



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2016 – 04:07 PM EDT

PDB ID : 5EMN
Title : Crystal Structure of Human NADPH-Cytochrome P450 Reductase(A287P mutant)
Authors : Xia, C.; Marohnic, C.; Panda, S.; Masters, B.S.; Kim, J.J.K.
Deposited on : 2015-11-06
Resolution : 2.20 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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) : 1.9-1692
EDS : rb-20027939
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

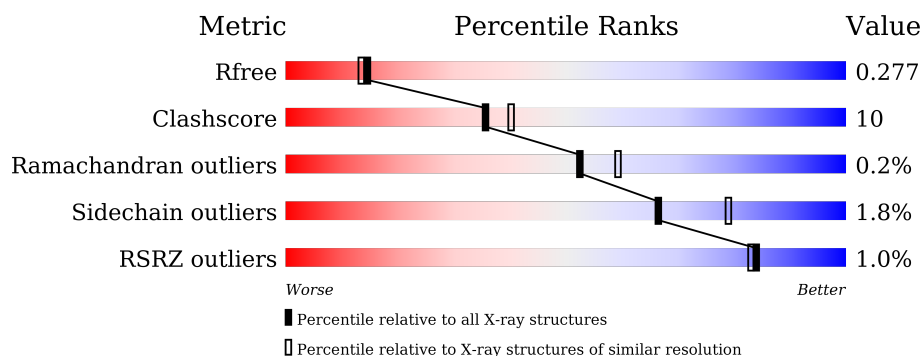
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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 ≥ 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.

Mol	Chain	Length	Quality of chain
1	A	618	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>17%</div> <div>.</div> </div> </div>
1	B	618	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>26%</div> <div>..</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10080 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.

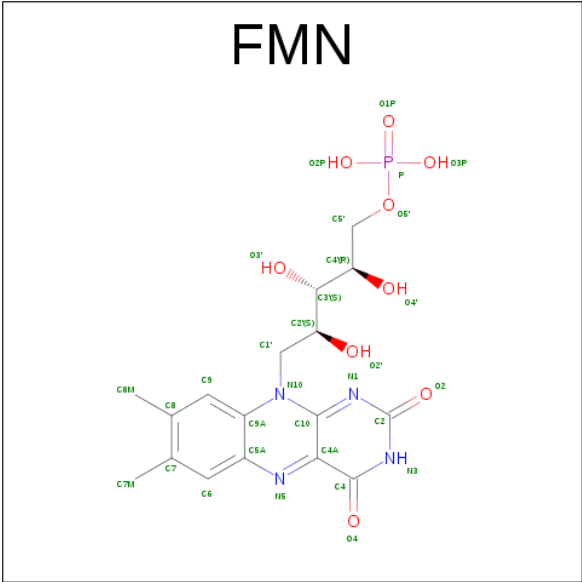
- Molecule 1 is a protein called NADPH–cytochrome P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	607	Total	C	N	O	S	0	0	0
			4835	3059	837	916	23			
1	B	597	Total	C	N	O	S	0	0	0
			4783	3030	827	903	23			

There are 14 discrepancies between the modelled and reference sequences:

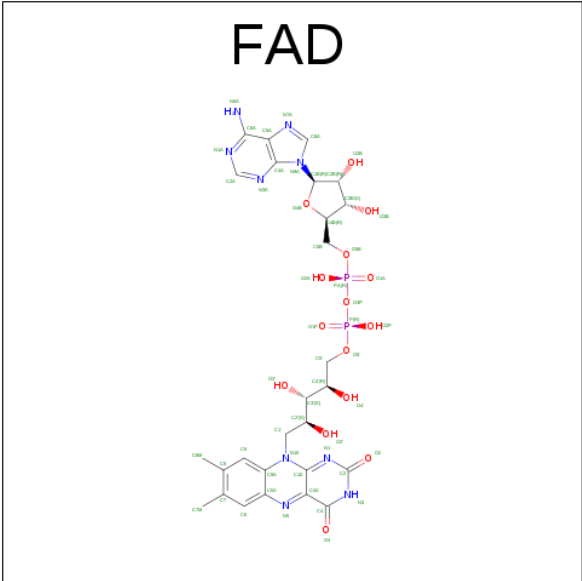
Chain	Residue	Modelled	Actual	Comment	Reference
A	63	GLY	-	expression tag	UNP P16435
A	64	SER	-	expression tag	UNP P16435
A	65	HIS	-	expression tag	UNP P16435
A	66	MET	-	expression tag	UNP P16435
A	228	LEU	PRO	engineered mutation	UNP P16435
A	287	PRO	ALA	engineered mutation	UNP P16435
A	503	VAL	ALA	engineered mutation	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	engineered mutation	UNP P16435
B	287	PRO	ALA	engineered mutation	UNP P16435
B	503	VAL	ALA	engineered mutation	UNP P16435

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



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

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



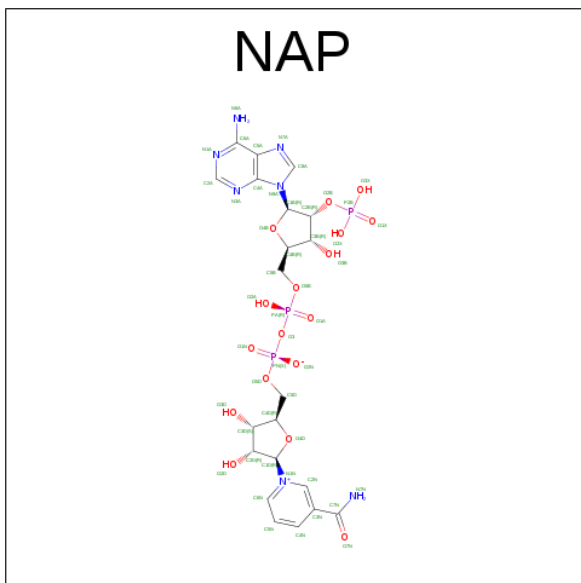
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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

- 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
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

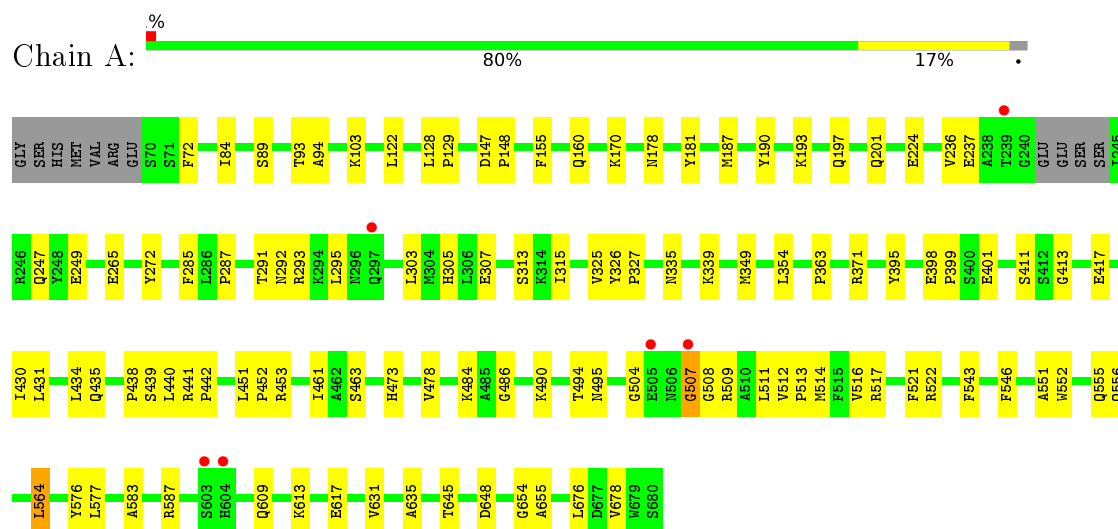
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	150	Total	O	0	0
			150	150		
5	B	82	Total	O	0	0
			82	82		

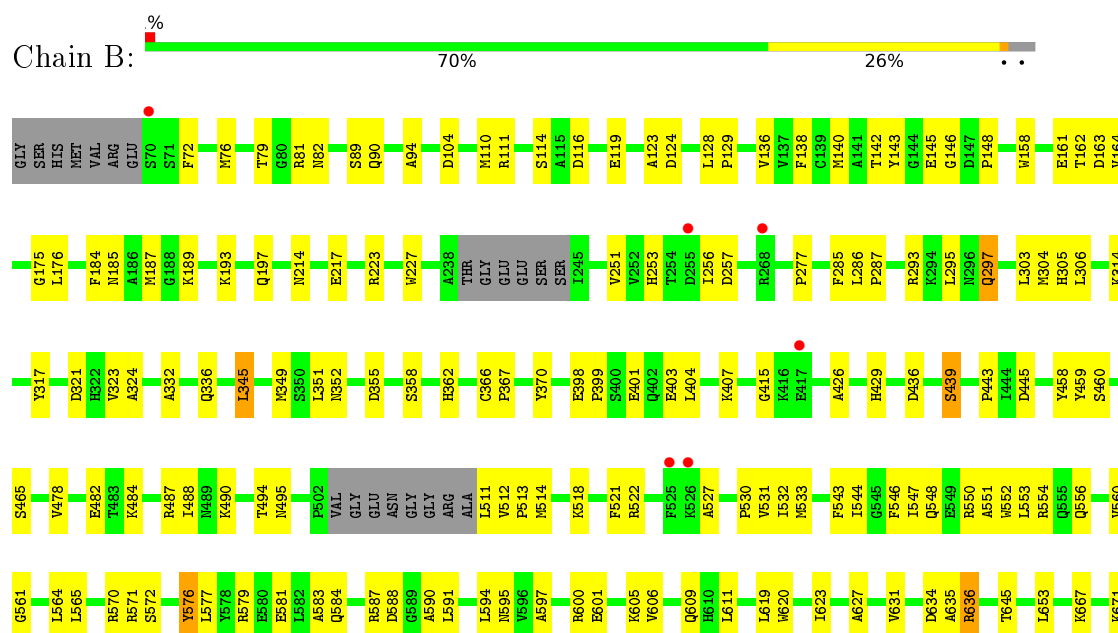
3 Residue-property plots

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.

- Molecule 1: NADPH-cytochrome P450 reductase



- Molecule 1: NADPH-cytochrome P450 reductase



1676	1677	1678	1679	1680
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.73Å 118.07Å 157.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.18 – 2.20 39.18 – 2.19	Depositor EDS
% Data completeness (in resolution range)	89.6 (39.18-2.20) 88.8 (39.18-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.18Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.222 , 0.277 0.222 , 0.277	Depositor DCC
R_{free} test set	3005 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	40.6	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10080	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.41	0/4945	0.64	0/6693
1	B	0.37	0/4892	0.60	1/6620 (0.0%)
All	All	0.39	0/9837	0.62	1/13313 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	145	GLU	N-CA-CB	6.04	121.47	110.60

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	4835	0	4696	68	0
1	B	4783	0	4659	119	0
2	A	31	0	19	0	0
2	B	31	0	19	0	0
3	A	53	0	31	0	0
3	B	53	0	31	0	0
4	A	31	0	11	1	0
4	B	31	0	11	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	150	0	0	3	0
5	B	82	0	0	0	0
All	All	10080	0	9477	187	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (187) 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:401:GLU:OE1	1:B:439:SER:HB3	1.68	0.91
1:A:103:LYS:HE2	1:A:247:GLN:OE1	1.83	0.79
1:A:613:LYS:HG3	1:A:645:THR:HG23	1.68	0.76
1:B:332:ALA:O	1:B:336:GLN:HG3	1.89	0.73
1:B:303:LEU:HD22	1:B:577:LEU:HD11	1.71	0.73
1:B:482:GLU:HG2	1:B:488:ILE:CD1	2.19	0.72
1:B:544:ILE:O	1:B:548:GLN:HG3	1.89	0.71
1:A:511:LEU:O	1:A:511:LEU:HD12	1.91	0.70
1:A:224:GLU:OE2	1:A:411:SER:HB2	1.93	0.69
1:A:303:LEU:HD22	1:A:577:LEU:HD21	1.77	0.66
1:A:178:ASN:HB3	1:A:181:TYR:HD2	1.60	0.66
1:A:438:PRO:HA	1:A:441:ARG:HH21	1.61	0.65
1:B:631:VAL:HB	1:B:676:LEU:HD23	1.78	0.65
1:B:667:LYS:HE3	1:B:671:LYS:HE2	1.79	0.64
1:B:552:TRP:O	1:B:556:GLN:HG2	1.98	0.64
1:A:325:VAL:HG12	1:A:514:MET:HB3	1.78	0.63
1:B:251:VAL:HG21	1:B:352:ASN:ND2	2.14	0.62
1:A:236:VAL:O	1:A:237:GLU:HG3	2.00	0.62
1:A:631:VAL:HB	1:A:676:LEU:HD23	1.81	0.61
1:B:304:MET:HG3	1:B:306:LEU:HD11	1.83	0.61
1:B:286:LEU:HD12	1:B:513:PRO:HA	1.82	0.60
1:B:571:ARG:HG3	1:B:571:ARG:HH11	1.66	0.60
1:B:286:LEU:HD11	1:B:513:PRO:HG3	1.85	0.59
1:B:407:LYS:HG3	1:B:415:GLY:HA2	1.83	0.59
1:B:162:THR:OG1	1:B:164:VAL:HG13	2.02	0.59
1:A:193:LYS:O	1:A:197:GLN:HG3	2.02	0.59
1:B:355:ASP:OD2	1:B:358:SER:HB2	2.03	0.58
1:A:401:GLU:OE2	1:A:438:PRO:HD2	2.03	0.58
1:A:287:PRO:HD2	1:A:512:VAL:O	2.03	0.58
1:A:478:VAL:HA	1:A:494:THR:HB	1.86	0.57
1:B:193:LYS:O	1:B:197:GLN:HG3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:TYR:HB2	1:A:513:PRO:HB2	1.86	0.57
1:B:295:LEU:HD11	1:B:305:HIS:HB2	1.86	0.57
1:A:249:GLU:HB3	1:A:354:LEU:HD21	1.86	0.57
1:A:543:PHE:HA	1:A:546:PHE:HB2	1.87	0.57
1:A:564:LEU:N	1:A:564:LEU:HD12	2.21	0.56
1:B:620:TRP:CD1	1:B:653:LEU:HB3	2.40	0.56
1:B:571:ARG:HE	1:B:600:ARG:CB	2.19	0.56
1:B:317:TYR:O	1:B:465:SER:HB3	2.06	0.54
1:B:551:ALA:HB2	1:B:590:ALA:HB1	1.89	0.54
1:B:564:LEU:HD12	1:B:564:LEU:N	2.22	0.54
1:A:178:ASN:HB3	1:A:181:TYR:CD2	2.40	0.54
1:B:253:HIS:HB3	1:B:256:ILE:HB	1.89	0.54
1:B:323:VAL:HG13	1:B:459:TYR:HB2	1.88	0.54
1:A:635:ALA:HB2	1:A:678:VAL:HB	1.89	0.54
1:B:576:TYR:CE1	1:B:579:ARG:HA	2.43	0.54
1:B:81:ARG:HG3	1:B:81:ARG:HH11	1.72	0.53
1:B:572:SER:HA	1:B:576:TYR:HB2	1.89	0.53
1:B:128:LEU:N	1:B:129:PRO:CD	2.72	0.53
1:B:277:PRO:HG3	1:B:314:LYS:HE2	1.91	0.53
1:B:82:ASN:OD1	1:B:110:MET:HB3	2.09	0.52
1:A:193:LYS:NZ	5:A:802:HOH:O	2.39	0.52
1:A:89:SER:HB2	1:A:94:ALA:HB3	1.91	0.52
1:A:265:GLU:HA	1:A:272:TYR:CZ	2.45	0.51
1:A:295:LEU:HD11	1:A:305:HIS:HB2	1.92	0.51
1:B:304:MET:HG3	1:B:306:LEU:CD1	2.40	0.51
1:A:160:GLN:HG2	1:A:190:TYR:OH	2.10	0.51
1:B:584:GLN:HG3	1:B:588:ASP:OD2	2.11	0.51
1:A:363:PRO:O	1:A:453:ARG:HD3	2.10	0.51
1:A:371:ARG:HG3	1:A:371:ARG:HH11	1.76	0.51
1:B:551:ALA:HB2	1:B:590:ALA:CB	2.41	0.51
1:B:404:LEU:O	1:B:407:LYS:HG2	2.11	0.50
1:B:527:ALA:HB2	1:B:553:LEU:HD13	1.92	0.50
1:B:543:PHE:HA	1:B:546:PHE:HB2	1.94	0.50
1:A:609:GLN:OE1	4:A:703:NAP:H2A	2.12	0.50
1:A:461:ILE:HG22	1:A:463:SER:H	1.77	0.49
1:B:323:VAL:CG1	1:B:459:TYR:HB2	2.42	0.49
1:B:482:GLU:HG2	1:B:488:ILE:HD12	1.93	0.49
1:A:398:GLU:H	1:A:439:SER:HB2	1.77	0.49
1:A:307:GLU:HG2	1:A:473:HIS:CD2	2.47	0.49
1:B:436:ASP:OD1	1:B:487:ARG:NH1	2.45	0.49
1:B:345:LEU:HA	1:B:370:TYR:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:LYS:HB2	1:B:518:LYS:NZ	2.27	0.49
1:B:546:PHE:O	1:B:550:ARG:HG2	2.12	0.49
1:B:609:GLN:HB2	1:B:645:THR:OG1	2.13	0.49
1:B:148:PRO:HB3	1:B:187:MET:SD	2.52	0.49
1:B:399:PRO:O	1:B:403:GLU:HG2	2.12	0.49
1:B:572:SER:N	1:B:601:GLU:OE1	2.42	0.48
1:A:431:LEU:O	1:A:435:GLN:HG3	2.13	0.48
1:B:443:PRO:HB2	1:B:445:ASP:OD1	2.13	0.48
1:B:426:ALA:HA	1:B:484:LYS:HB3	1.95	0.48
1:B:571:ARG:NH1	1:B:571:ARG:HG3	2.27	0.48
1:B:581:GLU:OE1	1:B:581:GLU:N	2.47	0.48
1:A:122:LEU:HG	1:A:155:PHE:CD1	2.49	0.48
1:A:552:TRP:O	1:A:556:GLN:HG2	2.13	0.48
1:B:79:THR:O	1:B:111:ARG:NH1	2.47	0.48
1:A:128:LEU:N	1:A:129:PRO:CD	2.76	0.48
1:B:214:ASN:OD1	1:B:217:GLU:HG2	2.14	0.48
1:B:398:GLU:OE2	1:B:399:PRO:HD2	2.14	0.48
1:B:597:ALA:HB1	1:B:606:VAL:O	2.13	0.47
1:A:170:LYS:HE2	1:A:201:GLN:OE1	2.14	0.47
1:A:484:LYS:C	1:A:486:GLY:H	2.17	0.47
1:B:185:ASN:O	1:B:189:LYS:HG3	2.15	0.47
1:B:317:TYR:O	1:B:465:SER:CB	2.63	0.47
1:B:577:LEU:N	1:B:577:LEU:CD1	2.78	0.47
1:B:89:SER:HB2	1:B:94:ALA:HB3	1.96	0.47
1:B:482:GLU:HA	1:B:488:ILE:HD13	1.97	0.47
1:B:570:ARG:O	1:B:571:ARG:HD3	2.13	0.47
1:A:617:GLU:HB2	5:A:851:HOH:O	2.15	0.47
1:B:193:LYS:HB3	1:B:193:LYS:NZ	2.30	0.46
1:B:482:GLU:HG2	1:B:488:ILE:HD11	1.94	0.46
1:A:645:THR:O	1:A:648:ASP:HB2	2.15	0.46
1:A:398:GLU:OE2	1:A:399:PRO:HD2	2.16	0.46
1:A:434:LEU:HD23	1:A:440:LEU:HD23	1.98	0.46
1:B:136:VAL:HG22	1:B:138:PHE:CE1	2.51	0.45
1:B:478:VAL:HA	1:B:494:THR:HB	1.98	0.45
1:A:551:ALA:O	1:A:555:GLN:HG3	2.17	0.45
1:B:72:PHE:CE1	1:B:124:ASP:HB2	2.52	0.45
1:A:236:VAL:C	1:A:237:GLU:HG3	2.36	0.45
1:B:351:LEU:O	1:B:362:HIS:HD2	2.00	0.45
1:A:398:GLU:H	1:A:439:SER:CB	2.29	0.45
1:B:176:LEU:N	1:B:176:LEU:HD12	2.32	0.45
1:B:184:PHE:O	1:B:189:LYS:HE3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:560:VAL:HG12	1:B:561:GLY:O	2.17	0.45
1:B:583:ALA:O	1:B:587:ARG:HG3	2.17	0.45
1:A:313:SER:C	1:A:315:ILE:H	2.20	0.45
1:B:321:ASP:OD1	1:B:518:LYS:HA	2.16	0.45
1:B:251:VAL:HG21	1:B:352:ASN:HD22	1.82	0.45
1:B:577:LEU:CD1	1:B:577:LEU:H	2.30	0.45
1:B:571:ARG:HE	1:B:600:ARG:HB2	1.82	0.45
1:B:306:LEU:HD12	1:B:306:LEU:N	2.30	0.44
1:B:543:PHE:O	1:B:547:ILE:HG13	2.17	0.44
1:B:554:ARG:NH2	1:B:588:ASP:O	2.50	0.44
1:B:487:ARG:O	1:B:488:ILE:HD13	2.17	0.44
1:B:530:PRO:HB2	1:B:627:ALA:HB2	1.99	0.44
1:B:72:PHE:O	1:B:76:MET:HG3	2.17	0.44
1:B:531:VAL:HG12	1:B:533:MET:HG3	2.00	0.44
1:A:613:LYS:HG3	1:A:645:THR:CG2	2.45	0.44
1:A:451:LEU:HA	1:A:452:PRO:HD3	1.79	0.43
1:B:90:GLN:HG2	1:B:143:TYR:CE1	2.52	0.43
1:B:591:LEU:CD2	1:B:594:LEU:HB2	2.49	0.43
1:A:72:PHE:CD1	1:A:84:ILE:HD13	2.53	0.43
1:B:533:MET:O	1:B:565:LEU:HD12	2.18	0.43
1:A:148:PRO:HB3	1:A:187:MET:SD	2.59	0.43
1:A:504:GLY:C	1:A:507:GLY:H	2.22	0.43
1:B:293:ARG:HG2	1:B:293:ARG:HH11	1.84	0.43
1:A:511:LEU:HD12	1:A:513:PRO:HD3	2.00	0.43
1:B:635:ALA:HB2	1:B:678:VAL:HB	2.01	0.43
1:A:293:ARG:NH2	5:A:810:HOH:O	2.51	0.43
1:B:584:GLN:OE1	1:B:584:GLN:HA	2.19	0.43
1:A:521:PHE:O	1:A:522:ARG:HG2	2.19	0.42
1:B:142:THR:CG2	1:B:146:GLY:HA2	2.50	0.42
1:A:147:ASP:HB3	1:A:148:PRO:HD2	2.01	0.42
1:B:297:GLN:HB3	1:B:297:GLN:HE21	1.69	0.42
1:B:128:LEU:HD23	1:B:128:LEU:HA	1.92	0.42
1:B:256:ILE:O	1:B:256:ILE:HG23	2.19	0.42
1:B:287:PRO:HD2	1:B:512:VAL:O	2.18	0.42
1:B:595:ASN:HB3	1:B:611:LEU:HD23	2.01	0.42
1:B:634:ASP:OD1	1:B:636:ARG:HG2	2.19	0.42
1:B:605:LYS:NZ	4:B:703:NAP:O1X	2.52	0.42
1:A:490:LYS:HD3	1:A:495:ASN:OD1	2.20	0.42
1:B:398:GLU:HA	1:B:399:PRO:HD3	1.94	0.42
1:A:413:GLY:O	1:A:417:GLU:HG2	2.20	0.42
1:B:123:ALA:HA	1:B:158:TRP:CZ2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:521:PHE:C	1:B:522:ARG:HG2	2.40	0.42
1:B:285:PHE:HE1	1:B:287:PRO:HB3	1.84	0.42
1:B:90:GLN:NE2	1:B:143:TYR:CE2	2.73	0.42
1:B:148:PRO:HB3	1:B:187:MET:CE	2.50	0.42
1:B:577:LEU:N	1:B:577:LEU:HD12	2.35	0.42
1:A:224:GLU:OE2	1:A:411:SER:CB	2.63	0.41
1:A:440:LEU:HG	1:A:442:PRO:HD3	2.02	0.41
1:A:285:PHE:O	1:A:287:PRO:HD3	2.19	0.41
1:B:116:ASP:O	1:B:119:GLU:HG2	2.20	0.41
1:B:352:ASN:OD1	1:B:362:HIS:NE2	2.45	0.41
1:A:335:ASN:O	1:A:339:LYS:HG3	2.20	0.41
1:B:366:CYS:HA	1:B:367:PRO:C	2.39	0.41
1:A:516:VAL:HG12	1:A:517:ARG:N	2.35	0.41
1:A:371:ARG:NH1	1:A:371:ARG:HG3	2.36	0.41
1:B:351:LEU:HD23	1:B:351:LEU:HA	1.92	0.41
1:B:591:LEU:HD21	1:B:594:LEU:HD13	2.03	0.41
1:B:532:ILE:HD13	1:B:619:LEU:HD22	2.01	0.41
1:B:619:LEU:O	1:B:623:ILE:HG13	2.20	0.41
1:A:508:GLY:O	1:A:509:ARG:C	2.59	0.41
1:A:291:THR:HG22	1:A:292:ASN:N	2.36	0.40
1:A:395:TYR:CD2	1:A:442:PRO:HB3	2.56	0.40
1:A:654:GLY:O	1:A:655:ALA:HB3	2.20	0.40
1:B:324:ALA:HB2	1:B:458:TYR:CE1	2.56	0.40
1:B:490:LYS:HB3	1:B:495:ASN:ND2	2.36	0.40
1:B:104:ASP:HB2	1:B:227:TRP:CZ2	2.55	0.40
1:B:81:ARG:HD3	1:B:111:ARG:HB3	2.03	0.40
1:A:583:ALA:O	1:A:587:ARG:HG3	2.22	0.40
1:B:285:PHE:CE1	1:B:287:PRO:HB3	2.57	0.40
1:B:597:ALA:HB1	1:B:606:VAL:HG12	2.04	0.40
1:A:430:ILE:HG23	1:A:431:LEU:N	2.37	0.40
1:B:104:ASP:OD1	1:B:223:ARG:NH2	2.55	0.40
1:B:140:MET:O	1:B:175:GLY:HA2	2.22	0.40
1:B:571:ARG:HE	1:B:600:ARG:C	2.25	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	603/618 (98%)	571 (95%)	31 (5%)	1 (0%)	52	59
1	B	591/618 (96%)	553 (94%)	37 (6%)	1 (0%)	52	59
All	All	1194/1236 (97%)	1124 (94%)	68 (6%)	2 (0%)	52	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	345	LEU
1	A	507	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	513/527 (97%)	508 (99%)	5 (1%)	82	91
1	B	511/527 (97%)	498 (98%)	13 (2%)	55	67
All	All	1024/1054 (97%)	1006 (98%)	18 (2%)	66	79

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	THR
1	A	327	PRO
1	A	349	MET
1	A	564	LEU

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Mol	Chain	Res	Type
1	A	576	TYR
1	B	114	SER
1	B	161	GLU
1	B	163	ASP
1	B	257	ASP
1	B	297	GLN
1	B	349	MET
1	B	429	HIS
1	B	439	SER
1	B	460	SER
1	B	511	LEU
1	B	514	MET
1	B	576	TYR
1	B	636	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	473	HIS
1	B	470	ASN
1	B	644	ASN

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](#)

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	FMN	A	701	-	32,33,33	2.89	15 (46%)	34,50,50	3.70	14 (41%)
3	FAD	A	702	-	52,58,58	2.14	11 (21%)	52,89,89	2.58	10 (19%)
4	NAP	A	703	-	28,33,52	1.56	4 (14%)	35,52,80	2.63	4 (11%)
2	FMN	B	701	-	32,33,33	2.99	13 (40%)	34,50,50	3.58	13 (38%)
3	FAD	B	702	-	52,58,58	2.15	11 (21%)	52,89,89	2.54	9 (17%)
4	NAP	B	703	-	28,33,52	1.55	3 (10%)	35,52,80	2.68	5 (14%)

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	FMN	A	701	-	-	0/18/18/18	0/3/3/3
3	FAD	A	702	-	-	0/30/50/50	0/6/6/6
4	NAP	A	703	-	-	0/17/37/67	0/3/3/5
2	FMN	B	701	-	-	0/18/18/18	0/3/3/3
3	FAD	B	702	-	-	0/30/50/50	0/6/6/6
4	NAP	B	703	-	-	0/17/37/67	0/3/3/5

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	FMN	C8M-C8	-6.59	1.37	1.51
2	A	701	FMN	C8M-C8	-6.26	1.38	1.51
3	B	702	FAD	C8M-C8	-5.85	1.39	1.51
3	A	702	FAD	C7M-C7	-5.80	1.39	1.51
3	B	702	FAD	C7M-C7	-5.80	1.39	1.51
3	A	702	FAD	C8M-C8	-5.80	1.39	1.51
3	B	702	FAD	C10-N10	-4.10	1.34	1.39
3	A	702	FAD	C10-N10	-4.08	1.34	1.39
2	A	701	FMN	C1'-N10	-3.09	1.45	1.48
4	B	703	NAP	C5A-C4A	-3.06	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	703	NAP	C5A-C4A	-3.00	1.33	1.40
3	B	702	FAD	C9A-N10	-2.98	1.34	1.38
3	A	702	FAD	C9A-N10	-2.98	1.34	1.38
3	B	702	FAD	C5A-C4A	-2.91	1.33	1.40
3	A	702	FAD	C5A-C4A	-2.89	1.34	1.40
2	B	701	FMN	C1'-N10	-2.52	1.45	1.48
4	A	703	NAP	O4B-C1B	2.03	1.44	1.41
2	A	701	FMN	C7M-C7	2.05	1.55	1.51
2	A	701	FMN	C6-C5A	2.10	1.45	1.41
3	A	702	FAD	O4B-C1B	2.10	1.44	1.41
2	B	701	FMN	C10-N1	2.15	1.39	1.35
3	B	702	FAD	O4B-C1B	2.17	1.44	1.41
2	A	701	FMN	C9A-C5A	2.43	1.47	1.42
2	A	701	FMN	C10-N1	2.44	1.39	1.35
2	B	701	FMN	C4'-C3'	2.45	1.58	1.53
2	B	701	FMN	O2'-C2'	2.49	1.48	1.43
2	A	701	FMN	C4'-C3'	2.57	1.58	1.53
2	B	701	FMN	C9A-C5A	2.59	1.48	1.42
2	A	701	FMN	C9-C9A	2.75	1.46	1.40
3	A	702	FAD	C10-N1	2.79	1.40	1.35
2	A	701	FMN	O2'-C2'	2.82	1.49	1.43
3	B	702	FAD	C10-N1	2.84	1.40	1.35
2	B	701	FMN	C9-C9A	2.88	1.47	1.40
2	A	701	FMN	C5A-N5	3.12	1.40	1.35
2	B	701	FMN	C5A-N5	3.14	1.40	1.35
2	A	701	FMN	C8-C7	3.28	1.49	1.41
3	A	702	FAD	C2A-N1A	3.29	1.40	1.33
4	B	703	NAP	C2A-N1A	3.31	1.40	1.33
3	B	702	FAD	C2A-N1A	3.34	1.40	1.33
4	A	703	NAP	C2A-N1A	3.34	1.40	1.33
2	B	701	FMN	C8-C7	3.59	1.50	1.41
2	A	701	FMN	C4-N3	3.92	1.40	1.33
3	A	702	FAD	C4-N3	4.13	1.40	1.33
3	B	702	FAD	C4-N3	4.16	1.40	1.33
3	A	702	FAD	C2A-N3A	4.62	1.40	1.32
3	B	702	FAD	C2A-N3A	4.62	1.40	1.32
4	A	703	NAP	C2A-N3A	4.63	1.40	1.32
4	B	703	NAP	C2A-N3A	4.66	1.40	1.32
2	B	701	FMN	C4-N3	4.86	1.41	1.33
2	A	701	FMN	C9A-N10	5.79	1.47	1.38
2	A	701	FMN	C4A-N5	6.05	1.42	1.33
2	B	701	FMN	C4A-N5	6.07	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	FMN	C9A-N10	6.64	1.48	1.38
3	B	702	FAD	C8A-N7A	6.98	1.48	1.34
3	A	702	FAD	C8A-N7A	7.01	1.48	1.34
2	A	701	FMN	C10-N10	7.11	1.47	1.39
2	B	701	FMN	C10-N10	7.31	1.47	1.39

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	FAD	N3A-C2A-N1A	-14.69	117.33	128.87
3	B	702	FAD	N3A-C2A-N1A	-14.59	117.41	128.87
4	A	703	NAP	N3A-C2A-N1A	-14.00	117.87	128.87
4	B	703	NAP	N3A-C2A-N1A	-13.94	117.92	128.87
2	A	701	FMN	C4-C4A-C10	-8.22	114.68	119.94
2	B	701	FMN	C4-C4A-C10	-7.54	115.11	119.94
2	A	701	FMN	N3-C2-N1	-6.66	116.47	127.69
2	B	701	FMN	N3-C2-N1	-6.32	117.04	127.69
2	A	701	FMN	C4A-C10-N10	-5.99	116.17	120.52
2	B	701	FMN	C4A-C4-N3	-5.52	116.30	123.52
2	B	701	FMN	C4A-C10-N10	-5.52	116.51	120.52
2	A	701	FMN	C4A-C4-N3	-5.01	116.97	123.52
3	A	702	FAD	N3-C2-N1	-4.73	119.72	127.69
3	B	702	FAD	N3-C2-N1	-4.72	119.74	127.69
4	B	703	NAP	C4B-O4B-C1B	-4.01	105.39	109.64
3	A	702	FAD	C4B-O4B-C1B	-3.51	105.92	109.64
2	A	701	FMN	O4'-C4'-C3'	-3.06	101.09	108.96
2	B	701	FMN	O4'-C4'-C3'	-3.06	101.09	108.96
4	A	703	NAP	C4B-O4B-C1B	-2.93	106.54	109.64
3	B	702	FAD	C2B-C3B-C4B	-2.91	96.69	102.64
2	B	701	FMN	C6-C5A-N5	-2.87	115.33	118.92
3	A	702	FAD	C4X-C4-N3	-2.81	119.85	123.52
3	B	702	FAD	C4B-O4B-C1B	-2.76	106.72	109.64
3	B	702	FAD	C4X-C4-N3	-2.67	120.03	123.52
2	A	701	FMN	C4A-N5-C5A	-2.61	113.65	116.72
4	A	703	NAP	C3B-C2B-C1B	-2.60	97.66	102.63
2	A	701	FMN	O4'-C4'-C5'	-2.52	104.59	110.09
4	B	703	NAP	O4B-C1B-C2B	-2.48	102.14	106.60
2	A	701	FMN	C6-C5A-N5	-2.43	115.89	118.92
2	B	701	FMN	C4A-N5-C5A	-2.40	113.89	116.72
2	B	701	FMN	C5A-C9A-N10	-2.39	115.79	117.58
2	B	701	FMN	O4'-C4'-C5'	-2.38	104.91	110.09
3	A	702	FAD	C2B-C3B-C4B	-2.29	97.94	102.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	FMN	C5A-C9A-N10	-2.21	115.92	117.58
2	A	701	FMN	O3P-P-O5'	-2.13	100.50	106.72
3	B	702	FAD	C1B-N9A-C4A	-2.06	124.50	126.81
3	A	702	FAD	C1B-N9A-C4A	-2.04	124.53	126.81
4	B	703	NAP	O3X-P2B-O2X	2.03	114.91	107.44
4	A	703	NAP	O4B-C1B-N9A	2.15	112.17	108.11
4	B	703	NAP	O4B-C1B-N9A	2.35	112.54	108.11
2	A	701	FMN	C8M-C8-C7	2.46	126.02	120.73
2	B	701	FMN	C8M-C8-C7	2.54	126.19	120.73
3	A	702	FAD	C4X-N5-C5X	2.57	119.75	116.72
2	A	701	FMN	C9A-C5A-N5	2.64	126.48	122.18
3	A	702	FAD	C1'-N10-C9A	2.69	121.95	118.83
2	B	701	FMN	O2P-P-O1P	2.71	119.48	110.63
2	A	701	FMN	O2P-P-O1P	2.72	119.51	110.63
2	B	701	FMN	C9A-C5A-N5	2.73	126.62	122.18
3	B	702	FAD	C4X-N5-C5X	2.82	120.05	116.72
3	B	702	FAD	C5X-C9A-N10	2.83	119.70	117.58
3	A	702	FAD	C5X-C9A-N10	2.83	119.70	117.58
3	B	702	FAD	C4-N3-C2	5.77	119.97	115.16
3	A	702	FAD	C4-N3-C2	5.93	120.11	115.16
2	B	701	FMN	C4-N3-C2	14.02	126.86	115.16
2	A	701	FMN	C4-N3-C2	14.70	127.42	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	703	NAP	1	0
4	B	703	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 [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	607/618 (98%)	-0.26	6 (0%) 84 83	31, 45, 68, 87	0
1	B	597/618 (96%)	-0.12	6 (1%) 84 83	31, 54, 75, 93	0
All	All	1204/1236 (97%)	-0.19	12 (0%) 84 83	31, 49, 72, 93	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	297	GLN	3.5
1	B	268	ARG	3.4
1	A	604	HIS	3.3
1	A	603	SER	3.2
1	B	255	ASP	3.2
1	B	526	LYS	2.9
1	B	525	PHE	2.8
1	B	70	SER	2.7
1	A	239	THR	2.5
1	A	505	GLU	2.5
1	A	507	GLY	2.3
1	B	417	GLU	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	NAP	A	703	31/48	0.79	0.21	1.57	99,104,112,115	0
3	FAD	A	702	53/53	0.95	0.15	0.73	33,38,51,52	0
2	FMN	A	701	31/31	0.97	0.14	0.26	34,40,45,48	0
2	FMN	B	701	31/31	0.96	0.14	0.05	41,48,53,54	0
3	FAD	B	702	53/53	0.94	0.16	-0.00	40,54,65,67	0
4	NAP	B	703	31/48	0.93	0.14	-0.13	55,67,84,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.