



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 05:23 pm BST

PDB ID : 2XVH  
Title : Crystal structure of bacterial flavin containing monooxygenase in complex with NADP  
Authors : Cho, H.J.; Kang, B.S.  
Deposited on : 2010-10-26  
Resolution : 2.54 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (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

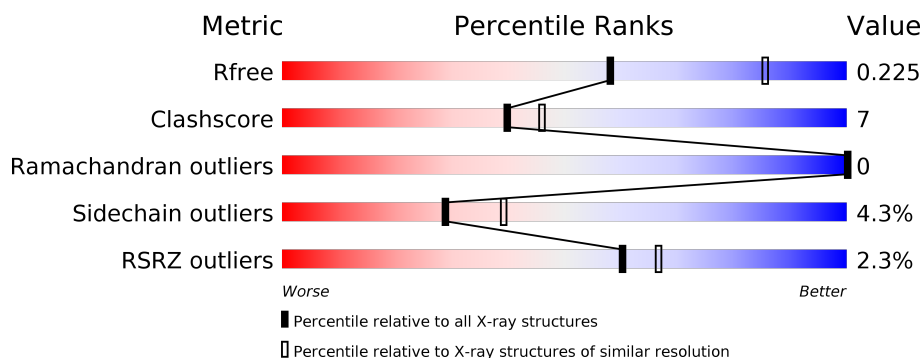
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.54 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	464	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 16%, green 78%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>78%</span> <span>16%</span> <span>• •</span> </div> </div>
1	B	464	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 14%, green 80%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>80%</span> <span>14%</span> <span>• •</span> </div> </div>
1	C	464	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, orange 1%, yellow 15%, green 80%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>5%</span> <span>80%</span> <span>15%</span> <span>• •</span> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11325 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 FLAVIN-CONTAINING MONOOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	0	0
			3637	2333	602	682	20			
1	B	445	Total	C	N	O	S	0	1	0
			3624	2325	599	680	20			
1	C	446	Total	C	N	O	S	0	1	0
			3544	2265	587	672	20			

There are 24 discrepancies between the modelled and reference sequences:

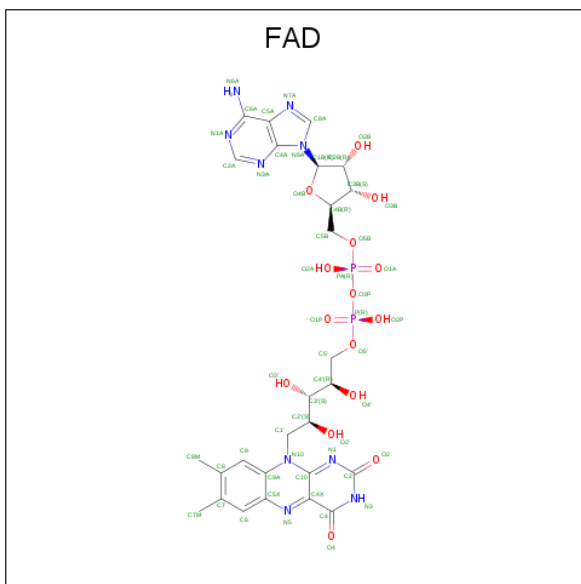
Chain	Residue	Modelled	Actual	Comment	Reference
A	457	LEU	-	expression tag	UNP Q83XK4
A	458	GLU	-	expression tag	UNP Q83XK4
A	459	HIS	-	expression tag	UNP Q83XK4
A	460	HIS	-	expression tag	UNP Q83XK4
A	461	HIS	-	expression tag	UNP Q83XK4
A	462	HIS	-	expression tag	UNP Q83XK4
A	463	HIS	-	expression tag	UNP Q83XK4
A	464	HIS	-	expression tag	UNP Q83XK4
B	457	LEU	-	expression tag	UNP Q83XK4
B	458	GLU	-	expression tag	UNP Q83XK4
B	459	HIS	-	expression tag	UNP Q83XK4
B	460	HIS	-	expression tag	UNP Q83XK4
B	461	HIS	-	expression tag	UNP Q83XK4
B	462	HIS	-	expression tag	UNP Q83XK4
B	463	HIS	-	expression tag	UNP Q83XK4
B	464	HIS	-	expression tag	UNP Q83XK4
C	457	LEU	-	expression tag	UNP Q83XK4
C	458	GLU	-	expression tag	UNP Q83XK4
C	459	HIS	-	expression tag	UNP Q83XK4
C	460	HIS	-	expression tag	UNP Q83XK4
C	461	HIS	-	expression tag	UNP Q83XK4
C	462	HIS	-	expression tag	UNP Q83XK4
C	463	HIS	-	expression tag	UNP Q83XK4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	464	HIS	-	expression tag	UNP Q83XK4

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$ ).



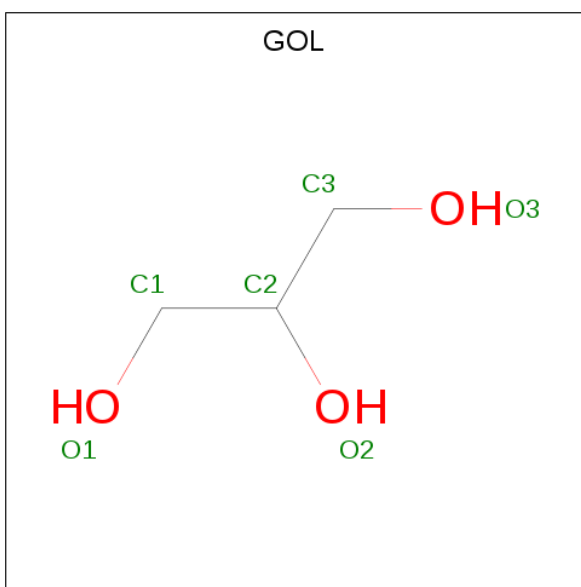
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	C	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula:  $\text{C}_{21}\text{H}_{28}\text{N}_7\text{O}_{17}\text{P}_3$ ).



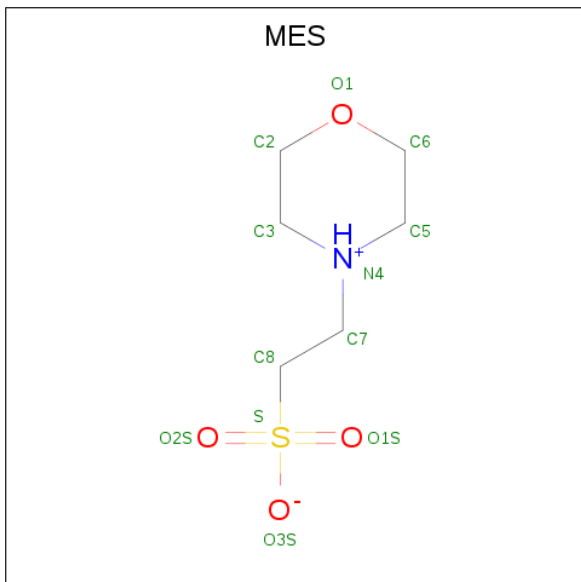
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	C	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).



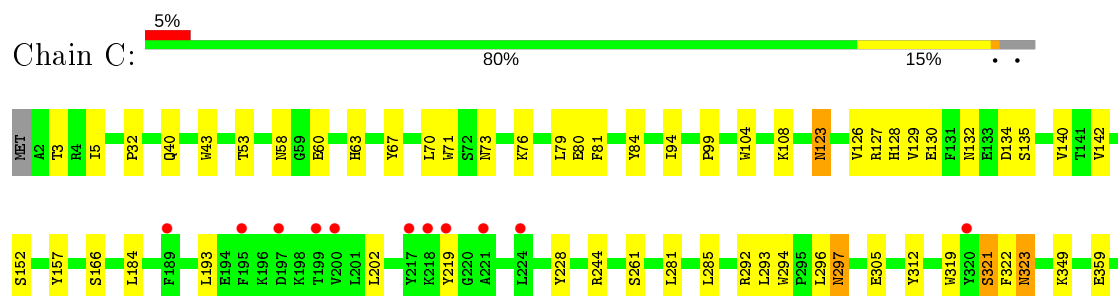
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

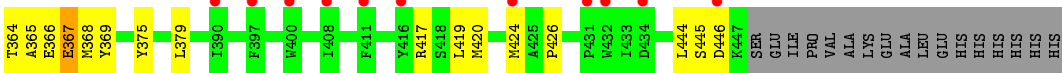
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	59	Total	O	0	0
			59	59		
6	B	84	Total	O	0	0
			84	84		
6	C	56	Total	O	0	0
			56	56		



- Molecule 1: FLAVIN-CONTAINING MONOOXYGENASE







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	159.21Å 71.14Å 141.36Å 90.00° 90.05° 90.00°	Depositor
Resolution (Å)	50.01 – 2.54 47.83 – 2.54	Depositor EDS
% Data completeness (in resolution range)	98.4 (50.01-2.54) 93.0 (47.83-2.54)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	307.43 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, $R_{free}$	0.184 , 0.226 0.184 , 0.225	Depositor DCC
$R_{free}$ test set	2482 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.4	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 35.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11325	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.63	2/3751 (0.1%)	0.57	0/5098
1	B	0.64	4/3741 (0.1%)	0.59	0/5089
1	C	0.60	1/3655 (0.0%)	0.58	0/4982
All	All	0.63	7/11147 (0.1%)	0.58	0/15169

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	320	TYR	CD1-CE1	-7.51	1.28	1.39
1	B	67	TYR	CE2-CZ	-6.80	1.29	1.38
1	B	67	TYR	CD1-CE1	-5.85	1.30	1.39
1	B	69	TYR	CD2-CE2	-5.84	1.30	1.39
1	B	68	ARG	CG-CD	-5.33	1.38	1.51
1	C	321	SER	CB-OG	-5.28	1.35	1.42
1	A	280	PHE	CD1-CE1	-5.15	1.28	1.39

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	3637	0	3395	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3624	0	3365	63	0
1	C	3544	0	3222	46	0
2	A	53	0	31	2	0
2	B	53	0	31	2	0
2	C	53	0	31	0	0
3	A	48	0	25	4	0
3	B	48	0	25	1	0
3	C	48	0	25	2	0
4	B	6	0	8	1	0
5	C	12	0	12	0	0
6	A	59	0	0	1	0
6	B	84	0	0	2	0
6	C	56	0	0	1	0
All	All	11325	0	10170	155	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 7.

All (155) 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:68:ARG:HH11	1:B:68:ARG:HG2	0.97	1.09
1:B:68:ARG:HH11	1:B:68:ARG:CG	1.84	0.91
1:C:58:ASN:HD21	1:C:123:ASN:HD21	1.19	0.90
1:B:383:THR:HG22	1:B:385:TYR:H	1.35	0.90
1:B:365:ALA:HA	1:B:368:MET:HE2	1.54	0.89
1:C:79:LEU:HD12	1:C:79:LEU:C	1.94	0.88
1:B:68:ARG:HG2	1:B:68:ARG:NH1	1.68	0.82
1:B:15:MET:HE1	1:B:44:GLY:N	2.02	0.75
1:C:80:GLU:HG2	1:C:420:MET:HG3	1.67	0.74
1:B:383:THR:CG2	1:B:385:TYR:H	2.00	0.73
1:B:319:TRP:CZ2	1:B:368:MET:HE3	2.26	0.71
1:B:233:MET:HE2	1:B:237:TRP:CZ2	2.28	0.69
1:B:122:PHE:HB2	4:B:1448:GOL:H11	1.73	0.69
1:C:60:GLU:OE2	1:C:127:ARG:NH2	2.24	0.69
1:A:226:SER:HB2	1:A:243:GLU:HG2	1.74	0.69
1:A:43:TRP:CH2	1:A:111:VAL:HG12	2.28	0.68
1:A:60:GLU:OE2	1:A:127:ARG:NH2	2.27	0.68
1:A:43:TRP:CZ3	1:A:111:VAL:CG1	2.78	0.67
1:B:233:MET:CE	1:B:237:TRP:CZ2	2.79	0.66
1:C:58:ASN:HD21	1:C:123:ASN:ND2	1.91	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:THR:HG22	1:B:385:TYR:N	2.10	0.66
1:C:445:SER:OG	1:C:446:ASP:N	2.29	0.65
1:A:376:ILE:O	1:A:380:ILE:HG12	1.96	0.65
1:A:445:SER:OG	1:A:446:ASP:N	2.30	0.64
1:C:79:LEU:CD1	1:C:79:LEU:C	2.67	0.64
1:B:60:GLU:OE2	1:B:127:ARG:NH2	2.30	0.64
1:C:305:GLU:OE1	1:C:349:LYS:HE2	1.98	0.64
1:A:251:ASP:OD1	1:A:252:THR:N	2.30	0.63
1:A:296:LEU:O	1:A:297:ASN:HB2	1.99	0.63
1:C:73:ASN:HB3	3:C:1450:NAP:N7N	2.14	0.62
1:B:408:ILE:HG23	1:B:409:MET:CE	2.29	0.62
1:A:67:TYR:OH	3:A:1449:NAP:H4N	2.01	0.60
1:A:103:LEU:O	1:A:107:ILE:HD13	2.01	0.60
1:C:321:SER:OG	1:C:322:PHE:N	2.33	0.60
1:C:244:ARG:NH2	1:C:261:SER:OG	2.37	0.58
1:B:408:ILE:HG23	1:B:409:MET:HE3	1.86	0.57
1:A:95:ALA:HB3	1:A:443:TYR:OH	2.05	0.56
1:B:177[B]:GLU:CD	1:B:177[B]:GLU:H	2.07	0.56
1:A:43:TRP:CH2	1:A:111:VAL:CG1	2.89	0.56
1:A:107:ILE:HD11	1:A:322:PHE:CE2	2.42	0.55
1:A:227:CYS:HA	1:A:244:ARG:O	2.06	0.55
1:B:290:ASN:ND2	6:B:2067:HOH:O	2.39	0.54
1:B:40:GLN:NE2	6:B:2007:HOH:O	2.40	0.54
1:C:375:TYR:CZ	1:C:379:LEU:HD11	2.42	0.54
1:C:71:TRP:HA	1:C:99:PRO:HA	1.90	0.54
1:C:128:HIS:NE2	1:C:130:GLU:HG3	2.22	0.54
1:B:290:ASN:H	1:B:290:ASN:HD22	1.55	0.54
1:B:70:LEU:HD11	2:B:1447:FAD:H6	1.90	0.53
1:A:71:TRP:HA	1:A:99:PRO:HA	1.90	0.53
1:B:244:ARG:NH1	1:B:261:SER:OG	2.42	0.53
1:B:330:TRP:HB3	1:B:383:THR:HG21	1.90	0.53
1:B:293:LEU:HD11	1:B:368:MET:HG2	1.91	0.52
1:B:319:TRP:HZ2	1:B:368:MET:HE3	1.70	0.52
1:A:82:ALA:HA	1:A:420:MET:CE	2.40	0.52
1:B:28:GLY:HA2	1:C:296:LEU:HD11	1.92	0.52
1:C:79:LEU:HD12	1:C:79:LEU:O	2.10	0.51
1:C:104:TRP:CE2	1:C:108:LYS:HD2	2.45	0.51
1:A:299:TYR:HB3	1:A:303:VAL:HB	1.93	0.51
1:B:233:MET:HE3	1:B:237:TRP:CZ2	2.46	0.51
1:A:5:ILE:HD11	1:A:336:ILE:HG21	1.93	0.50
1:C:364:THR:OG1	1:C:367:GLU:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:ASN:ND2	1:C:323:ASN:H	2.08	0.50
1:A:82:ALA:HA	1:A:420:MET:HE2	1.93	0.50
1:B:67:TYR:OH	3:B:1449:NAP:H4N	2.11	0.50
1:B:233:MET:HE2	1:B:237:TRP:HZ2	1.76	0.50
1:B:290:ASN:H	1:B:290:ASN:ND2	2.09	0.50
1:C:292:ARG:HD3	1:C:359:GLU:OE2	2.12	0.49
1:A:251:ASP:OD1	1:A:251:ASP:C	2.52	0.48
1:B:299:TYR:HB3	1:B:303:VAL:HB	1.94	0.48
1:C:228:TYR:CD2	1:C:244:ARG:O	2.65	0.48
1:C:73:ASN:ND2	3:C:1450:NAP:H2N	2.28	0.48
1:C:76:LYS:HE2	1:C:94:ILE:HG13	1.95	0.48
1:B:10:ALA:O	1:B:15:MET:HE2	2.12	0.48
1:B:211:ASP:O	1:B:215:GLN:HG2	2.14	0.48
1:A:282:ASN:O	1:A:286:ARG:HB2	2.13	0.48
1:C:126:VAL:HA	1:C:142:VAL:HG12	1.95	0.47
1:B:408:ILE:HG23	1:B:409:MET:HE2	1.96	0.47
1:C:79:LEU:CD1	1:C:79:LEU:O	2.62	0.47
1:B:182:ARG:NH1	1:B:194:GLU:OE1	2.37	0.47
1:C:293:LEU:HD21	1:C:319:TRP:CD1	2.50	0.47
1:A:94:ILE:O	1:A:426:PRO:HD2	2.14	0.47
1:C:5:ILE:HG13	1:C:157:TYR:HB2	1.95	0.47
1:A:84:TYR:CE2	1:A:89:HIS:HB2	2.50	0.46
1:C:366:GLU:HA	1:C:369:TYR:CE2	2.50	0.46
1:C:444:LEU:HD23	1:C:444:LEU:HA	1.54	0.46
1:B:365:ALA:HA	1:B:368:MET:CE	2.34	0.46
1:C:81:PHE:HB2	1:C:84:TYR:O	2.16	0.46
1:B:17:GLN:HE21	1:B:159:VAL:HG11	1.80	0.46
1:B:319:TRP:CZ2	1:B:368:MET:CE	2.99	0.46
1:A:124:THR:CG2	1:A:142:VAL:HG13	2.46	0.46
1:B:324:MET:O	1:B:328:GLN:HG3	2.15	0.46
1:B:15:MET:HE1	1:B:44:GLY:CA	2.45	0.46
1:C:297:ASN:O	1:C:305:GLU:HG3	2.16	0.45
1:A:124:THR:HG23	1:A:142:VAL:HG13	1.99	0.45
1:C:67:TYR:CZ	1:C:70:LEU:HD12	2.51	0.45
1:B:129:VAL:HB	1:B:281:LEU:HD23	1.97	0.45
1:A:164:HIS:HD2	6:A:2014:HOH:O	1.99	0.45
1:B:17:GLN:HA	1:B:329:ALA:HB1	1.98	0.45
1:B:65:SER:HB2	2:B:1447:FAD:HM82	1.98	0.45
1:A:17:GLN:HA	1:A:329:ALA:HB1	1.97	0.45
1:B:5:ILE:HD12	1:B:157:TYR:HB2	1.98	0.45
1:C:58:ASN:ND2	1:C:123:ASN:HD21	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:TYR:HH	1:B:400:TRP:HD1	1.66	0.44
1:A:272:THR:HA	3:A:1449:NAP:O4B	2.17	0.44
1:A:5:ILE:CD1	1:A:336:ILE:HG21	2.48	0.44
1:C:285:LEU:O	1:C:312:TYR:OH	2.33	0.44
1:A:182:ARG:NH1	1:A:194:GLU:OE1	2.51	0.44
1:B:131:PHE:HE2	1:B:133:GLU:OE2	2.00	0.44
1:A:207:TYR:HB2	3:A:1449:NAP:H2D	2.00	0.44
1:B:319:TRP:HZ2	1:B:368:MET:CE	2.30	0.44
1:B:380:ILE:HD12	1:B:387:SER:HA	1.99	0.43
1:A:15:MET:HE1	1:A:44:GLY:HA2	2.00	0.43
1:B:383:THR:CG2	1:B:384:ASP:N	2.81	0.43
1:C:3:THR:HB	1:C:32:PRO:HB3	1.98	0.43
1:B:415:SER:HB3	1:B:425:ALA:O	2.19	0.43
1:C:193:LEU:HD12	1:C:219:TYR:HB3	2.00	0.43
1:C:228:TYR:CE2	1:C:244:ARG:O	2.71	0.43
1:C:80:GLU:OE2	1:C:420:MET:HB2	2.17	0.43
1:A:375:TYR:CZ	1:A:379:LEU:HD11	2.53	0.43
1:C:292:ARG:HD2	1:C:294:TRP:O	2.19	0.43
1:B:289:THR:OG1	1:B:290:ASN:N	2.51	0.43
1:A:259:ASP:OD1	1:A:261:SER:HB3	2.19	0.43
1:A:201:LEU:HD23	1:A:268:ILE:HG12	2.01	0.42
1:B:68:ARG:NH1	1:B:68:ARG:CG	2.50	0.42
1:B:368:MET:HE2	1:B:368:MET:HB2	1.94	0.42
1:C:417:ARG:CZ	1:C:424:MET:HB2	2.50	0.42
1:A:446:ASP:O	1:A:447:LYS:CB	2.66	0.42
1:B:15:MET:HE1	1:B:44:GLY:H	1.80	0.42
1:B:226:SER:HB2	1:B:243:GLU:HG2	2.01	0.42
1:B:384:ASP:OD1	1:B:384:ASP:N	2.52	0.42
1:B:310:PHE:HE1	1:B:312:TYR:CE2	2.38	0.42
1:A:391:PRO:O	1:A:395:LYS:HD2	2.20	0.42
1:C:140:VAL:O	1:C:152:SER:HA	2.20	0.41
1:C:134:ASP:OD1	1:C:135:SER:N	2.54	0.41
1:B:104:TRP:CD2	1:B:108:LYS:HE2	2.56	0.41
1:B:179:PHE:HB2	1:B:250:VAL:HG11	2.02	0.41
1:C:63:HIS:CE1	1:C:166:SER:OG	2.74	0.41
1:A:12:PRO:HG2	2:A:1448:FAD:H4'	2.03	0.41
1:B:226:SER:O	1:B:243:GLU:HA	2.21	0.41
1:B:97:TYR:CD1	1:B:412:ARG:HA	2.55	0.41
1:A:293:LEU:HD11	1:A:368:MET:HB3	2.03	0.41
1:A:208:SER:HA	3:A:1449:NAP:H5N	2.02	0.41
1:B:6:ALA:HB2	1:B:155:PHE:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:PRO:HD3	1:A:443:TYR:CE1	2.56	0.41
1:B:102:VAL:HG21	1:B:443:TYR:CD2	2.56	0.41
1:A:190:ARG:HD3	1:A:190:ARG:HA	1.92	0.41
1:C:129:VAL:HB	1:C:281:LEU:HD23	2.02	0.41
1:C:365:ALA:HA	1:C:368:MET:HE3	2.03	0.40
1:A:380:ILE:HD12	1:A:385:TYR:HD2	1.87	0.40
1:B:93:PRO:HB2	1:B:426:PRO:HD3	2.03	0.40
1:A:127:ARG:HH21	1:A:143:GLN:NE2	2.20	0.40
1:A:69:TYR:HA	1:A:438:ASP:OD1	2.21	0.40
1:A:67:TYR:CZ	1:A:70:LEU:HD12	2.56	0.40
1:A:45:GLY:HA2	2:A:1448:FAD:O3B	2.21	0.40
1:C:40:GLN:NE2	6:C:2005:HOH:O	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	443/464 (96%)	430 (97%)	13 (3%)	0	100	100
1	B	444/464 (96%)	429 (97%)	15 (3%)	0	100	100
1	C	445/464 (96%)	427 (96%)	18 (4%)	0	100	100
All	All	1332/1392 (96%)	1286 (96%)	46 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	382/405 (94%)	362 (95%)	20 (5%)	23	30
1	B	378/405 (93%)	360 (95%)	18 (5%)	25	34
1	C	360/405 (89%)	349 (97%)	11 (3%)	40	54
All	All	1120/1215 (92%)	1071 (96%)	49 (4%)	29	38

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	43	TRP
1	A	69	TYR
1	A	111	VAL
1	A	132	ASN
1	A	205	SER
1	A	208	SER
1	A	230	THR
1	A	242	ASP
1	A	250	VAL
1	A	292	ARG
1	A	297	ASN
1	A	323	ASN
1	A	357	GLU
1	A	387	SER
1	A	395	LYS
1	A	402	HIS
1	A	419	LEU
1	A	420	MET
1	A	446	ASP
1	B	43	TRP
1	B	53	THR
1	B	68	ARG
1	B	177[A]	GLU
1	B	177[B]	GLU
1	B	184	LEU
1	B	230	THR
1	B	233	MET
1	B	250	VAL
1	B	290	ASN
1	B	297	ASN

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Mol	Chain	Res	Type
1	B	330	TRP
1	B	368	MET
1	B	383	THR
1	B	384	ASP
1	B	419	LEU
1	B	436	LEU
1	B	446	ASP
1	C	43	TRP
1	C	53	THR
1	C	123	ASN
1	C	132	ASN
1	C	184	LEU
1	C	202	LEU
1	C	297	ASN
1	C	323	ASN
1	C	367	GLU
1	C	419	LEU
1	C	426	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	25	GLN
1	A	40	GLN
1	A	48	ASN
1	A	143	GLN
1	A	164	HIS
1	A	282	ASN
1	A	290	ASN
1	A	377	GLN
1	B	17	GLN
1	B	25	GLN
1	B	40	GLN
1	B	48	ASN
1	B	132	ASN
1	B	290	ASN
1	B	297	ASN
1	C	40	GLN
1	C	48	ASN
1	C	123	ASN
1	C	136	GLN

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Mol	Chain	Res	Type
1	C	297	ASN
1	C	323	ASN
1	C	428	HIS
1	C	429	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](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	MES	C	1449	-	12,12,12	2.24	1 (8%)	14,16,16	2.51	6 (42%)
2	FAD	A	1448	-	51,58,58	1.41	6 (11%)	60,89,89	1.69	9 (15%)
2	FAD	C	1448	-	51,58,58	1.33	5 (9%)	60,89,89	1.87	9 (15%)
3	NAP	B	1449	-	45,52,52	1.74	4 (8%)	56,80,80	1.09	2 (3%)
4	GOL	B	1448	-	5,5,5	0.38	0	5,5,5	0.42	0
3	NAP	A	1449	-	45,52,52	1.71	4 (8%)	56,80,80	1.16	3 (5%)
3	NAP	C	1450	-	45,52,52	1.77	4 (8%)	56,80,80	1.09	3 (5%)
2	FAD	B	1447	-	51,58,58	1.26	5 (9%)	60,89,89	1.81	10 (16%)

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
5	MES	C	1449	-	-	6/6/14/14	0/1/1/1
2	FAD	A	1448	-	-	4/30/50/50	0/6/6/6
2	FAD	C	1448	-	-	5/30/50/50	0/6/6/6
3	NAP	B	1449	-	-	8/31/67/67	0/5/5/5
4	GOL	B	1448	-	-	4/4/4/4	-
3	NAP	A	1449	-	-	1/31/67/67	0/5/5/5
3	NAP	C	1450	-	-	7/31/67/67	0/5/5/5
2	FAD	B	1447	-	-	5/30/50/50	0/6/6/6

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1450	NAP	O7N-C7N	9.28	1.41	1.24
3	B	1449	NAP	O7N-C7N	9.14	1.41	1.24
3	A	1449	NAP	O7N-C7N	8.84	1.41	1.24
5	C	1449	MES	C8-S	-7.22	1.67	1.77
3	C	1450	NAP	C2A-N3A	4.19	1.38	1.32
2	A	1448	FAD	C10-N1	4.19	1.38	1.33
2	A	1448	FAD	C4X-N5	4.08	1.39	1.33
2	A	1448	FAD	C2A-N3A	4.03	1.38	1.32
2	C	1448	FAD	C10-N1	4.01	1.38	1.33
2	C	1448	FAD	C4X-N5	3.96	1.39	1.33
3	A	1449	NAP	C2A-N3A	3.95	1.38	1.32
3	B	1449	NAP	C2A-N3A	3.86	1.38	1.32
2	B	1447	FAD	C10-N1	3.72	1.38	1.33
2	C	1448	FAD	C2A-N3A	3.70	1.38	1.32
2	B	1447	FAD	C2A-N3A	3.39	1.37	1.32
2	B	1447	FAD	C4X-N5	3.21	1.37	1.33
2	A	1448	FAD	C1'-N10	3.18	1.51	1.48
2	C	1448	FAD	C4-N3	2.91	1.38	1.33
3	C	1450	NAP	C2A-N1A	2.78	1.39	1.33
3	B	1449	NAP	C2N-N1N	2.77	1.38	1.35
2	A	1448	FAD	C4-N3	2.74	1.37	1.33
2	B	1447	FAD	C4-N3	2.74	1.37	1.33
2	B	1447	FAD	C1'-N10	2.68	1.51	1.48
3	A	1449	NAP	C2A-N1A	2.57	1.38	1.33
3	A	1449	NAP	C2N-N1N	2.55	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1449	NAP	C2A-N1A	2.54	1.38	1.33
2	A	1448	FAD	C2A-N1A	2.41	1.38	1.33
3	C	1450	NAP	C2N-N1N	2.39	1.37	1.35
2	C	1448	FAD	C2A-N1A	2.19	1.38	1.33

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1448	FAD	C1'-N10-C9A	6.91	123.73	118.29
2	B	1447	FAD	N3A-C2A-N1A	-6.58	118.40	128.68
2	C	1448	FAD	C4-N3-C2	6.46	120.60	115.14
2	A	1448	FAD	C4-N3-C2	6.19	120.37	115.14
3	A	1449	NAP	N3A-C2A-N1A	-5.91	119.44	128.68
2	B	1447	FAD	C1'-N10-C9A	5.86	122.90	118.29
2	C	1448	FAD	N3A-C2A-N1A	-5.72	119.73	128.68
2	A	1448	FAD	N3A-C2A-N1A	-5.72	119.74	128.68
3	B	1449	NAP	N3A-C2A-N1A	-5.62	119.89	128.68
2	B	1447	FAD	C4-N3-C2	5.60	119.87	115.14
3	C	1450	NAP	N3A-C2A-N1A	-5.35	120.32	128.68
5	C	1449	MES	C5-N4-C3	5.23	120.60	108.83
2	A	1448	FAD	C1'-N10-C9A	4.19	121.59	118.29
2	B	1447	FAD	C4X-N5-C5X	4.00	120.77	116.77
2	A	1448	FAD	C4X-N5-C5X	3.91	120.68	116.77
2	C	1448	FAD	P-O3P-PA	-3.55	120.66	132.83
5	C	1449	MES	C2-C3-N4	-3.50	104.80	110.10
2	C	1448	FAD	C4X-N5-C5X	3.39	120.15	116.77
5	C	1449	MES	C7-N4-C3	3.36	119.83	111.23
5	C	1449	MES	C7-N4-C5	3.26	119.57	111.23
5	C	1449	MES	O3S-S-C8	3.05	110.70	105.77
2	A	1448	FAD	C5X-C9A-N10	3.04	119.92	117.72
2	C	1448	FAD	C1'-N10-C10	-2.94	115.78	118.41
2	B	1447	FAD	C4X-C4-N3	-2.83	119.56	123.43
2	A	1448	FAD	C4X-C4-N3	-2.63	119.83	123.43
2	B	1447	FAD	C5X-C9A-N10	2.56	119.57	117.72
2	A	1448	FAD	C10-C4X-N5	-2.53	119.50	121.26
5	C	1449	MES	C6-C5-N4	-2.48	106.34	110.10
2	A	1448	FAD	P-O3P-PA	-2.31	124.89	132.83
2	B	1447	FAD	P-O3P-PA	-2.30	124.95	132.83
3	B	1449	NAP	C3N-C7N-N7N	2.28	120.49	117.75
2	B	1447	FAD	C1B-N9A-C4A	-2.22	122.75	126.64
3	A	1449	NAP	C3N-C7N-N7N	2.20	120.39	117.75
2	B	1447	FAD	C10-C4X-N5	-2.19	119.74	121.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1448	FAD	C1'-C2'-C3'	2.15	115.81	109.79
2	C	1448	FAD	O2'-C2'-C1'	-2.15	104.42	109.59
3	C	1450	NAP	C3D-C2D-C1D	2.14	104.21	100.98
2	C	1448	FAD	C4X-C4-N3	-2.14	120.50	123.43
3	C	1450	NAP	C6N-N1N-C2N	-2.13	120.03	121.97
2	B	1447	FAD	C9A-N10-C10	-2.08	119.19	121.91
3	A	1449	NAP	O7N-C7N-N7N	-2.08	119.62	122.58
2	A	1448	FAD	C9A-N10-C10	-2.01	119.27	121.91

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1449	MES	N4-C7-C8-S
2	A	1448	FAD	N10-C1'-C2'-O2'
2	C	1448	FAD	N10-C1'-C2'-O2'
3	B	1449	NAP	C5D-O5D-PN-O3
4	B	1448	GOL	C1-C2-C3-O3
3	C	1450	NAP	C2B-O2B-P2B-O1X
3	C	1450	NAP	C5D-O5D-PN-O3
3	C	1450	NAP	C5D-O5D-PN-O1N
3	C	1450	NAP	C5D-O5D-PN-O2N
3	C	1450	NAP	O4D-C1D-N1N-C2N
2	B	1447	FAD	N10-C1'-C2'-O2'
5	C	1449	MES	C7-C8-S-O3S
4	B	1448	GOL	O1-C1-C2-C3
4	B	1448	GOL	O1-C1-C2-O2
4	B	1448	GOL	O2-C2-C3-O3
3	B	1449	NAP	O4B-C4B-C5B-O5B
5	C	1449	MES	C8-C7-N4-C3
2	C	1448	FAD	C5'-O5'-P-O3P
3	B	1449	NAP	C5B-O5B-PA-O3
3	C	1450	NAP	O4B-C4B-C5B-O5B
5	C	1449	MES	C7-C8-S-O1S
5	C	1449	MES	C7-C8-S-O2S
2	A	1448	FAD	N10-C1'-C2'-C3'
2	C	1448	FAD	N10-C1'-C2'-C3'
2	B	1447	FAD	N10-C1'-C2'-C3'
3	B	1449	NAP	C3B-C4B-C5B-O5B
5	C	1449	MES	C8-C7-N4-C5
2	B	1447	FAD	O3'-C3'-C4'-C5'
2	A	1448	FAD	PA-O3P-P-O5'

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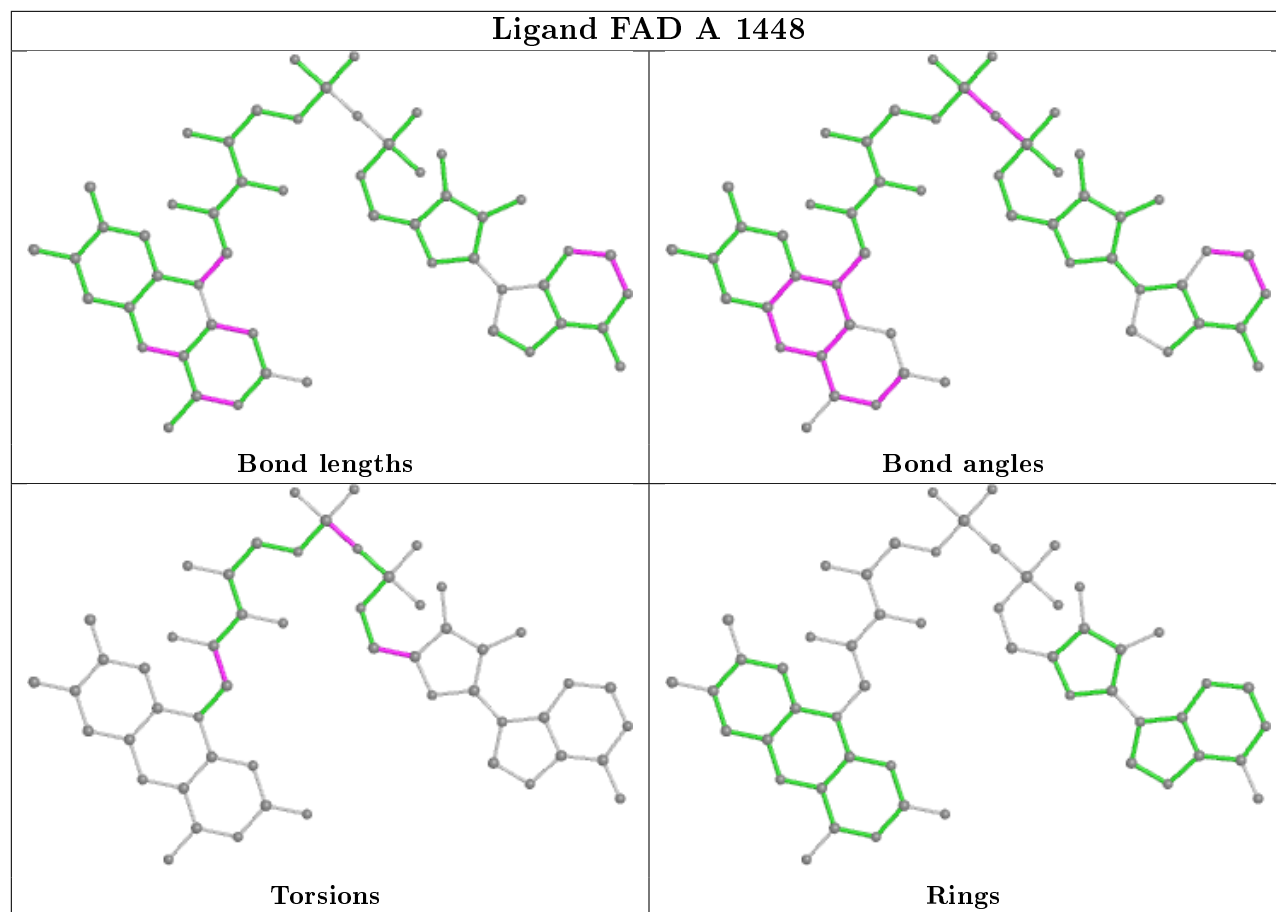
Mol	Chain	Res	Type	Atoms
3	A	1449	NAP	O4B-C4B-C5B-O5B
2	B	1447	FAD	C5'-O5'-P-O3P
2	C	1448	FAD	O4B-C4B-C5B-O5B
3	C	1450	NAP	O4D-C4D-C5D-O5D
2	B	1447	FAD	O4B-C4B-C5B-O5B
3	B	1449	NAP	C4N-C3N-C7N-N7N
2	C	1448	FAD	C3'-C4'-C5'-O5'
3	B	1449	NAP	C5B-O5B-PA-O1A
3	B	1449	NAP	C5D-O5D-PN-O1N
2	A	1448	FAD	O4B-C4B-C5B-O5B
3	B	1449	NAP	C4N-C3N-C7N-O7N

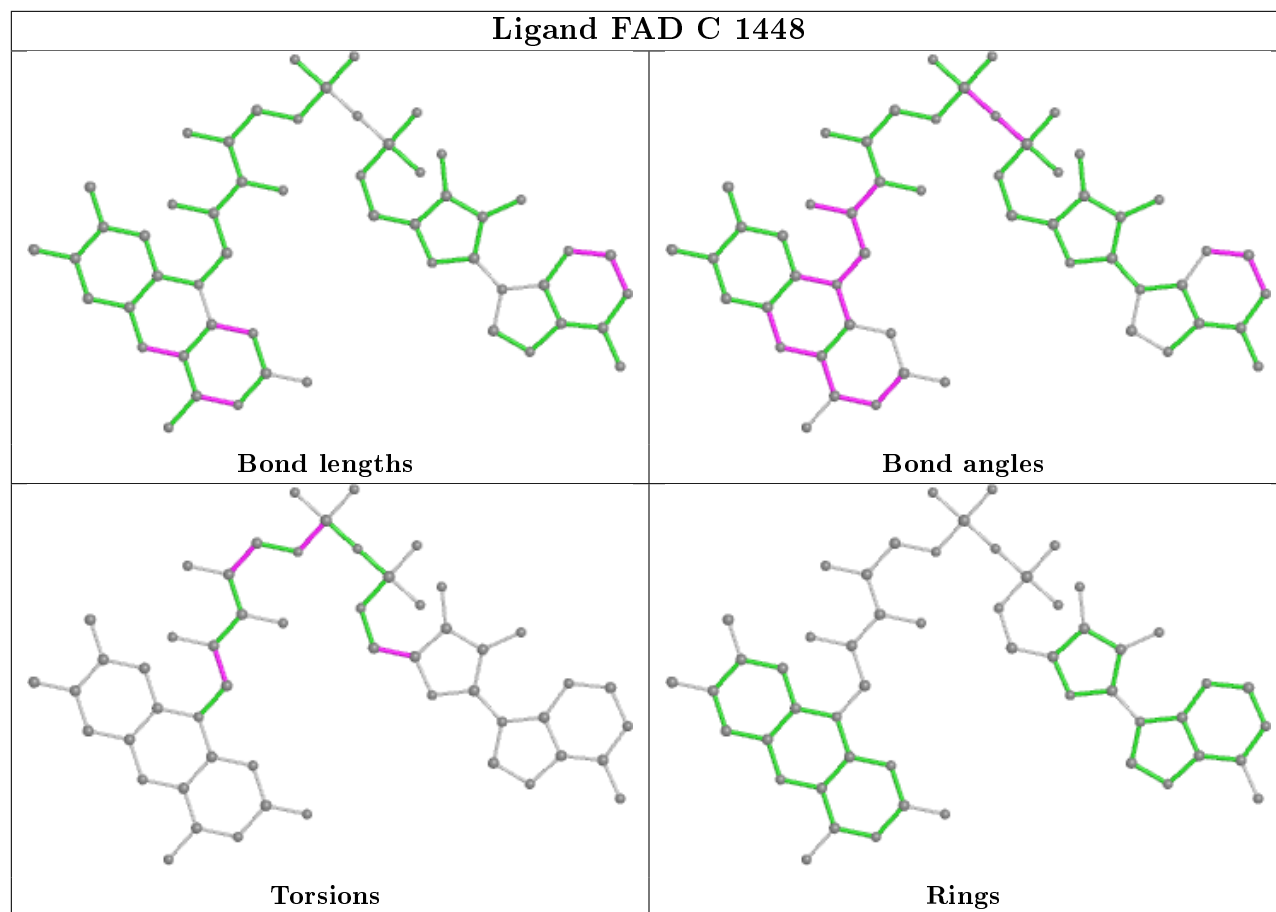
There are no ring outliers.

6 monomers are involved in 12 short contacts:

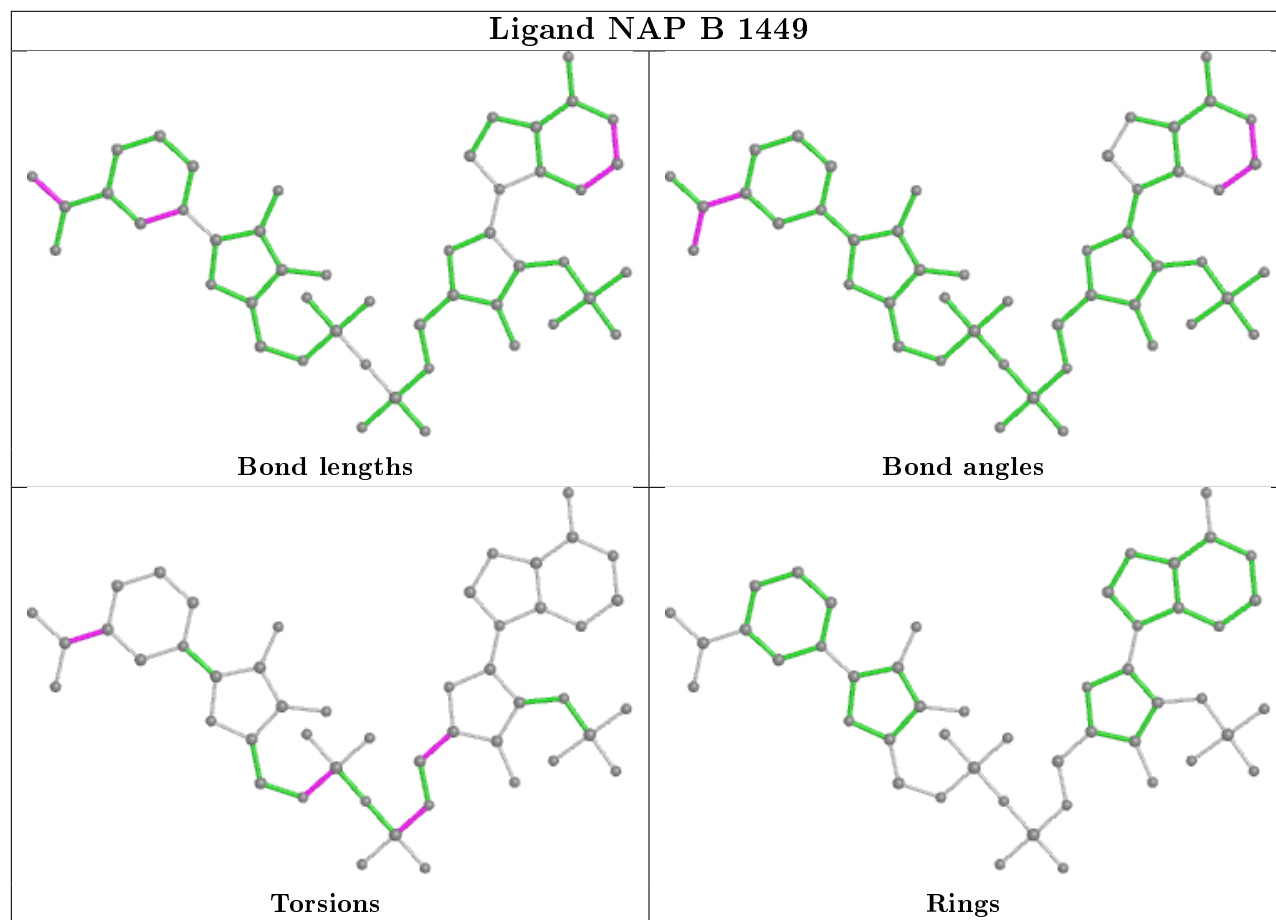
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1448	FAD	2	0
3	B	1449	NAP	1	0
4	B	1448	GOL	1	0
3	A	1449	NAP	4	0
3	C	1450	NAP	2	0
2	B	1447	FAD	2	0

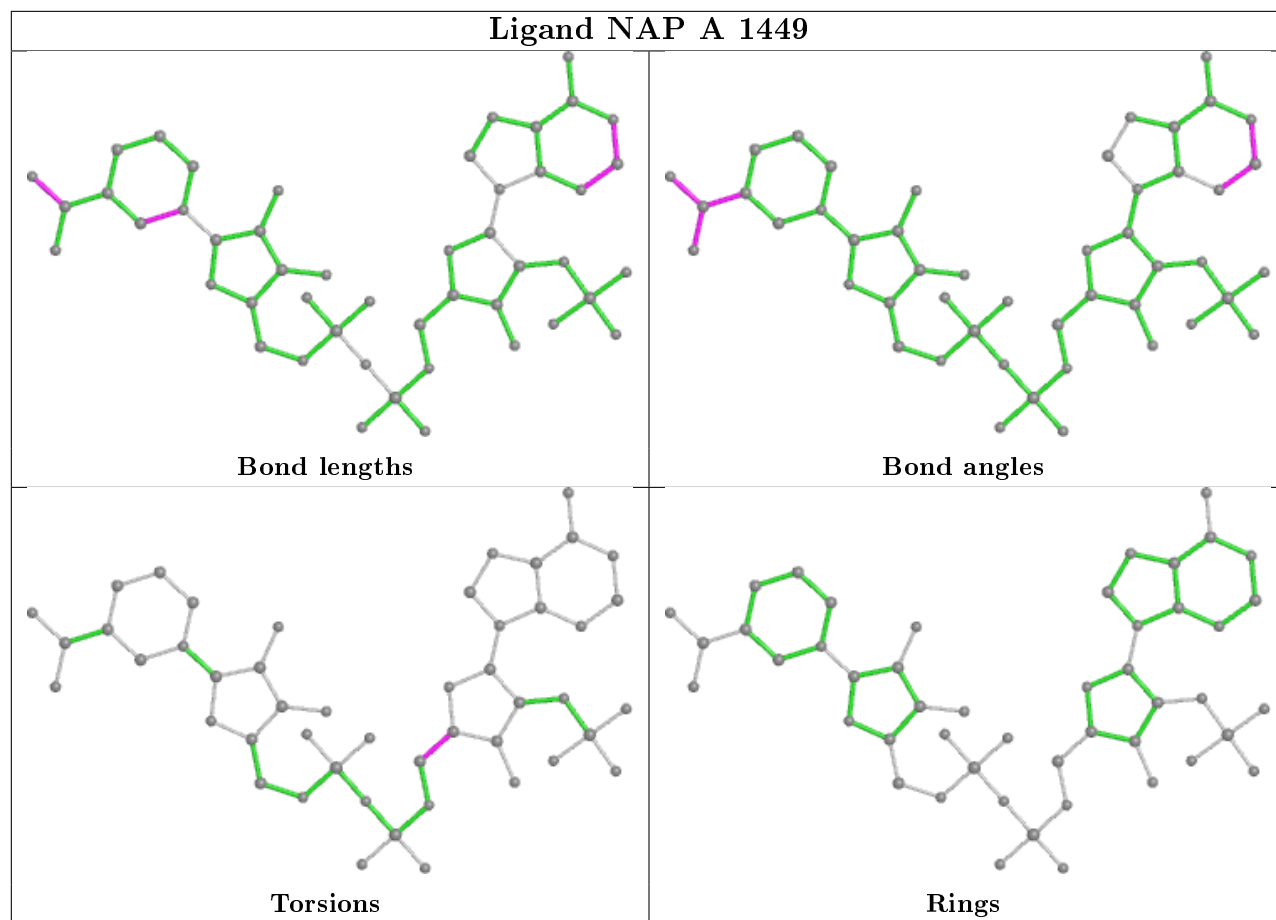
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

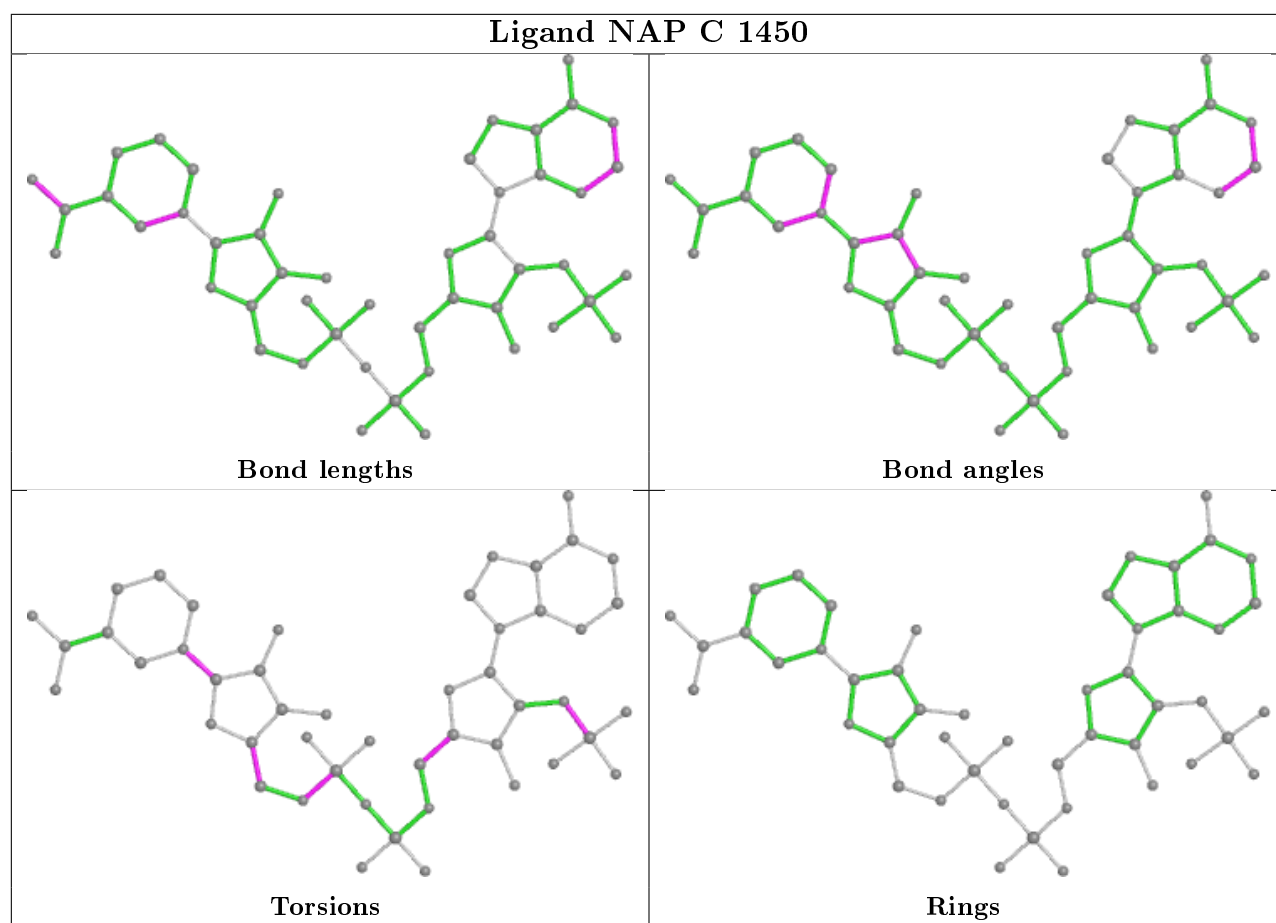


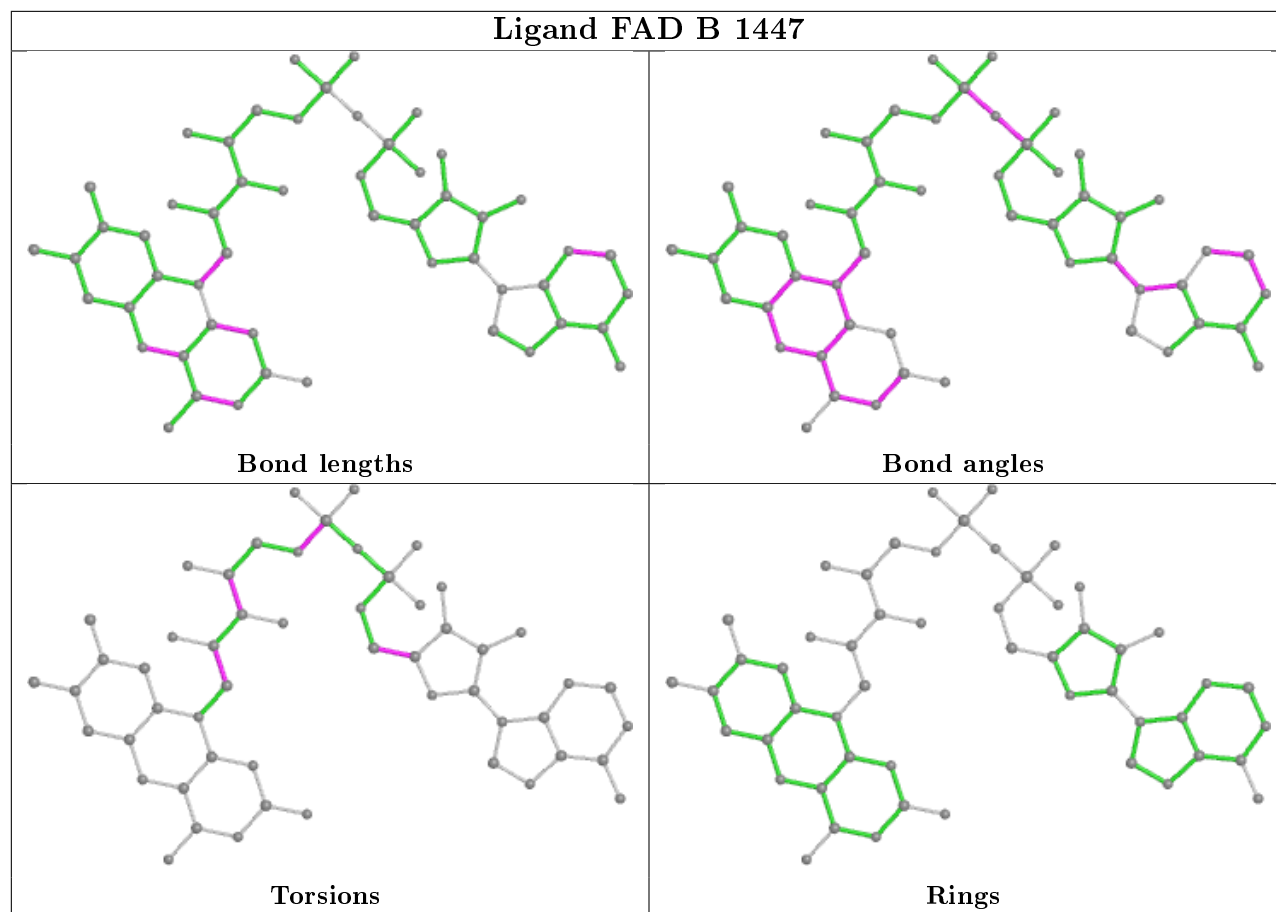












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	445/464 (95%)	0.01	6 (1%) 77 82	26, 50, 72, 85	0
1	B	445/464 (95%)	-0.10	3 (0%) 87 90	23, 43, 66, 77	0
1	C	446/464 (96%)	0.10	22 (4%) 29 35	24, 56, 94, 117	0
All	All	1336/1392 (95%)	0.01	31 (2%) 60 67	23, 48, 84, 117	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	197	ASP	4.6
1	C	221	ALA	3.9
1	A	28	GLY	3.8
1	C	408	ILE	3.8
1	C	200	VAL	3.7
1	C	431	PRO	3.4
1	C	195	PHE	3.4
1	C	217	TYR	3.3
1	C	199	THR	3.2
1	C	432	TRP	3.2
1	A	21	PHE	3.1
1	C	189	PHE	3.0
1	C	411	PHE	2.9
1	C	218	LYS	2.9
1	C	219	TYR	2.8
1	C	416	TYR	2.5
1	B	348	MET	2.4
1	C	397	PHE	2.4
1	C	400	TRP	2.4
1	C	434	ASP	2.3
1	B	355	TRP	2.3
1	B	343	PRO	2.3
1	A	424	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	424	MET	2.3
1	C	224	LEU	2.3
1	A	5	ILE	2.2
1	A	241	TRP	2.1
1	C	446	ASP	2.1
1	A	417	ARG	2.0
1	C	320	TYR	2.0
1	C	390	ILE	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

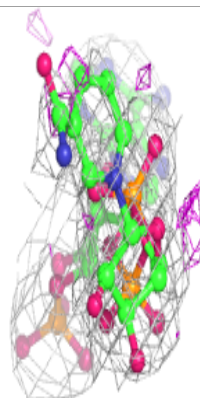
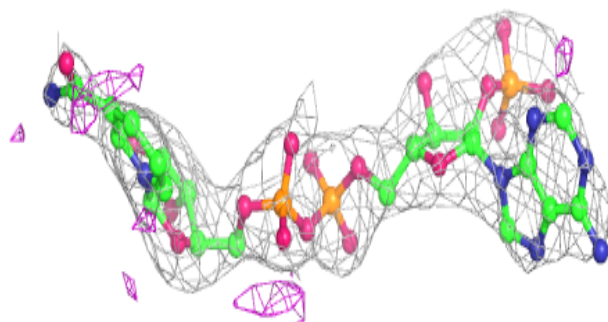
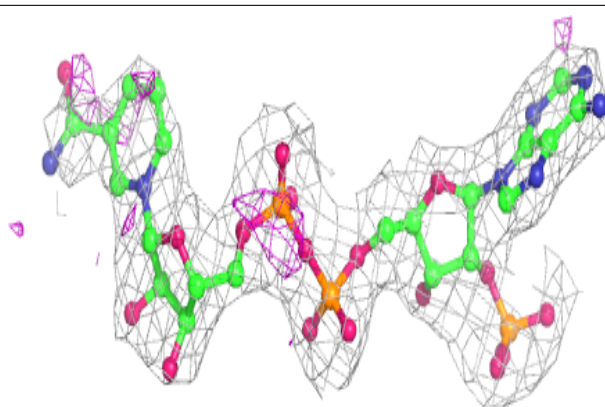
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	MES	C	1449	12/12	0.68	0.35	135,135,136,136	0
4	GOL	B	1448	6/6	0.76	0.33	58,61,61,61	0
3	NAP	C	1450	48/48	0.91	0.17	65,70,78,78	0
3	NAP	A	1449	48/48	0.95	0.13	44,49,56,57	0
3	NAP	B	1449	48/48	0.97	0.13	34,41,45,46	0
2	FAD	C	1448	53/53	0.97	0.15	23,34,38,40	0
2	FAD	A	1448	53/53	0.98	0.14	25,32,36,37	0
2	FAD	B	1447	53/53	0.98	0.15	21,26,31,33	0

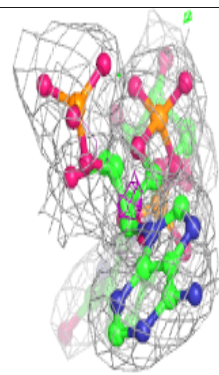
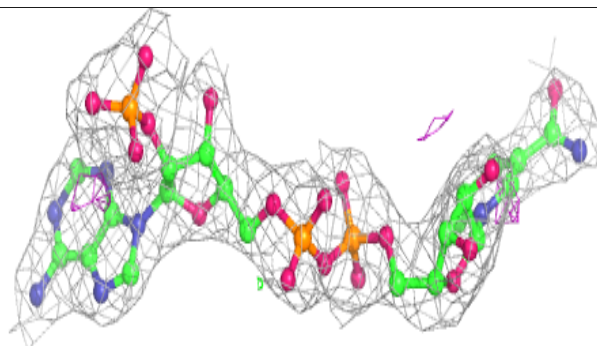
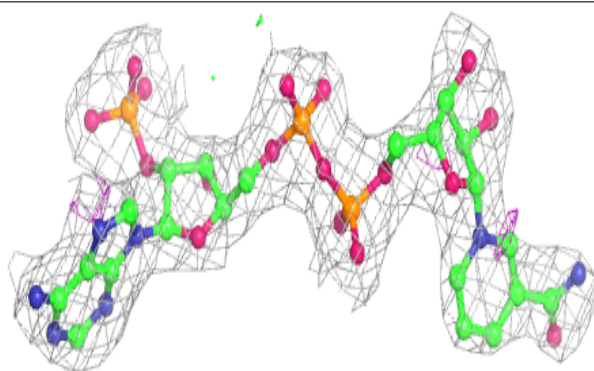
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAP C 1450:**

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

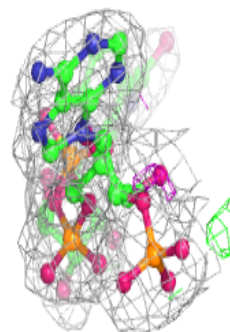
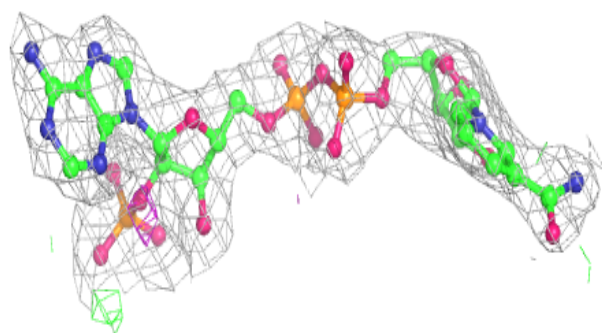
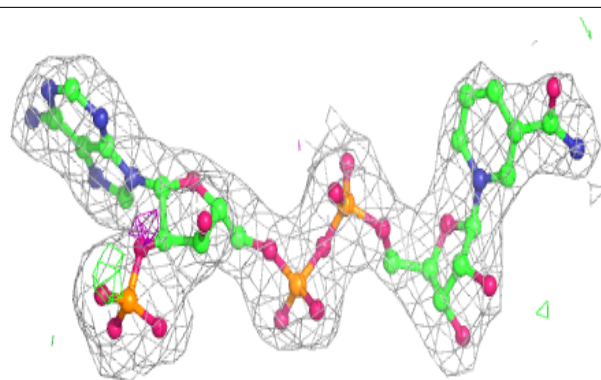
**Electron density around NAP A 1449:**

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

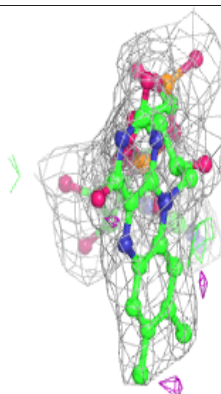
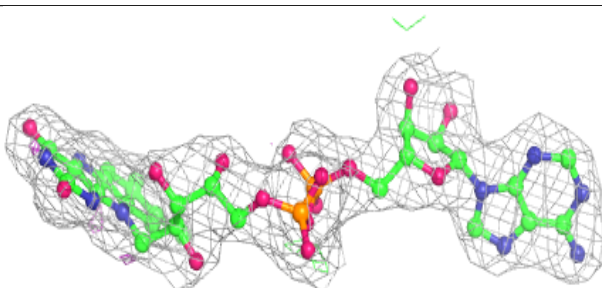
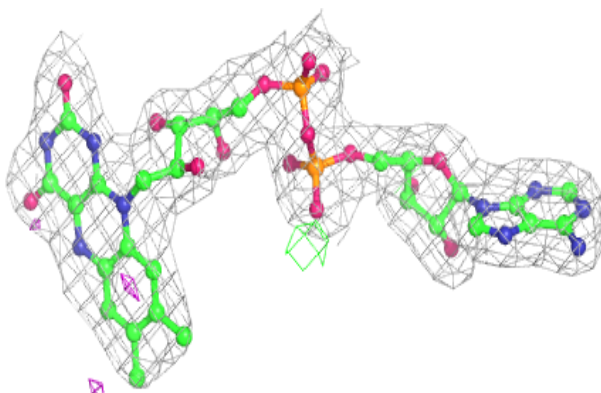


**Electron density around NAP B 1449:**

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

**Electron density around FAD C 1448:**

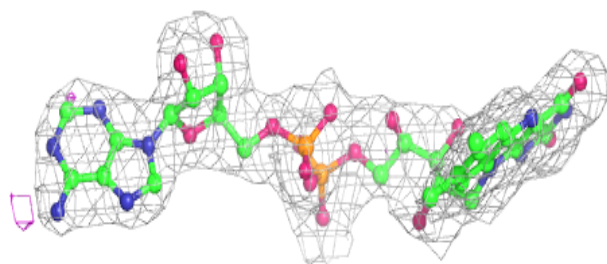
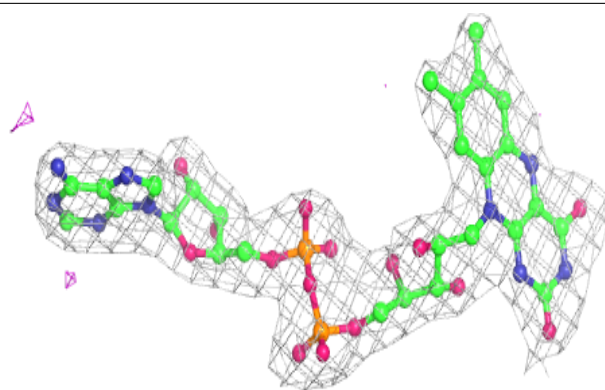
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



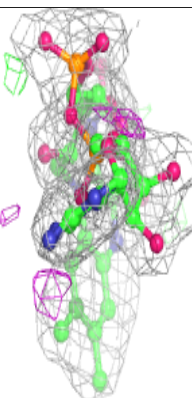
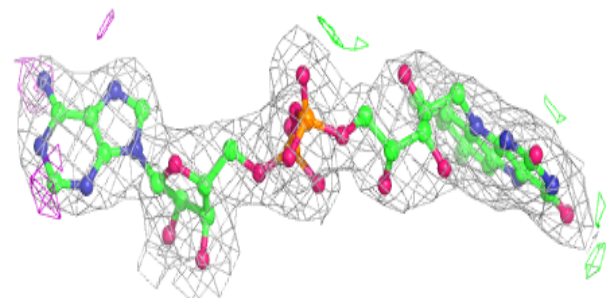
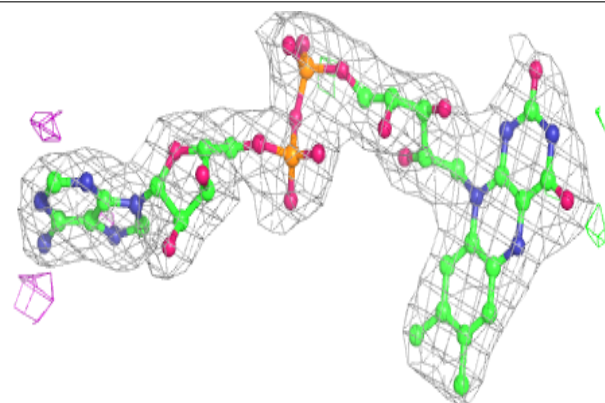


**Electron density around FAD A 1448:**

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

**Electron density around FAD B 1447:**

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



## 6.5 Other polymers

There are no such residues in this entry.