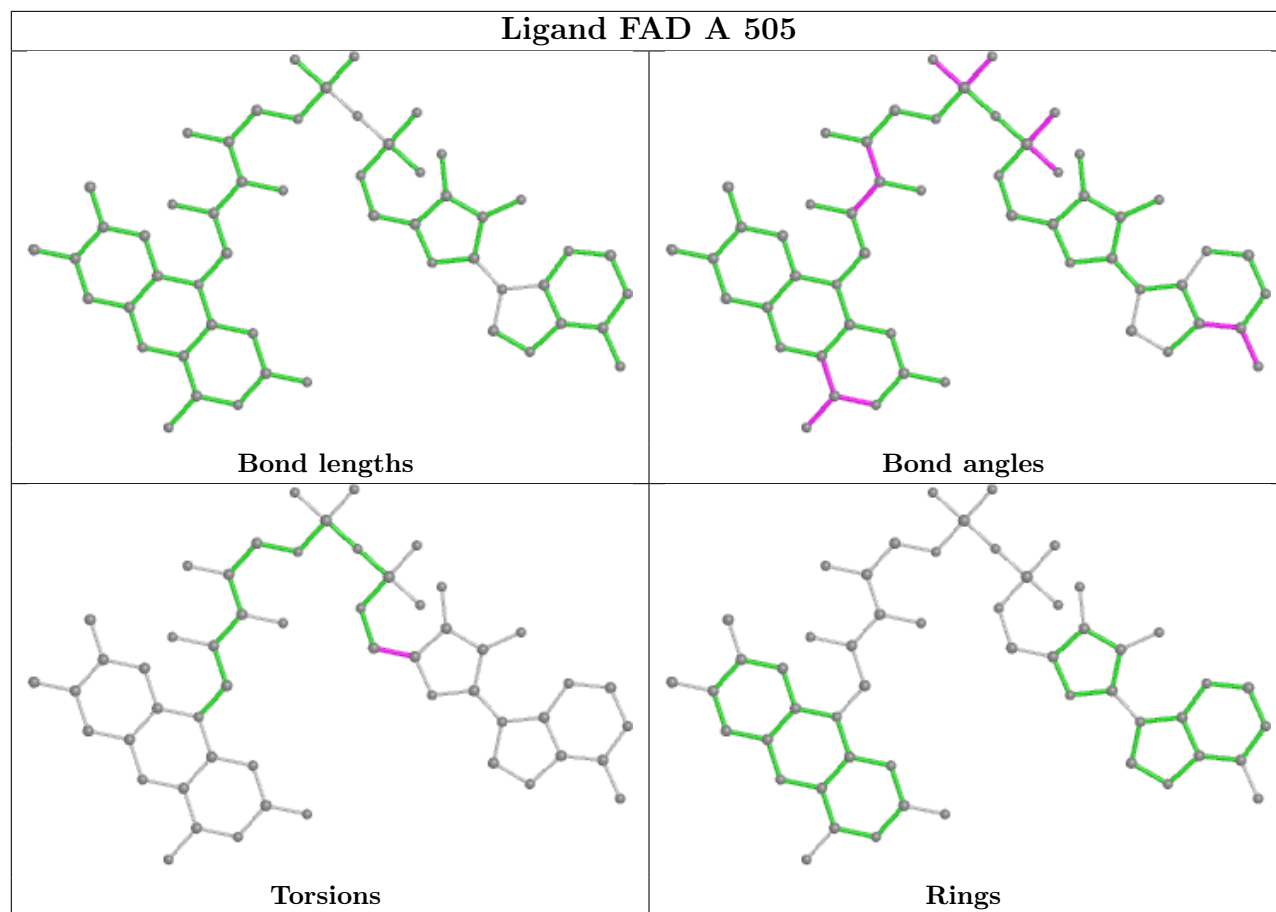
There are no ring outliers.

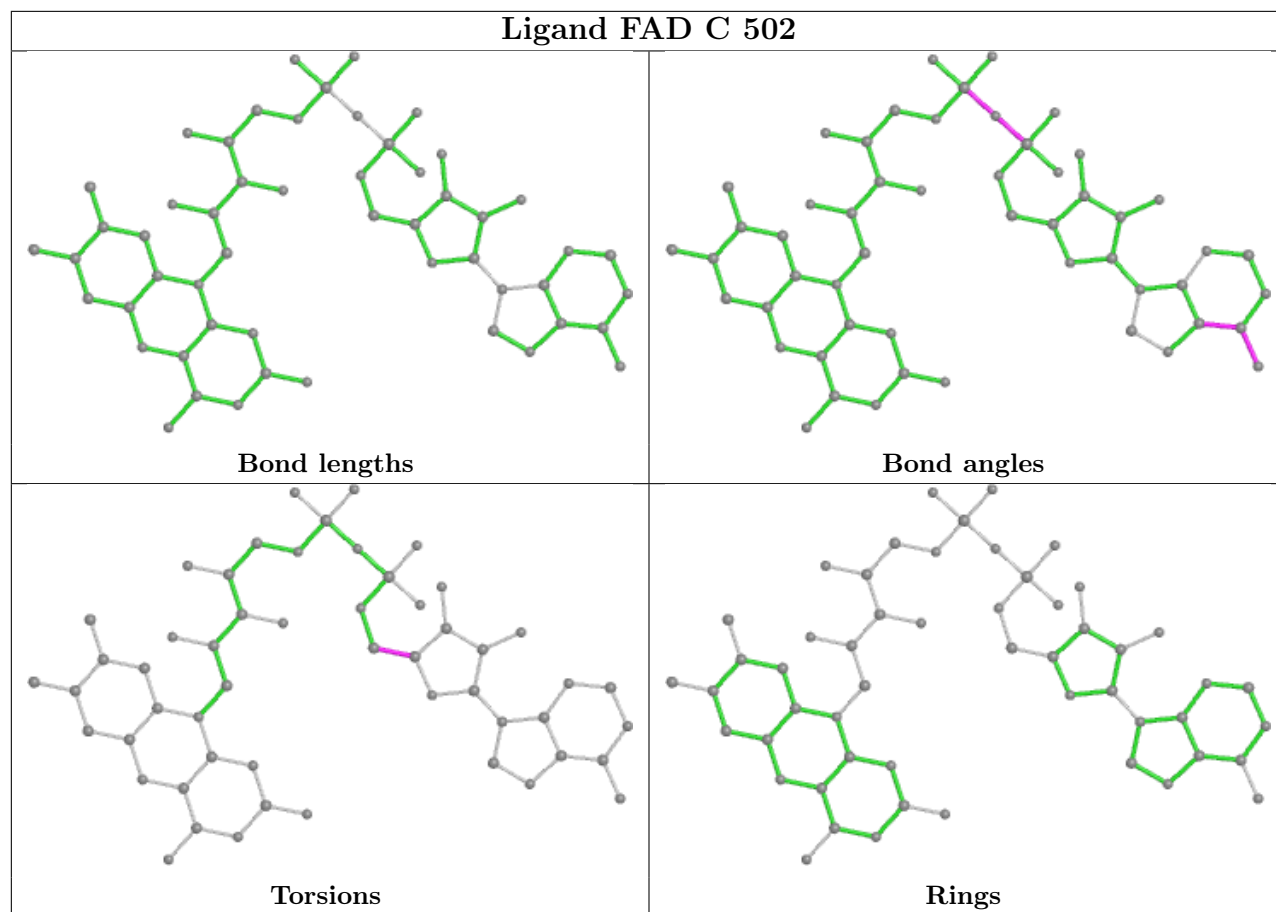
9 monomers are involved in 13 short contacts:

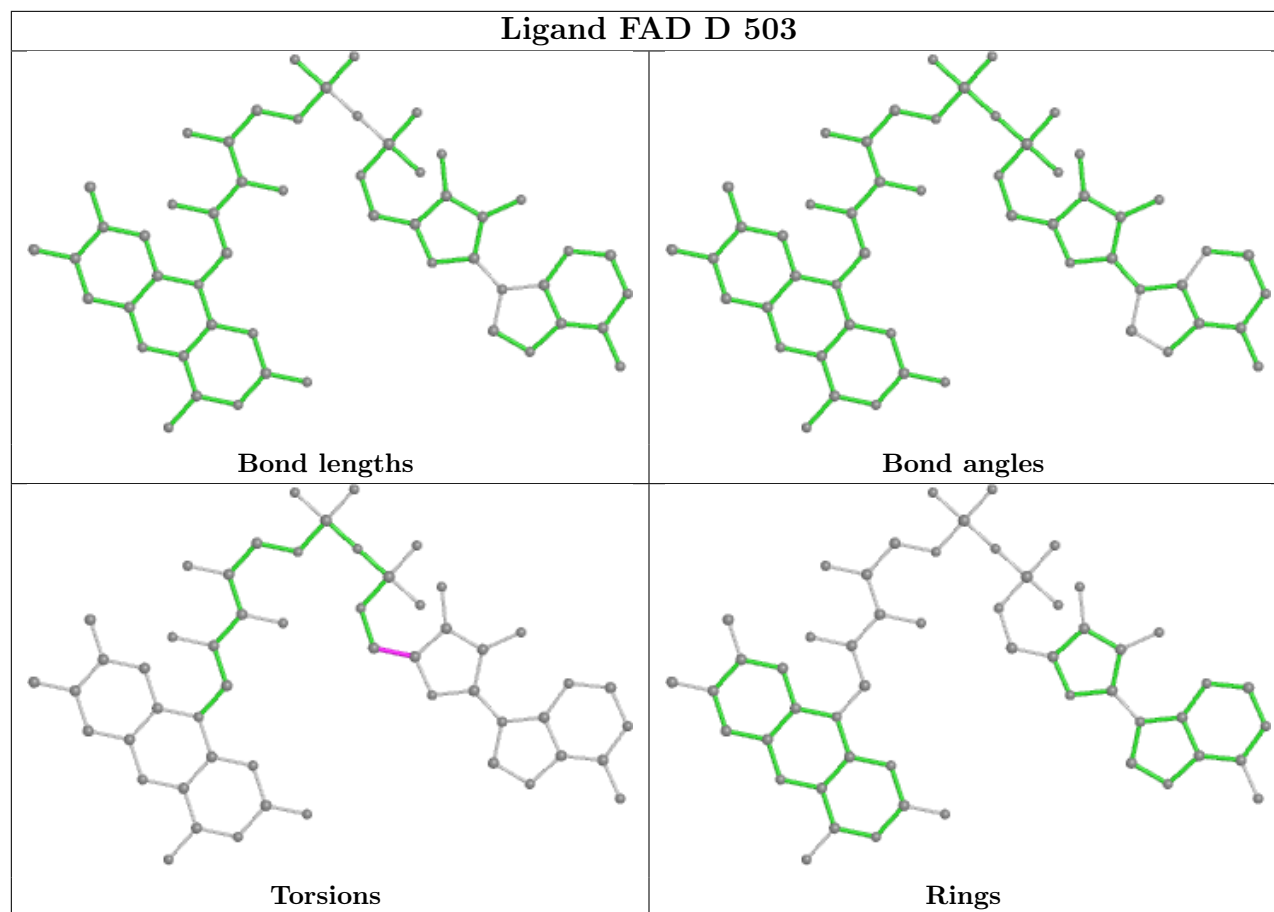
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	505	PO4	2	0
2	B	504	PO4	1	0
3	B	509	FAD	2	0
3	A	505	FAD	1	0
3	C	502	FAD	2	0
2	A	503	PO4	1	0
2	A	504	PO4	1	0
3	D	503	FAD	2	0
2	A	501	PO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	480/497 (96%)	-0.06	21 (4%) 34 41	12, 29, 62, 79	0
1	B	491/497 (98%)	-0.21	13 (2%) 56 63	8, 23, 49, 84	0
1	C	471/497 (94%)	0.34	20 (4%) 36 43	16, 40, 64, 76	0
1	D	484/497 (97%)	-0.22	8 (1%) 70 76	10, 24, 47, 78	0
All	All	1926/1988 (96%)	-0.04	62 (3%) 47 54	8, 29, 58, 84	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	454	PRO	5.6
1	B	451	THR	4.7
1	A	399	LEU	4.3
1	D	141	ASP	4.1
1	D	140	ALA	3.6
1	A	227	THR	3.6
1	A	192	PHE	3.5
1	A	244	GLY	3.4
1	D	227	THR	3.2
1	C	427	ASP	3.2
1	A	459	HIS	3.1
1	C	169	PHE	3.1
1	B	227	THR	3.1
1	A	400	VAL	3.0
1	C	36	ARG	3.0
1	C	400	VAL	3.0
1	C	483	ALA	3.0
1	C	225	ASN	2.9
1	B	455	ASP	2.9
1	C	133	VAL	2.8
1	B	209	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	384	ALA	2.8
1	C	210	VAL	2.8
1	B	450	HIS	2.8
1	B	406	SER	2.6
1	A	347	GLU	2.6
1	B	187	ASP	2.6
1	C	129	ASP	2.6
1	D	138	ARG	2.6
1	C	158	ARG	2.6
1	A	407	GLY	2.6
1	C	448	THR	2.5
1	C	164	ALA	2.5
1	A	226	SER	2.5
1	C	4	ILE	2.5
1	A	187	ASP	2.5
1	C	315	GLU	2.5
1	D	406	SER	2.4
1	C	143	GLU	2.4
1	D	131	THR	2.4
1	A	250	GLY	2.4
1	C	171	GLY	2.3
1	C	37	LEU	2.3
1	A	2	ASN	2.3
1	C	28	ASN	2.3
1	B	453	ASP	2.3
1	C	11	VAL	2.3
1	A	228	GLU	2.3
1	B	198	PRO	2.3
1	A	478	ALA	2.2
1	A	428	ASP	2.2
1	D	192[A]	PHE	2.2
1	A	456	ASP	2.2
1	A	198	PRO	2.2
1	A	430	ALA	2.2
1	A	427	ASP	2.2
1	C	226	SER	2.2
1	D	439	THR	2.1
1	B	68	GLU	2.1
1	B	222	GLY	2.1
1	B	210	VAL	2.1
1	A	68	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](#)

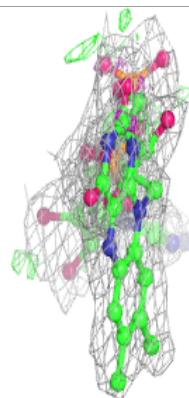
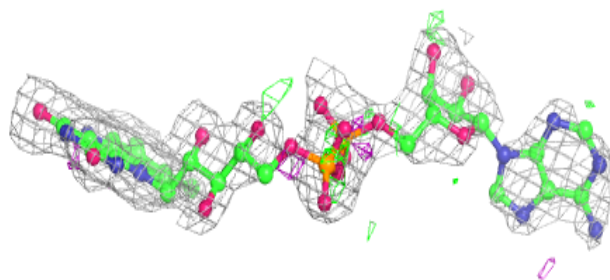
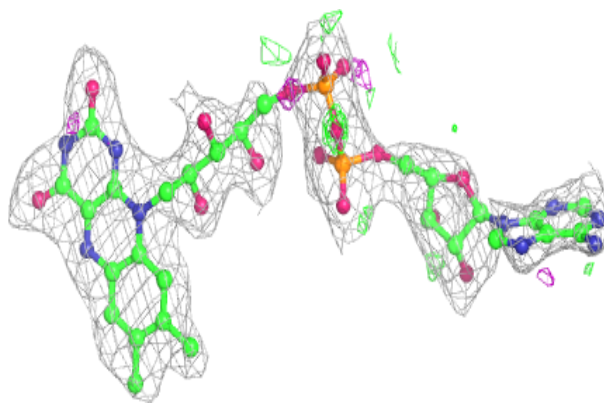
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PO4	B	502	5/5	0.80	0.32	61,68,76,80	0
2	PO4	D	501	5/5	0.84	0.30	45,54,64,71	0
2	PO4	B	507	5/5	0.85	0.26	41,45,58,58	0
2	PO4	B	505	5/5	0.86	0.22	42,43,51,54	0
2	PO4	A	501	5/5	0.86	0.21	61,63,72,80	0
2	PO4	B	506	5/5	0.88	0.21	70,71,75,82	0
2	PO4	C	501	5/5	0.89	0.27	59,63,67,69	0
3	FAD	C	502	53/53	0.91	0.16	24,37,69,70	0
2	PO4	B	503	5/5	0.92	0.14	21,27,28,30	0
2	PO4	A	504	5/5	0.92	0.20	58,59,70,71	0
2	PO4	D	502	5/5	0.92	0.19	43,45,50,61	0
2	PO4	A	502	5/5	0.94	0.23	31,34,37,41	0
2	PO4	A	503	5/5	0.94	0.18	29,33,38,39	0
2	PO4	B	501	5/5	0.95	0.28	43,44,53,59	0
3	FAD	D	503	53/53	0.96	0.10	13,19,36,37	0
3	FAD	A	505	53/53	0.96	0.09	12,17,27,33	0
2	PO4	B	504	5/5	0.96	0.17	42,42,44,55	0
3	FAD	B	509	53/53	0.97	0.08	11,14,26,28	0
4	NA	B	508	1/1	0.97	0.09	30,30,30,30	0

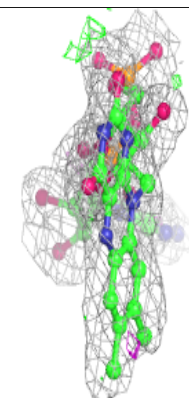
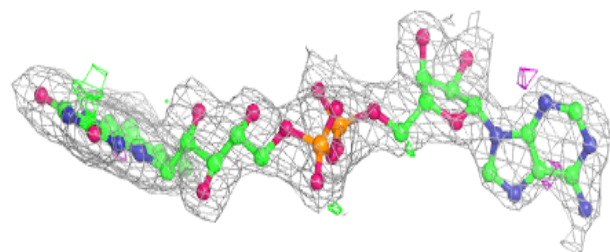
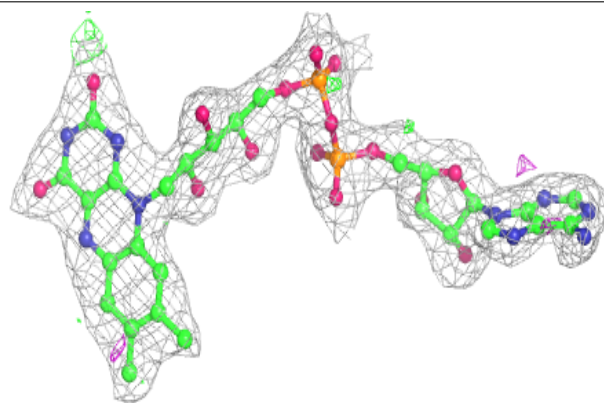
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD C 502:

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

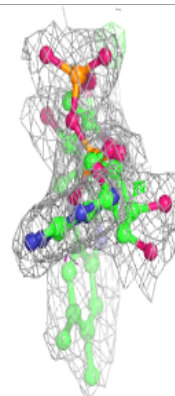
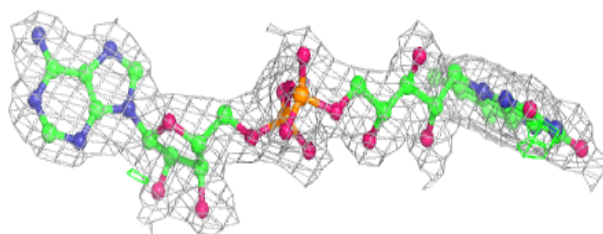
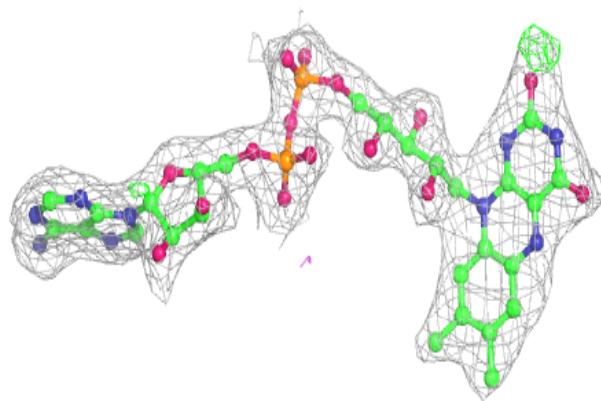
**Electron density around FAD D 503:**

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

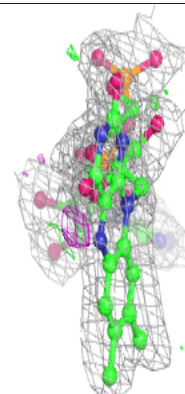
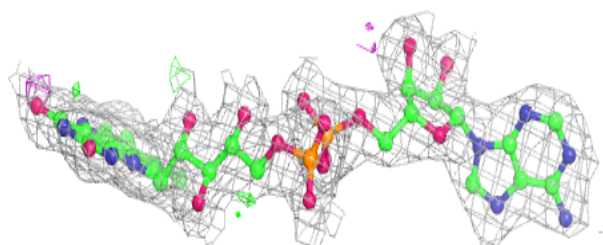
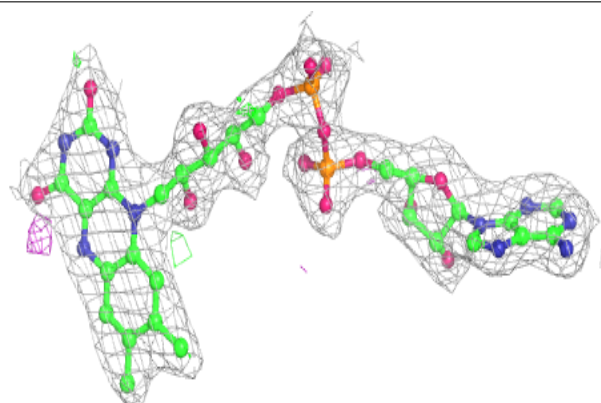


Electron density around FAD A 505:

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

**Electron density around FAD B 509:**

$2mF_o-DF_c$ (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.