Full wwPDB X-ray Structure Validation Report (i)

Sep 2, 2023 – 03:21 PM EDT

PDB ID	:	3QE2
Title	:	Crystal Structure of Human NADPH-Cytochrome P450 Reductase
Authors	:	Xia, C.; Marohnic, C.; Panda, S.P.; Masters, B.S.; Kim, J.-J.P.
Deposited on	:	2011-01-19
Resolution	:	1.75 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 (i) 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 (i)) were used in the production of this report:

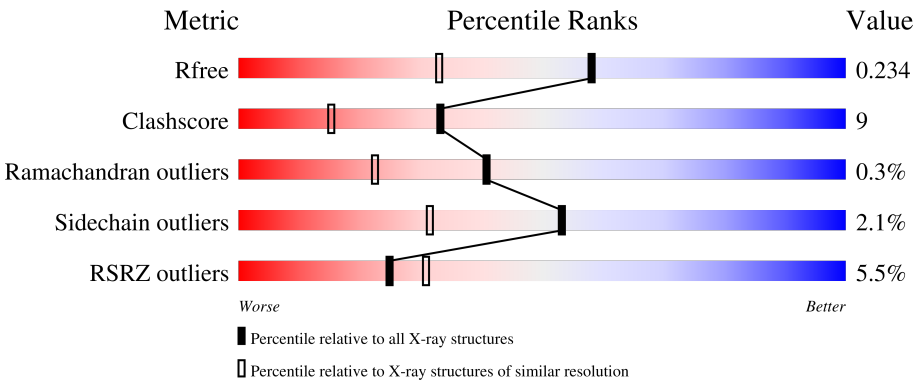
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 <=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	618	4% 81% 15% • •
1	B	618	7% 80% 17% • •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10859 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 NADPH–cytochrome P450 reductase.

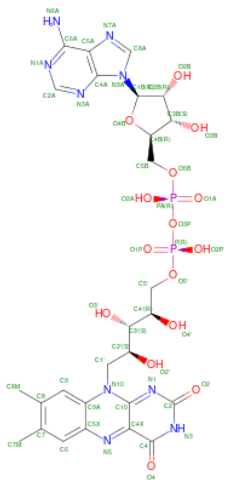
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	604	4836	3059	837	917	23	0	0	0
1	B	606	4826	3053	836	914	23	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	GLY	-	expression tag	UNP P16435
A	64	SER	-	expression tag	UNP P16435
A	65	HIS	-	expression tag	UNP P16435
A	66	MET	-	expression tag	UNP P16435
A	228	LEU	PRO	SEE REMARK 999	UNP P16435
A	503	VAL	ALA	SEE REMARK 999	UNP P16435
B	63	GLY	-	expression tag	UNP P16435
B	64	SER	-	expression tag	UNP P16435
B	65	HIS	-	expression tag	UNP P16435
B	66	MET	-	expression tag	UNP P16435
B	228	LEU	PRO	SEE REMARK 999	UNP P16435
B	503	VAL	ALA	SEE REMARK 999	UNP P16435

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

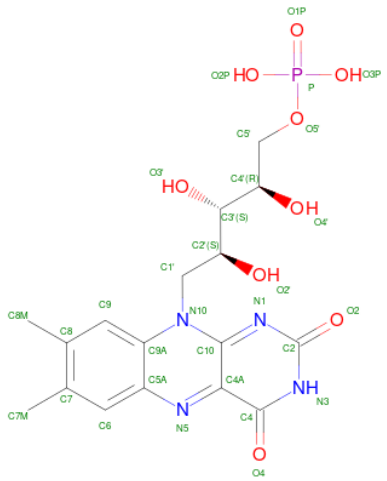
FAD



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

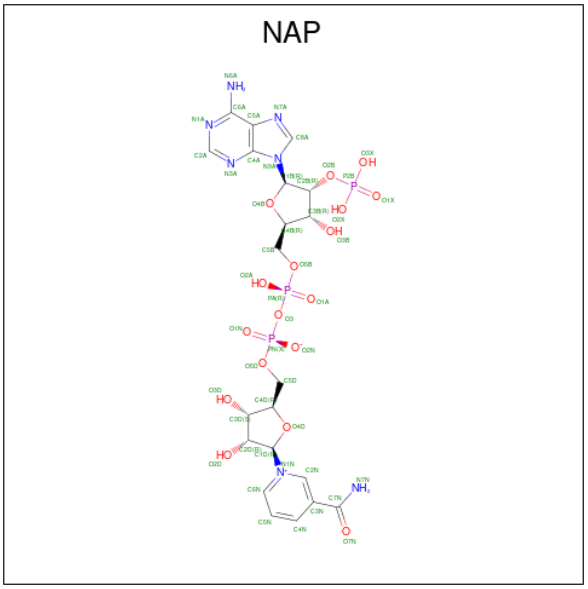
- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

FMN



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	31	17	4	9	1	0	0
			Total	C	N	O	P		
3	B	1	31	17	4	9	1	0	0

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	31	10	5	13	3	0	0
			Total	C	N	O	P		
4	B	1	31	10	5	13	3	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
5	A	1	1	1	0	0

- Molecule 6 is water.

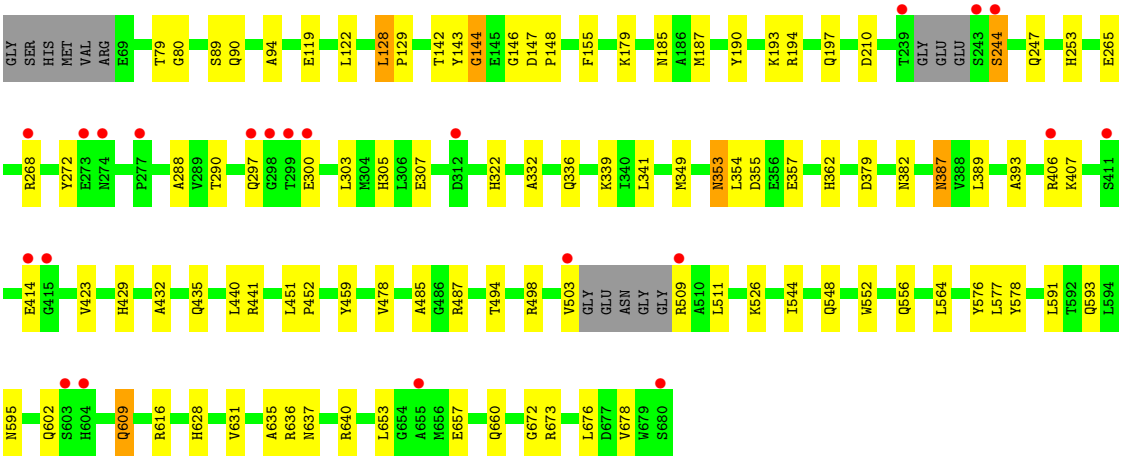
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	596	596	596	0	0
			Total	O		
6	B	370	370	370	0	0

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.

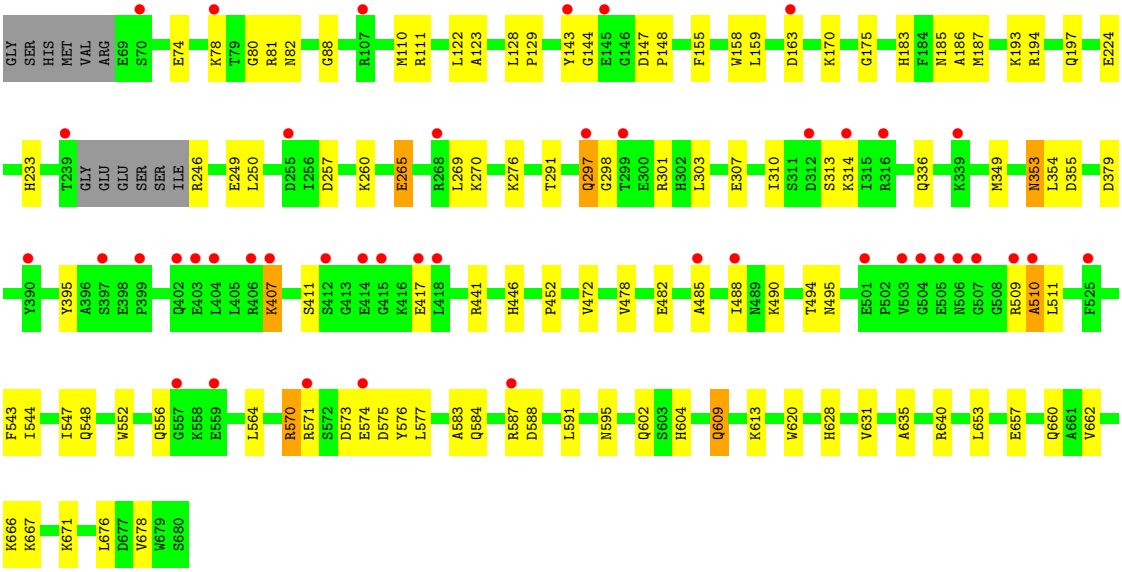
• Molecule 1: NADPH–cytochrome P450 reductase

Chain A:



• Molecule 1: NADPH–cytochrome P450 reductase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	70.14Å 117.78Å 156.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.10 – 1.75 45.10 – 1.75	Depositor EDS
% Data completeness (in resolution range)	95.4 (45.10-1.75) 95.3 (45.10-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.67 (at 1.75Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.211 , 0.239 0.206 , 0.234	Depositor DCC
R_{free} test set	6299 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	22.4	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 46.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10859	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: FMN, NAP, FAD, CA

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	0.32	0/4944	0.59	0/6689
1	B	0.29	0/4935	0.55	1/6679 (0.0%)
All	All	0.30	0/9879	0.57	1/13368 (0.0%)

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	88	GLY	N-CA-C	-5.44	99.49	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	459	TYR	Sidechain

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	4836	0	4711	83	0
1	B	4826	0	4684	83	0
2	A	53	0	31	0	0
2	B	53	0	31	1	0
3	A	31	0	19	0	0
3	B	31	0	19	1	0
4	A	31	0	11	1	0
4	B	31	0	11	1	0
5	A	1	0	0	0	0
6	A	596	0	0	17	0
6	B	370	0	0	12	0
All	All	10859	0	9517	166	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 9.

All (166) 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:609:GLN:H	1:A:609:GLN:HE21	1.09	0.99
1:B:640:ARG:HH11	1:B:640:ARG:HB3	1.32	0.94
1:B:509:ARG:O	1:B:511:LEU:HG	1.69	0.93
1:A:247:GLN:HE21	1:A:353:ASN:HD21	1.24	0.84
1:A:609:GLN:HE22	4:A:753:NAP:H2A	1.42	0.82
1:A:609:GLN:H	1:A:609:GLN:NE2	1.79	0.80
1:A:407:LYS:HD3	1:A:414:GLU:HG3	1.63	0.80
1:B:609:GLN:HE22	4:B:753:NAP:H2A	1.48	0.79
1:B:82:ASN:HD21	1:B:110:MET:HB3	1.47	0.78
1:A:609:GLN:HE21	1:A:609:GLN:N	1.82	0.77
1:B:482:GLU:HG2	1:B:488:ILE:CD1	2.15	0.76
1:A:509:ARG:HD3	1:A:511:LEU:HD21	1.68	0.75
1:B:640:ARG:HB3	1:B:640:ARG:NH1	2.01	0.74
1:A:440:LEU:O	1:A:441:ARG:HD3	1.87	0.74
1:A:339:LYS:NZ	1:A:339:LYS:HB3	2.02	0.73
1:B:657:GLU:H	1:B:660:GLN:HE21	1.35	0.73
1:A:247:GLN:HE21	1:A:353:ASN:ND2	1.87	0.72
1:B:609:GLN:H	1:B:609:GLN:HE21	1.38	0.71
1:A:268:ARG:HB2	1:A:268:ARG:NH1	2.05	0.71
1:A:244:SER:HA	6:A:957:HOH:O	1.90	0.71
1:B:379:ASP:HB3	1:B:452:PRO:HG2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:ASN:HD22	1:A:640:ARG:HH11	1.40	0.68
1:A:435:GLN:HE21	1:A:487:ARG:HH11	1.42	0.66
1:A:657:GLU:H	1:A:660:GLN:HE21	1.43	0.66
1:B:613:LYS:HE3	6:B:905:HOH:O	1.95	0.65
1:B:570:ARG:HD3	1:B:575:ASP:OD2	1.96	0.65
1:A:247:GLN:NE2	1:A:353:ASN:HD21	1.94	0.64
1:B:81:ARG:HG3	1:B:81:ARG:HH11	1.61	0.64
1:A:451:LEU:HD22	6:A:963:HOH:O	1.98	0.64
1:A:429:HIS:HD2	1:A:432:ALA:H	1.48	0.62
1:B:170:LYS:NZ	1:B:233:HIS:HE1	1.98	0.62
1:B:482:GLU:HG2	1:B:488:ILE:HD13	1.82	0.61
1:B:631:VAL:HB	1:B:676:LEU:HD23	1.82	0.61
1:B:298:GLY:HA3	1:B:574:GLU:OE1	2.01	0.61
1:A:389:LEU:HD11	1:A:423:VAL:HG21	1.83	0.60
1:B:666:LYS:HE3	6:B:977:HOH:O	2.02	0.60
1:B:303:LEU:CD2	1:B:577:LEU:HD21	2.32	0.59
1:B:303:LEU:HD22	1:B:577:LEU:HD21	1.84	0.59
1:B:609:GLN:H	1:B:609:GLN:NE2	2.01	0.59
1:B:260:LYS:HG3	6:B:1030:HOH:O	2.02	0.59
1:B:662:VAL:CG1	1:B:666:LYS:HE2	2.33	0.58
1:A:552:TRP:O	1:A:556:GLN:HG2	2.03	0.58
1:A:526:LYS:HE2	6:A:826:HOH:O	2.04	0.57
1:A:179:LYS:HE2	1:A:210:ASP:OD2	2.04	0.57
1:A:353:ASN:ND2	1:A:355:ASP:H	2.02	0.57
1:B:353:ASN:HD22	1:B:354:LEU:N	2.03	0.57
1:A:79:THR:HG22	1:A:357:GLU:OE1	2.04	0.56
1:A:485:ALA:HB3	6:A:896:HOH:O	2.05	0.56
1:A:303:LEU:HD22	1:A:577:LEU:HD21	1.87	0.55
1:A:407:LYS:HD3	1:A:414:GLU:CG	2.35	0.55
1:A:89:SER:HB2	1:A:94:ALA:HB3	1.87	0.55
1:A:80:GLY:HA2	6:A:733:HOH:O	2.05	0.55
1:A:429:HIS:CD2	1:A:432:ALA:H	2.25	0.55
1:B:662:VAL:HG12	1:B:666:LYS:HE2	1.89	0.55
1:A:305:HIS:HD2	1:A:578:TYR:OH	1.89	0.55
1:A:119:GLU:HG3	6:A:965:HOH:O	2.07	0.54
1:B:544:ILE:O	1:B:548:GLN:HG3	2.07	0.54
1:B:81:ARG:HD3	1:B:111:ARG:HB3	1.90	0.54
1:B:257:ASP:HB2	1:B:260:LYS:NZ	2.23	0.54
1:B:552:TRP:O	1:B:556:GLN:HG2	2.07	0.54
1:B:571:ARG:HB2	1:B:574:GLU:HB2	1.89	0.54
1:A:379:ASP:HB3	1:A:452:PRO:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:609:GLN:HE21	1:B:609:GLN:N	2.04	0.53
1:B:564:LEU:N	1:B:564:LEU:HD12	2.23	0.53
1:A:322:HIS:HD2	6:A:906:HOH:O	1.91	0.53
1:A:353:ASN:HD22	1:A:354:LEU:N	2.06	0.53
1:B:640:ARG:HH11	1:B:640:ARG:CB	2.15	0.53
1:A:268:ARG:HH11	1:A:268:ARG:CB	2.22	0.52
1:B:301:ARG:NH1	1:B:570:ARG:NE	2.58	0.52
1:A:268:ARG:HB2	1:A:268:ARG:HH11	1.74	0.51
1:A:435:GLN:NE2	1:A:487:ARG:HH11	2.06	0.51
1:B:662:VAL:O	1:B:666:LYS:HG3	2.10	0.51
1:A:387:ASN:HD22	1:A:387:ASN:H	1.57	0.51
1:B:74:GLU:O	1:B:78:LYS:HG2	2.11	0.51
1:B:407:LYS:HB3	1:B:407:LYS:NZ	2.26	0.51
1:B:269:LEU:O	1:B:270:LYS:HB2	2.11	0.51
1:A:593:GLN:HE21	1:A:595:ASN:HD21	1.59	0.50
1:B:395:TYR:OH	1:B:446:HIS:HD2	1.93	0.50
1:A:339:LYS:HB3	1:A:339:LYS:HZ2	1.75	0.50
1:A:353:ASN:HD22	1:A:355:ASP:H	1.59	0.50
1:A:407:LYS:CD	1:A:414:GLU:HG3	2.37	0.50
1:B:159:LEU:HB3	1:B:194:ARG:HG2	1.94	0.50
1:B:571:ARG:HB2	1:B:574:GLU:CB	2.42	0.50
1:B:291:THR:HB	1:B:307:GLU:HB2	1.94	0.49
1:B:583:ALA:O	1:B:587:ARG:HG3	2.12	0.49
1:A:498:ARG:HD3	6:A:909:HOH:O	2.11	0.49
1:A:628:HIS:HE1	6:A:1063:HOH:O	1.94	0.49
1:B:353:ASN:ND2	1:B:355:ASP:H	2.10	0.49
1:A:253:HIS:HD2	6:A:1042:HOH:O	1.95	0.49
1:A:339:LYS:HB3	1:A:339:LYS:HZ3	1.75	0.49
1:A:478:VAL:HA	1:A:494:THR:HB	1.95	0.49
1:A:190:TYR:CZ	1:A:194:ARG:HG3	2.48	0.48
1:B:148:PRO:HB3	1:B:187:MET:SD	2.53	0.48
1:A:414:GLU:OE2	1:B:276:LYS:HE3	2.13	0.48
1:B:257:ASP:HB2	1:B:260:LYS:HE2	1.94	0.48
1:A:564:LEU:HD12	1:A:564:LEU:N	2.28	0.48
1:B:170:LYS:HZ2	1:B:233:HIS:HE1	1.62	0.48
1:B:246:ARG:HD3	1:B:446:HIS:CD2	2.49	0.47
1:B:301:ARG:HH11	1:B:570:ARG:NE	2.12	0.47
1:A:673:ARG:HD3	6:A:1188:HOH:O	2.14	0.47
1:B:441:ARG:HD2	6:B:965:HOH:O	2.14	0.47
1:B:635:ALA:HB2	1:B:678:VAL:HB	1.97	0.47
1:A:290:THR:HA	1:A:503:VAL:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:GLU:HG2	6:B:696:HOH:O	2.14	0.47
1:A:341:LEU:HD23	6:A:930:HOH:O	2.15	0.47
1:B:667:LYS:O	1:B:671:LYS:HG2	2.15	0.47
1:A:305:HIS:HE1	1:A:307:GLU:OE1	1.98	0.47
1:B:620:TRP:HB2	1:B:653:LEU:HD12	1.97	0.46
1:A:144:GLY:O	1:A:147:ASP:OD2	2.33	0.46
1:B:122:LEU:HG	1:B:155:PHE:CD1	2.50	0.46
1:B:249:GLU:HB3	1:B:354:LEU:HD21	1.97	0.46
1:A:268:ARG:NH1	1:A:268:ARG:CB	2.77	0.46
1:A:193:LYS:O	1:A:197:GLN:HG3	2.16	0.46
1:B:478:VAL:HA	1:B:494:THR:HB	1.98	0.46
1:B:584:GLN:NE2	1:B:584:GLN:HA	2.31	0.45
1:B:602:GLN:HG2	1:B:604:HIS:O	2.17	0.45
1:B:82:ASN:ND2	1:B:111:ARG:H	2.15	0.45
1:B:183:HIS:HB3	1:B:186:ALA:HB2	1.99	0.45
1:A:382:ASN:ND2	6:A:776:HOH:O	2.50	0.45
1:B:81:ARG:HG3	1:B:81:ARG:NH1	2.29	0.45
1:B:224:GLU:OE2	1:B:411:SER:HB3	2.16	0.44
1:B:657:GLU:H	1:B:660:GLN:NE2	2.10	0.44
1:B:310:ILE:HD13	1:B:472:VAL:HG23	1.99	0.44
1:A:142:THR:CG2	1:A:146:GLY:HA2	2.47	0.43
1:A:636:ARG:HB2	1:A:636:ARG:NH1	2.32	0.43
1:A:637:ASN:HD22	1:A:640:ARG:NH1	2.10	0.43
1:B:193:LYS:O	1:B:197:GLN:HG3	2.18	0.43
1:B:257:ASP:HB2	1:B:260:LYS:CE	2.48	0.43
1:B:80:GLY:HA2	6:B:964:HOH:O	2.17	0.43
1:B:595:ASN:ND2	6:B:845:HOH:O	2.51	0.43
1:B:297:GLN:HG3	1:B:573:ASP:O	2.18	0.43
2:B:752:FAD:HM83	3:B:751:FMN:HM71	2.00	0.43
1:A:362:HIS:HE1	6:A:692:HOH:O	2.02	0.43
1:B:128:LEU:N	1:B:129:PRO:CD	2.81	0.43
1:B:175:GLY:C	1:B:185:ASN:HD21	2.22	0.43
1:B:313:SER:O	1:B:314:LYS:HB2	2.19	0.43
1:A:631:VAL:HB	1:A:676:LEU:HD23	2.01	0.43
1:A:544:ILE:O	1:A:548:GLN:HG3	2.18	0.42
1:A:635:ALA:HB2	1:A:678:VAL:HB	2.02	0.42
1:B:509:ARG:O	1:B:510:ALA:C	2.58	0.42
1:A:288:ALA:HB2	1:A:509:ARG:HD3	2.00	0.42
1:B:490:LYS:HB3	1:B:495:ASN:ND2	2.34	0.42
1:A:393:ALA:HB1	1:A:406:ARG:HG3	2.02	0.42
1:A:393:ALA:HB1	1:A:406:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ASP:HB3	6:B:908:HOH:O	2.19	0.42
1:A:90:GLN:HB3	1:A:143:TYR:CZ	2.54	0.42
1:B:224:GLU:HG3	6:B:730:HOH:O	2.19	0.42
1:A:672:GLY:HA2	6:A:717:HOH:O	2.20	0.42
1:B:628:HIS:HD2	6:B:879:HOH:O	2.02	0.42
1:A:148:PRO:HB3	1:A:187:MET:SD	2.60	0.41
1:A:332:ALA:O	1:A:336:GLN:HG3	2.20	0.41
1:A:122:LEU:HG	1:A:155:PHE:CD1	2.55	0.41
1:B:485:ALA:HB3	6:B:779:HOH:O	2.20	0.41
1:B:543:PHE:O	1:B:547:ILE:HG13	2.20	0.41
1:A:247:GLN:HG2	6:A:918:HOH:O	2.21	0.41
1:A:509:ARG:CD	1:A:511:LEU:HD21	2.44	0.41
1:A:616:ARG:HG3	1:A:653:LEU:HD11	2.02	0.41
1:A:297:GLN:N	1:A:297:GLN:CD	2.74	0.41
1:B:123:ALA:HA	1:B:158:TRP:CZ2	2.55	0.41
1:B:143:TYR:O	1:B:147:ASP:HB2	2.20	0.41
1:B:336:GLN:NE2	6:B:854:HOH:O	2.53	0.41
1:A:265:GLU:HA	1:A:272:TYR:CZ	2.56	0.41
1:A:616:ARG:HD2	6:A:18:HOH:O	2.20	0.41
1:A:640:ARG:HG2	1:A:640:ARG:HH21	1.85	0.40
1:A:628:HIS:CE1	1:A:673:ARG:HG2	2.56	0.40
1:A:128:LEU:N	1:A:129:PRO:CD	2.83	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	598/618 (97%)	579 (97%)	17 (3%)	2 (0%)	41 22
1	B	602/618 (97%)	582 (97%)	18 (3%)	2 (0%)	41 22
All	All	1200/1236 (97%)	1161 (97%)	35 (3%)	4 (0%)	41 22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	GLY
1	B	144	GLY
1	A	244	SER
1	B	510	ALA

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	517/526 (98%)	507 (98%)	10 (2%)	57	37
1	B	511/526 (97%)	499 (98%)	12 (2%)	50	28
All	All	1028/1052 (98%)	1006 (98%)	22 (2%)	53	31

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	LEU
1	A	185	ASN
1	A	300	GLU
1	A	349	MET
1	A	353	ASN
1	A	387	ASN
1	A	576	TYR
1	A	591	LEU
1	A	602	GLN
1	A	609	GLN
1	B	250	LEU
1	B	265	GLU
1	B	297	GLN
1	B	349	MET
1	B	353	ASN
1	B	407	LYS
1	B	417	GLU
1	B	570	ARG
1	B	576	TYR

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Mol	Chain	Res	Type
1	B	588	ASP
1	B	591	LEU
1	B	609	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	185	ASN
1	A	253	HIS
1	A	283	ASN
1	A	305	HIS
1	A	322	HIS
1	A	353	ASN
1	A	362	HIS
1	A	387	ASN
1	A	429	HIS
1	A	435	GLN
1	A	455	GLN
1	A	468	HIS
1	A	489	ASN
1	A	555	GLN
1	A	586	HIS
1	A	593	GLN
1	A	602	GLN
1	A	609	GLN
1	A	628	HIS
1	A	637	ASN
1	A	658	HIS
1	A	660	GLN
1	B	82	ASN
1	B	183	HIS
1	B	185	ASN
1	B	233	HIS
1	B	283	ASN
1	B	336	GLN
1	B	353	ASN
1	B	362	HIS
1	B	382	ASN
1	B	387	ASN
1	B	394	GLN
1	B	446	HIS

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Mol	Chain	Res	Type
1	B	455	GLN
1	B	470	ASN
1	B	489	ASN
1	B	520	GLN
1	B	555	GLN
1	B	584	GLN
1	B	586	HIS
1	B	609	GLN
1	B	660	GLN

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 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FMN	B	751	-	33,33,33	2.29	11 (33%)	48,50,50	1.45	7 (14%)
2	FAD	B	752	-	53,58,58	2.62	19 (35%)	68,89,89	1.63	14 (20%)
2	FAD	A	752	-	53,58,58	2.55	19 (35%)	68,89,89	1.60	12 (17%)
4	NAP	A	753	-	27,33,52	2.38	5 (18%)	35,52,80	1.34	5 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FMN	A	751	-	33,33,33	2.36	11 (33%)	48,50,50	1.46	6 (12%)
4	NAP	B	753	-	27,33,52	2.49	7 (25%)	35,52,80	1.39	6 (17%)

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	FMN	B	751	-	-	0/18/18/18	0/3/3/3
2	FAD	B	752	-	-	2/30/50/50	0/6/6/6
2	FAD	A	752	-	-	1/30/50/50	0/6/6/6
4	NAP	A	753	-	-	1/17/37/67	0/3/3/5
3	FMN	A	751	-	-	0/18/18/18	0/3/3/3
4	NAP	B	753	-	-	4/17/37/67	0/3/3/5

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	753	NAP	C4A-N3A	10.59	1.50	1.35
4	A	753	NAP	C4A-N3A	10.19	1.49	1.35
2	B	752	FAD	C4A-N3A	7.50	1.46	1.35
2	A	752	FAD	C1'-C2'	7.13	1.62	1.52
2	A	752	FAD	C4A-N3A	7.04	1.45	1.35
2	B	752	FAD	C1'-C2'	5.89	1.61	1.52
3	B	751	FMN	C4A-N5	5.54	1.41	1.30
3	A	751	FMN	C4A-N5	5.47	1.41	1.30
3	A	751	FMN	C10-N10	5.36	1.49	1.37
2	A	752	FAD	C5'-C4'	-5.32	1.44	1.51
2	B	752	FAD	C9A-C5X	5.30	1.50	1.41
2	B	752	FAD	C5'-C4'	-5.30	1.44	1.51
2	B	752	FAD	C4X-N5	5.16	1.40	1.30
3	B	751	FMN	C10-N10	5.03	1.48	1.37
2	B	752	FAD	C9A-N10	5.01	1.50	1.41
3	A	751	FMN	C9-C9A	4.86	1.47	1.39
2	A	752	FAD	C9A-C5X	4.67	1.49	1.41
3	A	751	FMN	C9A-N10	4.55	1.49	1.41
2	A	752	FAD	C4X-N5	4.53	1.39	1.30
2	A	752	FAD	C9A-N10	4.48	1.49	1.41
3	B	751	FMN	C9A-N10	4.32	1.48	1.41
2	A	752	FAD	C6-C5X	4.21	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	752	FAD	C2'-C3'	4.11	1.61	1.53
3	B	751	FMN	C9-C9A	4.09	1.46	1.39
2	A	752	FAD	C2'-C3'	4.05	1.61	1.53
2	B	752	FAD	C6-C5X	3.99	1.46	1.40
3	B	751	FMN	C9A-C5A	3.69	1.47	1.41
2	B	752	FAD	C2A-N3A	3.62	1.37	1.32
3	A	751	FMN	C9A-C5A	3.61	1.47	1.41
2	B	752	FAD	C10-N1	3.58	1.40	1.33
2	A	752	FAD	C2A-N3A	3.53	1.37	1.32
3	B	751	FMN	C8-C7	3.49	1.49	1.40
2	B	752	FAD	C8-C7	3.47	1.49	1.40
3	A	751	FMN	C6-C5A	3.39	1.45	1.40
4	A	753	NAP	P2B-O1X	3.37	1.61	1.50
2	B	752	FAD	C9-C9A	3.36	1.45	1.39
2	A	752	FAD	C10-N1	3.34	1.40	1.33
2	B	752	FAD	O4B-C1B	3.27	1.45	1.41
2	A	752	FAD	C8-C7	3.26	1.49	1.40
3	A	751	FMN	C8-C7	3.24	1.49	1.40
2	A	752	FAD	O4B-C1B	3.22	1.45	1.41
4	B	753	NAP	P2B-O1X	3.20	1.60	1.50
3	B	751	FMN	C1'-C2'	3.19	1.57	1.52
3	B	751	FMN	C6-C5A	3.14	1.44	1.40
2	A	752	FAD	O2'-C2'	3.03	1.49	1.43
2	B	752	FAD	O2'-C2'	3.01	1.49	1.43
2	A	752	FAD	C9-C9A	2.99	1.44	1.39
3	A	751	FMN	C1'-C2'	2.93	1.56	1.52
2	B	752	FAD	C6-C7	2.88	1.43	1.39
4	B	753	NAP	PA-O5B	-2.78	1.48	1.59
2	A	752	FAD	C6-C7	2.73	1.43	1.39
4	A	753	NAP	PA-O5B	-2.67	1.48	1.59
2	B	752	FAD	PA-O5B	-2.65	1.48	1.59
2	B	752	FAD	C8A-N7A	2.64	1.39	1.34
2	B	752	FAD	C4-N3	2.57	1.43	1.38
4	B	753	NAP	C5A-C4A	2.54	1.47	1.40
4	B	753	NAP	P2B-O2B	2.46	1.64	1.59
2	A	752	FAD	C4-N3	2.41	1.43	1.38
2	A	752	FAD	C8A-N7A	2.39	1.39	1.34
2	A	752	FAD	PA-O5B	-2.39	1.49	1.59
4	A	753	NAP	C5A-C4A	2.38	1.47	1.40
4	B	753	NAP	C2A-N3A	2.33	1.35	1.32
3	B	751	FMN	O4'-C4'	2.29	1.48	1.43
3	A	751	FMN	C8M-C8	2.29	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	751	FMN	C10-N1	2.24	1.37	1.33
4	B	753	NAP	C2A-N1A	2.24	1.38	1.33
2	A	752	FAD	P-O5'	-2.20	1.50	1.59
4	A	753	NAP	C2A-N1A	2.16	1.37	1.33
3	B	751	FMN	C10-N1	2.14	1.37	1.33
2	B	752	FAD	P-O5'	-2.10	1.50	1.59
3	B	751	FMN	C8M-C8	2.03	1.55	1.51
3	A	751	FMN	O4'-C4'	2.02	1.47	1.43

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	752	FAD	C2A-N1A-C6A	5.36	127.92	118.75
2	A	752	FAD	C2A-N1A-C6A	5.25	127.74	118.75
2	B	752	FAD	N3A-C2A-N1A	-4.34	121.90	128.68
2	A	752	FAD	N3A-C2A-N1A	-4.29	121.97	128.68
3	A	751	FMN	C9A-C5A-N5	3.92	126.70	122.43
3	B	751	FMN	C9A-C5A-N5	3.79	126.55	122.43
4	A	753	NAP	C4A-C5A-N7A	3.50	113.04	109.40
4	B	753	NAP	C4A-C5A-N7A	3.40	112.95	109.40
2	A	752	FAD	C1B-N9A-C4A	-3.33	120.80	126.64
2	B	752	FAD	C1B-N9A-C4A	-3.06	121.27	126.64
4	B	753	NAP	N3A-C2A-N1A	-3.02	123.96	128.68
4	A	753	NAP	N3A-C2A-N1A	-2.99	124.01	128.68
4	B	753	NAP	PA-O3-PN	-2.98	122.60	132.83
3	A	751	FMN	O4-C4-N3	-2.96	114.44	120.12
2	B	752	FAD	O2'-C2'-C1'	2.90	116.81	109.80
2	A	752	FAD	O2'-C2'-C1'	2.87	116.74	109.80
3	B	751	FMN	O4-C4-N3	-2.86	114.64	120.12
4	B	753	NAP	O2N-PN-O3	2.86	114.21	104.64
2	B	752	FAD	O2-C2-N3	2.82	124.13	118.65
2	A	752	FAD	O2-C2-N3	2.81	124.12	118.65
3	A	751	FMN	C9-C9A-N10	2.77	125.58	121.84
2	B	752	FAD	P-O3P-PA	-2.64	123.76	132.83
4	A	753	NAP	O2N-PN-O3	2.63	113.47	104.64
2	B	752	FAD	C10-N1-C2	2.62	122.13	116.90
2	B	752	FAD	C9-C9A-N10	2.60	125.35	121.84
2	A	752	FAD	C10-N1-C2	2.56	122.03	116.90
4	A	753	NAP	PA-O3-PN	-2.52	124.19	132.83
3	B	751	FMN	P-O5'-C5'	2.50	125.18	118.30
3	A	751	FMN	C5A-C9A-N10	-2.43	115.45	117.95
2	A	752	FAD	O5'-C5'-C4'	2.42	115.82	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	753	NAP	C2A-N1A-C6A	2.39	122.84	118.75
2	A	752	FAD	C9A-C5X-N5	2.38	125.01	122.43
2	B	752	FAD	C9A-C5X-N5	2.37	125.01	122.43
2	B	752	FAD	C5X-C9A-N10	-2.32	115.56	117.95
3	B	751	FMN	C9-C9A-N10	2.31	124.96	121.84
2	A	752	FAD	C9-C9A-N10	2.29	124.94	121.84
2	B	752	FAD	O5'-C5'-C4'	2.27	115.43	109.36
4	A	753	NAP	C2A-N1A-C6A	2.27	122.64	118.75
2	B	752	FAD	C1'-N10-C9A	2.27	124.30	120.51
2	B	752	FAD	C5A-C6A-N1A	-2.23	115.31	120.35
2	A	752	FAD	C8M-C8-C9	-2.18	115.45	119.49
2	A	752	FAD	C5A-C6A-N1A	-2.18	115.41	120.35
3	B	751	FMN	C8M-C8-C7	2.17	125.18	120.74
3	B	751	FMN	O3P-P-O5'	-2.15	101.01	106.73
3	A	751	FMN	P-O5'-C5'	2.14	124.19	118.30
2	B	752	FAD	C8M-C8-C9	-2.10	115.61	119.49
2	A	752	FAD	C5X-C9A-N10	-2.09	115.79	117.95
3	A	751	FMN	O4'-C4'-C3'	-2.07	104.06	109.10
4	B	753	NAP	O4B-C1B-C2B	-2.06	103.02	106.59
3	B	751	FMN	C5A-C9A-N10	-2.03	115.86	117.95

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	753	NAP	PA-O3-PN-O2N
4	B	753	NAP	PA-O3-PN-O5D
2	A	752	FAD	PA-O3P-P-O2P
2	B	752	FAD	PA-O3P-P-O2P
4	B	753	NAP	C2B-O2B-P2B-O1X
4	B	753	NAP	PA-O3-PN-O1N
2	B	752	FAD	PA-O3P-P-O1P
4	A	753	NAP	C5B-O5B-PA-O1A

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	751	FMN	1	0
2	B	752	FAD	1	0
4	A	753	NAP	1	0

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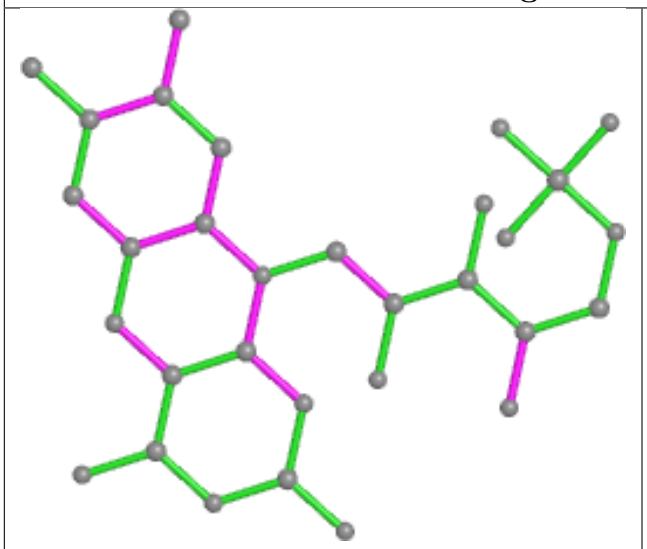
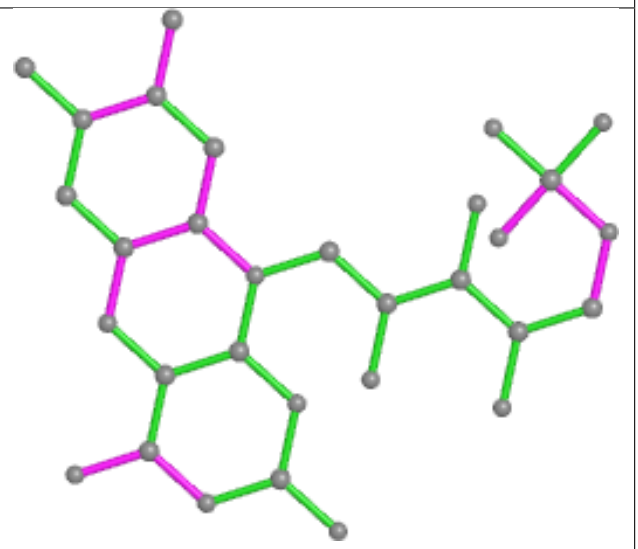
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	753	NAP	1	0

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 then 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.

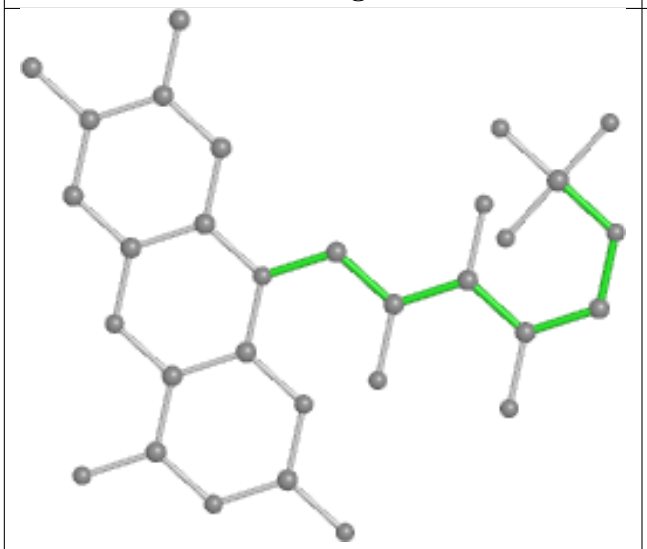
Ligand FMN B 751



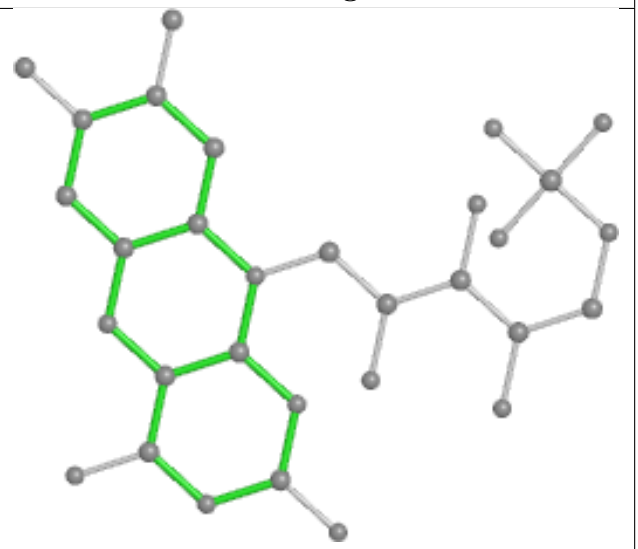
Bond lengths



Bond angles

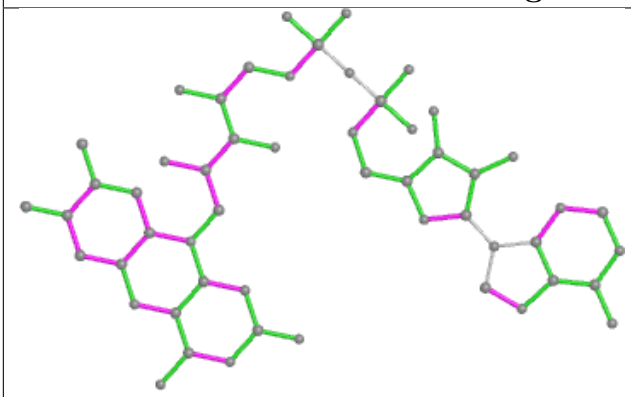


Torsions

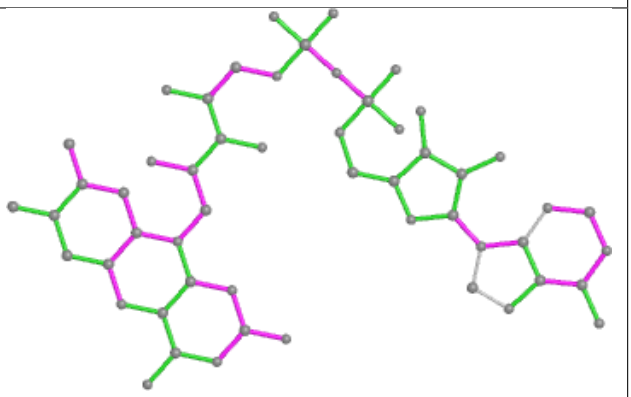


Rings

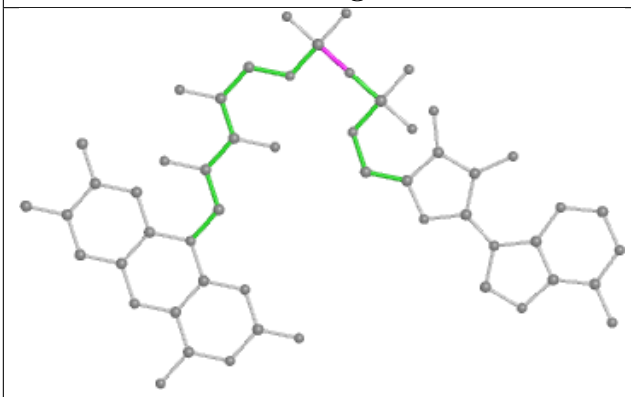
Ligand FAD B 752



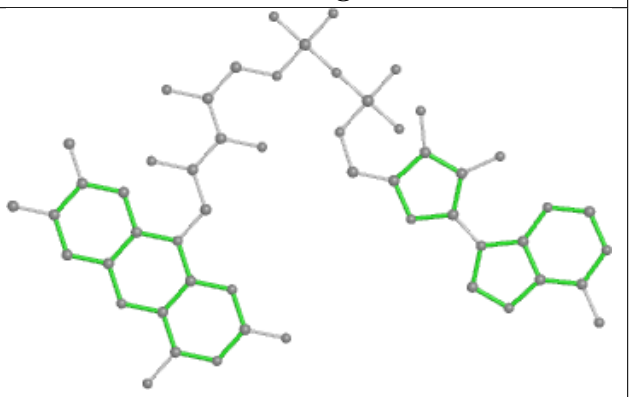
Bond lengths



Bond angles

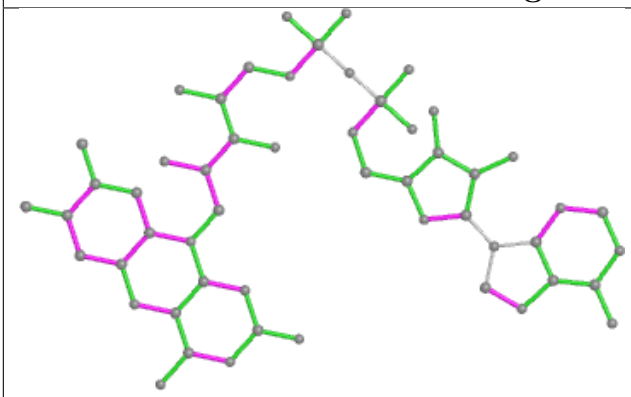


Torsions

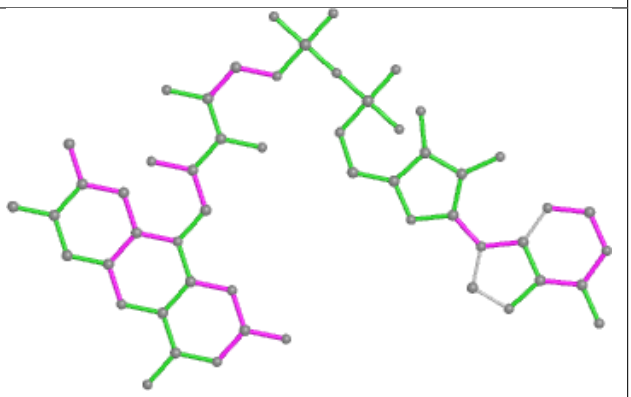


Rings

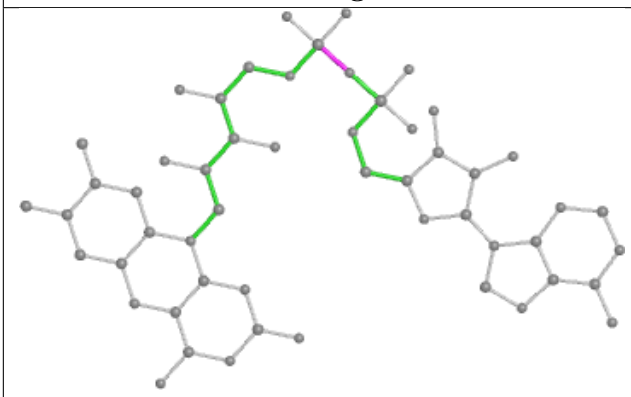
Ligand FAD A 752



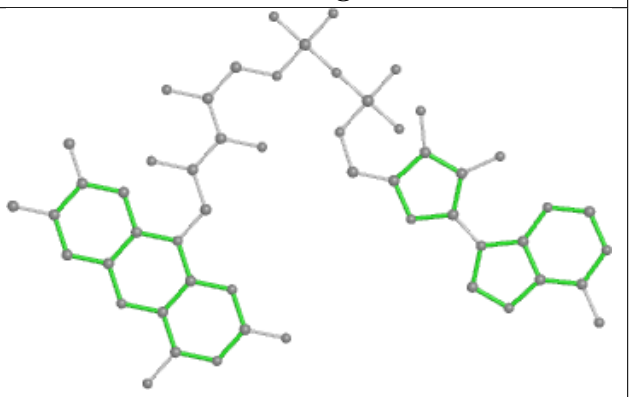
Bond lengths



Bond angles

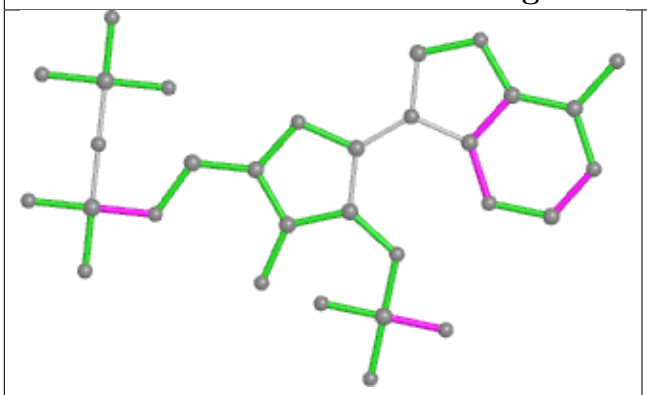


Torsions

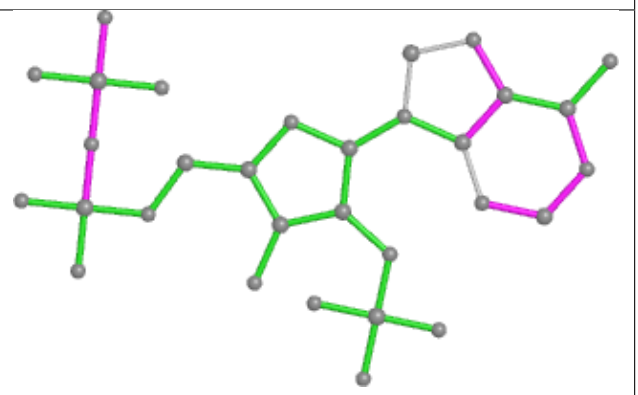


Rings

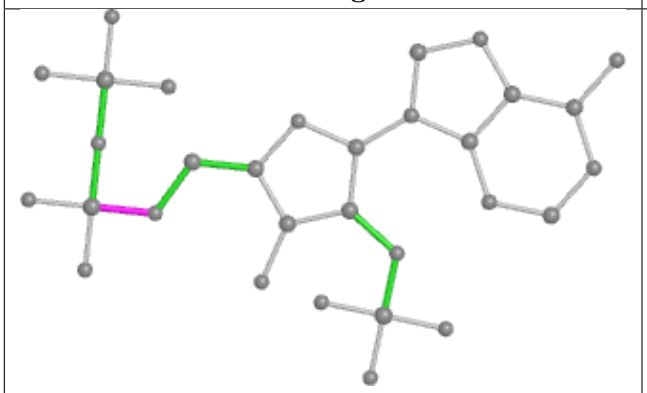
Ligand NAP A 753



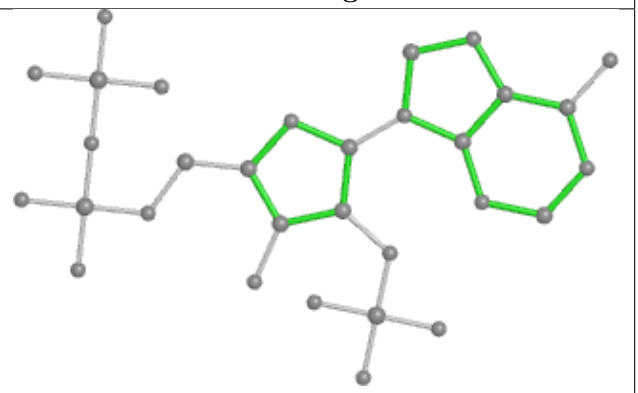
Bond lengths



Bond angles

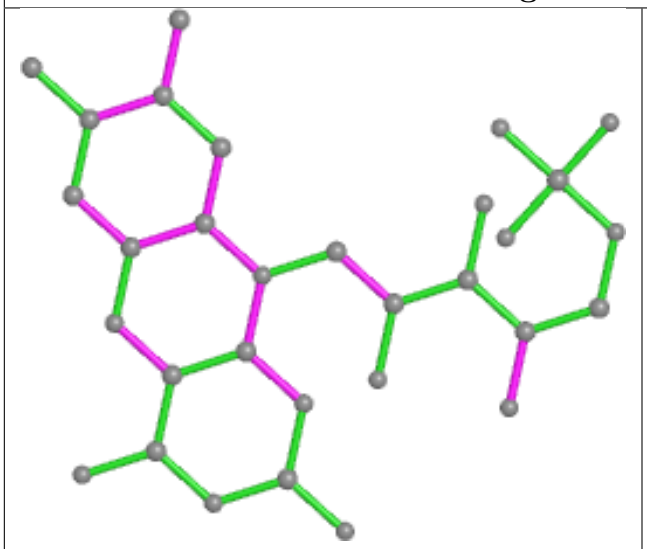


Torsions

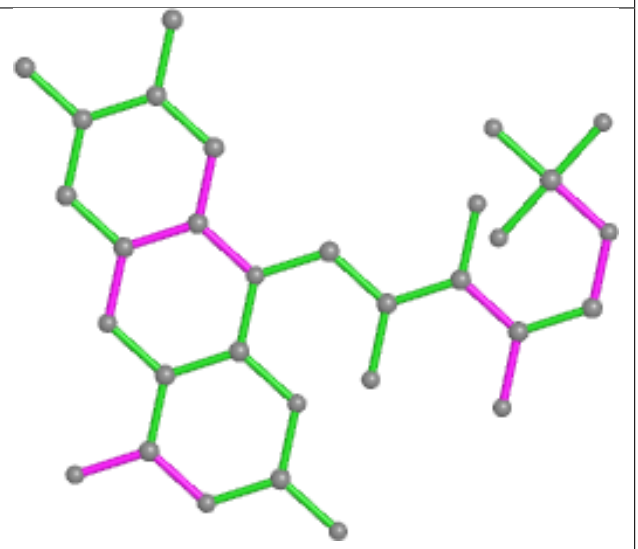


Rings

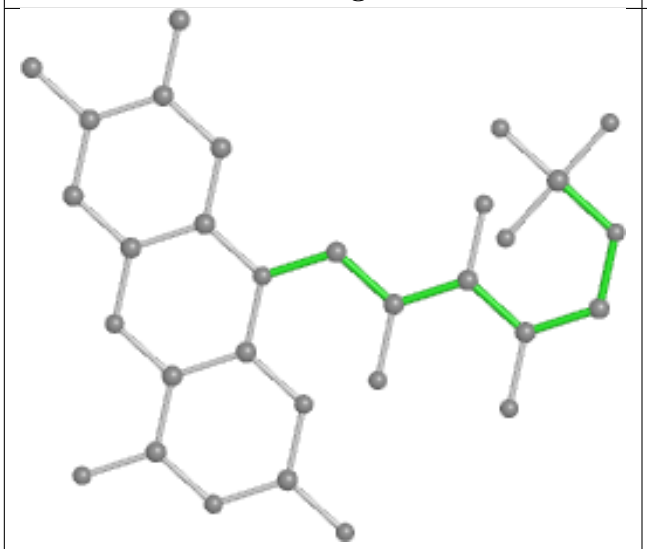
Ligand FMN A 751



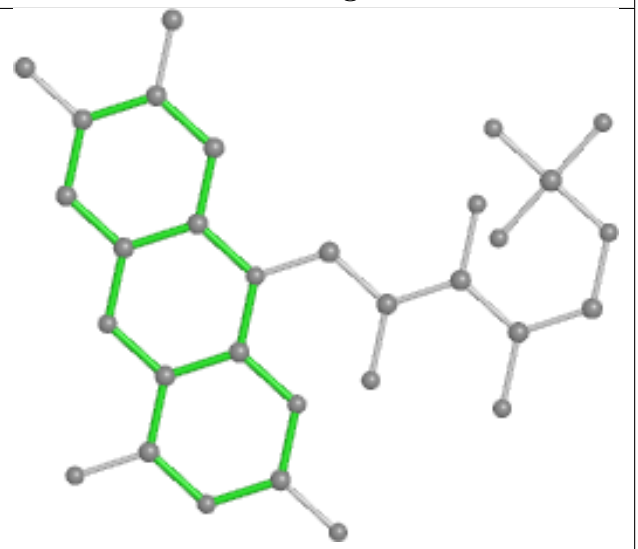
Bond lengths



Bond angles

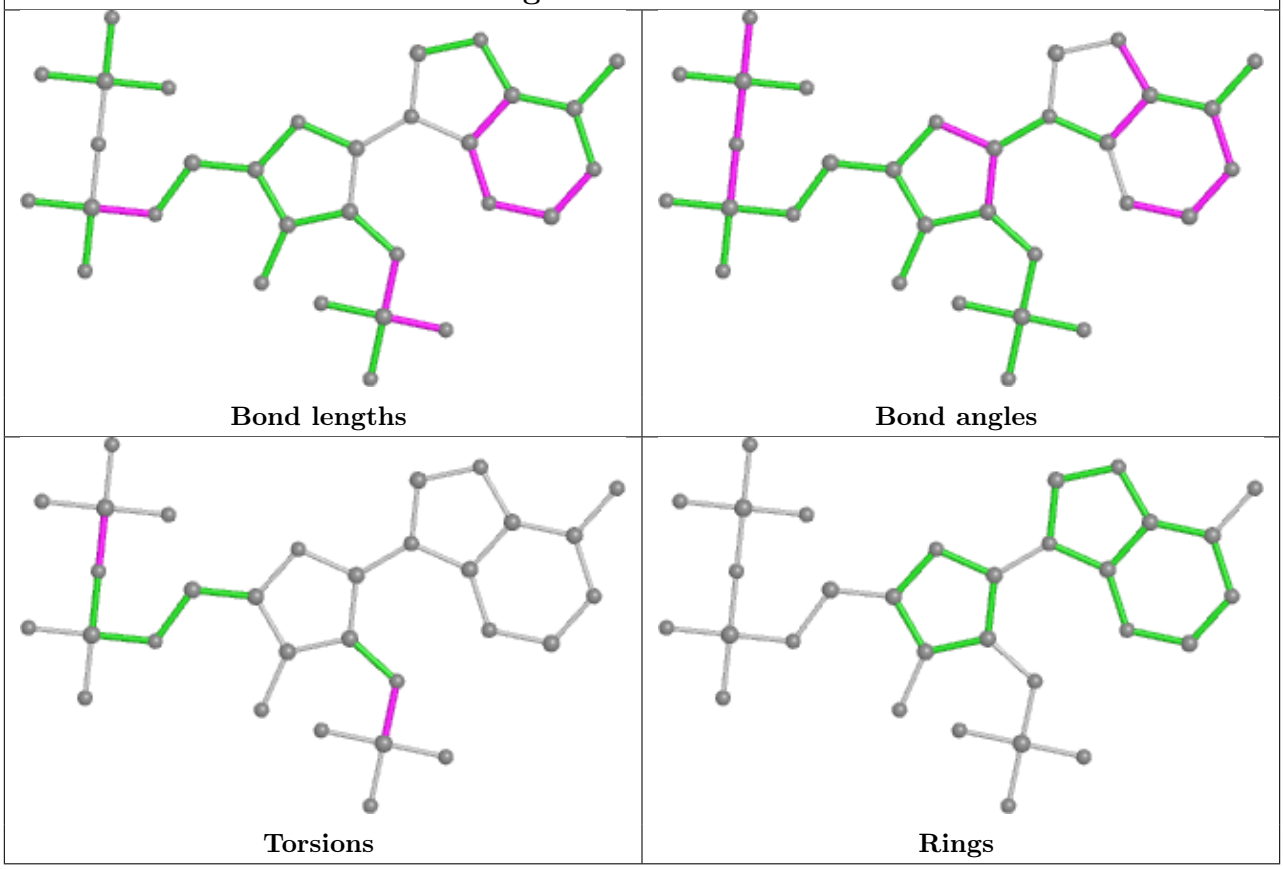


Torsions



Rings

Ligand NAP B 753



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	604/618 (97%)	0.21	22 (3%)	42	49	13, 22, 37, 51	0
1	B	606/618 (98%)	0.57	44 (7%)	15	20	17, 30, 45, 51	0
All	All	1210/1236 (97%)	0.39	66 (5%)	25	31	13, 26, 43, 51	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	525	PHE	6.6
1	A	243	SER	6.0
1	B	70	SER	5.9
1	A	509	ARG	5.7
1	B	143	TYR	5.6
1	B	414	GLU	5.2
1	B	255	ASP	5.0
1	B	268	ARG	4.9
1	B	507	GLY	4.8
1	A	503	VAL	4.6
1	A	244	SER	4.6
1	B	404	LEU	4.6
1	B	418	LEU	4.5
1	B	503	VAL	4.5
1	B	505	GLU	4.4
1	B	239	THR	4.4
1	A	655	ALA	4.0
1	B	417	GLU	4.0
1	A	297	GLN	3.8
1	B	510	ALA	3.8
1	B	504	GLY	3.7
1	A	239	THR	3.4
1	B	485	ALA	3.2
1	A	299	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	412	SER	3.1
1	B	415	GLY	3.1
1	B	107	ARG	3.0
1	B	163	ASP	2.9
1	B	587	ARG	2.9
1	A	415	GLY	2.8
1	A	273	GLU	2.8
1	B	145	GLU	2.8
1	B	571	ARG	2.8
1	B	403	GLU	2.8
1	B	501	GLU	2.7
1	B	402	GLN	2.7
1	B	299	THR	2.7
1	B	574	GLU	2.7
1	B	407	LYS	2.6
1	A	414	GLU	2.6
1	B	390	TYR	2.5
1	B	316	ARG	2.5
1	B	406	ARG	2.4
1	A	680	SER	2.4
1	B	557	GLY	2.4
1	B	509	ARG	2.4
1	A	274	ASN	2.4
1	B	559	GLU	2.4
1	B	488	ILE	2.3
1	B	399	PRO	2.3
1	B	314	LYS	2.3
1	B	78	LYS	2.3
1	A	298	GLY	2.3
1	A	312	ASP	2.3
1	B	297	GLN	2.2
1	B	397	SER	2.2
1	A	300	GLU	2.2
1	B	506	ASN	2.2
1	A	277	PRO	2.2
1	A	603	SER	2.1
1	B	312	ASP	2.1
1	A	406	ARG	2.1
1	B	339	LYS	2.1
1	A	411	SER	2.1
1	A	604	HIS	2.1
1	A	268	ARG	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)

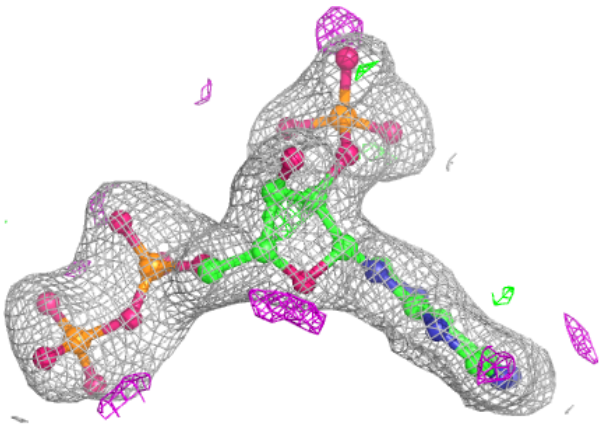
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

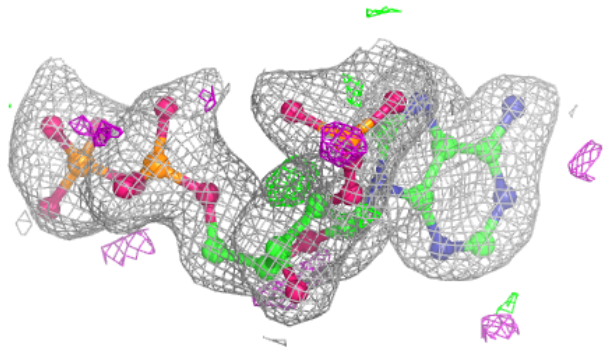
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAP	B	753	31/48	0.93	0.10	22,27,48,52	0
3	FMN	B	751	31/31	0.94	0.11	23,27,32,33	0
4	NAP	A	753	31/48	0.95	0.10	15,21,37,40	0
2	FAD	B	752	53/53	0.95	0.11	19,24,43,44	0
3	FMN	A	751	31/31	0.96	0.14	17,19,24,26	0
2	FAD	A	752	53/53	0.96	0.13	12,16,27,30	0
5	CA	A	762	1/1	0.98	0.05	31,31,31,31	0

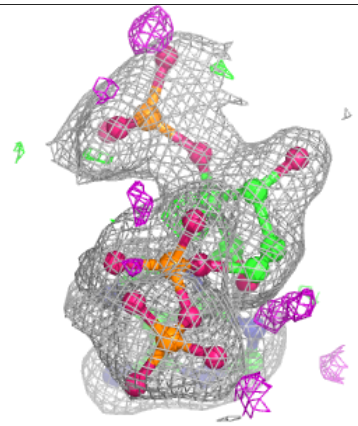
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP B 753:

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

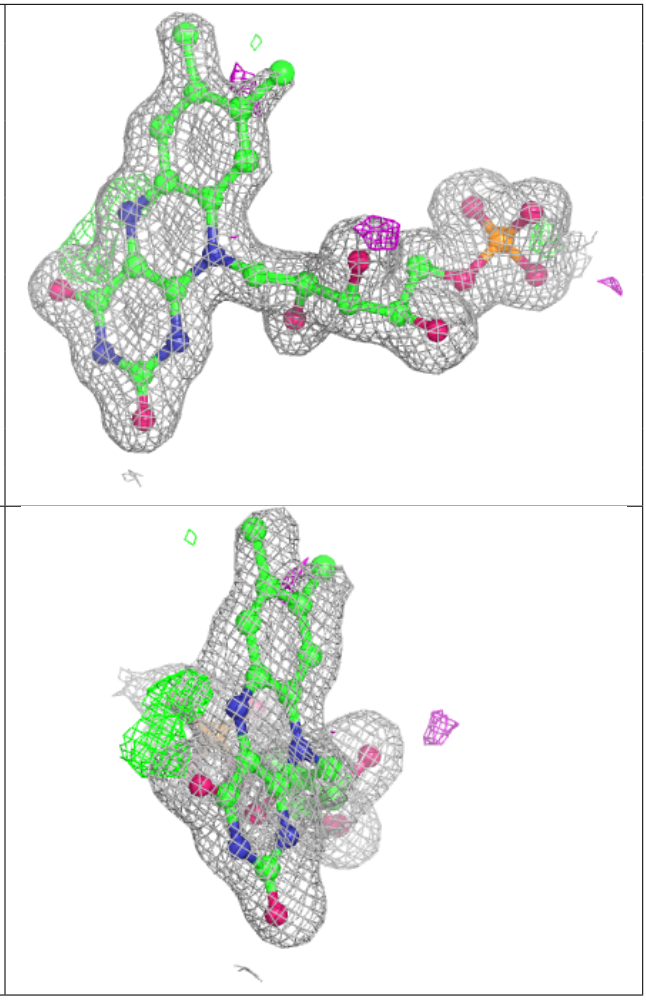






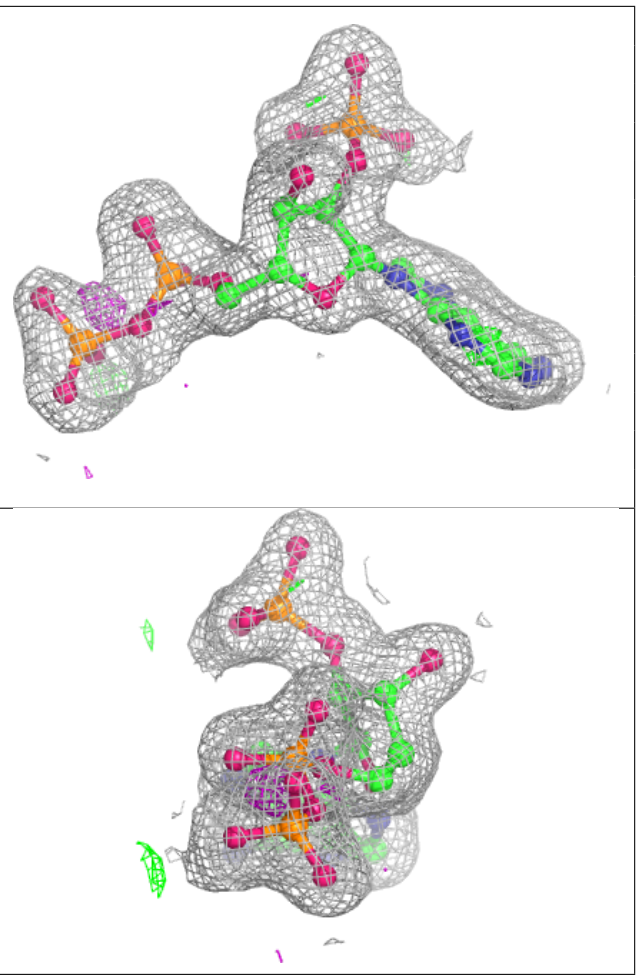
Electron density around FMN B 751:

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



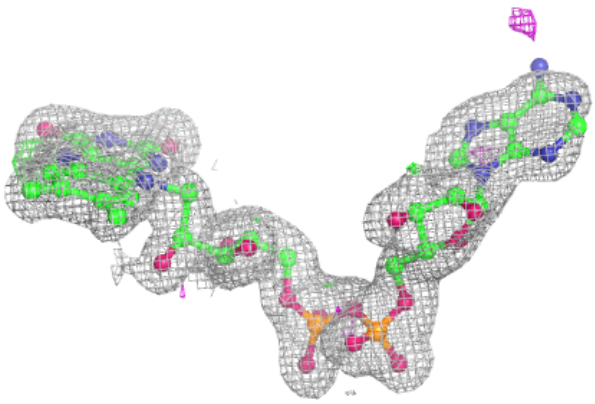
Electron density around NAP A 753:

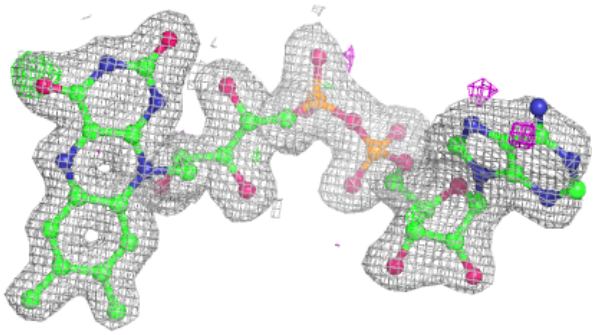
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

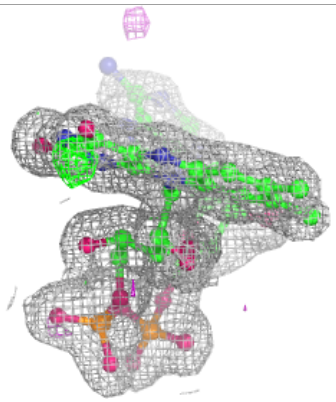


Electron density around FAD B 752:

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

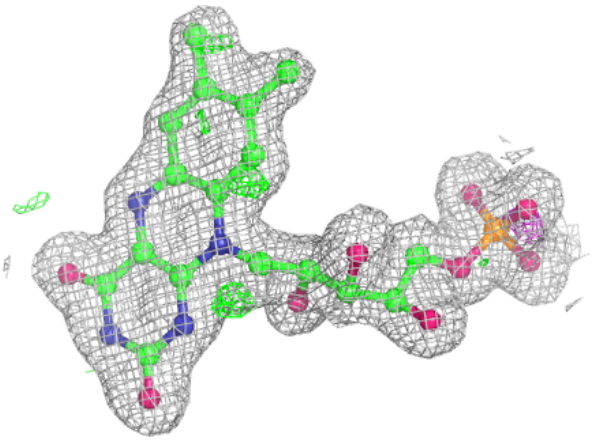


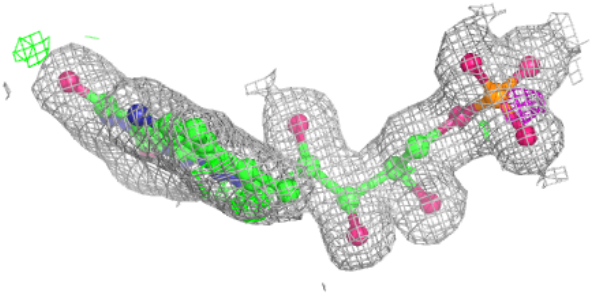


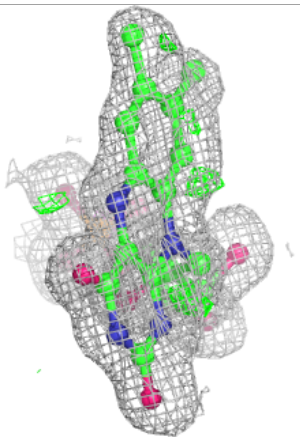


Electron density around FMN A 751:

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

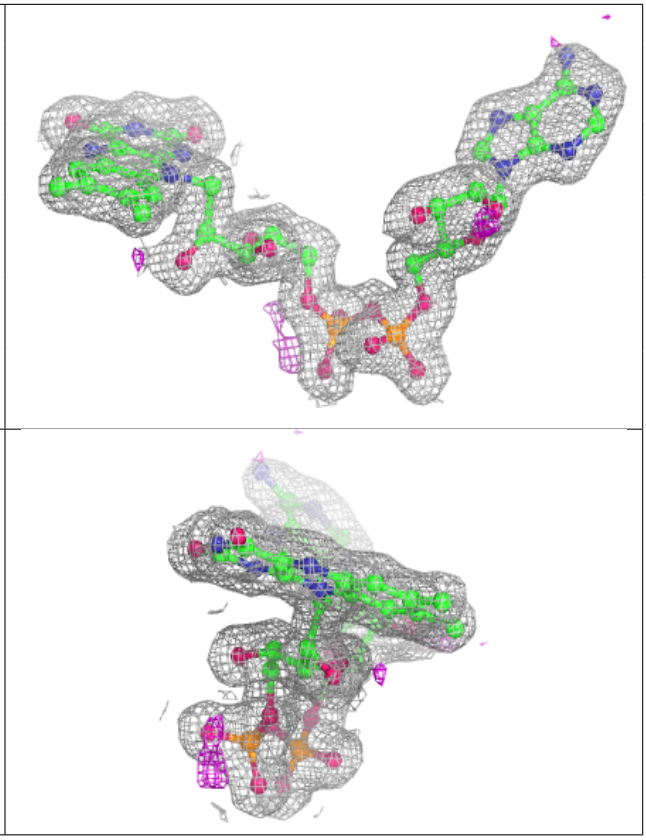






Electron density around FAD A 752:

$2mF_o$-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.