



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 13, 2016 – 06:09 PM EDT

PDB ID : 4YAF  
Title : rat CYPOR with 2'-AMP  
Authors : Xia, C.; Kim, J.J.P.  
Deposited on : 2015-02-17  
Resolution : 1.91 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) : 1.9-1692  
EDS : rb-20027790  
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-20027790

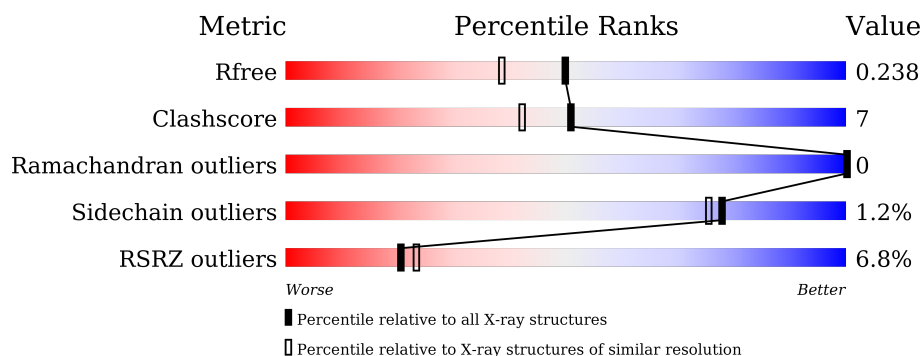
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.91 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	5832 (1.94-1.90)
Clashscore	102246	6540 (1.94-1.90)
Ramachandran outliers	100387	6464 (1.94-1.90)
Sidechain outliers	100360	6465 (1.94-1.90)
RSRZ outliers	91569	5846 (1.94-1.90)

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.

Mol	Chain	Length	Quality of chain
1	A	622	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>.</div> </div> </div>
1	B	622	<div> <div>11%</div> <div> <div></div> <div>79%</div> <div>18%</div> <div>.</div> </div> </div>

## 2 Entry composition [i](#)

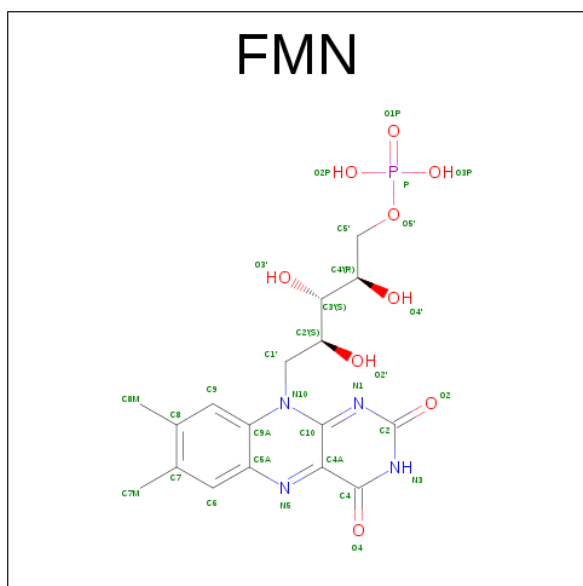
There are 6 unique types of molecules in this entry. The entry contains 10977 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

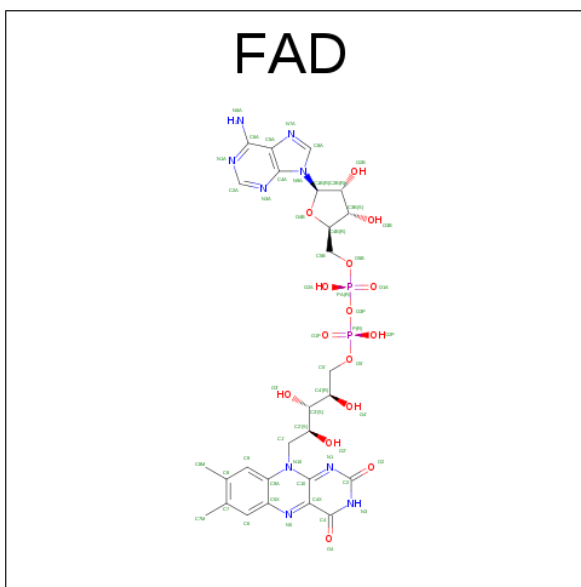
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	609	Total	C	N	O	S	0	0	0
			4867	3087	835	922	23			
1	B	605	Total	C	N	O	S	0	0	0
			4804	3045	830	906	23			

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).



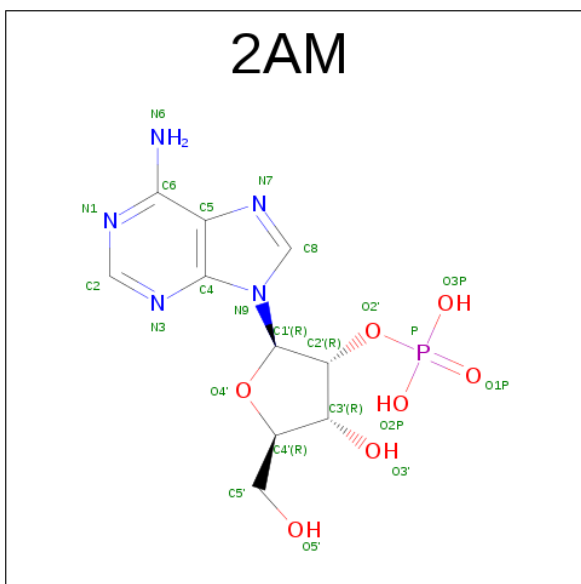
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



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

- Molecule 4 is ADENOSINE-2'-MONOPHOSPHATE (three-letter code: 2AM) (formula:  $\text{C}_{10}\text{H}_{14}\text{N}_5\text{O}_7\text{P}$ ).



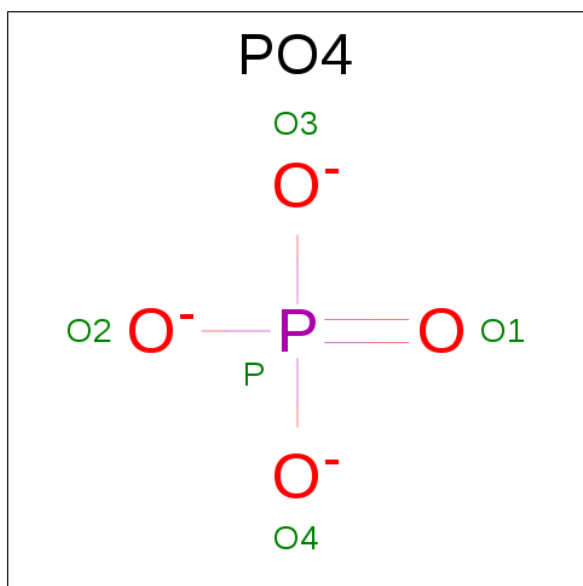
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			5	4	1		

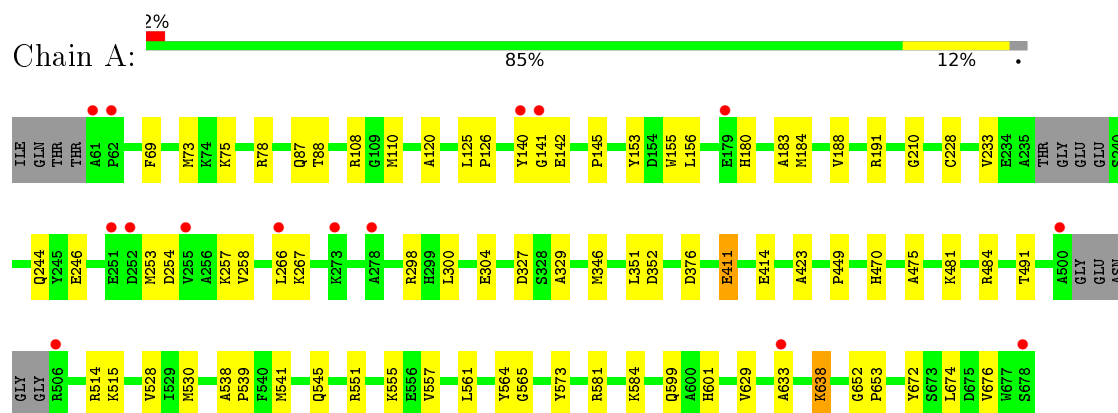
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	596	Total	O	0	0
			596	596		
6	B	491	Total	O	0	0
			491	491		

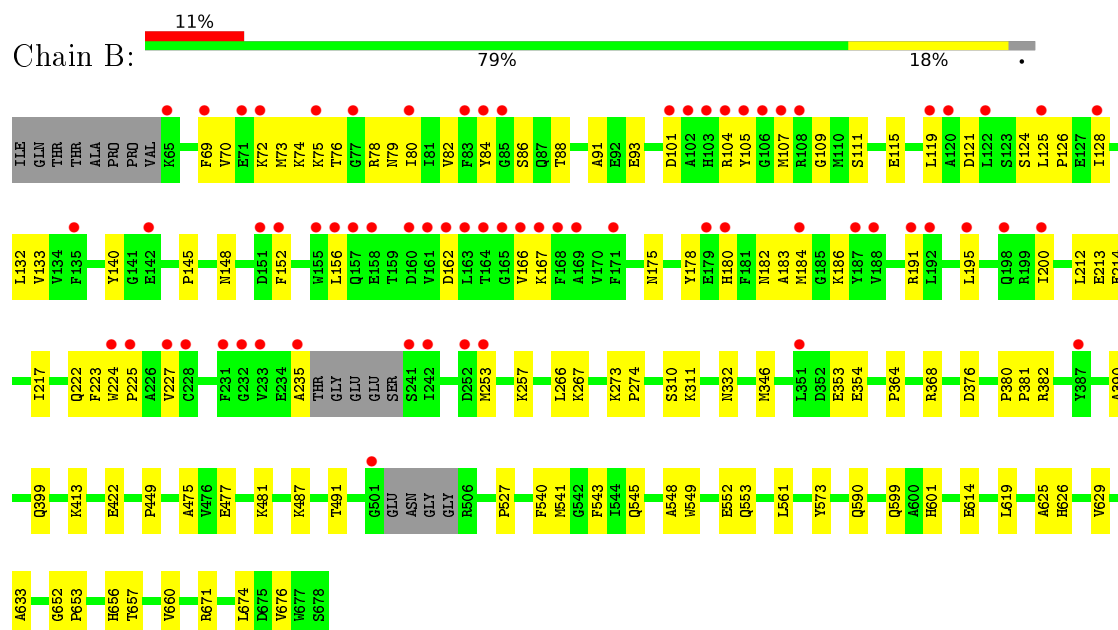
### 3 Residue-property plots

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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.04Å 115.29Å 118.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.24 – 1.91 46.24 – 1.91	Depositor EDS
% Data completeness (in resolution range)	99.2 (46.24-1.91) 99.3 (46.24-1.91)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.10 (at 1.91Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.205 , 0.239 0.205 , 0.238	Depositor DCC
$R_{free}$ test set	5432 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.3	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 48.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.008 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10977	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.25% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, PO4, 2AM, 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	0.35	0/4984	0.59	2/6747 (0.0%)
1	B	0.31	0/4919	0.58	3/6657 (0.0%)
All	All	0.33	0/9903	0.58	5/13404 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	TYR	CB-CA-C	6.88	124.16	110.40
1	B	140	TYR	CB-CA-C	5.91	122.22	110.40
1	A	210	GLY	N-CA-C	-5.30	99.84	113.10
1	B	128	ILE	N-CA-C	5.28	125.27	111.00
1	B	128	ILE	CB-CA-C	-5.14	101.31	111.60

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	4867	0	4709	57	0
1	B	4804	0	4610	76	0
2	A	31	0	19	1	0
2	B	31	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	53	0	31	0	0
3	B	53	0	31	0	0
4	A	23	0	12	0	0
4	B	23	0	12	0	0
5	B	5	0	0	0	0
6	A	596	0	0	8	0
6	B	491	0	0	9	0
All	All	10977	0	9443	133	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (133) 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:581:ARG:HH21	1:A:584:LYS:HD3	1.37	0.89
1:B:72:LYS:HD2	1:B:354:GLU:HB3	1.58	0.85
1:B:119:LEU:HG	1:B:152:PHE:CD1	2.22	0.75
1:A:254:ASP:HB2	1:A:257:LYS:HE2	1.71	0.71
1:A:581:ARG:NH2	1:A:584:LYS:HD3	2.06	0.71
1:B:477:GLU:HG3	1:B:487:LYS:HD2	1.72	0.70
1:A:184:MET:HE2	1:A:184:MET:O	1.91	0.70
1:A:376:ASP:HB3	1:A:449:PRO:HG2	1.75	0.67
1:B:115:GLU:OE1	1:B:148:ASN:HA	1.95	0.67
1:B:86:SER:HB2	1:B:91:ALA:HB3	1.77	0.65
1:A:633:ALA:HB2	1:A:676:VAL:HB	1.78	0.65
1:A:253:MET:HE2	1:A:257:LYS:HE3	1.79	0.65
1:A:629:VAL:HB	1:A:674:LEU:HD23	1.78	0.65
1:A:257:LYS:HA	1:A:266:LEU:HD21	1.79	0.64
1:B:156:LEU:HB3	1:B:191:ARG:HG2	1.79	0.63
1:B:376:ASP:HB3	1:B:449:PRO:HG2	1.79	0.63
1:B:70:VAL:HG12	1:B:74:LYS:HE3	1.81	0.62
1:B:69:PHE:CE1	1:B:121:ASP:HB2	2.35	0.61
1:B:76:THR:HG21	1:B:78:ARG:HE	1.65	0.61
1:B:561:LEU:HD22	1:B:590:GLN:HB2	1.82	0.60
1:A:638:LYS:HE3	1:A:638:LYS:HA	1.82	0.60
1:A:88:THR:HB	2:A:701:FMN:O1P	2.02	0.59
1:B:222:GLN:C	1:B:225:PRO:HD2	2.23	0.58
1:B:548:ALA:O	1:B:552:GLU:HG2	2.05	0.56
1:A:551:ARG:HG3	1:A:557:VAL:HG21	1.87	0.56
1:B:191:ARG:NE	1:B:195:LEU:HD11	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ARG:HH11	1:A:78:ARG:HG3	1.69	0.56
1:A:228:CYS:HA	1:A:233:VAL:CG2	2.36	0.55
1:B:125:LEU:N	1:B:126:PRO:HD2	2.21	0.55
1:A:75:LYS:HD2	6:A:1357:HOH:O	2.06	0.55
1:B:422:GLU:HG3	1:B:481:LYS:CE	2.37	0.55
1:B:223:PHE:O	1:B:227:VAL:HG23	2.07	0.55
1:A:555:LYS:HE2	6:A:1340:HOH:O	2.06	0.55
1:B:167:LYS:HG3	1:B:200:ILE:HD11	1.89	0.54
1:B:390:ALA:O	1:B:399:GLN:HG3	2.07	0.54
1:A:78:ARG:HH11	1:A:78:ARG:CG	2.21	0.53
1:B:76:THR:CG2	1:B:78:ARG:HE	2.21	0.52
1:B:167:LYS:CG	1:B:200:ILE:HD11	2.38	0.52
1:A:228:CYS:HA	1:A:233:VAL:HG22	1.90	0.52
1:B:191:ARG:O	1:B:195:LEU:HD13	2.09	0.52
1:B:481:LYS:HE3	6:B:1133:HOH:O	2.08	0.52
1:A:423:ALA:HA	1:A:481:LYS:HB2	1.91	0.52
1:A:244:GLN:HG2	6:A:1099:HOH:O	2.10	0.51
1:B:162:ASP:HA	1:B:195:LEU:O	2.10	0.51
1:A:156:LEU:HB3	1:A:191:ARG:HG2	1.93	0.51
1:A:145:PRO:HG3	1:A:184:MET:SD	2.51	0.51
1:B:93:GLU:OE1	1:B:93:GLU:HA	2.11	0.50
1:B:549:TRP:O	1:B:553:GLN:HG2	2.10	0.50
1:A:298:ARG:HD3	6:A:1109:HOH:O	2.10	0.50
1:B:126:PRO:HD3	1:B:166:VAL:HG22	1.92	0.50
1:A:145:PRO:HG2	1:A:153:TYR:CG	2.46	0.50
1:B:167:LYS:HD2	1:B:167:LYS:N	2.27	0.50
1:B:222:GLN:O	1:B:225:PRO:HD2	2.11	0.50
1:B:310:SER:O	1:B:311:LYS:HB2	2.12	0.49
1:A:514:ARG:HH11	1:A:514:ARG:HG2	1.75	0.49
1:A:541:MET:O	1:A:545:GLN:HG3	2.12	0.49
1:B:657:THR:HG23	6:B:1147:HOH:O	2.11	0.49
1:A:69:PHE:O	1:A:73:MET:HG3	2.13	0.49
1:B:652:GLY:N	1:B:653:PRO:HA	2.28	0.48
1:B:541:MET:O	1:B:545:GLN:HG3	2.14	0.48
1:B:656:HIS:O	1:B:660:VAL:HG23	2.14	0.48
1:A:246:GLU:HB3	1:A:351:LEU:HD21	1.96	0.48
1:B:633:ALA:HB2	1:B:676:VAL:HB	1.95	0.48
1:B:119:LEU:HD22	1:B:119:LEU:N	2.28	0.48
1:B:266:LEU:HG	1:B:267:LYS:HG2	1.96	0.48
1:B:182:ASN:O	1:B:186:LYS:HG2	2.13	0.47
1:B:70:VAL:HG21	1:B:124:SER:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:PRO:HB3	1:B:184:MET:SD	2.55	0.47
1:B:253:MET:SD	1:B:364:PRO:HG3	2.54	0.47
1:B:332:ASN:OD1	1:B:368:ARG:NH1	2.47	0.47
1:B:88:THR:HG22	6:B:899:HOH:O	2.14	0.47
1:A:561:LEU:HD12	1:A:561:LEU:N	2.30	0.46
1:B:133:VAL:HG13	1:B:133:VAL:O	2.16	0.46
1:A:88:THR:O	1:A:88:THR:HG22	2.16	0.46
1:B:614:GLU:HG2	6:B:1218:HOH:O	2.16	0.46
1:B:180:HIS:HB3	1:B:183:ALA:HB2	1.96	0.46
1:B:629:VAL:HB	1:B:674:LEU:HD23	1.97	0.46
1:B:132:LEU:HD12	1:B:167:LYS:O	2.15	0.46
1:B:76:THR:HB	1:B:78:ARG:HG2	1.98	0.46
1:A:254:ASP:HB2	1:A:257:LYS:CE	2.43	0.46
1:A:411:GLU:HA	1:A:414:GLU:OE1	2.16	0.46
1:B:82:VAL:O	1:B:111:SER:HA	2.15	0.46
1:A:515:LYS:HE3	6:A:1336:HOH:O	2.16	0.46
1:B:101:ASP:HB2	1:B:224:TRP:CZ2	2.51	0.45
1:A:184:MET:CE	1:A:188:VAL:HG23	2.47	0.45
1:A:184:MET:HE2	1:A:188:VAL:HG23	1.98	0.45
1:B:599:GLN:HG3	1:B:601:HIS:CE1	2.51	0.45
1:B:148:ASN:HB3	6:B:1236:HOH:O	2.16	0.45
1:B:382:ARG:CZ	6:B:932:HOH:O	2.64	0.45
1:B:75:LYS:HD2	6:B:1252:HOH:O	2.17	0.45
1:B:175:ASN:HB3	1:B:178:TYR:CD1	2.52	0.45
1:A:120:ALA:HA	1:A:155:TRP:CZ2	2.52	0.45
1:A:528:VAL:HG12	1:A:530:MET:HG3	1.99	0.44
1:B:104:ARG:O	1:B:235:ALA:HA	2.17	0.44
1:A:78:ARG:HD3	1:A:110:MET:HB3	1.99	0.44
1:B:93:GLU:HG3	6:B:938:HOH:O	2.17	0.44
1:A:78:ARG:NH2	1:A:352:ASP:OD2	2.51	0.44
1:B:475:ALA:HA	1:B:491:THR:HB	1.99	0.44
1:B:186:LYS:HE2	1:B:186:LYS:HB3	1.85	0.44
1:B:80:ILE:O	1:B:109:GLY:HA2	2.18	0.44
1:B:167:LYS:HD3	6:B:968:HOH:O	2.16	0.44
1:A:253:MET:CE	1:A:257:LYS:HE3	2.46	0.44
1:A:304:GLU:HG2	1:A:470:HIS:CD2	2.53	0.44
1:B:105:TYR:O	1:B:107:MET:HG3	2.18	0.44
1:B:167:LYS:HB3	1:B:200:ILE:CG1	2.48	0.44
1:A:652:GLY:N	1:A:653:PRO:HA	2.32	0.43
1:B:540:PHE:HA	1:B:543:PHE:HB2	1.99	0.43
1:B:84:TYR:CD1	1:B:84:TYR:O	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:ALA:HB3	1:A:539:PRO:CD	2.49	0.43
1:B:214:GLU:OE1	1:B:413:LYS:HE3	2.19	0.43
1:B:380:PRO:HA	1:B:381:PRO:HD3	1.92	0.43
1:A:180:HIS:HB3	1:A:183:ALA:HB2	2.01	0.43
1:A:599:GLN:HG2	1:A:601:HIS:O	2.19	0.42
1:A:125:LEU:N	1:A:126:PRO:CD	2.81	0.42
1:B:257:LYS:HA	1:B:266:LEU:HD21	2.01	0.42
1:A:141:GLY:O	1:A:142:GLU:HB2	2.19	0.42
1:A:267:LYS:HA	6:A:1245:HOH:O	2.18	0.42
1:A:551:ARG:HG3	1:A:557:VAL:CG2	2.49	0.42
1:B:273:LYS:HA	1:B:274:PRO:HD3	1.89	0.41
1:B:626:HIS:CD2	1:B:671:ARG:HG2	2.55	0.41
1:A:638:LYS:CE	1:A:638:LYS:HA	2.50	0.41
1:B:79:ASN:ND2	1:B:80:ILE:HG13	2.35	0.41
1:B:213:GLU:O	1:B:217:ILE:HG13	2.20	0.41
1:B:73:MET:HB3	1:B:78:ARG:HB2	2.03	0.41
1:A:108:ARG:HH11	1:A:108:ARG:HG3	1.85	0.41
1:A:253:MET:HG2	1:A:258:VAL:CG2	2.51	0.41
1:A:564:TYR:CG	1:A:565:GLY:N	2.88	0.41
1:A:475:ALA:HA	1:A:491:THR:HB	2.03	0.40
1:A:514:ARG:NH1	6:A:818:HOH:O	2.54	0.40
1:B:266:LEU:O	1:B:267:LYS:HB2	2.21	0.40
1:A:327:ASP:OD1	1:A:329:ALA:HB3	2.21	0.40
1:A:87:GLN:HG2	6:A:810:HOH:O	2.21	0.40
1:B:527:PRO:HB2	1:B:625:ALA:HB2	2.03	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	603/622 (97%)	590 (98%)	13 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	599/622 (96%)	570 (95%)	29 (5%)	0	100	100
All	All	1202/1244 (97%)	1160 (96%)	42 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	518/531 (98%)	511 (99%)	7 (1%)	74	70
1	B	502/531 (94%)	497 (99%)	5 (1%)	82	80
All	All	1020/1062 (96%)	1008 (99%)	12 (1%)	78	75

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	300	LEU
1	A	346	MET
1	A	411	GLU
1	A	484	ARG
1	A	573	TYR
1	A	638	LYS
1	A	672	TYR
1	B	212	LEU
1	B	346	MET
1	B	353	GLU
1	B	573	TYR
1	B	619	LEU

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	399	GLN

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Mol	Chain	Res	Type
1	A	486	ASN
1	B	356	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

7 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	2.98	14 (43%)	34,50,50	3.61	13 (38%)
3	FAD	A	702	-	52,58,58	2.14	11 (21%)	52,89,89	2.58	10 (19%)
4	2AM	A	703	-	21,25,25	1.70	3 (14%)	25,38,38	3.14	5 (20%)
2	FMN	B	701	-	32,33,33	3.01	14 (43%)	34,50,50	3.68	13 (38%)
3	FAD	B	702	-	52,58,58	2.14	11 (21%)	52,89,89	2.56	9 (17%)
4	2AM	B	703	-	21,25,25	1.71	4 (19%)	25,38,38	3.12	3 (12%)
5	PO4	B	704	-	4,4,4	1.99	2 (50%)	6,6,6	0.25	0

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	2AM	A	703	-	-	0/7/27/27	0/3/3/3
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	2AM	B	703	-	-	0/7/27/27	0/3/3/3
5	PO4	B	704	-	-	0/0/0/0	0/0/0/0

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	FMN	C8M-C8	-6.42	1.38	1.51
2	A	701	FMN	C8M-C8	-6.21	1.38	1.51
3	A	702	FAD	C7M-C7	-5.80	1.39	1.51
3	A	702	FAD	C8M-C8	-5.79	1.39	1.51
3	B	702	FAD	C8M-C8	-5.77	1.39	1.51
3	B	702	FAD	C7M-C7	-5.76	1.39	1.51
3	A	702	FAD	C10-N10	-4.07	1.34	1.39
3	B	702	FAD	C10-N10	-4.06	1.34	1.39
4	B	703	2AM	C5-C4	-3.05	1.33	1.40
3	A	702	FAD	C9A-N10	-3.03	1.34	1.38
4	A	703	2AM	C5-C4	-3.02	1.33	1.40
3	B	702	FAD	C9A-N10	-2.96	1.34	1.38
3	B	702	FAD	C5A-C4A	-2.94	1.33	1.40
3	A	702	FAD	C5A-C4A	-2.89	1.34	1.40
2	A	701	FMN	C1'-N10	-2.43	1.45	1.48
2	B	701	FMN	C1'-N10	-2.40	1.45	1.48
5	B	704	PO4	P-O2	-2.26	1.46	1.53
5	B	704	PO4	P-O3	-2.02	1.47	1.53
4	B	703	2AM	O4'-C1'	2.03	1.44	1.41
2	B	701	FMN	C7M-C7	2.05	1.55	1.51
3	B	702	FAD	O4B-C1B	2.07	1.44	1.41
3	A	702	FAD	O4B-C1B	2.11	1.44	1.41
2	A	701	FMN	C7M-C7	2.13	1.55	1.51
2	A	701	FMN	C4'-C3'	2.19	1.57	1.53
2	B	701	FMN	C4'-C3'	2.24	1.57	1.53
2	A	701	FMN	C10-N1	2.42	1.39	1.35
2	B	701	FMN	C9A-C5A	2.45	1.47	1.42
2	B	701	FMN	C10-N1	2.46	1.39	1.35
2	B	701	FMN	O2'-C2'	2.46	1.48	1.43
2	A	701	FMN	O2'-C2'	2.48	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	FMN	C9A-C5A	2.49	1.47	1.42
3	A	702	FAD	C10-N1	2.78	1.40	1.35
3	B	702	FAD	C10-N1	2.81	1.40	1.35
2	A	701	FMN	C9-C9A	3.08	1.47	1.40
2	B	701	FMN	C9-C9A	3.14	1.47	1.40
3	A	702	FAD	C2A-N1A	3.29	1.40	1.33
3	B	702	FAD	C2A-N1A	3.29	1.40	1.33
2	A	701	FMN	C5A-N5	3.36	1.40	1.35
4	A	703	2AM	C2-N1	3.36	1.40	1.33
4	B	703	2AM	C2-N1	3.37	1.40	1.33
2	B	701	FMN	C5A-N5	3.39	1.40	1.35
2	B	701	FMN	C8-C7	3.45	1.50	1.41
2	A	701	FMN	C8-C7	3.50	1.50	1.41
3	A	702	FAD	C4-N3	4.13	1.40	1.33
3	B	702	FAD	C4-N3	4.15	1.40	1.33
2	B	701	FMN	C4-N3	4.18	1.40	1.33
2	A	701	FMN	C4-N3	4.58	1.41	1.33
4	A	703	2AM	C2-N3	4.59	1.40	1.32
4	B	703	2AM	C2-N3	4.61	1.40	1.32
3	A	702	FAD	C2A-N3A	4.63	1.40	1.32
3	B	702	FAD	C2A-N3A	4.69	1.40	1.32
2	A	701	FMN	C4A-N5	5.66	1.42	1.33
2	B	701	FMN	C4A-N5	5.75	1.42	1.33
2	B	701	FMN	C9A-N10	6.77	1.48	1.38
2	A	701	FMN	C9A-N10	6.89	1.48	1.38
3	B	702	FAD	C8A-N7A	6.94	1.48	1.34
3	A	702	FAD	C8A-N7A	7.01	1.48	1.34
2	A	701	FMN	C10-N10	7.46	1.47	1.39
2	B	701	FMN	C10-N10	8.07	1.48	1.39

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	FAD	N3A-C2A-N1A	-14.64	117.37	128.87
3	B	702	FAD	N3A-C2A-N1A	-14.45	117.52	128.87
4	B	703	2AM	N3-C2-N1	-14.25	117.68	128.87
4	A	703	2AM	N3-C2-N1	-14.22	117.70	128.87
2	B	701	FMN	C4-C4A-C10	-7.80	114.95	119.94
2	A	701	FMN	C4-C4A-C10	-7.75	114.98	119.94
2	B	701	FMN	N3-C2-N1	-6.57	116.62	127.69
2	A	701	FMN	N3-C2-N1	-6.52	116.72	127.69
2	B	701	FMN	C4A-C10-N10	-5.69	116.39	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	FMN	C4A-C10-N10	-5.45	116.56	120.52
2	A	701	FMN	C4A-C4-N3	-5.35	116.53	123.52
2	B	701	FMN	C4A-C4-N3	-5.31	116.58	123.52
3	B	702	FAD	N3-C2-N1	-4.84	119.54	127.69
3	A	702	FAD	N3-C2-N1	-4.75	119.69	127.69
3	B	702	FAD	C4B-O4B-C1B	-3.59	105.84	109.64
3	A	702	FAD	C4B-O4B-C1B	-3.48	105.96	109.64
2	A	701	FMN	O4'-C4'-C3'	-3.17	100.79	108.96
4	A	703	2AM	C4'-O4'-C1'	-3.17	106.28	109.64
2	B	701	FMN	O4'-C4'-C3'	-3.16	100.83	108.96
2	A	701	FMN	C6-C5A-N5	-2.86	115.35	118.92
2	B	701	FMN	C6-C5A-N5	-2.85	115.36	118.92
2	A	701	FMN	C5A-C9A-N10	-2.85	115.44	117.58
3	A	702	FAD	C4X-C4-N3	-2.81	119.85	123.52
2	B	701	FMN	C5A-C9A-N10	-2.80	115.48	117.58
4	B	703	2AM	C4'-O4'-C1'	-2.74	106.74	109.64
3	B	702	FAD	C4X-C4-N3	-2.71	119.98	123.52
4	A	703	2AM	O4'-C1'-C2'	-2.43	102.22	106.60
2	B	701	FMN	O3P-P-O5'	-2.41	99.68	106.72
3	B	702	FAD	C2B-C3B-C4B	-2.38	97.76	102.64
3	A	702	FAD	C2B-C3B-C4B	-2.27	97.99	102.64
2	A	701	FMN	C4A-N5-C5A	-2.25	114.08	116.72
2	B	701	FMN	C4A-N5-C5A	-2.22	114.11	116.72
4	A	703	2AM	C5'-C4'-C3'	-2.14	109.97	115.08
4	A	703	2AM	C1'-N9-C4	-2.08	124.49	126.81
3	A	702	FAD	C1B-N9A-C4A	-2.07	124.49	126.81
4	B	703	2AM	C3'-C2'-C1'	-2.06	98.68	102.63
2	A	701	FMN	O4'-C4'-C5'	-2.02	105.70	110.09
2	A	701	FMN	C8M-C8-C7	2.44	125.97	120.73
3	B	702	FAD	C1'-N10-C9A	2.44	121.66	118.83
2	B	701	FMN	C8M-C8-C7	2.44	125.99	120.73
3	A	702	FAD	C4X-N5-C5X	2.58	119.77	116.72
2	A	701	FMN	C9A-C5A-N5	2.72	126.60	122.18
3	A	702	FAD	C1'-N10-C9A	2.74	122.00	118.83
3	B	702	FAD	C5X-C9A-N10	2.76	119.65	117.58
2	B	701	FMN	C9A-C5A-N5	2.78	126.71	122.18
3	B	702	FAD	C4X-N5-C5X	2.82	120.04	116.72
2	B	701	FMN	O2P-P-O1P	2.82	119.83	110.63
2	A	701	FMN	O2P-P-O1P	2.82	119.83	110.63
3	A	702	FAD	C5X-C9A-N10	2.88	119.73	117.58
3	A	702	FAD	C4-N3-C2	5.95	120.12	115.16
3	B	702	FAD	C4-N3-C2	6.02	120.18	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	FMN	C4-N3-C2	14.35	127.13	115.16
2	B	701	FMN	C4-N3-C2	14.69	127.41	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	FMN	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 ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	609/622 (97%)	0.12	15 (2%) 61 65	22, 32, 49, 64	0
1	B	605/622 (97%)	0.59	67 (11%) 7 8	19, 37, 76, 90	0
All	All	1214/1244 (97%)	0.35	82 (6%) 20 23	19, 34, 70, 90	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	195	LEU	6.2
1	B	104	ARG	5.5
1	B	163	LEU	5.5
1	B	192	LEU	5.2
1	B	161	VAL	4.9
1	B	125	LEU	4.8
1	A	61	ALA	4.7
1	B	242	ILE	4.6
1	B	106	GLY	4.6
1	B	103	HIS	4.6
1	B	120	ALA	4.4
1	B	200	ILE	4.4
1	B	119	LEU	4.4
1	B	191	ARG	4.2
1	B	252	ASP	4.0
1	B	231	PHE	3.9
1	B	105	TYR	3.8
1	A	500	ALA	3.8
1	B	187	TYR	3.7
1	B	80	ILE	3.7
1	B	233	VAL	3.6
1	B	160	ASP	3.6
1	B	501	GLY	3.5
1	B	155	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	224	TRP	3.5
1	B	166	VAL	3.4
1	A	678	SER	3.4
1	B	65	LYS	3.3
1	B	180	HIS	3.3
1	B	168	PHE	3.3
1	B	171	PHE	3.2
1	B	85	GLY	3.2
1	B	227	VAL	3.2
1	B	135	PHE	3.2
1	B	188	VAL	3.2
1	B	162	ASP	3.1
1	B	235	ALA	3.1
1	B	152	PHE	3.1
1	B	102	ALA	3.0
1	B	151	ASP	3.0
1	B	128	ILE	2.9
1	B	108	ARG	2.8
1	B	101	ASP	2.7
1	B	142	GLU	2.7
1	A	506	ARG	2.7
1	A	273	LYS	2.7
1	A	140	TYR	2.6
1	B	351	LEU	2.6
1	B	75	LYS	2.6
1	B	241	SER	2.6
1	B	69	PHE	2.6
1	B	157	GLN	2.6
1	B	167	LYS	2.6
1	B	164	THR	2.6
1	A	255	VAL	2.5
1	B	232	GLY	2.5
1	A	141	GLY	2.5
1	B	165	GLY	2.5
1	B	107	MET	2.5
1	B	179	GLU	2.4
1	A	266	LEU	2.4
1	A	62	PRO	2.4
1	B	77	GLY	2.4
1	B	228	CYS	2.4
1	B	158	GLU	2.3
1	A	278	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	83	PHE	2.3
1	B	225	PRO	2.3
1	B	72	LYS	2.3
1	B	387	TYR	2.2
1	A	179	GLU	2.2
1	B	84	TYR	2.2
1	A	252	ASP	2.2
1	B	71	GLU	2.2
1	A	251	GLU	2.1
1	B	198	GLN	2.1
1	A	633	ALA	2.1
1	B	184	MET	2.1
1	B	169	ALA	2.1
1	B	253	MET	2.1
1	B	122	LEU	2.0
1	B	156	LEU	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 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	FAD	B	702	53/53	0.98	0.15	0.72	18,22,30,32	0
4	2AM	A	703	23/23	0.97	0.09	-0.28	26,27,29,38	0
3	FAD	A	702	53/53	0.98	0.10	-0.36	20,24,30,33	0
4	2AM	B	703	23/23	0.97	0.10	-0.41	25,27,31,38	0
2	FMN	A	701	31/31	0.94	0.12	-0.43	33,39,43,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FMN	B	701	31/31	0.93	0.13	-0.68	49,60,63,63	0
5	PO4	B	704	5/5	0.83	0.18	-	68,71,71,71	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.