



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 08:21 PM UTC

PDB ID : 5O8R / pdb_00005o8r
Title : The crystal structure of DfoA bound to FAD and NADP; the desferrioxamine biosynthetic pathway cadaverine monooxygenase from the fire blight disease pathogen *Erwinia amylovora*
Authors : Salomone-Stagni, M.; Bartho, J.D.; Polsinelli, I.; Bellini, D.; Walsh, M.A.; Demitri, N.; Benini, S.
Deposited on : 2017-06-14
Resolution : 2.80 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](#) ①) were used in the production of this report:

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

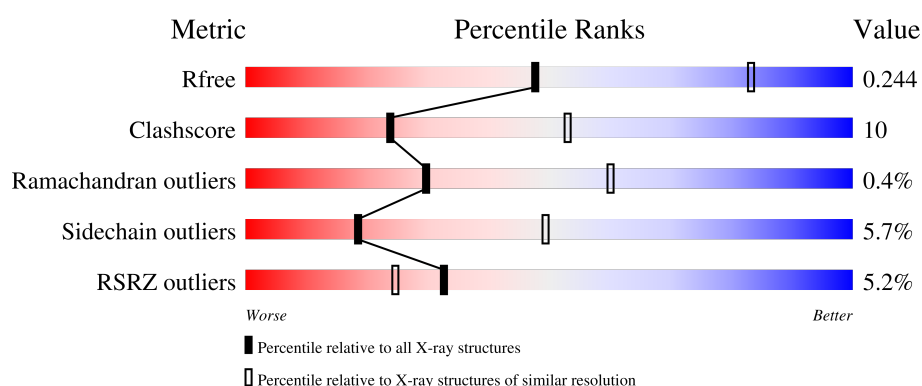
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	433	7% 74% 22% ..
1	B	433	3% 76% 20% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7379 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.

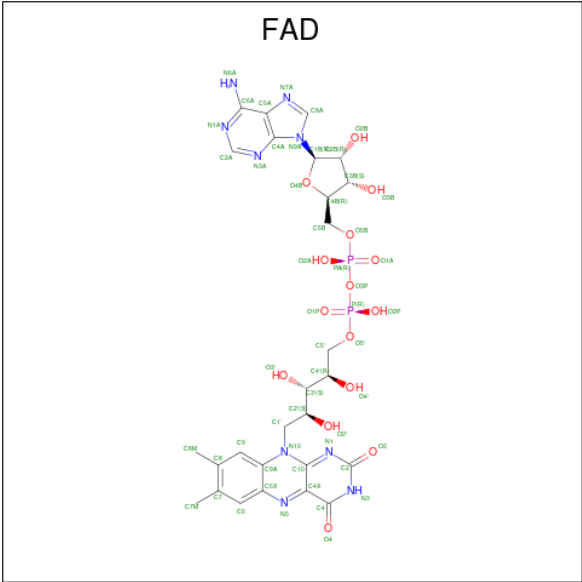
- Molecule 1 is a protein called L-lysine 6-monooxygenase involved in desferrioxamine biosynthesis.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	3	0
			3549	2263	613	659	14			
1	B	427	Total	C	N	O	S	0	3	0
			3547	2263	610	659	15			

There are 8 discrepancies between the modelled and reference sequences:

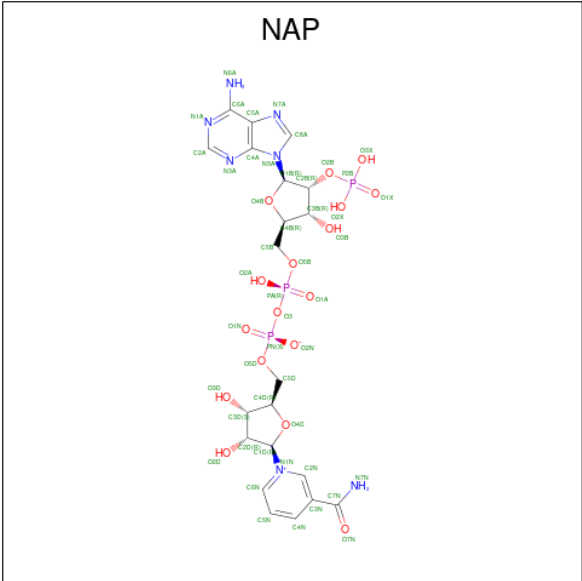
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP D4I246
A	-1	ALA	-	expression tag	UNP D4I246
A	0	MET	-	expression tag	UNP D4I246
A	1	ALA	-	expression tag	UNP D4I246
B	-2	GLY	-	expression tag	UNP D4I246
B	-1	ALA	-	expression tag	UNP D4I246
B	0	MET	-	expression tag	UNP D4I246
B	1	ALA	-	expression tag	UNP D4I246

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



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

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

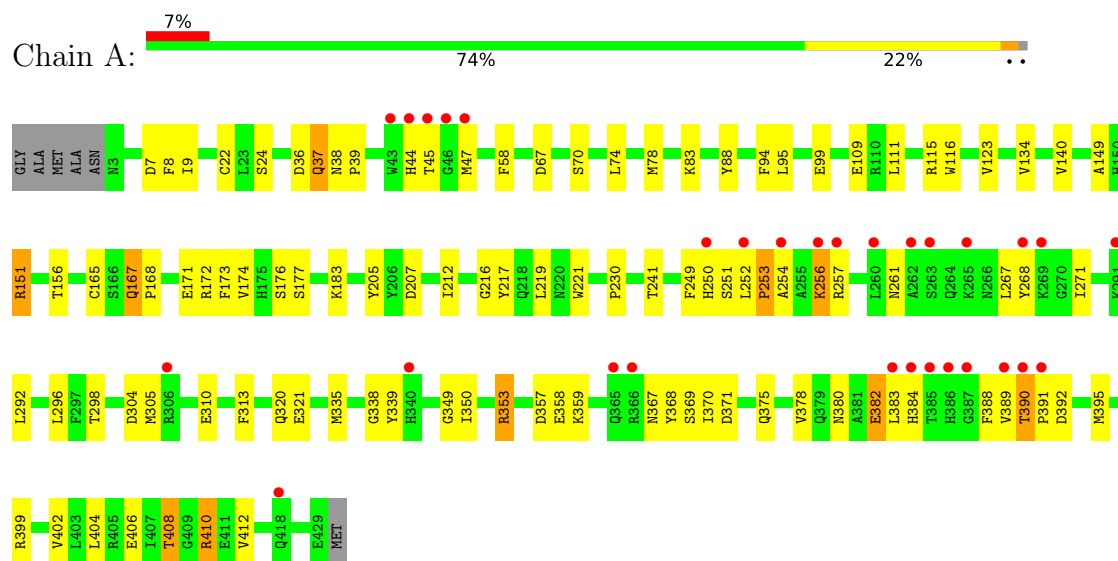
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	43	Total	O	0	1
			43	43		
4	B	38	Total	O	0	0
			38	38		

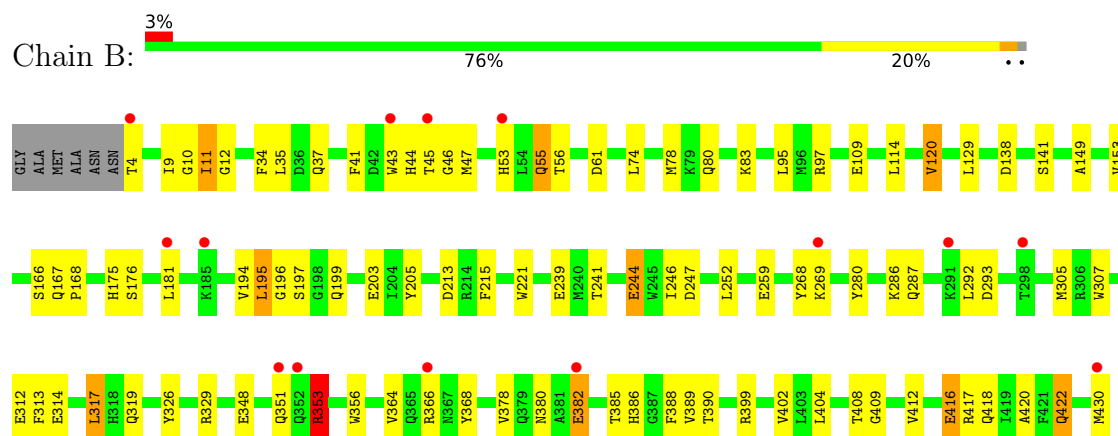
3 Residue-property plots

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: L-lysine 6-monooxygenase involved in desferrioxamine biosynthesis



- Molecule 1: L-lysine 6-monooxygenase involved in desferrioxamine biosynthesis



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	163.94Å 163.94Å 166.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.59 – 2.80 47.59 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.59-2.80) 99.9 (47.59-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.187 , 0.240 0.194 , 0.244	Depositor DCC
R_{free} test set	2895 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	56.4	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.021 for -h,l,k 0.000 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7379	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.68% 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

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.19	3/3644 (0.1%)	1.21	16/4942 (0.3%)
1	B	1.10	4/3642 (0.1%)	1.20	13/4939 (0.3%)
All	All	1.14	7/7286 (0.1%)	1.21	29/9881 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	12	GLY	N-CA	5.99	1.52	1.45
1	B	138	ASP	C-O	-5.23	1.17	1.24
1	A	24	SER	CA-C	-5.12	1.45	1.52
1	A	298	THR	CA-C	5.08	1.58	1.52
1	A	67	ASP	C-N	-5.05	1.28	1.34
1	B	10	GLY	CA-C	-5.04	1.48	1.52
1	B	293	ASP	N-CA	-5.04	1.40	1.46

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	217	TYR	N-CA-C	8.62	122.08	110.35
1	A	253	PRO	N-CA-C	-7.79	104.70	114.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	SER	CA-C-N	-7.29	112.29	119.87
1	A	70	SER	C-N-CA	-7.29	112.29	119.87
1	B	120	VAL	N-CA-CB	7.18	118.36	110.53
1	B	408	THR	N-CA-C	-6.73	101.85	110.53
1	B	46	GLY	N-CA-C	6.34	121.65	114.67
1	B	252	LEU	CA-C-N	6.23	126.26	119.90
1	B	252	LEU	C-N-CA	6.23	126.26	119.90
1	A	37	GLN	CB-CA-C	-6.16	100.38	110.85
1	A	251	SER	N-CA-C	-6.13	97.19	107.80
1	B	215	PHE	N-CA-C	-6.04	101.04	110.17
1	B	196	GLY	CA-C-O	-5.91	118.38	122.22
1	B	417	ARG	N-CA-C	-5.76	106.39	113.41
1	A	252	LEU	CA-C-N	5.58	127.30	120.94
1	A	252	LEU	C-N-CA	5.58	127.30	120.94
1	A	292	LEU	N-CA-C	-5.41	100.89	109.76
1	A	384	HIS	N-CA-C	5.38	119.00	112.23
1	A	151	ARG	N-CA-C	5.33	117.49	109.23
1	B	353	ARG	N-CA-C	5.33	119.62	113.18
1	B	197	SER	CB-CA-C	-5.24	103.00	111.28
1	B	11	ILE	N-CA-C	5.22	116.30	111.45
1	A	353	ARG	N-CA-C	5.21	119.48	113.18
1	B	382	GLU	CB-CA-C	-5.16	101.84	110.56
1	B	412	VAL	CB-CA-C	-5.15	105.38	111.97
1	A	94	PHE	N-CA-C	5.12	117.08	108.73
1	A	412	VAL	N-CA-C	-5.11	107.16	111.56
1	A	88	TYR	CA-CB-CG	5.06	123.00	113.90
1	A	321	GLU	N-CA-C	-5.05	106.80	113.12

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	216	GLY	Peptide
1	B	409	GLY	Peptide

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	3549	0	3413	70	0
1	B	3547	0	3411	67	0
2	A	53	0	31	11	0
2	B	53	0	31	12	0
3	A	48	0	25	0	0
3	B	48	0	25	3	0
4	A	43	0	0	1	0
4	B	38	0	0	2	0
All	All	7379	0	6936	144	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 10.

All (144) 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:246:ILE:CG2	1:B:366:ARG:HH12	1.07	1.58
1:B:246:ILE:HG22	1:B:366:ARG:NH1	1.07	1.34
1:B:246:ILE:CG2	1:B:366:ARG:NH1	1.78	1.15
1:B:246:ILE:CB	1:B:366:ARG:HH12	1.75	0.99
1:B:246:ILE:HG22	1:B:366:ARG:HH11	1.23	0.92
1:B:246:ILE:HG21	1:B:366:ARG:HH12	1.37	0.88
1:A:253:PRO:HG3	1:A:257:ARG:HG3	1.61	0.81
1:A:305:MET:CE	1:A:313:PHE:CE1	2.64	0.79
1:B:364:VAL:HB	1:B:385:THR:HG21	1.67	0.77
1:B:74:LEU:HD13	1:B:95:LEU:HD11	1.67	0.77
2:A:501:FAD:C3'	2:A:501:FAD:H9	2.14	0.76
1:A:404:LEU:O	1:A:408:THR:HB	1.85	0.76
2:A:501:FAD:H9	2:A:501:FAD:H3'	1.70	0.73
1:B:246:ILE:HG21	1:B:366:ARG:NH1	1.94	0.72
2:B:501:FAD:H9	2:B:501:FAD:C3'	2.20	0.72
1:A:253:PRO:CG	1:A:257:ARG:HG3	2.20	0.71
1:A:371:ASP:OD2	1:A:375:GLN:HG3	1.92	0.69
1:B:44:HIS:CE1	2:B:501:FAD:HM81	2.27	0.69
1:B:166:SER:O	1:B:168:PRO:O	2.11	0.68
1:B:378:VAL:HG23	1:B:382:GLU:OE2	1.94	0.68
1:A:44[A]:HIS:NE2	1:A:339:TYR:OH	2.25	0.68
1:A:9:ILE:HD12	1:A:149:ALA:HB2	1.76	0.67
1:B:244:GLU:OE1	1:B:420:ALA:HB3	1.96	0.66
1:B:55:GLN:CA	1:B:55:GLN:HE21	2.08	0.65
1:B:55:GLN:HE21	1:B:55:GLN:HA	1.62	0.65
1:A:268:TYR:CE2	1:A:383:LEU:HD11	2.32	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44[A]:HIS:HE1	1:A:47:MET:SD	2.19	0.65
1:A:249:PHE:O	1:A:257:ARG:NH1	2.31	0.64
1:A:44[A]:HIS:ND1	2:A:501:FAD:C7M	2.61	0.63
1:B:53[B]:HIS:HD2	4:B:635:HOH:O	1.80	0.63
1:A:391:PRO:O	2:A:501:FAD:H1'2	1.98	0.63
2:A:501:FAD:H3'	2:A:501:FAD:C9	2.28	0.63
1:A:183:LYS:HE3	1:A:207:ASP:OD2	1.99	0.62
1:B:246:ILE:HB	1:B:366:ARG:HH22	1.64	0.61
1:A:173:PHE:C	1:A:173:PHE:CD1	2.78	0.60
2:B:501:FAD:C9	2:B:501:FAD:H3'	2.31	0.60
1:A:305:MET:HE3	1:A:313:PHE:CD1	2.36	0.60
1:B:74:LEU:CD1	1:B:95:LEU:HD11	2.32	0.59
1:B:348:GLU:HA	1:B:351:GLN:HB2	1.84	0.58
1:B:247:ASP:OD1	1:B:366:ARG:NH2	2.37	0.57
1:A:37:GLN:HG3	2:A:501:FAD:C2A	2.34	0.57
1:A:183:LYS:CE	1:A:207:ASP:OD2	2.54	0.56
1:A:380:ASN:N	1:A:382:GLU:OE1	2.39	0.56
1:B:74:LEU:HD11	1:B:95:LEU:HD21	1.87	0.55
1:A:58:PHE:HB2	1:A:74:LEU:HD22	1.88	0.55
1:A:249:PHE:CE2	1:A:257:ARG:HD2	2.42	0.55
1:A:305:MET:HE1	1:A:313:PHE:CE1	2.42	0.55
1:A:367:ASN:HD22	1:A:406:GLU:CD	2.14	0.55
1:A:253:PRO:HB2	1:A:256:LYS:HB2	1.88	0.54
1:B:305:MET:CE	1:B:313:PHE:CE1	2.91	0.54
1:A:83:LYS:NZ	1:A:99:GLU:OE2	2.40	0.54
1:A:8:PHE:HA	1:A:151:ARG:O	2.07	0.53
1:A:370:ILE:HD11	1:A:378:VAL:HB	1.91	0.53
1:A:44[A]:HIS:CE1	1:A:47:MET:SD	3.02	0.52
1:A:305:MET:HE3	1:A:313:PHE:CE1	2.44	0.52
1:B:287[B]:GLN:O	1:B:287[B]:GLN:HG3	2.07	0.51
1:A:253:PRO:HD3	1:A:257:ARG:NH1	2.26	0.51
2:B:501:FAD:H9	2:B:501:FAD:H3'	1.90	0.51
1:B:416:GLU:H	1:B:416:GLU:CD	2.18	0.51
1:A:44[A]:HIS:CE1	2:A:501:FAD:HM71	2.46	0.51
1:A:268:TYR:CD1	1:A:388:PHE:HB2	2.46	0.51
1:A:151:ARG:HG2	1:A:375:GLN:CB	2.42	0.50
1:B:53[B]:HIS:CD2	4:B:626:HOH:O	2.63	0.50
1:B:34:PHE:HB2	1:B:114:LEU:HD23	1.92	0.49
1:A:172:ARG:HG3	1:B:141:SER:HB2	1.95	0.49
1:A:230:PRO:HA	1:A:271:ILE:O	2.13	0.49
1:B:385:THR:HG23	1:B:386:HIS:ND1	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:MET:CE	1:A:313:PHE:HE1	2.23	0.49
1:B:167:GLN:N	1:B:168:PRO:HD2	2.28	0.49
1:B:368:TYR:CE2	1:B:399:ARG:HG3	2.48	0.49
1:A:389:VAL:CG1	1:A:395:MET:CG	2.90	0.49
1:A:389:VAL:CG1	1:A:395:MET:HG3	2.42	0.49
1:A:44[A]:HIS:CE1	2:A:501:FAD:C7M	2.96	0.49
1:A:47:MET:HE2	1:A:176:SER:OG	2.13	0.49
1:B:61:ASP:OD1	1:B:61:ASP:C	2.55	0.48
2:B:501:FAD:C3'	2:B:501:FAD:C9	2.89	0.48
1:A:357:ASP:O	1:A:359:LYS:N	2.46	0.48
1:B:11:ILE:O	1:B:35:LEU:O	2.31	0.48
1:A:123:VAL:O	1:A:349:GLY:HA3	2.14	0.47
2:B:501:FAD:H9	2:B:501:FAD:O3'	2.15	0.47
1:B:213:ASP:OD1	1:B:213:ASP:N	2.39	0.47
1:A:22:CYS:HA	1:A:111:LEU:HD21	1.97	0.47
1:B:199:GLN:O	1:B:203:GLU:HG3	2.14	0.46
1:B:78:MET:HG3	1:B:83:LYS:HG3	1.98	0.46
1:B:246:ILE:HD11	1:B:389:VAL:HG21	1.97	0.46
1:A:151:ARG:HG2	1:A:375:GLN:HA	1.98	0.46
1:B:287[A]:GLN:O	1:B:287[A]:GLN:HG3	2.15	0.46
1:A:74:LEU:HD13	1:A:95:LEU:HD11	1.98	0.45
1:B:380:ASN:ND2	2:B:501:FAD:O4'	2.49	0.45
1:A:241:THR:O	1:A:241:THR:OG1	2.19	0.45
1:B:74:LEU:HD21	1:B:78:MET:CE	2.47	0.45
1:B:41:PHE:CE2	1:B:43:TRP:HB2	2.52	0.45
1:A:78:MET:SD	1:A:83:LYS:HD2	2.57	0.44
1:B:175[A]:HIS:O	1:B:176:SER:C	2.60	0.44
1:B:269:LYS:HE3	3:B:502:NAP:O2A	2.16	0.44
1:A:123:VAL:HG22	1:A:134:VAL:HG22	1.99	0.44
1:B:312:GLU:OE1	1:B:329:ARG:HD3	2.16	0.44
1:A:47:MET:HE2	1:A:176:SER:CB	2.48	0.44
1:B:241:THR:O	1:B:241:THR:HG22	2.18	0.44
1:A:36:ASP:HB3	1:A:116:TRP:CE3	2.53	0.44
1:A:44[A]:HIS:CE1	1:A:47:MET:CE	3.01	0.44
1:B:74:LEU:HD21	1:B:78:MET:HE3	2.00	0.43
2:B:501:FAD:C5X	3:B:502:NAP:C2N	2.96	0.43
1:A:392:ASP:HA	2:A:501:FAD:O2	2.18	0.43
1:B:47:MET:HE2	1:B:176:SER:HB2	2.00	0.43
1:B:195:LEU:HD22	1:B:195:LEU:HA	1.88	0.43
1:A:38:ASN:OD1	2:A:501:FAD:O2B	2.27	0.43
1:A:408:THR:CG2	1:A:410:ARG:HG3	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:ARG:HD2	3:B:502:NAP:O7N	2.18	0.43
1:B:37:GLN:HB3	2:B:501:FAD:C2A	2.48	0.43
1:A:151:ARG:HG2	1:A:375:GLN:CA	2.48	0.43
1:B:80:GLN:HA	1:B:80:GLN:OE1	2.19	0.43
1:B:286:LYS:HB3	1:B:292:LEU:HD21	2.01	0.42
1:B:368:TYR:CZ	1:B:399:ARG:HG3	2.54	0.42
1:B:43:TRP:HE1	2:B:501:FAD:H5'1	1.83	0.42
1:A:250:HIS:HE1	4:A:612:HOH:O	2.02	0.42
1:B:351:GLN:HG3	1:B:356:TRP:CZ2	2.54	0.42
1:A:249:PHE:CD2	1:A:257:ARG:HD2	2.54	0.42
1:B:307:TRP:CE3	1:B:312:GLU:O	2.72	0.42
1:A:408:THR:HG22	1:A:410:ARG:H	1.84	0.42
1:A:39:PRO:HG2	1:B:129:LEU:HD22	2.02	0.41
1:A:167:GLN:N	1:A:168:PRO:HD2	2.35	0.41
1:A:382:GLU:OE2	1:A:390:THR:HB	2.20	0.41
1:B:205:TYR:CE1	1:B:221:TRP:HB2	2.56	0.41
1:B:268:TYR:CD1	1:B:388:PHE:HB2	2.55	0.41
1:A:221:TRP:O	1:A:296:LEU:HA	2.20	0.41
1:A:257:ARG:O	1:A:261:ASN:ND2	2.54	0.41
1:B:239:GLU:OE1	1:B:422:GLN:HG2	2.21	0.41
1:A:44[A]:HIS:ND1	2:A:501:FAD:HM73	2.34	0.41
1:B:9:ILE:HD12	1:B:149:ALA:HB2	2.03	0.41
1:B:37:GLN:OE1	2:B:501:FAD:C4A	2.69	0.41
1:B:47:MET:SD	2:B:501:FAD:HM72	2.61	0.41
1:B:353:ARG:HH11	1:B:353:ARG:HG2	1.86	0.41
1:A:7:ASP:O	1:A:151:ARG:HB2	2.20	0.41
1:A:335:MET:HE2	1:A:335:MET:HB2	1.90	0.41
1:B:317:LEU:HD12	1:B:326:TYR:CE2	2.55	0.41
1:B:418:GLN:O	1:B:418:GLN:CG	2.67	0.41
1:A:212:ILE:HG21	1:A:212:ILE:HD13	1.83	0.40
1:A:368:TYR:CE2	1:A:399:ARG:HG3	2.56	0.40
1:B:404:LEU:HD23	1:B:404:LEU:HA	1.91	0.40
1:A:44[A]:HIS:CE1	1:A:47:MET:HE3	2.56	0.40
1:B:280:TYR:CD1	1:B:280:TYR:C	2.99	0.40
1:A:205:TYR:CE1	1:A:219:LEU:HG	2.56	0.40
1:A:338:GLY:C	1:A:339:TYR:CD1	3.00	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	428/433 (99%)	395 (92%)	30 (7%)	3 (1%)	18	47
1	B	428/433 (99%)	407 (95%)	21 (5%)	0	100	100
All	All	856/866 (99%)	802 (94%)	51 (6%)	3 (0%)	30	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	358	GLU
1	A	254	ALA
1	A	165	CYS

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	381/381 (100%)	359 (94%)	22 (6%)	18	49
1	B	381/381 (100%)	360 (94%)	21 (6%)	19	51
All	All	762/762 (100%)	719 (94%)	43 (6%)	18	50

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	THR
1	A	109	GLU
1	A	115	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	140	VAL
1	A	156	THR
1	A	167	GLN
1	A	171	GLU
1	A	174	VAL
1	A	177	SER
1	A	256	LYS
1	A	267	LEU
1	A	304	ASP
1	A	310	GLU
1	A	320	GLN
1	A	350	ILE
1	A	353	ARG
1	A	369	SER
1	A	382	GLU
1	A	390	THR
1	A	402	VAL
1	A	408	THR
1	A	410	ARG
1	B	4	THR
1	B	45	THR
1	B	55	GLN
1	B	56	THR
1	B	109	GLU
1	B	120	VAL
1	B	153	VAL
1	B	181	LEU
1	B	194	VAL
1	B	195	LEU
1	B	244	GLU
1	B	259	GLU
1	B	314	GLU
1	B	317	LEU
1	B	319	GLN
1	B	353	ARG
1	B	390	THR
1	B	402	VAL
1	B	416	GLU
1	B	422	GLN
1	B	430	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	144	GLN
1	A	295	ASN
1	A	320	GLN
1	B	31	ASN
1	B	44	HIS
1	B	55	GLN
1	B	272	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	A	501	-	58,58,58	2.29	14 (24%)	85,89,89	1.96	26 (30%)
2	FAD	B	501	-	58,58,58	2.10	16 (27%)	85,89,89	2.27	37 (43%)
3	NAP	A	502	-	50,52,52	1.44	7 (14%)	71,80,80	1.94	21 (29%)
3	NAP	B	502	-	50,52,52	1.68	9 (18%)	71,80,80	1.83	21 (29%)

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	501	-	-	14/34/50/50	0/6/6/6
2	FAD	B	501	-	-	13/34/50/50	0/6/6/6
3	NAP	A	502	-	-	17/35/67/67	0/5/5/5
3	NAP	B	502	-	-	7/35/67/67	0/5/5/5

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FAD	PA-O3P	9.12	1.69	1.59
2	A	501	FAD	P-O3P	6.55	1.66	1.59
2	B	501	FAD	C9A-C5X	6.30	1.51	1.41
2	A	501	FAD	C9A-C5X	5.79	1.50	1.41
2	B	501	FAD	C1'-C2'	5.41	1.60	1.52
2	B	501	FAD	PA-O3P	5.31	1.65	1.59
3	B	502	NAP	C5A-C4A	5.14	1.48	1.39
2	A	501	FAD	C5A-C4A	5.05	1.48	1.39
3	A	502	NAP	C5A-C4A	4.97	1.48	1.39
3	B	502	NAP	PA-O3	4.70	1.64	1.59
3	B	502	NAP	PN-O3	4.04	1.63	1.59
2	B	501	FAD	C5A-C4A	4.04	1.46	1.39
2	B	501	FAD	P-O3P	3.98	1.63	1.59
3	B	502	NAP	O4D-C1D	3.76	1.45	1.40
2	B	501	FAD	C10-N10	3.70	1.45	1.37
3	A	502	NAP	C8A-N7A	3.42	1.38	1.31
2	B	501	FAD	C8-C7	3.33	1.49	1.40
2	A	501	FAD	C8-C7	3.21	1.48	1.40
2	A	501	FAD	C2'-C3'	3.17	1.59	1.53
2	A	501	FAD	C8A-N7A	3.09	1.37	1.31
2	B	501	FAD	O2B-C2B	2.99	1.50	1.43
3	B	502	NAP	C5A-C6A	2.96	1.49	1.41
2	A	501	FAD	C10-N10	2.90	1.43	1.37
2	B	501	FAD	C4X-C10	2.88	1.52	1.44
2	A	501	FAD	C1'-C2'	2.88	1.56	1.52
2	B	501	FAD	C5A-N7A	-2.81	1.33	1.39
2	B	501	FAD	C4X-N5	2.81	1.36	1.30
2	A	501	FAD	C4X-C10	2.78	1.52	1.44
2	A	501	FAD	C4X-N5	2.71	1.36	1.30
3	B	502	NAP	C8A-N7A	2.63	1.36	1.31
2	B	501	FAD	C2'-C3'	2.57	1.57	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	NAP	PA-O3	2.56	1.62	1.59
2	A	501	FAD	C5A-C6A	2.52	1.48	1.41
3	A	502	NAP	C5A-N7A	-2.52	1.34	1.39
2	A	501	FAD	C7M-C7	-2.49	1.46	1.51
3	A	502	NAP	C4A-N3A	2.48	1.39	1.34
2	A	501	FAD	C9-C8	-2.37	1.36	1.39
3	B	502	NAP	P2B-O2B	2.32	1.63	1.59
2	B	501	FAD	C8A-N7A	2.26	1.36	1.31
3	A	502	NAP	C4A-N9A	-2.16	1.33	1.37
2	B	501	FAD	C10-N1	2.11	1.37	1.33
3	B	502	NAP	C2N-C3N	2.11	1.42	1.39
3	B	502	NAP	C4A-N3A	2.10	1.38	1.34
2	B	501	FAD	C5A-C6A	2.03	1.46	1.41
2	B	501	FAD	C9-C8	-2.02	1.36	1.39
3	A	502	NAP	C2N-N1N	2.01	1.37	1.35

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FAD	C5A-C4A-N3A	-5.40	119.29	126.72
2	B	501	FAD	C3B-C2B-C1B	-5.22	91.59	101.46
2	B	501	FAD	C5A-C4A-N3A	-5.08	119.72	126.72
2	A	501	FAD	N3A-C4A-N9A	4.77	135.28	127.17
2	B	501	FAD	N3A-C4A-N9A	4.55	134.90	127.17
2	B	501	FAD	O2B-C2B-C1B	4.52	125.66	110.10
3	A	502	NAP	N3A-C2A-N1A	-4.51	121.76	128.58
3	A	502	NAP	C4A-N9A-C8A	4.42	110.38	105.74
2	B	501	FAD	N3A-C2A-N1A	-4.31	122.05	128.58
2	B	501	FAD	C4'-C3'-C2'	4.28	120.70	113.57
3	B	502	NAP	C4A-N9A-C8A	4.19	110.14	105.74
3	B	502	NAP	C5A-C4A-N3A	-4.06	121.12	126.72
2	A	501	FAD	C9-C8-C7	-4.04	113.75	119.69
3	A	502	NAP	N3A-C4A-N9A	3.92	133.84	127.17
3	B	502	NAP	N3A-C2A-N1A	-3.92	122.65	128.58
3	B	502	NAP	C6N-N1N-C2N	-3.85	118.61	121.88
3	B	502	NAP	N3A-C4A-N9A	3.80	133.63	127.17
2	B	501	FAD	O3B-C3B-C4B	-3.79	100.19	111.08
2	B	501	FAD	C8M-C8-C7	3.79	128.49	120.76
3	A	502	NAP	C4A-N9A-C1B	-3.73	117.91	126.63
3	A	502	NAP	C5A-C4A-N3A	-3.72	121.60	126.72
3	A	502	NAP	O3-PA-O1A	-3.71	99.54	110.70
2	A	501	FAD	C2A-N3A-C4A	3.70	120.88	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	FAD	C2A-N3A-C4A	3.69	120.84	111.83
2	B	501	FAD	C1'-C2'-C3'	3.69	119.65	109.66
2	B	501	FAD	C5X-C9A-N10	3.65	121.27	117.97
2	A	501	FAD	N3A-C2A-N1A	-3.60	123.13	128.58
2	A	501	FAD	C9A-C9-C8	3.55	126.36	119.22
2	B	501	FAD	C4A-N9A-C8A	3.55	109.46	105.74
2	B	501	FAD	C9A-C9-C8	3.55	126.35	119.22
2	A	501	FAD	C1'-C2'-C3'	3.54	119.26	109.66
2	A	501	FAD	C8M-C8-C7	3.40	127.71	120.76
3	B	502	NAP	C2A-N3A-C4A	3.34	119.99	111.83
3	B	502	NAP	C6A-C5A-N7A	3.27	138.40	132.09
2	B	501	FAD	C4X-C10-N1	-3.20	116.75	124.59
2	B	501	FAD	N9A-C8A-N7A	-3.20	109.40	113.94
2	B	501	FAD	C5A-N7A-C8A	3.17	108.44	103.45
3	A	502	NAP	C2A-N3A-C4A	3.15	119.53	111.83
2	A	501	FAD	O4B-C1B-C2B	-3.08	100.02	106.62
2	B	501	FAD	O3P-PA-O1A	3.07	119.95	110.70
2	A	501	FAD	O4B-C1B-N9A	3.06	113.96	108.09
3	A	502	NAP	N9A-C8A-N7A	-3.01	109.66	113.94
3	B	502	NAP	N9A-C8A-N7A	-3.00	109.68	113.94
3	B	502	NAP	O2B-C2B-C1B	3.00	120.60	110.05
3	B	502	NAP	C4A-N9A-C1B	-2.96	119.70	126.63
2	B	501	FAD	C9A-N10-C10	-2.92	116.30	120.75
3	B	502	NAP	C4A-C5A-N7A	-2.90	107.26	110.58
3	A	502	NAP	O4B-C4B-C3B	2.89	110.90	105.15
3	A	502	NAP	O4B-C4B-C5B	-2.85	100.20	109.33
2	B	501	FAD	C4A-C5A-N7A	-2.84	107.33	110.58
2	A	501	FAD	C4X-C10-N1	-2.83	117.64	124.59
2	A	501	FAD	C2B-C1B-N9A	2.80	120.26	113.30
2	B	501	FAD	C2B-C3B-C4B	2.79	108.00	102.61
2	A	501	FAD	O2-C2-N1	-2.78	117.18	121.80
2	A	501	FAD	C5X-C9A-N10	2.78	120.48	117.97
2	B	501	FAD	O2A-PA-O3P	-2.76	99.83	107.27
3	A	502	NAP	C5A-C6A-N6A	-2.75	116.47	123.29
2	A	501	FAD	C4A-N9A-C8A	2.74	108.62	105.74
3	B	502	NAP	C3N-C7N-N7N	2.70	121.07	117.74
3	B	502	NAP	C5A-N7A-C8A	2.69	107.68	103.45
2	B	501	FAD	C6A-C5A-N7A	2.68	137.25	132.09
3	B	502	NAP	O4B-C4B-C3B	2.65	110.42	105.15
2	B	501	FAD	C9-C8-C7	-2.61	115.86	119.69
2	A	501	FAD	C6-C7-C8	2.61	123.52	119.69
2	B	501	FAD	C4A-N9A-C1B	-2.59	120.58	126.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FAD	O3'-C3'-C2'	2.56	114.75	108.93
2	B	501	FAD	C10-N1-C2	2.50	122.27	116.85
3	A	502	NAP	C6A-C5A-N7A	2.50	136.91	132.09
2	A	501	FAD	O5B-C5B-C4B	2.49	117.46	108.99
3	A	502	NAP	O4B-C1B-N9A	2.45	112.80	108.09
3	B	502	NAP	O3B-C3B-C4B	2.44	118.10	111.08
2	B	501	FAD	C6-C5X-N5	2.44	122.50	118.44
2	A	501	FAD	C9A-N10-C10	-2.41	117.08	120.75
3	A	502	NAP	C4D-O4D-C1D	-2.40	107.72	109.92
2	A	501	FAD	O3B-C3B-C4B	-2.38	104.24	111.08
3	B	502	NAP	C2B-C3B-C4B	-2.35	96.95	101.99
2	B	501	FAD	C2B-C1B-N9A	2.32	119.07	113.30
3	A	502	NAP	O7N-C7N-N7N	2.29	125.92	122.62
2	B	501	FAD	C2A-N1A-C6A	2.26	122.45	118.73
2	A	501	FAD	C6-C5X-N5	2.25	122.18	118.44
2	A	501	FAD	N3-C2-N1	2.23	124.25	119.50
2	B	501	FAD	C8M-C8-C9	-2.23	115.64	119.57
2	B	501	FAD	C4X-C4-N3	2.22	118.92	113.25
2	B	501	FAD	O3B-C3B-C2B	2.22	118.93	111.82
2	A	501	FAD	C4X-C10-N10	2.22	119.65	116.48
2	B	501	FAD	C4X-C10-N10	2.21	119.65	116.48
3	B	502	NAP	O5D-PN-O1N	2.21	117.69	108.94
3	A	502	NAP	O4D-C4D-C3D	2.20	109.51	105.15
2	B	501	FAD	C4-N3-C2	-2.19	121.76	125.64
3	A	502	NAP	C6A-C5A-C4A	-2.17	114.21	117.18
2	A	501	FAD	O2P-P-O3P	2.16	113.12	107.27
3	A	502	NAP	O3D-C3D-C4D	2.16	117.28	111.08
3	B	502	NAP	O7N-C7N-N7N	-2.16	119.50	122.62
3	A	502	NAP	O3-PN-O1N	-2.14	104.26	110.70
2	B	501	FAD	C5'-C4'-C3'	2.14	116.25	112.22
2	B	501	FAD	C4-C4X-N5	2.14	121.16	118.21
3	B	502	NAP	O2D-C2D-C3D	2.11	118.59	111.82
2	A	501	FAD	C6A-C5A-N7A	2.10	136.14	132.09
3	A	502	NAP	C2A-N1A-C6A	2.09	122.16	118.73
3	B	502	NAP	C6A-C5A-C4A	-2.08	114.33	117.18
3	A	502	NAP	C1B-N9A-C8A	2.07	131.69	127.09
3	B	502	NAP	P2B-O2B-C2B	-2.06	117.94	123.43
2	B	501	FAD	P-O5'-C5'	2.02	132.93	121.35
2	B	501	FAD	O2B-C2B-C3B	2.02	118.28	111.82
2	A	501	FAD	C4A-C5A-N7A	-2.01	108.28	110.58

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	FAD	N10-C1'-C2'-O2'
2	A	501	FAD	N10-C1'-C2'-C3'
2	A	501	FAD	C3'-C4'-C5'-O5'
2	A	501	FAD	C5'-O5'-P-O1P
2	B	501	FAD	C5B-O5B-PA-O2A
2	B	501	FAD	N10-C1'-C2'-O2'
2	B	501	FAD	N10-C1'-C2'-C3'
2	B	501	FAD	C3'-C4'-C5'-O5'
2	B	501	FAD	O4'-C4'-C5'-O5'
2	B	501	FAD	C4'-C5'-O5'-P
2	B	501	FAD	C5'-O5'-P-O3P
3	A	502	NAP	C5B-O5B-PA-O2A
3	A	502	NAP	C5B-O5B-PA-O3
3	A	502	NAP	C5D-O5D-PN-O1N
3	A	502	NAP	C5D-O5D-PN-O2N
3	A	502	NAP	C2D-C1D-N1N-C2N
3	A	502	NAP	C2D-C1D-N1N-C6N
3	B	502	NAP	C5B-O5B-PA-O3
3	B	502	NAP	O4B-C4B-C5B-O5B
3	B	502	NAP	C5D-O5D-PN-O3
3	B	502	NAP	C3B-C4B-C5B-O5B
2	A	501	FAD	O4B-C4B-C5B-O5B
3	A	502	NAP	O4B-C4B-C5B-O5B
3	A	502	NAP	C3B-C4B-C5B-O5B
2	A	501	FAD	O4'-C4'-C5'-O5'
2	A	501	FAD	C3B-C4B-C5B-O5B
3	A	502	NAP	C4D-C5D-O5D-PN
2	A	501	FAD	C4'-C5'-O5'-P
2	A	501	FAD	PA-O3P-P-O5'
2	B	501	FAD	PA-O3P-P-O5'
3	A	502	NAP	PN-O3-PA-O5B
3	A	502	NAP	PA-O3-PN-O2N
2	A	501	FAD	C5B-O5B-PA-O3P
2	B	501	FAD	C5B-O5B-PA-O1A
3	A	502	NAP	C5D-O5D-PN-O3
3	B	502	NAP	C5B-O5B-PA-O1A
2	B	501	FAD	O4B-C4B-C5B-O5B
2	B	501	FAD	C2B-C1B-N9A-C8A
3	A	502	NAP	C2B-O2B-P2B-O2X
3	B	502	NAP	C2B-O2B-P2B-O3X
3	A	502	NAP	C3B-C2B-O2B-P2B
2	B	501	FAD	C3B-C4B-C5B-O5B

Continued on next page...

Continued from previous page...

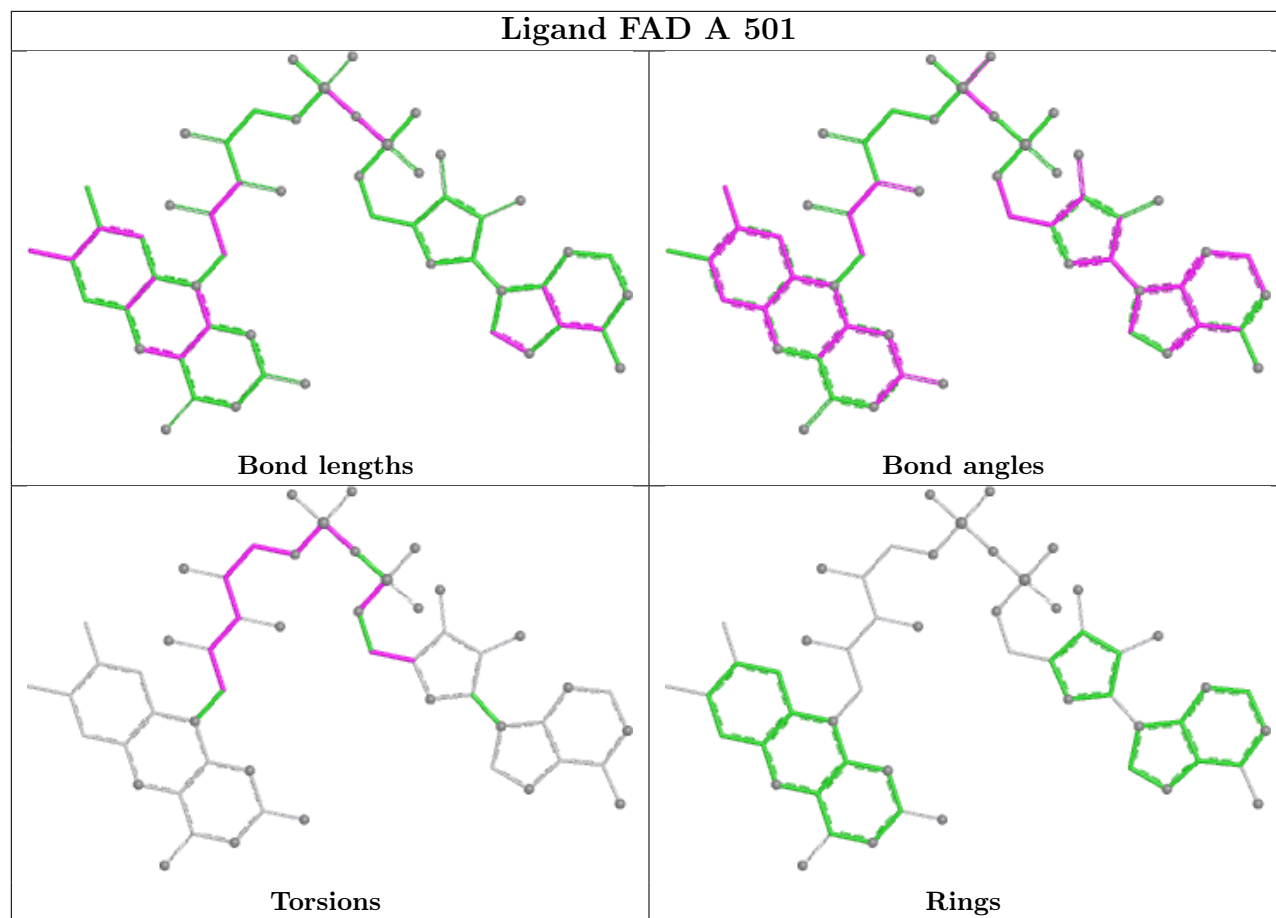
Mol	Chain	Res	Type	Atoms
3	A	502	NAP	C2B-O2B-P2B-O1X
2	A	501	FAD	O2'-C2'-C3'-O3'
2	B	501	FAD	O4B-C1B-N9A-C8A
2	A	501	FAD	C1'-C2'-C3'-O3'
2	A	501	FAD	C2'-C3'-C4'-C5'
3	A	502	NAP	C1B-C2B-O2B-P2B
3	B	502	NAP	C2B-O2B-P2B-O1X
2	A	501	FAD	PA-O3P-P-O2P
3	A	502	NAP	PA-O3-PN-O1N

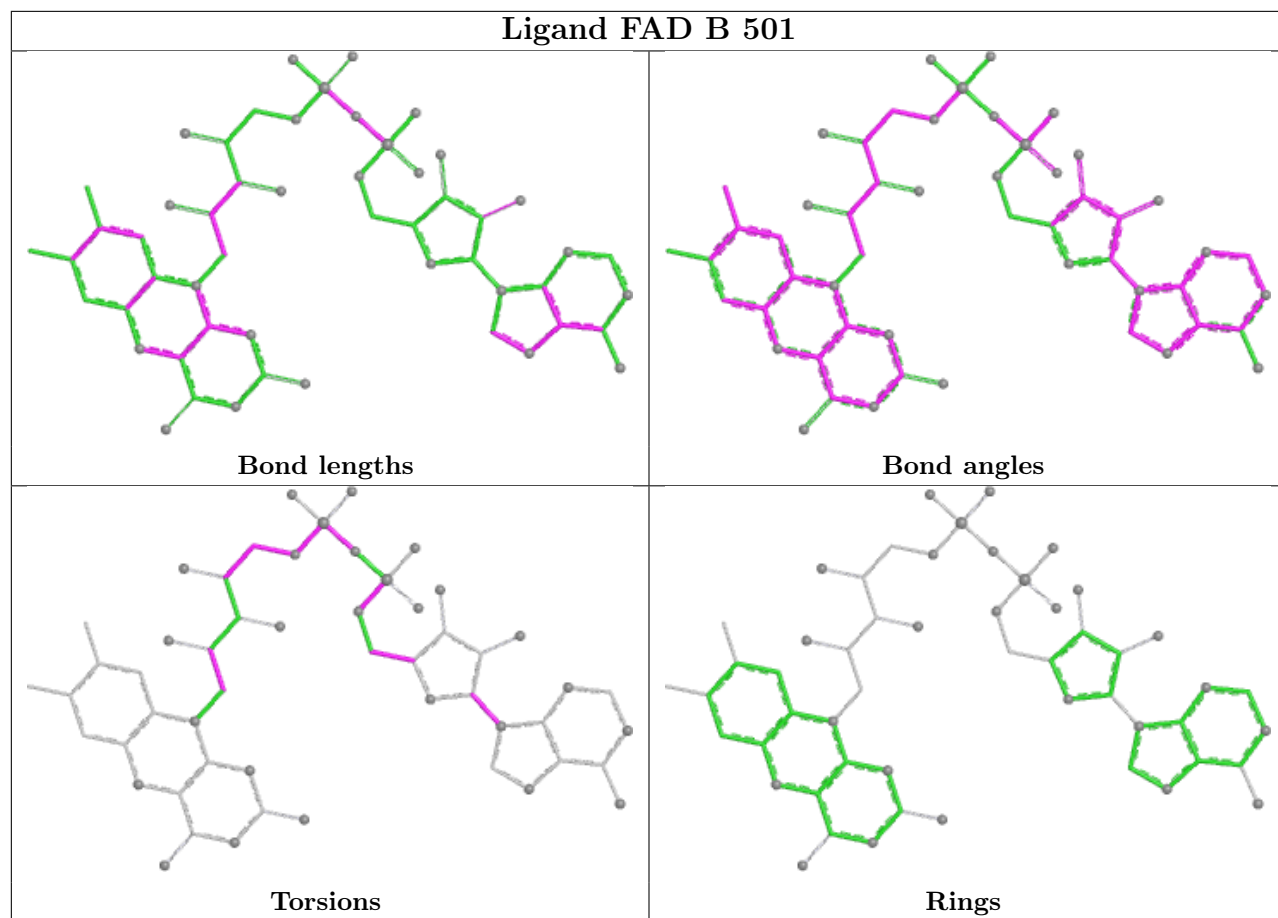
There are no ring outliers.

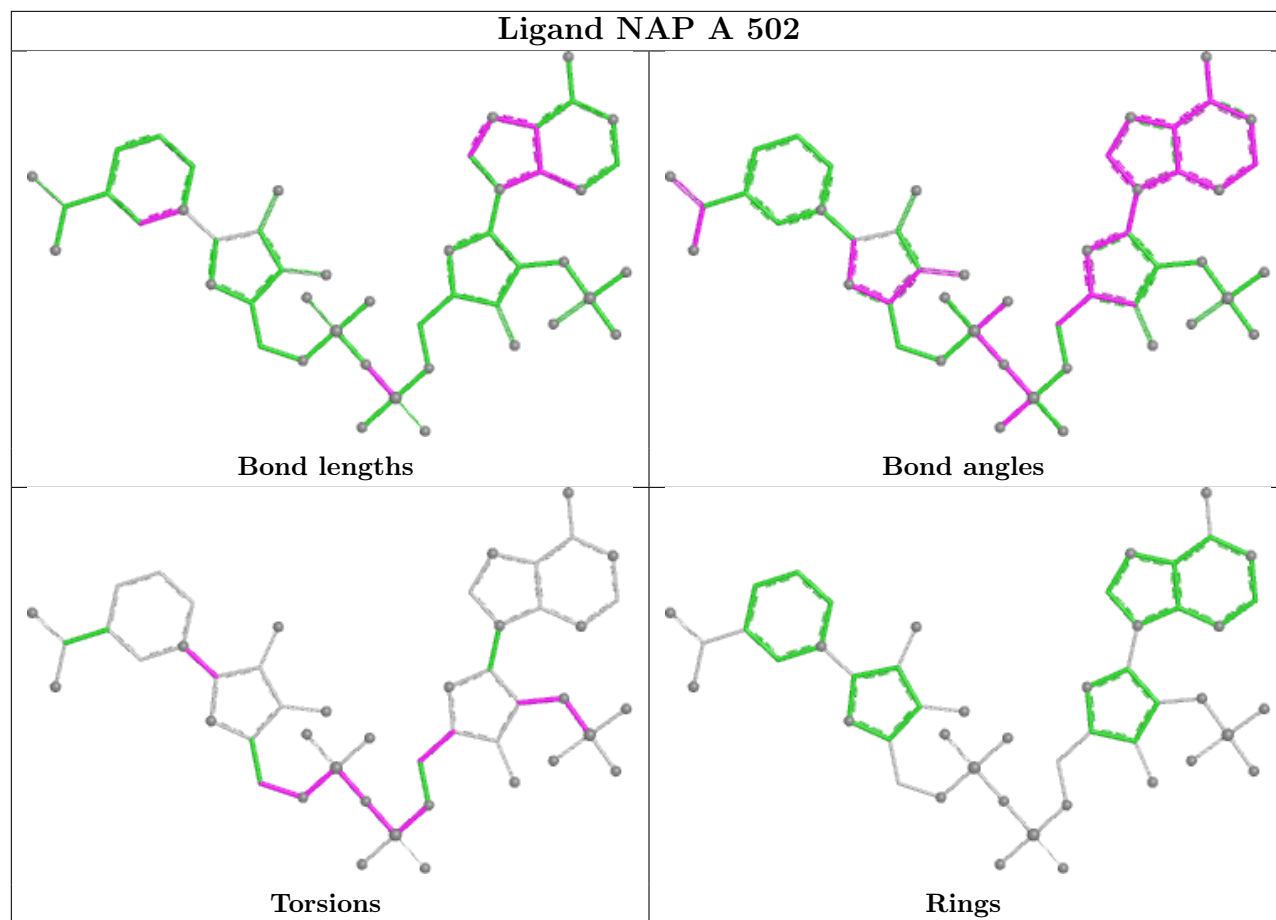
3 monomers are involved in 25 short contacts:

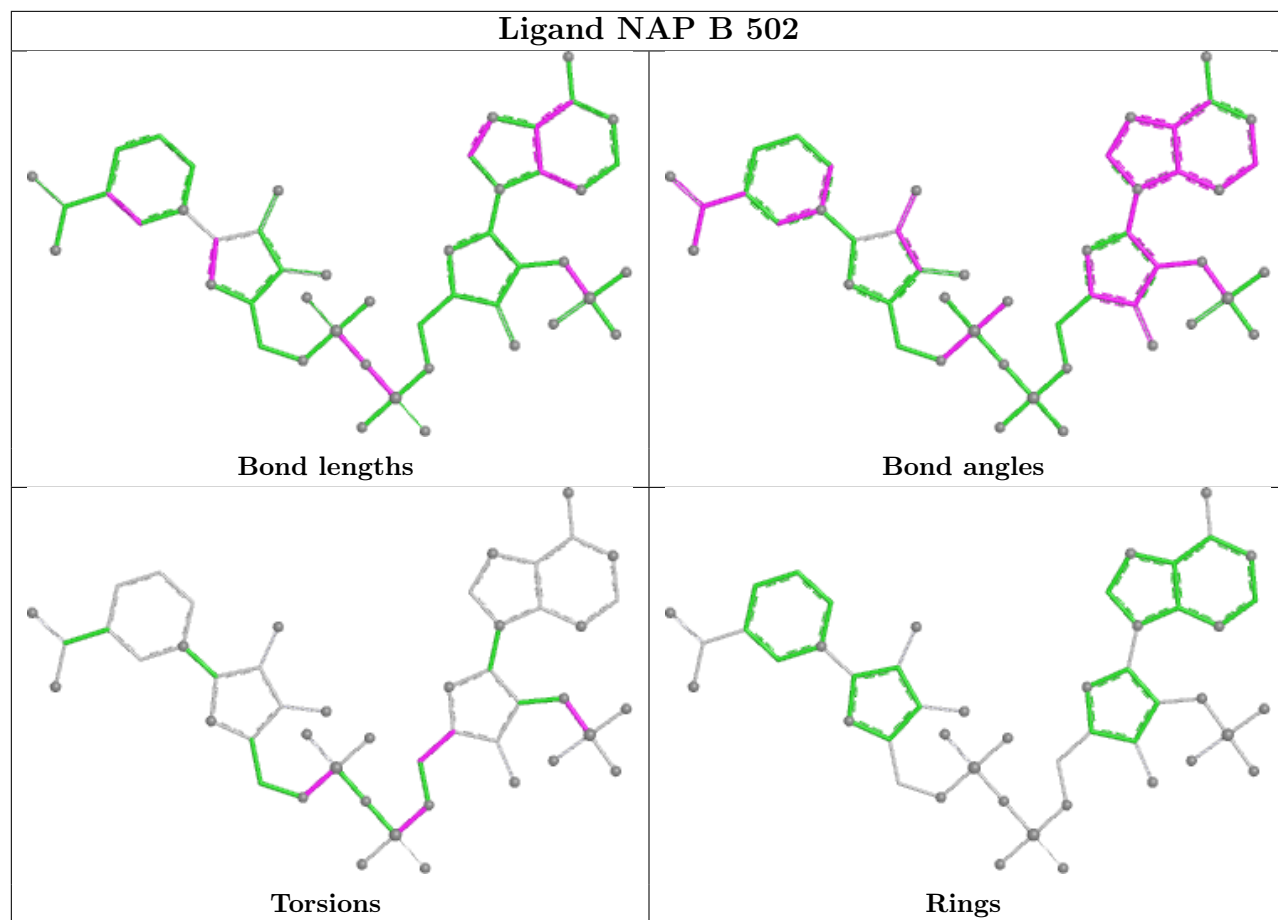
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	FAD	11	0
2	B	501	FAD	12	0
3	B	502	NAP	3	0

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	427/433 (98%)	-0.00	30 (7%)	22 16	15, 56, 126, 163	3 (0%)
1	B	427/433 (98%)	-0.20	14 (3%)	49 39	25, 57, 94, 115	3 (0%)
All	All	854/866 (98%)	-0.10	44 (5%)	33 25	15, 57, 108, 163	6 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	383	LEU	8.0
1	A	252	LEU	7.5
1	A	44[A]	HIS	7.0
1	A	254	ALA	5.5
1	A	340[A]	HIS	4.3
1	A	257	ARG	3.8
1	A	43	TRP	3.8
1	A	365	GLN	3.7
1	A	45	THR	3.5
1	B	430	MET	3.4
1	B	4	THR	3.4
1	A	389	VAL	3.4
1	A	268	TYR	3.2
1	B	181	LEU	3.1
1	A	385	THR	3.0
1	B	291	LYS	2.9
1	A	47	MET	2.9
1	A	269	LYS	2.9
1	A	262	ALA	2.9
1	B	366	ARG	2.8
1	A	46	GLY	2.8
1	A	260	LEU	2.7
1	A	250	HIS	2.7
1	A	418	GLN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	351	GLN	2.6
1	A	386	HIS	2.6
1	A	256	LYS	2.6
1	A	384	HIS	2.5
1	B	45	THR	2.5
1	A	387	GLY	2.5
1	A	263	SER	2.4
1	B	269	LYS	2.4
1	A	390	THR	2.4
1	A	291	LYS	2.4
1	A	306	ARG	2.4
1	A	366	ARG	2.3
1	B	43	TRP	2.3
1	A	391	PRO	2.2
1	B	298	THR	2.2
1	A	265	LYS	2.2
1	B	382	GLU	2.2
1	B	53[A]	HIS	2.2
1	B	185	LYS	2.2
1	B	352	GLN	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(Å ²)	Q<0.9
2	FAD	A	501	53/53	0.87	0.25	51,96,148,158	53
3	NAP	B	502	48/48	0.91	0.14	74,92,139,145	0
3	NAP	A	502	48/48	0.92	0.15	55,78,159,168	0

Continued on next page...

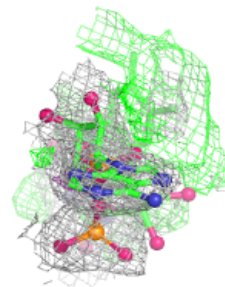
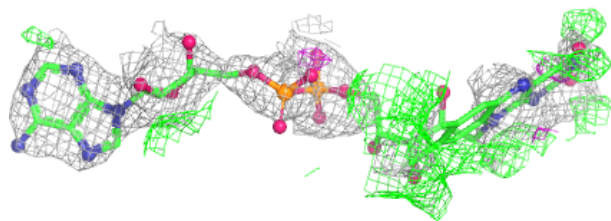
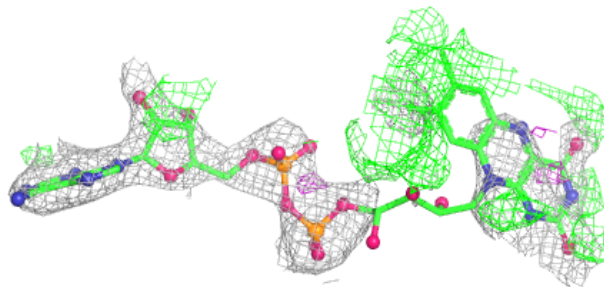
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	B	501	53/53	0.93	0.16	41,72,168,189	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.

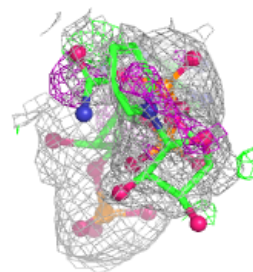
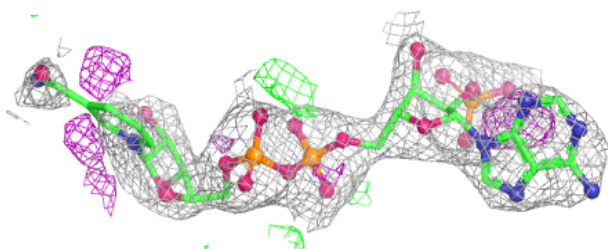
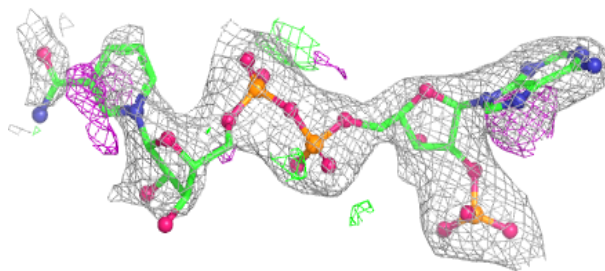
Electron density around FAD A 501:

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

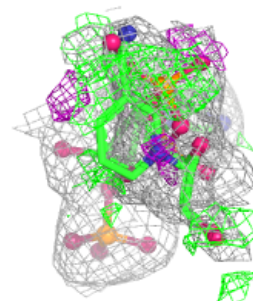
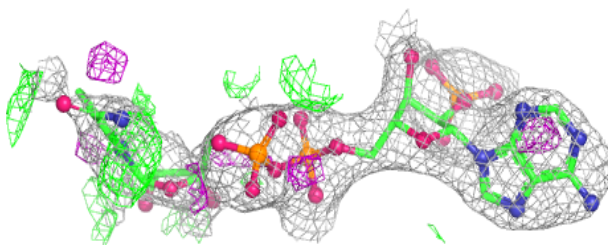
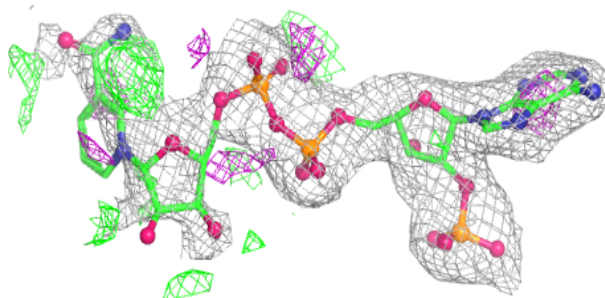


Electron density around NAP B 502:

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

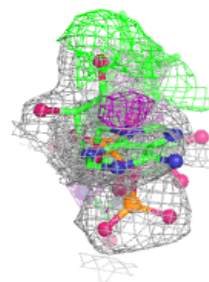
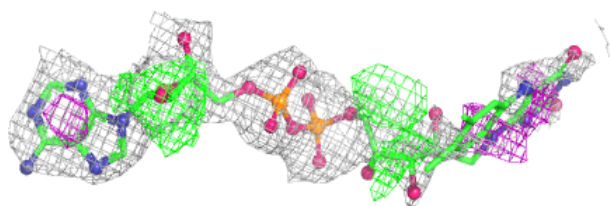
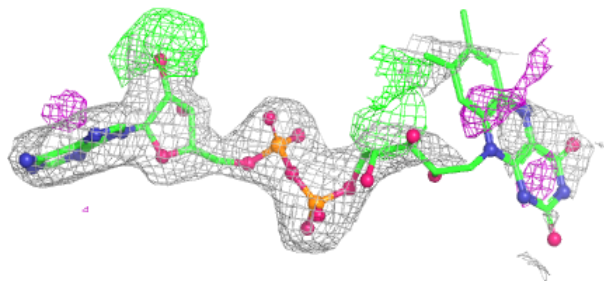
**Electron density around NAP A 502:**

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



Electron density around FAD B 501:

$2mF_o - DF_c$ (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.