



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 06:07 PM GMT

PDB ID : 1AMO  
Title : THREE-DIMENSIONAL STRUCTURE OF NADPH-CYTOCHROME P450  
REDUCTASE: PROTOTYPE FOR FMN-AND FAD-CONTAINING EN-  
ZYMES  
Authors : Wang, M.; Roberts, D.L.; Paschke, R.; Shea, T.M.; Masters, B.S.S.; Kim,  
J.J.P.  
Deposited on : 1997-06-17  
Resolution : 2.60 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  
<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

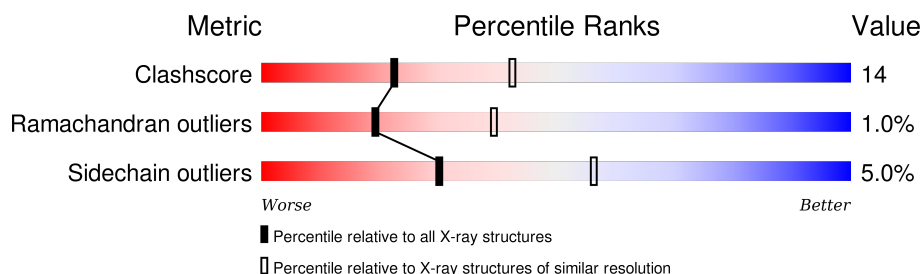
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	615	 67% 27% ...
1	B	615	 67% 28% ...

## 2 Entry composition [i](#)

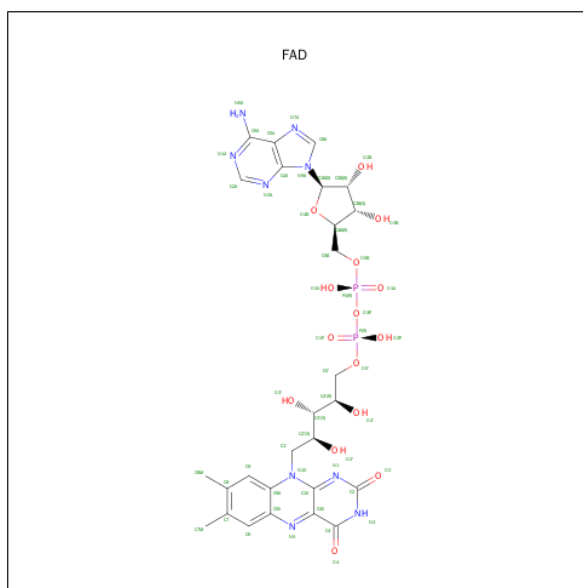
There are 5 unique types of molecules in this entry. The entry contains 10040 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

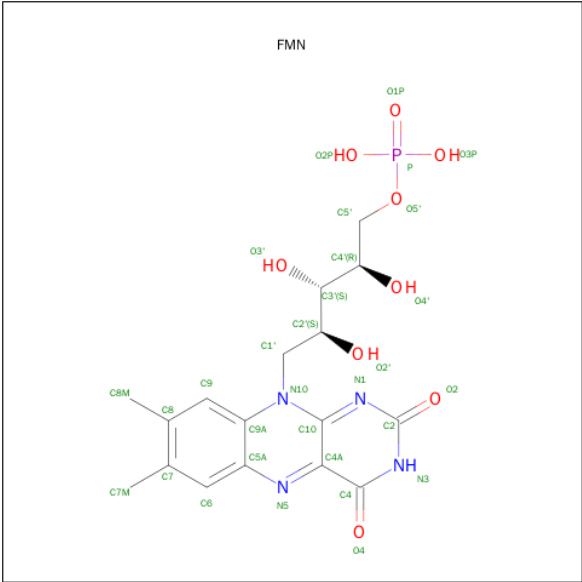
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	601	Total	C	N	O	S	0	0	0
			4830	3062	830	915	23			
1	B	601	Total	C	N	O	S	0	0	0
			4830	3062	830	915	23			

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



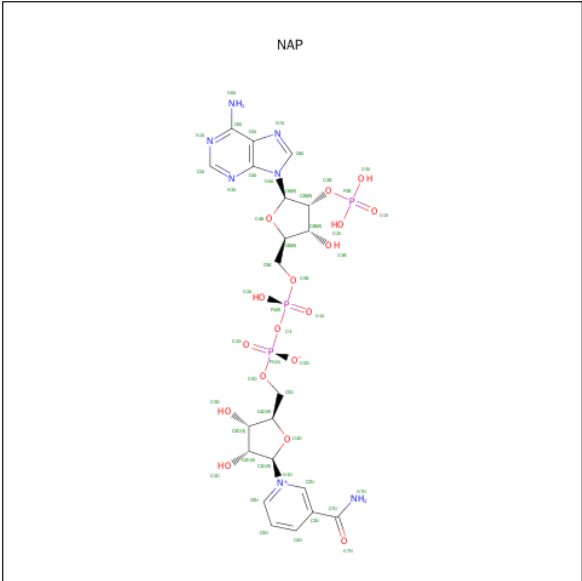
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			47	23	7	15	2		

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



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

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



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

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

- Molecule 5 is water.

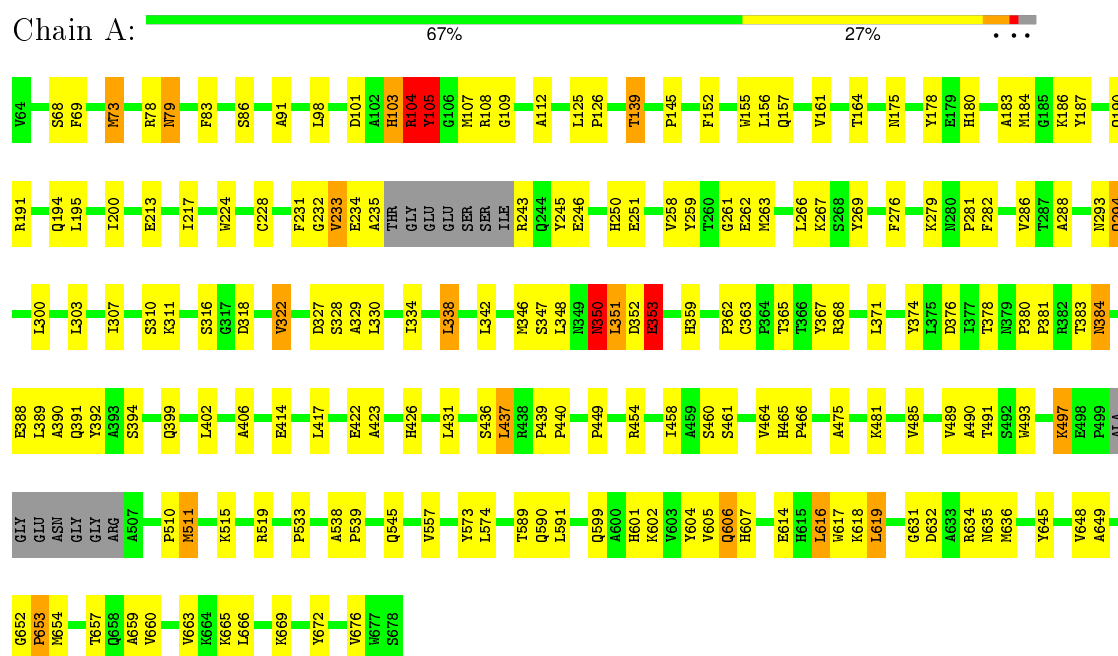
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	78	Total	O	0	0
			78	78		
5	B	78	Total	O	0	0
			78	78		

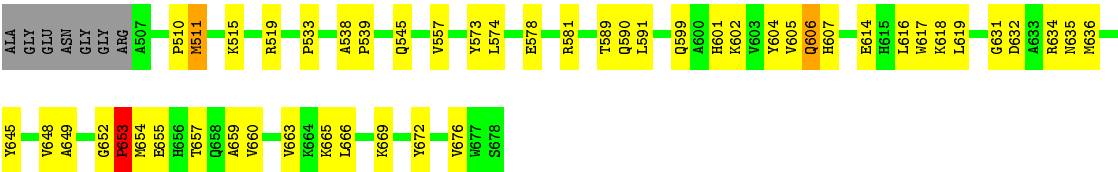
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

#### • Molecule 1: NADPH-CYTOCHROME P450 REDUCTASE





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.28Å 116.18Å 119.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.60	Depositor
% Data completeness (in resolution range)	91.5 (10.00-2.60)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.200 , 0.310	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10040	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.47	1/4945 (0.0%)	0.73	15/6691 (0.2%)
1	B	0.47	1/4945 (0.0%)	0.73	15/6691 (0.2%)
All	All	0.47	2/9890 (0.0%)	0.73	30/13382 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	350	ASN	C-N	10.97	1.59	1.34
1	B	350	ASN	C-N	10.96	1.59	1.34

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	350	ASN	C-N-CA	-9.61	97.67	121.70
1	B	350	ASN	C-N-CA	-9.60	97.69	121.70
1	A	652	GLY	N-CA-C	-8.79	91.12	113.10
1	B	652	GLY	N-CA-C	-8.79	91.12	113.10
1	A	231	PHE	C-N-CA	7.70	138.48	122.30
1	B	231	PHE	C-N-CA	7.67	138.41	122.30
1	A	243	ARG	NE-CZ-NH2	7.42	124.01	120.30
1	B	235	ALA	CB-CA-C	-7.39	99.01	110.10
1	B	243	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	A	235	ALA	CB-CA-C	-7.38	99.04	110.10
1	B	104	ARG	NE-CZ-NH2	6.88	123.74	120.30
1	A	104	ARG	NE-CZ-NH2	6.86	123.73	120.30
1	A	351	LEU	O-C-N	6.75	133.50	122.70
1	B	263	MET	CG-SD-CE	6.74	110.98	100.20
1	A	263	MET	CG-SD-CE	6.72	110.95	100.20
1	B	235	ALA	N-CA-C	6.71	129.13	111.00
1	B	351	LEU	O-C-N	6.71	133.44	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	ALA	N-CA-C	6.71	129.11	111.00
1	B	262	GLU	O-C-N	-6.37	112.50	122.70
1	A	652	GLY	CA-C-O	-6.35	109.17	120.60
1	A	262	GLU	O-C-N	-6.34	112.55	122.70
1	B	652	GLY	CA-C-O	-6.34	109.19	120.60
1	B	351	LEU	CA-C-N	-5.51	105.08	117.20
1	A	352	ASP	N-CA-C	-5.51	96.13	111.00
1	A	351	LEU	CA-C-N	-5.50	105.09	117.20
1	B	352	ASP	N-CA-C	-5.49	96.17	111.00
1	A	73	MET	CG-SD-CE	5.12	108.40	100.20
1	B	73	MET	CG-SD-CE	5.12	108.39	100.20
1	B	103	HIS	CA-CB-CG	-5.07	104.98	113.60
1	A	103	HIS	CA-CB-CG	-5.06	105.00	113.60

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4830	0	4678	129	3
1	B	4830	0	4678	130	10
2	A	53	0	31	2	0
2	B	47	0	22	9	0
3	A	31	0	19	1	0
3	B	31	0	19	1	0
4	A	31	0	11	1	0
4	B	31	0	11	1	0
5	A	78	0	0	10	0
5	B	78	0	0	11	2
All	All	10040	0	9469	266	11

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 14.

All (266) 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:353:GLU:OE1	1:A:353:GLU:HA	1.36	1.11
1:B:353:GLU:OE1	1:B:353:GLU:HA	1.36	1.08
2:B:750:FAD:C7	2:B:750:FAD:C9	2.39	1.00
2:B:750:FAD:C7	2:B:750:FAD:C5X	2.42	0.98
2:B:750:FAD:C7	2:B:750:FAD:C8M	2.50	0.90
2:B:750:FAD:C9	2:B:750:FAD:C8M	2.55	0.85
1:A:353:GLU:OE1	1:A:353:GLU:CA	2.25	0.84
1:A:402:LEU:HD11	1:A:437:LEU:HD21	1.63	0.81
1:B:353:GLU:OE1	1:B:353:GLU:CA	2.25	0.80
1:B:402:LEU:HD11	1:B:437:LEU:HD21	1.63	0.80
1:A:78:ARG:HG2	1:A:108:ARG:HG2	1.66	0.77
1:B:78:ARG:HG2	1:B:108:ARG:HG2	1.66	0.76
2:B:750:FAD:O4	2:B:750:FAD:C4X	2.33	0.76
1:B:461:SER:HB3	1:B:464:VAL:HG22	1.70	0.72
1:A:461:SER:HB3	1:A:464:VAL:HG22	1.70	0.71
1:B:665:LYS:HG3	1:B:669:LYS:HE3	1.77	0.66
1:A:665:LYS:HG3	1:A:669:LYS:HE3	1.77	0.65
1:A:261:GLY:HA2	1:A:374:TYR:CZ	2.32	0.64
1:B:261:GLY:HA2	1:B:374:TYR:CZ	2.32	0.64
1:A:378:THR:O	1:A:426:HIS:HB3	1.97	0.64
1:B:378:THR:O	1:B:426:HIS:HB3	1.97	0.63
1:A:86:SER:HB2	1:A:91:ALA:HB3	1.79	0.63
1:B:632:ASP:OD1	1:B:634:ARG:HG2	1.99	0.63
1:B:86:SER:HB2	1:B:91:ALA:HB3	1.79	0.62
1:A:632:ASP:OD1	1:A:634:ARG:HG2	1.99	0.62
1:A:604:TYR:H	1:A:607:HIS:CD2	2.17	0.62
1:B:156:LEU:HG	1:B:191:ARG:HG2	1.81	0.62
1:B:604:TYR:H	1:B:607:HIS:CD2	2.17	0.61
1:A:156:LEU:HG	1:A:191:ARG:HG2	1.81	0.61
1:B:213:GLU:O	1:B:217:ILE:HG13	2.00	0.61
2:B:750:FAD:C7	2:B:750:FAD:C9A	2.79	0.60
1:A:213:GLU:O	1:A:217:ILE:HG13	2.00	0.60
1:A:105:TYR:CE1	1:A:228:CYS:SG	2.95	0.60
1:B:105:TYR:CE1	1:B:228:CYS:SG	2.95	0.60
1:B:634:ARG:NH1	5:B:779:HOH:O	2.37	0.58
1:B:604:TYR:H	1:B:607:HIS:HD2	1.51	0.58
1:B:515:LYS:HD2	1:B:519:ARG:HH22	1.69	0.58
1:B:614:GLU:HG2	1:B:618:LYS:NZ	2.19	0.58
1:A:614:GLU:HG2	1:A:618:LYS:NZ	2.19	0.58
1:B:300:LEU:HD22	1:B:574:LEU:HD21	1.86	0.57
1:A:617:TRP:HZ3	1:A:648:VAL:HG22	1.69	0.57
1:A:604:TYR:H	1:A:607:HIS:HD2	1.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:LEU:HD11	1:A:439:PRO:HD2	1.87	0.57
1:A:515:LYS:HD2	1:A:519:ARG:HH22	1.69	0.57
1:A:634:ARG:NH1	5:A:823:HOH:O	2.37	0.57
1:B:617:TRP:HZ3	1:B:648:VAL:HG22	1.69	0.57
1:B:105:TYR:HE1	1:B:228:CYS:SG	2.28	0.57
1:A:300:LEU:HD22	1:A:574:LEU:HD21	1.86	0.56
1:A:79:ASN:HD21	1:A:107:MET:HB3	1.70	0.56
1:B:338:LEU:HD11	1:B:439:PRO:HD2	1.87	0.56
1:A:105:TYR:HE1	1:A:228:CYS:SG	2.28	0.56
1:B:383:THR:HG23	1:B:406:ALA:HA	1.87	0.56
1:A:383:THR:HG23	1:A:406:ALA:HA	1.87	0.56
1:A:657:THR:O	1:A:660:VAL:HG22	2.06	0.56
1:B:657:THR:O	1:B:660:VAL:HG22	2.06	0.56
1:A:279:LYS:H	1:A:279:LYS:HD2	1.71	0.55
1:B:659:ALA:O	1:B:663:VAL:HG23	2.07	0.55
1:A:334:ILE:O	1:A:338:LEU:HB2	2.07	0.55
1:B:145:PRO:HB3	1:B:184:MET:SD	2.47	0.55
1:A:186:LYS:O	1:A:190:GLN:HG2	2.06	0.55
1:B:186:LYS:O	1:B:190:GLN:HG2	2.06	0.55
2:B:750:FAD:C7M	2:B:750:FAD:C8M	2.84	0.55
1:A:145:PRO:HB3	1:A:184:MET:SD	2.47	0.55
1:A:557:VAL:HG11	5:A:816:HOH:O	2.07	0.55
1:B:557:VAL:HG11	5:B:772:HOH:O	2.07	0.55
1:A:390:ALA:HA	1:A:402:LEU:HD12	1.89	0.54
1:A:103:HIS:O	1:A:104:ARG:NE	2.30	0.54
1:A:659:ALA:O	1:A:663:VAL:HG23	2.07	0.54
1:A:79:ASN:HD22	1:A:79:ASN:N	2.05	0.54
1:B:279:LYS:H	1:B:279:LYS:HD2	1.71	0.54
1:A:342:LEU:HB3	1:A:368:ARG:HB2	1.89	0.54
1:B:390:ALA:HA	1:B:402:LEU:HD12	1.88	0.54
1:B:79:ASN:HD21	1:B:107:MET:HB3	1.70	0.54
1:B:334:ILE:O	1:B:338:LEU:HB2	2.07	0.54
1:B:347:SER:OG	1:B:363:CYS:HB3	2.07	0.54
1:B:293:ASN:HB2	1:B:300:LEU:H	1.72	0.54
1:B:342:LEU:HB3	1:B:368:ARG:HB2	1.89	0.54
1:B:376:ASP:HB3	1:B:449:PRO:HG2	1.89	0.54
1:A:293:ASN:HB2	1:A:300:LEU:H	1.72	0.54
1:B:79:ASN:HD22	1:B:79:ASN:N	2.05	0.54
1:A:376:ASP:HB3	1:A:449:PRO:HG2	1.89	0.54
1:A:634:ARG:HG3	1:A:635:ASN:N	2.23	0.54
1:B:634:ARG:HG3	1:B:635:ASN:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:GLN:O	1:B:194:GLN:HG3	2.08	0.53
1:A:232:GLY:O	1:A:234:GLU:HB2	2.08	0.53
1:B:232:GLY:O	1:B:234:GLU:HB2	2.08	0.53
1:A:190:GLN:O	1:A:194:GLN:HG3	2.08	0.53
1:B:103:HIS:CE1	1:B:108:ARG:HG3	2.44	0.53
1:A:589:THR:HG22	1:A:590:GLN:HG3	1.90	0.53
1:B:589:THR:HG22	1:B:590:GLN:HG3	1.90	0.53
1:B:101:ASP:O	1:B:105:TYR:HB2	2.09	0.53
1:B:348:LEU:O	1:B:359:HIS:HD2	1.92	0.53
1:A:347:SER:OG	1:A:363:CYS:HB3	2.07	0.53
1:B:103:HIS:O	1:B:104:ARG:NE	2.30	0.53
1:B:464:VAL:HG23	1:B:465:HIS:CD2	2.44	0.53
1:B:599:GLN:HG2	1:B:601:HIS:O	2.08	0.52
1:A:599:GLN:HG3	1:A:601:HIS:CE1	2.44	0.52
1:A:464:VAL:HG23	1:A:465:HIS:CD2	2.44	0.52
1:B:599:GLN:HG3	1:B:601:HIS:CE1	2.45	0.52
1:A:599:GLN:HG2	1:A:601:HIS:O	2.08	0.52
1:A:310:SER:O	1:A:311:LYS:HB2	2.09	0.52
1:A:103:HIS:CE1	1:A:108:ARG:HG3	2.44	0.52
1:A:368:ARG:HH11	1:A:368:ARG:HG3	1.74	0.52
1:A:101:ASP:O	1:A:105:TYR:HB2	2.09	0.52
1:B:368:ARG:HG3	1:B:368:ARG:HH11	1.74	0.52
1:B:310:SER:O	1:B:311:LYS:HB2	2.09	0.52
1:B:79:ASN:H	1:B:79:ASN:HD22	1.58	0.51
1:A:602:LYS:HD3	1:A:604:TYR:OH	2.10	0.51
1:A:604:TYR:HB3	1:A:606:GLN:OE1	2.10	0.51
1:B:604:TYR:HB3	1:B:606:GLN:OE1	2.10	0.51
1:A:68:SER:HA	5:A:775:HOH:O	2.11	0.51
1:A:348:LEU:O	1:A:359:HIS:HD2	1.92	0.51
1:B:68:SER:HA	5:B:809:HOH:O	2.11	0.51
1:A:322:VAL:HG13	1:A:493:TRP:HZ3	1.76	0.51
1:B:322:VAL:HG13	1:B:493:TRP:HZ3	1.76	0.51
1:B:602:LYS:HD3	1:B:604:TYR:OH	2.10	0.50
1:A:557:VAL:CG1	5:A:816:HOH:O	2.60	0.50
1:A:175:ASN:HB3	1:A:178:TYR:HD1	1.77	0.50
1:B:175:ASN:HB3	1:B:178:TYR:HD1	1.77	0.50
1:A:79:ASN:H	1:A:79:ASN:HD22	1.58	0.50
1:B:466:PRO:O	5:B:768:HOH:O	2.20	0.50
1:A:466:PRO:O	5:A:812:HOH:O	2.20	0.50
1:A:246:GLU:O	1:A:348:LEU:HA	2.12	0.49
1:B:125:LEU:N	1:B:126:PRO:HD2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:LEU:N	1:A:126:PRO:HD2	2.27	0.49
1:B:384:ASN:HD22	1:B:384:ASN:H	1.60	0.49
1:B:250:HIS:CE1	1:B:347:SER:HB2	2.48	0.49
1:B:246:GLU:O	1:B:348:LEU:HA	2.12	0.49
1:B:269:TYR:HE1	1:B:281:PRO:HG2	1.78	0.49
1:B:475:ALA:HA	1:B:491:THR:HB	1.95	0.49
1:A:533:PRO:HG3	1:A:636:MET:HG3	1.94	0.49
1:B:318:ASP:OD1	1:B:515:LYS:HA	2.13	0.48
1:A:250:HIS:CE1	1:A:347:SER:HB2	2.47	0.48
1:B:388:GLU:O	1:B:391:GLN:HG2	2.13	0.48
1:A:250:HIS:HE1	1:A:347:SER:HB2	1.78	0.48
1:A:388:GLU:O	1:A:391:GLN:HG2	2.13	0.48
1:A:475:ALA:HA	1:A:491:THR:HB	1.95	0.48
1:B:533:PRO:HG3	1:B:636:MET:HG3	1.94	0.48
1:B:515:LYS:HD2	1:B:519:ARG:NH2	2.29	0.48
1:B:557:VAL:CG1	5:B:772:HOH:O	2.60	0.48
1:A:269:TYR:HE1	1:A:281:PRO:HG2	1.78	0.48
1:A:318:ASP:OD1	1:A:515:LYS:HA	2.13	0.48
1:B:417:LEU:O	1:B:422:GLU:HB2	2.13	0.48
1:B:645:TYR:HD1	1:B:663:VAL:HG21	1.79	0.48
1:A:645:TYR:HD1	1:A:663:VAL:HG21	1.79	0.48
1:A:175:ASN:HB3	1:A:178:TYR:CD1	2.49	0.48
1:A:417:LEU:O	1:A:422:GLU:HB2	2.13	0.48
1:A:384:ASN:HD22	1:A:384:ASN:H	1.60	0.48
1:B:458:ILE:HG22	1:B:460:SER:H	1.79	0.48
1:A:606:GLN:OE1	4:A:752:NAP:H2A	2.14	0.48
1:B:606:GLN:OE1	4:B:752:NAP:H2A	2.14	0.48
1:A:458:ILE:HG22	1:A:460:SER:H	1.79	0.47
1:A:614:GLU:HB3	5:A:815:HOH:O	2.15	0.47
1:B:538:ALA:HB3	1:B:539:PRO:CD	2.44	0.47
1:A:515:LYS:HD2	1:A:519:ARG:NH2	2.29	0.47
1:B:250:HIS:HE1	1:B:347:SER:HB2	1.79	0.47
1:B:175:ASN:HB3	1:B:178:TYR:CD1	2.49	0.47
1:A:316:SER:HA	5:A:787:HOH:O	2.14	0.47
1:A:493:TRP:HH2	1:A:510:PRO:HD2	1.80	0.47
1:A:538:ALA:HB3	1:A:539:PRO:CD	2.44	0.47
1:B:493:TRP:HH2	1:B:510:PRO:HD2	1.80	0.47
1:A:489:VAL:HG23	2:A:750:FAD:O1A	2.15	0.47
1:A:286:VAL:HG21	1:A:497:LYS:HB3	1.96	0.47
1:A:155:TRP:HZ2	1:A:161:VAL:HG11	1.80	0.47
1:A:485:VAL:HG23	5:B:817:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:489:VAL:HG23	2:B:750:FAD:O1A	2.15	0.47
1:A:330:LEU:O	1:A:334:ILE:HG13	2.15	0.47
5:A:783:HOH:O	1:B:485:VAL:HG23	2.14	0.47
1:B:316:SER:HA	5:B:821:HOH:O	2.14	0.46
1:B:276:PHE:CE2	1:B:282:PHE:HD2	2.34	0.46
1:B:279:LYS:N	1:B:279:LYS:HD2	2.31	0.46
1:A:276:PHE:CE2	1:A:282:PHE:HD2	2.34	0.46
1:B:245:TYR:CE1	1:B:350:ASN:HB2	2.50	0.46
1:B:330:LEU:O	1:B:334:ILE:HG13	2.15	0.46
1:A:402:LEU:CD1	1:A:437:LEU:HD21	2.42	0.46
1:B:390:ALA:O	1:B:399:GLN:HG3	2.16	0.46
1:B:69:PHE:HD1	1:B:73:MET:HE2	1.80	0.46
1:B:98:LEU:O	1:B:224:TRP:HZ2	1.99	0.46
1:B:286:VAL:HG21	1:B:497:LYS:HB3	1.96	0.46
1:A:384:ASN:O	1:A:388:GLU:HG2	2.16	0.46
1:B:402:LEU:CD1	1:B:437:LEU:HD21	2.42	0.45
1:A:279:LYS:N	1:A:279:LYS:HD2	2.31	0.45
1:A:245:TYR:CE1	1:A:350:ASN:HB2	2.50	0.45
1:A:390:ALA:O	1:A:399:GLN:HG3	2.16	0.45
1:B:649:ALA:HA	1:B:654:MET:HB2	1.98	0.45
1:B:155:TRP:HZ2	1:B:161:VAL:HG11	1.80	0.45
1:A:649:ALA:HA	1:A:654:MET:HB2	1.98	0.45
1:A:98:LEU:O	1:A:224:TRP:HZ2	1.99	0.45
1:B:614:GLU:HB3	5:B:771:HOH:O	2.15	0.45
1:B:233:VAL:HG13	1:B:234:GLU:H	1.82	0.45
1:B:631:GLY:O	1:B:676:VAL:HA	2.17	0.45
1:A:631:GLY:O	1:A:676:VAL:HA	2.17	0.45
1:B:294:GLN:HE21	1:B:294:GLN:HB2	1.59	0.45
1:A:233:VAL:HG13	1:A:234:GLU:H	1.81	0.44
1:A:103:HIS:CD2	1:A:109:GLY:H	2.35	0.44
1:A:351:LEU:HD23	1:A:351:LEU:HA	1.90	0.44
1:A:490:ALA:O	1:A:493:TRP:HB3	2.18	0.44
1:B:327:ASP:OD2	1:B:329:ALA:HB3	2.18	0.44
1:B:103:HIS:CD2	1:B:109:GLY:H	2.35	0.44
1:B:423:ALA:HA	1:B:481:LYS:HB2	2.00	0.44
1:B:384:ASN:O	1:B:388:GLU:HG2	2.16	0.44
1:A:288:ALA:O	1:A:303:LEU:HA	2.18	0.43
1:A:104:ARG:HA	1:A:104:ARG:HD3	1.84	0.43
1:B:261:GLY:HA2	1:B:374:TYR:OH	2.19	0.43
1:B:338:LEU:HD13	1:B:431:LEU:HD13	2.01	0.43
1:A:157:GLN:HA	1:A:187:TYR:OH	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:PHE:HA	1:A:112:ALA:O	2.18	0.43
1:B:288:ALA:O	1:B:303:LEU:HA	2.18	0.43
1:A:423:ALA:HA	1:A:481:LYS:HB2	2.00	0.43
1:A:511:MET:C	1:A:511:MET:SD	2.97	0.43
1:B:511:MET:C	1:B:511:MET:SD	2.97	0.43
1:B:83:PHE:HA	1:B:112:ALA:O	2.18	0.43
1:A:180:HIS:HB3	1:A:183:ALA:HB2	2.00	0.43
1:A:327:ASP:OD2	1:A:329:ALA:HB3	2.18	0.43
1:B:105:TYR:CZ	1:B:224:TRP:HB3	2.54	0.43
1:B:157:GLN:HA	1:B:187:TYR:OH	2.18	0.43
1:A:338:LEU:HD13	1:A:431:LEU:HD13	2.01	0.43
1:B:328:SER:CB	5:B:766:HOH:O	2.66	0.43
1:A:261:GLY:HA2	1:A:374:TYR:OH	2.19	0.43
1:A:139:THR:HG23	3:A:751:FMN:C2	2.49	0.43
1:B:246:GLU:HB3	1:B:351:LEU:HD12	2.01	0.43
1:B:180:HIS:HB3	1:B:183:ALA:HB2	2.00	0.43
1:B:139:THR:HG23	3:B:751:FMN:C2	2.49	0.43
1:B:490:ALA:O	1:B:493:TRP:HB3	2.18	0.42
1:A:380:PRO:HA	1:A:381:PRO:HD3	1.94	0.42
1:A:605:VAL:HG13	5:A:807:HOH:O	2.18	0.42
1:A:105:TYR:CZ	1:A:224:TRP:HB3	2.54	0.42
1:A:307:ILE:O	1:A:307:ILE:HG13	2.19	0.42
1:A:464:VAL:HG21	1:A:545:GLN:HB3	2.00	0.42
1:A:294:GLN:HB2	1:A:294:GLN:HE21	1.59	0.42
1:A:246:GLU:HB3	1:A:351:LEU:HD12	2.01	0.42
1:A:328:SER:CB	5:A:810:HOH:O	2.66	0.42
1:B:303:LEU:HD12	1:B:303:LEU:N	2.35	0.42
1:A:69:PHE:HD1	1:A:73:MET:HE2	1.84	0.42
1:A:303:LEU:HD12	1:A:303:LEU:N	2.35	0.42
1:A:392:TYR:CE1	1:A:440:PRO:HD3	2.55	0.42
1:B:307:ILE:HG13	1:B:307:ILE:O	2.19	0.42
1:B:394:SER:H	1:B:436:SER:HB3	1.85	0.42
1:B:342:LEU:HA	1:B:367:TYR:HB2	2.01	0.42
1:B:389:LEU:HA	1:B:392:TYR:HD2	1.85	0.42
1:B:491:THR:HG23	2:B:750:FAD:O2P	2.20	0.41
1:B:605:VAL:HG13	5:B:763:HOH:O	2.18	0.41
1:B:464:VAL:HG21	1:B:545:GLN:HB3	2.00	0.41
1:B:392:TYR:CE1	1:B:440:PRO:HD3	2.55	0.41
1:A:152:PHE:CZ	1:A:156:LEU:HD22	2.56	0.41
1:B:450:ARG:NH1	5:B:776:HOH:O	2.40	0.41
1:A:394:SER:H	1:A:436:SER:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:VAL:HG13	1:A:493:TRP:CZ3	2.55	0.41
1:A:619:LEU:HD12	1:A:619:LEU:HA	1.86	0.41
1:B:663:VAL:O	1:B:666:LEU:HB2	2.20	0.41
1:A:389:LEU:HA	1:A:392:TYR:HD2	1.85	0.41
1:A:259:TYR:CE1	1:A:266:LEU:HG	2.56	0.41
1:A:342:LEU:HA	1:A:367:TYR:HB2	2.01	0.41
1:A:663:VAL:O	1:A:666:LEU:HB2	2.21	0.41
1:B:103:HIS:CD2	1:B:108:ARG:HA	2.57	0.40
1:B:617:TRP:CZ3	1:B:648:VAL:HA	2.56	0.40
1:A:491:THR:HG23	2:A:750:FAD:O2P	2.20	0.40
1:B:258:VAL:HG13	1:B:365:THR:HA	2.02	0.40
1:B:262:GLU:HB2	1:B:268:SER:OG	2.21	0.40
1:B:104:ARG:HD3	1:B:104:ARG:HA	1.83	0.40
1:B:152:PHE:CZ	1:B:156:LEU:HD22	2.56	0.40
1:B:139:THR:HG21	1:B:182:ASN:HA	2.03	0.40
1:A:258:VAL:HG13	1:A:365:THR:HA	2.02	0.40
1:B:380:PRO:HA	1:B:381:PRO:HD3	1.94	0.40
1:B:259:TYR:CE1	1:B:266:LEU:HG	2.56	0.40
1:A:616:LEU:HD12	1:A:616:LEU:HA	1.95	0.40

All (11) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:ASN:OD1	1:B:655:GLU:OE2[3_655]	1.58	0.62
1:B:271:ASN:CG	1:B:655:GLU:OE2[3_655]	1.63	0.57
1:A:669:LYS:O	1:B:251:GLU:OE1[3_545]	1.64	0.56
5:B:795:HOH:O	5:B:825:HOH:O[3_645]	1.70	0.50
1:B:271:ASN:ND2	1:B:655:GLU:OE2[3_655]	1.72	0.48
1:B:266:LEU:O	5:B:796:HOH:O[3_655]	1.73	0.47
1:A:164:THR:CG2	1:B:578:GLU:OE2[2_555]	1.86	0.34
1:B:266:LEU:CD1	1:B:653:PRO:CG[3_655]	2.03	0.17
1:B:271:ASN:ND2	1:B:655:GLU:CD[3_655]	2.07	0.13
1:A:195:LEU:CA	1:B:581:ARG:NH2[2_555]	2.12	0.08
1:B:271:ASN:ND2	1:B:655:GLU:OE1[3_655]	2.17	0.03

## 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	595/615 (97%)	547 (92%)	42 (7%)	6 (1%)	19	39
1	B	595/615 (97%)	546 (92%)	43 (7%)	6 (1%)	19	39
All	All	1190/1230 (97%)	1093 (92%)	85 (7%)	12 (1%)	19	39

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	353	GLU
1	B	353	GLU
1	A	497	LYS
1	A	653	PRO
1	B	497	LYS
1	B	653	PRO
1	A	105	TYR
1	B	105	TYR
1	A	437	LEU
1	B	437	LEU
1	A	233	VAL
1	B	233	VAL

### 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	516/525 (98%)	490 (95%)	26 (5%)	30	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	516/525 (98%)	490 (95%)	26 (5%)	30	56
All	All	1032/1050 (98%)	980 (95%)	52 (5%)	30	56

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	104	ARG
1	A	105	TYR
1	A	139	THR
1	A	200	ILE
1	A	251	GLU
1	A	267	LYS
1	A	294	GLN
1	A	322	VAL
1	A	338	LEU
1	A	346	MET
1	A	350	ASN
1	A	353	GLU
1	A	362	PRO
1	A	371	LEU
1	A	384	ASN
1	A	414	GLU
1	A	454	ARG
1	A	511	MET
1	A	573	TYR
1	A	591	LEU
1	A	606	GLN
1	A	616	LEU
1	A	619	LEU
1	A	653	PRO
1	A	672	TYR
1	B	79	ASN
1	B	104	ARG
1	B	105	TYR
1	B	139	THR
1	B	200	ILE
1	B	251	GLU
1	B	267	LYS
1	B	294	GLN
1	B	322	VAL
1	B	338	LEU

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Mol	Chain	Res	Type
1	B	346	MET
1	B	350	ASN
1	B	353	GLU
1	B	362	PRO
1	B	371	LEU
1	B	384	ASN
1	B	414	GLU
1	B	454	ARG
1	B	511	MET
1	B	573	TYR
1	B	591	LEU
1	B	606	GLN
1	B	616	LEU
1	B	619	LEU
1	B	653	PRO
1	B	672	TYR

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	79	ASN
1	A	180	HIS
1	A	250	HIS
1	A	293	ASN
1	A	294	GLN
1	A	302	HIS
1	A	350	ASN
1	A	384	ASN
1	A	399	GLN
1	A	465	HIS
1	A	486	ASN
1	A	607	HIS
1	B	79	ASN
1	B	180	HIS
1	B	250	HIS
1	B	293	ASN
1	B	294	GLN
1	B	302	HIS
1	B	350	ASN
1	B	384	ASN
1	B	399	GLN
1	B	465	HIS

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Mol	Chain	Res	Type
1	B	486	ASN
1	B	607	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

6 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	750	-	52,58,58	1.33	6 (11%)	52,89,89	3.06	14 (26%)
3	FMN	A	751	-	32,33,33	1.22	4 (12%)	34,50,50	3.48	10 (29%)
4	NAP	A	752	-	28,33,52	0.96	0	35,52,80	2.03	6 (17%)
2	FAD	B	750	-	40,46,58	2.54	6 (15%)	38,67,89	1.86	9 (23%)
3	FMN	B	751	-	32,33,33	1.22	4 (12%)	34,50,50	3.49	10 (29%)
4	NAP	B	752	-	28,33,52	0.96	0	35,52,80	2.03	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
2	FAD	A	750	-	-	0/30/50/50	0/6/6/6
3	FMN	A	751	-	-	0/18/18/18	0/3/3/3
4	NAP	A	752	-	-	0/17/37/67	0/3/3/5
2	FAD	B	750	-	-	0/30/50/50	0/4/4/6
3	FMN	B	751	-	-	0/18/18/18	0/3/3/3
4	NAP	B	752	-	-	0/17/37/67	0/3/3/5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	FAD	C5X-C9A	-8.00	1.41	1.51
2	B	750	FAD	C5X-N5	-7.80	1.36	1.46
2	B	750	FAD	C10-C4X	-3.64	1.39	1.49
2	B	750	FAD	C9-C9A	-2.99	1.43	1.52
2	A	750	FAD	C1'-N10	-2.80	1.45	1.48
3	A	751	FMN	P-O3P	-2.20	1.47	1.54
3	B	751	FMN	P-O3P	-2.18	1.47	1.54
3	B	751	FMN	P-O2P	-2.13	1.47	1.54
3	A	751	FMN	P-O2P	-2.13	1.47	1.54
2	B	750	FAD	P-O2P	-2.04	1.46	1.55
2	A	750	FAD	P-O2P	-2.03	1.46	1.55
3	B	751	FMN	C10-N10	2.54	1.42	1.39
3	A	751	FMN	C10-N10	2.55	1.42	1.39
2	A	750	FAD	C4X-N5	2.92	1.37	1.33
2	A	750	FAD	C9A-N10	3.05	1.43	1.38
3	B	751	FMN	C4-N3	3.38	1.39	1.33
3	A	751	FMN	C4-N3	3.39	1.39	1.33
2	A	750	FAD	C10-N10	3.98	1.43	1.39
2	A	750	FAD	C4-N3	4.18	1.40	1.33
2	B	750	FAD	C4X-N5	9.06	1.37	1.27

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	750	FAD	N3-C2-N1	-7.95	114.30	127.69
3	B	751	FMN	N3-C2-N1	-7.55	114.98	127.69
3	A	751	FMN	N3-C2-N1	-7.54	114.98	127.69
2	A	750	FAD	C4-C4X-C10	-7.16	115.36	119.94
4	A	752	NAP	C1B-N9A-C4A	-6.71	119.32	126.81
4	B	752	NAP	C1B-N9A-C4A	-6.70	119.33	126.81
4	A	752	NAP	N3A-C2A-N1A	-6.63	123.66	128.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	752	NAP	N3A-C2A-N1A	-6.61	123.68	128.87
3	B	751	FMN	C4A-C4-N3	-6.32	115.26	123.52
2	A	750	FAD	C4X-C10-N10	-6.31	115.94	120.52
3	A	751	FMN	C4A-C4-N3	-6.30	115.28	123.52
2	A	750	FAD	C4X-C4-N3	-5.15	116.79	123.52
3	B	751	FMN	C4-C4A-C10	-5.00	116.74	119.94
3	A	751	FMN	C4-C4A-C10	-4.97	116.76	119.94
3	B	751	FMN	C4A-N5-C5A	-4.49	111.43	116.72
3	A	751	FMN	C4A-N5-C5A	-4.49	111.44	116.72
3	B	751	FMN	C4A-C10-N10	-4.31	117.39	120.52
3	A	751	FMN	C4A-C10-N10	-4.28	117.41	120.52
2	B	750	FAD	C2'-C1'-N10	-4.06	105.18	112.06
2	B	750	FAD	C2B-C3B-C4B	-3.67	95.13	102.64
2	A	750	FAD	C2B-C3B-C4B	-3.65	95.18	102.64
2	A	750	FAD	C4X-N5-C5X	-3.40	112.71	116.72
3	A	751	FMN	C6-C5A-N5	-2.99	115.19	118.92
3	B	751	FMN	C6-C5A-N5	-2.97	115.21	118.92
2	A	750	FAD	C6-C5X-N5	-2.85	115.36	118.92
3	B	751	FMN	C4-C4A-N5	-2.68	115.44	118.70
3	A	751	FMN	C4-C4A-N5	-2.67	115.45	118.70
4	A	752	NAP	O5D-PN-O3	-2.63	95.95	104.29
4	B	752	NAP	O5D-PN-O3	-2.62	95.99	104.29
2	A	750	FAD	C5X-C9A-N10	-2.44	115.75	117.58
4	A	752	NAP	O2X-P2B-O2B	-2.13	100.24	106.62
4	B	752	NAP	O2X-P2B-O2B	-2.13	100.26	106.62
4	B	752	NAP	O3B-C3B-C4B	-2.06	104.87	111.01
4	A	752	NAP	O3B-C3B-C4B	-2.05	104.88	111.01
2	A	750	FAD	O2B-C2B-C3B	-2.04	105.26	111.86
2	B	750	FAD	O2B-C2B-C3B	-2.03	105.28	111.86
4	B	752	NAP	C2B-C1B-N9A	2.19	119.73	113.48
4	A	752	NAP	C2B-C1B-N9A	2.19	119.73	113.48
2	A	750	FAD	O3'-C3'-C2'	2.22	114.49	108.73
2	B	750	FAD	O3'-C3'-C2'	2.24	114.53	108.73
3	B	751	FMN	O3P-P-O2P	2.44	116.39	107.44
3	A	751	FMN	O3P-P-O2P	2.44	116.40	107.44
2	B	750	FAD	C2B-C1B-N9A	2.77	120.88	113.47
2	A	750	FAD	C2B-C1B-N9A	2.78	120.92	113.47
2	B	750	FAD	C5X-C9A-N10	3.00	115.76	107.74
2	B	750	FAD	C9-C9A-N10	3.07	124.39	112.10
2	A	750	FAD	C1'-N10-C9A	3.08	122.40	118.83
3	B	751	FMN	C9A-C5A-N5	3.18	127.36	122.18
3	A	751	FMN	C9A-C5A-N5	3.21	127.40	122.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	750	FAD	C9A-C5X-N5	3.29	127.53	122.18
2	B	750	FAD	C1'-N10-C9A	4.17	122.38	113.39
2	B	750	FAD	C10-N10-C1'	4.61	117.52	111.00
2	A	750	FAD	C4-N3-C2	13.99	126.83	115.16
3	A	751	FMN	C4-N3-C2	14.17	126.98	115.16
3	B	751	FMN	C4-N3-C2	14.20	127.00	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	750	FAD	2	0
3	A	751	FMN	1	0
4	A	752	NAP	1	0
2	B	750	FAD	9	0
3	B	751	FMN	1	0
4	B	752	NAP	1	0

## 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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers

EDS was not executed - this section will therefore be empty.