



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2018 – 03:33 PM EST

PDB ID : 4Y9U  
Title : rat CYPOR mutant - G143del  
Authors : Xia, C.; Kim, J.J.P.  
Deposited on : 2015-02-17  
Resolution : 1.95 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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-20030736

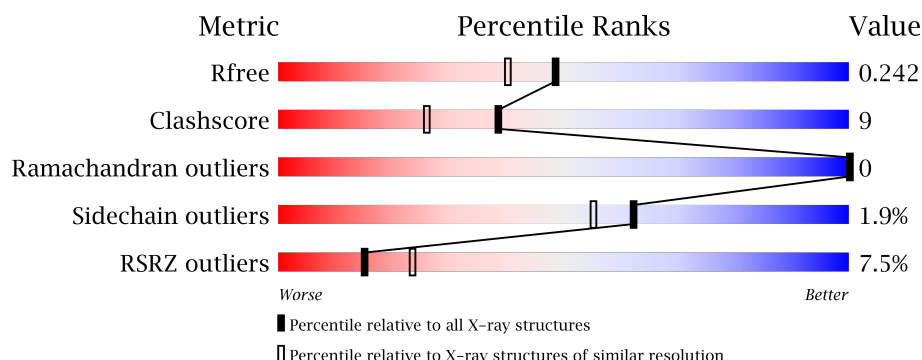
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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))
$R_{free}$	100719	2004 (1.96-1.96)
Clashscore	112137	2136 (1.96-1.96)
Ramachandran outliers	110173	2117 (1.96-1.96)
Sidechain outliers	110143	2117 (1.96-1.96)
RSRZ outliers	101464	2018 (1.96-1.96)

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	621	<div> <div>2%</div> <div>83%</div> <div>14%</div> <div>..</div> </div>
1	B	621	<div> <div>12%</div> <div>78%</div> <div>17%</div> <div>..</div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10985 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	608	Total	C	N	O	S	0	0	0
			4872	3090	840	919	23			
1	B	600	Total	C	N	O	S	0	0	0
			4804	3049	832	900	23			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLY	deletion	UNP P00388
B	?	-	GLY	deletion	UNP P00388

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



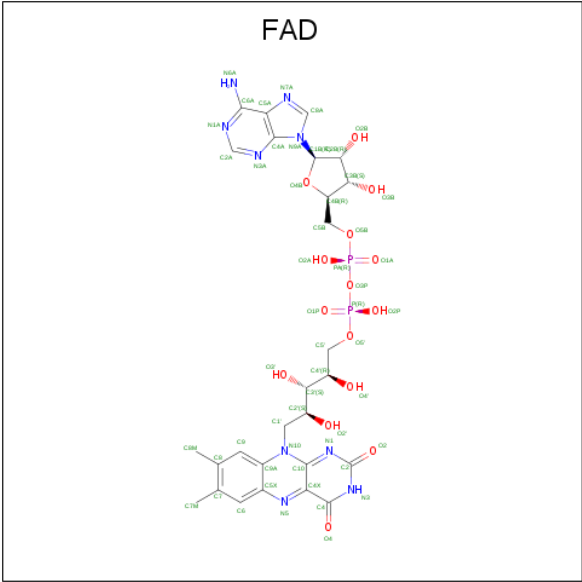
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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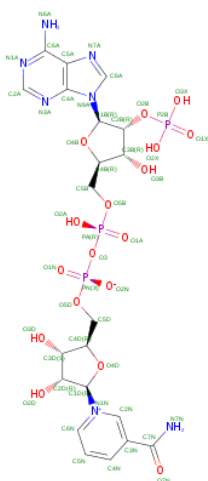
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



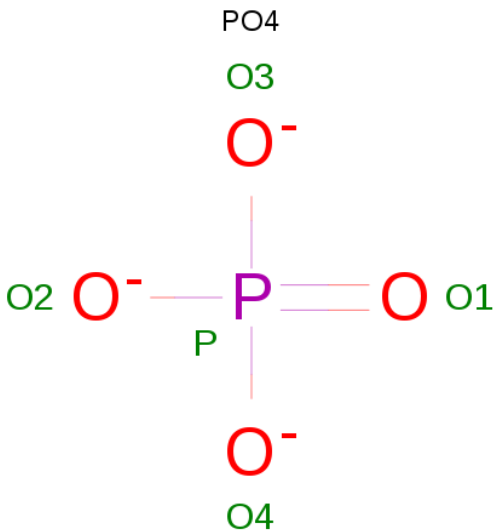
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<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 31	C 10	N 5	O 13	P 3	0	0
4	B	1	Total 31	C 10	N 5	O 13	P 3	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula:  $\text{O}_4\text{P}$ ).



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	609	Total 609	O 609	0	0
6	B	465	Total 465	O 465	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.79Å 115.05Å 119.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.02 – 1.95 47.02 – 1.94	Depositor EDS
% Data completeness (in resolution range)	95.5 (47.02-1.95) 94.9 (47.02-1.94)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.23 (at 1.94Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.203 , 0.241 0.204 , 0.242	Depositor DCC
$R_{free}$ test set	4923 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.6	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 48.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10985	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 18.90% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, PO4, 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	0.36	0/4988	0.58	2/6747 (0.0%)
1	B	0.33	0/4918	0.57	1/6651 (0.0%)
All	All	0.35	0/9906	0.58	3/13398 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	GLY	N-CA-C	-5.38	99.65	113.10
1	B	158	GLU	N-CA-C	5.24	125.15	111.00
1	A	158	GLU	N-CA-C	5.05	124.64	111.00

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4872	0	4724	77	0
1	B	4804	0	4650	90	0
2	A	31	0	19	0	0
2	B	31	0	19	2	0
3	A	53	0	31	0	0
3	B	53	0	31	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	31	0	11	0	0
4	B	31	0	11	0	0
5	B	5	0	0	0	0
6	A	609	0	0	9	0
6	B	465	0	0	9	0
All	All	10985	0	9496	167	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 (167) 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:159:THR:OG1	1:A:161:VAL:HG13	1.56	1.05
1:B:70:VAL:HA	1:B:73:MET:HE2	1.50	0.93
1:A:257:LYS:HA	1:A:266:LEU:HD21	1.53	0.90
1:B:86:SER:HB3	1:B:91:ALA:HB3	1.61	0.83
1:A:159:THR:HG1	1:A:161:VAL:HG13	1.44	0.79
1:A:108:ARG:HD2	6:A:1329:HOH:O	1.87	0.74
1:B:125:LEU:HD23	1:B:166:VAL:HG13	1.70	0.72
1:A:551:ARG:HG3	1:A:557:VAL:HG21	1.71	0.72
1:A:254:ASP:O	1:A:257:LYS:HG2	1.90	0.72
1:B:358:LYS:HD2	1:B:358:LYS:H	1.56	0.70
1:A:228:CYS:HA	1:A:233:VAL:HG12	1.74	0.69
1:A:250:HIS:HB3	1:A:253:MET:HG3	1.74	0.68
1:A:254:ASP:HB2	1:A:257:LYS:HD2	1.74	0.68
1:A:638:LYS:HE3	1:A:638:LYS:HA	1.74	0.68
1:B:86:SER:HB2	2:B:701:FMN:O3P	1.96	0.66
1:B:665:LYS:HG2	1:B:669:LYS:HE2	1.78	0.66
1:A:458:ILE:HG23	1:A:469:VAL:HG13	1.80	0.63
1:A:246:GLU:HB3	1:A:351:LEU:HD21	1.81	0.63
1:B:629:VAL:HB	1:B:674:LEU:HD23	1.80	0.62
1:B:81:ILE:HD12	1:B:110:MET:HG3	1.81	0.62
1:B:167:LYS:HB3	1:B:200:ILE:CG1	2.30	0.62
1:B:70:VAL:HG21	1:B:124:SER:HB2	1.82	0.61
1:B:104:ARG:HD2	6:B:1007:HOH:O	1.99	0.61
1:B:70:VAL:HG12	1:B:74:LYS:HE3	1.83	0.61
1:B:70:VAL:HA	1:B:73:MET:CE	2.29	0.60
1:A:180:HIS:HB3	1:A:183:ALA:HB2	1.82	0.60
1:A:551:ARG:HG3	1:A:557:VAL:CG2	2.31	0.59
1:B:561:LEU:HD22	1:B:590:GLN:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:THR:HB	2:B:701:FMN:O1P	2.03	0.58
1:B:123:SER:O	1:B:126:PRO:HD2	2.03	0.58
1:A:400:GLU:OE2	1:A:404:LYS:HE3	2.04	0.58
1:A:257:LYS:HB2	6:A:899:HOH:O	2.04	0.58
1:B:665:LYS:O	1:B:669:LYS:HD3	2.04	0.58
1:B:69:PHE:O	1:B:73:MET:HG3	2.03	0.58
1:A:321:ALA:HB2	1:A:455:TYR:CE1	2.39	0.57
1:B:69:PHE:CE1	1:B:121:ASP:HB2	2.39	0.57
1:A:285:ALA:HB1	1:A:506:ARG:HE	1.68	0.57
1:A:105:TYR:HD1	1:A:235:ALA:HA	1.69	0.57
1:B:438:ARG:HG3	1:B:438:ARG:HH21	1.69	0.57
1:B:119:LEU:HD22	1:B:152:PHE:CD1	2.40	0.56
1:A:139:THR:O	1:A:140:TYR:CD1	2.59	0.56
1:A:629:VAL:HB	1:A:674:LEU:HD23	1.87	0.56
1:A:228:CYS:HA	1:A:233:VAL:CG1	2.35	0.56
1:B:477:GLU:HG3	1:B:487:LYS:HD2	1.88	0.55
1:B:527:PRO:HB2	1:B:625:ALA:HB2	1.89	0.55
1:B:126:PRO:HA	6:B:818:HOH:O	2.07	0.55
1:A:561:LEU:HD12	1:A:561:LEU:N	2.22	0.54
1:B:86:SER:HB3	1:B:91:ALA:CB	2.34	0.54
1:A:300:LEU:HD22	1:A:574:LEU:HD21	1.89	0.54
1:A:84:TYR:OH	1:A:113:ASP:HB2	2.07	0.54
1:A:254:ASP:HB2	1:A:257:LYS:CD	2.37	0.53
1:B:449:PRO:HG3	6:B:1233:HOH:O	2.08	0.53
1:B:481:LYS:HE3	6:B:1093:HOH:O	2.08	0.53
1:A:156:LEU:HB3	1:A:191:ARG:HG2	1.90	0.53
1:A:184:MET:HE2	1:A:184:MET:O	2.09	0.53
1:A:449:PRO:HG3	6:A:1382:HOH:O	2.10	0.52
1:B:353:GLU:H	1:B:353:GLU:CD	2.13	0.52
1:B:660:VAL:HG12	1:B:664:LYS:HE3	1.90	0.52
1:B:175:ASN:HB3	1:B:178:TYR:CD2	2.44	0.52
1:B:175:ASN:HB3	1:B:178:TYR:HD2	1.75	0.52
1:A:257:LYS:NZ	1:A:257:LYS:HB3	2.25	0.51
1:B:358:LYS:N	1:B:358:LYS:HD2	2.25	0.51
1:B:101:ASP:HB2	1:B:224:TRP:CZ2	2.45	0.51
1:B:475:ALA:HA	1:B:491:THR:HB	1.92	0.51
1:B:78:ARG:HG2	1:B:78:ARG:HH11	1.75	0.51
1:A:285:ALA:CB	1:A:506:ARG:HE	2.24	0.51
1:B:119:LEU:HD22	1:B:152:PHE:CE1	2.46	0.51
1:B:633:ALA:HB2	1:B:676:VAL:HB	1.94	0.50
1:A:159:THR:OG1	1:A:161:VAL:CG1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:HIS:CB	1:A:253:MET:HG3	2.41	0.50
1:A:130:LYS:HG3	1:A:231:PHE:CD1	2.47	0.50
1:B:119:LEU:HD12	1:B:119:LEU:N	2.27	0.49
1:B:83:PHE:HB2	1:B:135:PHE:CD1	2.47	0.49
1:B:222:GLN:C	1:B:225:PRO:HD2	2.32	0.49
1:B:555:LYS:HB3	1:B:555:LYS:NZ	2.27	0.49
1:A:105:TYR:CD1	1:A:235:ALA:HA	2.47	0.49
1:B:385:VAL:O	1:B:389:LEU:HG	2.12	0.49
1:B:670:GLY:HA2	6:B:903:HOH:O	2.12	0.49
1:B:137:MET:HG3	1:B:188:VAL:HG21	1.95	0.49
1:A:652:GLY:N	1:A:653:PRO:HA	2.28	0.49
1:B:547:ARG:O	1:B:551:ARG:HG3	2.14	0.48
1:B:167:LYS:HB3	1:B:200:ILE:HG13	1.96	0.48
1:B:266:LEU:HG	1:B:267:LYS:HD3	1.95	0.48
1:B:76:THR:HG21	1:B:352:ASP:OD1	2.13	0.48
1:B:610:LYS:HE3	6:B:801:HOH:O	2.12	0.48
1:B:80:ILE:O	1:B:109:GLY:HA2	2.14	0.48
1:B:184:MET:O	1:B:188:VAL:HG23	2.14	0.48
1:B:549:TRP:O	1:B:553:GLN:HG2	2.14	0.47
1:A:105:TYR:O	1:A:233:VAL:HG21	2.14	0.47
1:B:246:GLU:HB2	1:B:351:LEU:HD21	1.96	0.47
1:B:132:LEU:HD12	1:B:167:LYS:O	2.15	0.47
1:B:167:LYS:HD2	1:B:200:ILE:HD11	1.97	0.47
1:B:595:PHE:HB3	1:B:598:GLU:HG3	1.96	0.47
1:B:253:MET:HE2	1:B:364:PRO:HG3	1.97	0.47
1:B:678:SER:HA	6:B:889:HOH:O	2.14	0.47
1:A:540:PHE:HA	1:A:543:PHE:HB2	1.97	0.47
1:B:506:ARG:HG2	1:B:506:ARG:HH11	1.80	0.47
1:A:80:ILE:HG23	1:A:109:GLY:HA3	1.97	0.47
1:A:78:ARG:CD	1:A:110:MET:HB3	2.45	0.47
1:B:253:MET:CE	1:B:364:PRO:HG3	2.45	0.46
1:B:79:ASN:O	1:B:131:SER:HA	2.16	0.46
1:A:157:GLN:HG2	1:A:187:TYR:OH	2.15	0.46
1:A:610:LYS:HE2	1:A:613:ARG:HD3	1.96	0.46
1:B:245:TYR:CE2	1:B:360:PRO:HD3	2.51	0.46
1:A:506:ARG:HH11	1:A:506:ARG:HG2	1.80	0.46
1:A:78:ARG:HD3	1:A:110:MET:HB3	1.97	0.46
1:A:233:VAL:HG22	1:A:234:GLU:N	2.30	0.46
1:A:62:PRO:HD3	6:A:1367:HOH:O	2.16	0.46
1:B:438:ARG:HG3	1:B:438:ARG:NH2	2.31	0.46
1:B:358:LYS:CD	1:B:358:LYS:H	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:SER:HB2	1:A:91:ALA:HB3	1.99	0.45
1:B:191:ARG:HD3	1:B:191:ARG:O	2.16	0.45
1:A:402:LEU:HD11	1:A:437:LEU:HD22	1.97	0.45
1:A:213:GLU:OE1	1:A:382:ARG:HD2	2.16	0.45
1:A:484:ARG:HD2	1:A:484:ARG:N	2.32	0.45
1:A:500:ALA:HB2	1:A:506:ARG:HA	1.97	0.45
1:A:633:ALA:HB2	1:A:676:VAL:HB	1.99	0.45
1:B:664:LYS:HG3	6:B:845:HOH:O	2.16	0.45
1:B:222:GLN:O	1:B:225:PRO:HD2	2.17	0.45
1:A:71:GLU:O	1:A:75:LYS:HG2	2.17	0.44
1:B:70:VAL:O	1:B:74:LYS:HG3	2.18	0.44
1:B:382:ARG:CZ	6:B:852:HOH:O	2.65	0.44
1:A:257:LYS:HZ3	1:A:257:LYS:HB3	1.80	0.44
1:A:559:GLU:HB3	1:A:561:LEU:HD11	1.99	0.44
1:A:125:LEU:N	1:A:126:PRO:CD	2.81	0.44
1:A:257:LYS:CB	1:A:257:LYS:NZ	2.80	0.44
1:B:245:TYR:CD2	1:B:360:PRO:HD3	2.52	0.44
1:B:266:LEU:O	1:B:267:LYS:HB2	2.17	0.44
1:A:76:THR:HB	1:A:78:ARG:NH1	2.32	0.44
1:A:253:MET:CE	1:A:257:LYS:HG3	2.48	0.43
1:A:500:ALA:CB	1:A:506:ARG:HA	2.48	0.43
1:A:88:THR:HG22	6:A:801:HOH:O	2.17	0.43
1:A:475:ALA:HA	1:A:491:THR:HB	2.00	0.43
1:A:257:LYS:HA	1:A:266:LEU:CD2	2.38	0.43
1:B:149:ALA:O	1:B:153:TYR:N	2.41	0.43
1:B:537:ILE:O	1:B:537:ILE:HG13	2.18	0.43
1:B:300:LEU:HD22	1:B:574:LEU:HD21	1.99	0.43
1:B:81:ILE:CD1	1:B:110:MET:HG3	2.48	0.42
1:A:253:MET:HE1	1:A:257:LYS:HG3	2.01	0.42
1:A:568:ARG:HD2	6:A:1336:HOH:O	2.19	0.42
1:B:652:GLY:N	1:B:653:PRO:HA	2.33	0.42
1:A:139:THR:C	1:A:140:TYR:CD1	2.92	0.42
1:A:84:TYR:CE1	1:A:112:ALA:C	2.93	0.42
1:B:458:ILE:HG23	1:B:469:VAL:HG13	2.02	0.42
1:B:526:THR:HA	1:B:527:PRO:HD3	1.86	0.42
1:A:526:THR:HA	1:A:527:PRO:HD3	1.89	0.42
1:A:651:PHE:O	1:A:652:GLY:C	2.57	0.42
1:A:155:TRP:O	1:A:159:THR:HG22	2.20	0.42
1:A:328:SER:HB3	6:A:1284:HOH:O	2.20	0.42
1:B:359:HIS:HB3	1:B:360:PRO:HD2	2.02	0.42
1:B:120:ALA:HA	1:B:155:TRP:CZ2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ASP:HB2	6:A:1220:HOH:O	2.19	0.41
1:A:401:HIS:O	1:A:405:MET:HG2	2.20	0.41
1:B:133:VAL:O	1:B:133:VAL:HG13	2.21	0.41
1:B:167:LYS:HB3	1:B:200:ILE:HD11	2.02	0.41
1:A:581:ARG:NH1	1:A:585:ASP:OD2	2.54	0.41
1:A:266:LEU:HG	1:A:267:LYS:HG2	2.03	0.41
1:B:125:LEU:N	1:B:126:PRO:CD	2.84	0.41
1:B:139:THR:OG1	1:B:182:ASN:HA	2.21	0.41
1:B:538:ALA:HB3	1:B:539:PRO:CD	2.50	0.41
1:A:279:LYS:HG2	6:A:1302:HOH:O	2.21	0.41
1:B:360:PRO:O	1:B:450:ARG:HD3	2.21	0.41
1:B:610:LYS:HE2	1:B:613:ARG:HD3	2.03	0.41
1:A:481:LYS:NZ	1:A:481:LYS:HB3	2.36	0.40
1:B:157:GLN:HG2	1:B:187:TYR:OH	2.21	0.40
1:B:292:LEU:HD11	1:B:302:HIS:HB2	2.03	0.40
1:B:395:GLU:HA	1:B:396:PRO:HD2	1.90	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	600/621 (97%)	586 (98%)	14 (2%)	0	100	100
1	B	592/621 (95%)	570 (96%)	22 (4%)	0	100	100
All	All	1192/1242 (96%)	1156 (97%)	36 (3%)	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	519/531 (98%)	508 (98%)	11 (2%)	59	50
1	B	507/531 (96%)	499 (98%)	8 (2%)	68	63
All	All	1026/1062 (97%)	1007 (98%)	19 (2%)	62	55

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	LYS
1	A	234	GLU
1	A	253	MET
1	A	254	ASP
1	A	257	LYS
1	A	346	MET
1	A	484	ARG
1	A	506	ARG
1	A	573	TYR
1	A	610	LYS
1	A	638	LYS
1	B	191	ARG
1	B	212	LEU
1	B	267	LYS
1	B	346	MET
1	B	353	GLU
1	B	555	LYS
1	B	573	TYR
1	B	669	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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	-	31,33,33	2.86	11 (35%)	38,50,50	3.34	16 (42%)
3	FAD	A	702	-	51,58,58	2.21	10 (19%)	54,89,89	2.32	9 (16%)
4	NAP	A	703	-	28,33,52	1.61	3 (10%)	32,52,80	2.57	4 (12%)
2	FMN	B	701	-	31,33,33	2.87	13 (41%)	38,50,50	3.38	15 (39%)
3	FAD	B	702	-	51,58,58	2.20	10 (19%)	54,89,89	2.30	9 (16%)
4	NAP	B	703	-	28,33,52	1.62	4 (14%)	32,52,80	2.56	4 (12%)
5	PO4	B	704	-	4,4,4	1.35	0	6,6,6	0.39	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	-	-	0/16/18/18	0/3/3/3
3	FAD	A	702	-	-	0/28/50/50	0/6/6/6
4	NAP	A	703	-	-	0/17/37/67	0/3/3/5
2	FMN	B	701	-	-	0/16/18/18	0/3/3/3
3	FAD	B	702	-	-	0/28/50/50	0/6/6/6
4	NAP	B	703	-	-	0/17/37/67	0/3/3/5
5	PO4	B	704	-	-	0/0/0/0	0/0/0/0



All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	FMN	C8M-C8	-6.54	1.38	1.51
2	A	701	FMN	C8M-C8	-6.21	1.38	1.51
3	A	702	FAD	C8M-C8	-5.87	1.39	1.51
3	B	702	FAD	C7M-C7	-5.84	1.39	1.51
3	A	702	FAD	C7M-C7	-5.83	1.39	1.51
3	B	702	FAD	C8M-C8	-5.79	1.39	1.51
3	A	702	FAD	C9A-N10	-3.16	1.34	1.38
3	B	702	FAD	C9A-N10	-3.12	1.34	1.38
4	B	703	NAP	C5A-C4A	-3.07	1.33	1.40
4	A	703	NAP	C5A-C4A	-3.03	1.33	1.40
3	A	702	FAD	C5A-C4A	-2.93	1.33	1.40
3	B	702	FAD	C5A-C4A	-2.91	1.33	1.40
2	B	701	FMN	C1'-N10	-2.50	1.45	1.48
4	B	703	NAP	O4B-C1B	2.04	1.44	1.41
2	B	701	FMN	C7M-C7	2.06	1.55	1.51
3	A	702	FAD	O4B-C1B	2.07	1.44	1.41
3	B	702	FAD	O4B-C1B	2.17	1.44	1.41
2	B	701	FMN	C4'-C3'	2.21	1.57	1.53
2	B	701	FMN	O2'-C2'	2.45	1.48	1.43
2	A	701	FMN	O2'-C2'	2.50	1.48	1.43
2	B	701	FMN	C9A-C5A	2.54	1.47	1.42
2	A	701	FMN	C4'-C3'	2.61	1.58	1.53
2	A	701	FMN	C9A-C5A	2.79	1.48	1.42
2	A	701	FMN	C9-C9A	3.11	1.47	1.40
2	B	701	FMN	C9-C9A	3.20	1.47	1.40
2	A	701	FMN	C5A-N5	3.32	1.40	1.35
2	B	701	FMN	C5A-N5	3.34	1.40	1.35
3	B	702	FAD	C2A-N1A	3.36	1.40	1.33
3	A	702	FAD	C2A-N1A	3.38	1.40	1.33
4	B	703	NAP	C2A-N1A	3.40	1.40	1.33
4	A	703	NAP	C2A-N1A	3.49	1.40	1.33
2	B	701	FMN	C8-C7	3.69	1.50	1.41
2	A	701	FMN	C8-C7	3.89	1.50	1.41
3	A	702	FAD	C4-N3	4.09	1.40	1.33
3	B	702	FAD	C4-N3	4.16	1.40	1.33
2	B	701	FMN	C4-N3	4.17	1.40	1.33
2	A	701	FMN	C4-N3	4.42	1.41	1.33
2	A	701	FMN	C10-N1	4.48	1.39	1.33
2	B	701	FMN	C10-N1	4.56	1.39	1.33
4	A	703	NAP	C2A-N3A	4.90	1.40	1.32
3	A	702	FAD	C2A-N3A	4.91	1.40	1.32
4	B	703	NAP	C2A-N3A	4.92	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	FAD	C2A-N3A	4.93	1.40	1.32
3	B	702	FAD	C10-N1	5.05	1.40	1.33
3	A	702	FAD	C10-N1	5.10	1.40	1.33
2	A	701	FMN	C4A-N5	6.02	1.42	1.33
2	B	701	FMN	C4A-N5	6.08	1.42	1.33
3	B	702	FAD	C8A-N7A	7.13	1.48	1.34
3	A	702	FAD	C8A-N7A	7.18	1.48	1.34
2	A	701	FMN	C9A-N10	7.37	1.48	1.38
2	B	701	FMN	C9A-N10	7.38	1.48	1.38

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	FAD	N3A-C2A-N1A	-13.22	117.34	128.86
3	B	702	FAD	N3A-C2A-N1A	-12.98	117.55	128.86
4	A	703	NAP	N3A-C2A-N1A	-12.82	117.69	128.86
4	B	703	NAP	N3A-C2A-N1A	-12.82	117.70	128.86
2	B	701	FMN	C4-C4A-C10	-6.28	114.88	119.96
2	A	701	FMN	C4-C4A-C10	-6.24	114.92	119.96
2	B	701	FMN	C4A-C10-N10	-5.83	116.47	120.52
2	A	701	FMN	C4A-C10-N10	-5.54	116.67	120.52
2	B	701	FMN	C4A-C4-N3	-4.89	116.52	123.48
2	A	701	FMN	C4A-C4-N3	-4.86	116.56	123.48
3	A	702	FAD	C4B-O4B-C1B	-3.71	105.82	109.77
3	B	702	FAD	C4B-O4B-C1B	-3.45	106.10	109.77
4	A	703	NAP	C4B-O4B-C1B	-3.38	106.18	109.77
2	A	701	FMN	O4'-C4'-C3'	-3.30	100.91	109.09
2	B	701	FMN	O4'-C4'-C3'	-3.26	101.01	109.09
2	A	701	FMN	C6-C5A-N5	-3.11	115.32	118.97
4	B	703	NAP	C4B-O4B-C1B	-3.08	106.49	109.77
2	B	701	FMN	C6-C5A-N5	-3.04	115.40	118.97
2	B	701	FMN	C5A-C9A-N10	-3.01	115.42	117.66
2	A	701	FMN	C5A-C9A-N10	-2.95	115.47	117.66
2	B	701	FMN	O3P-P-O5'	-2.85	99.15	106.73
2	A	701	FMN	C4A-N5-C5A	-2.63	113.99	116.76
3	B	702	FAD	C4X-C4-N3	-2.60	119.78	123.48
3	A	702	FAD	C4X-C4-N3	-2.57	119.82	123.48
3	B	702	FAD	C2B-C3B-C4B	-2.48	97.79	102.62
2	B	701	FMN	C4A-N5-C5A	-2.47	114.15	116.76
3	A	702	FAD	C2B-C3B-C4B	-2.46	97.82	102.62
2	A	701	FMN	O3P-P-O5'	-2.34	100.49	106.73
4	B	703	NAP	C3B-C2B-C1B	-2.30	98.25	102.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	NAP	C3B-C2B-C1B	-2.11	98.61	102.75
3	A	702	FAD	C5A-C6A-N6A	-2.07	116.25	120.47
2	A	701	FMN	C4'-C3'-C2'	-2.06	108.98	113.41
3	B	702	FAD	C5A-C6A-N6A	-2.05	116.30	120.47
4	B	703	NAP	O2N-PN-O1N	2.16	118.93	110.50
4	A	703	NAP	O2N-PN-O1N	2.20	119.09	110.50
2	B	701	FMN	C1'-N10-C9A	2.21	120.38	118.35
2	A	701	FMN	O2P-P-O1P	2.31	119.54	110.50
2	B	701	FMN	O2P-P-O1P	2.40	119.91	110.50
2	B	701	FMN	C8M-C8-C7	2.51	125.98	120.72
2	A	701	FMN	C8M-C8-C7	2.58	126.14	120.72
3	B	702	FAD	C5X-C9A-N10	2.78	119.72	117.66
3	A	702	FAD	C5X-C9A-N10	2.80	119.74	117.66
2	A	701	FMN	C1'-N10-C9A	2.88	120.99	118.35
2	A	701	FMN	C9A-C5A-N5	2.95	126.63	122.24
2	B	701	FMN	C9A-C5A-N5	2.96	126.64	122.24
3	A	702	FAD	C4X-N5-C5X	3.06	120.00	116.76
3	B	702	FAD	C4X-N5-C5X	3.15	120.09	116.76
2	A	701	FMN	P-O5'-C5'	3.16	127.00	118.30
3	B	702	FAD	C1'-N10-C9A	3.23	121.31	118.35
3	A	702	FAD	C1'-N10-C9A	3.41	121.47	118.35
2	B	701	FMN	P-O5'-C5'	3.63	128.30	118.30
2	B	701	FMN	C10-C4A-N5	5.62	127.05	120.59
2	A	701	FMN	C10-C4A-N5	5.73	127.18	120.59
3	A	702	FAD	C4-N3-C2	5.74	120.18	115.16
3	B	702	FAD	C4-N3-C2	5.89	120.31	115.16
2	A	701	FMN	C4-N3-C2	13.75	127.19	115.16
2	B	701	FMN	C4-N3-C2	14.03	127.43	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	FMN	2	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	608/621 (97%)	0.23	14 (2%) 61 71	22, 32, 52, 81	0
1	B	600/621 (96%)	0.72	76 (12%) 4 7	22, 36, 71, 101	0
All	All	1208/1242 (97%)	0.47	90 (7%) 15 23	22, 33, 67, 101	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	200	ILE	7.6
1	B	195	LEU	6.7
1	B	104	ARG	6.3
1	B	192	LEU	6.1
1	A	235	ALA	6.0
1	B	233	VAL	6.0
1	B	252	ASP	5.6
1	A	505	GLY	5.5
1	B	128	ILE	5.5
1	B	106	GLY	5.3
1	B	155	TRP	5.3
1	B	105	TYR	5.2
1	B	191	ARG	5.2
1	B	166	VAL	5.1
1	B	161	VAL	4.6
1	B	181	PHE	4.5
1	A	140	TYR	4.5
1	B	255	VAL	4.4
1	B	231	PHE	4.4
1	A	500	ALA	4.4
1	B	146	THR	4.4
1	B	125	LEU	4.3
1	B	140	TYR	4.3
1	B	228	CYS	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	205	LEU	4.2
1	B	187	TYR	4.1
1	B	129	ASP	4.1
1	A	179	GLU	4.0
1	B	77	GLY	4.0
1	B	180	HIS	3.9
1	B	103	HIS	3.9
1	B	131	SER	3.9
1	A	506	ARG	3.7
1	B	198	GLN	3.7
1	B	149	ALA	3.7
1	B	253	MET	3.7
1	A	180	HIS	3.7
1	B	157	GLN	3.6
1	B	227	VAL	3.6
1	B	163	LEU	3.6
1	B	76	THR	3.6
1	A	254	ASP	3.5
1	B	78	ARG	3.5
1	B	152	PHE	3.5
1	B	230	PHE	3.5
1	B	197	ALA	3.3
1	B	500	ALA	3.3
1	B	254	ASP	3.2
1	B	153	TYR	3.1
1	B	168	PHE	3.1
1	B	352	ASP	3.1
1	B	160	ASP	3.1
1	B	119	LEU	3.0
1	B	159	THR	3.0
1	B	194	GLN	3.0
1	B	151	ASP	3.0
1	B	242	ILE	2.9
1	B	176	LYS	2.8
1	B	403	HIS	2.8
1	A	252	ASP	2.8
1	B	107	MET	2.8
1	B	120	ALA	2.7
1	B	665	LYS	2.7
1	B	226	ALA	2.6
1	B	387	TYR	2.6
1	B	184	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	135	PHE	2.5
1	A	153	TYR	2.5
1	B	108	ARG	2.5
1	B	147	ASP	2.5
1	B	130	LYS	2.5
1	B	224	TRP	2.5
1	B	102	ALA	2.5
1	B	165	GLY	2.5
1	B	351	LEU	2.5
1	B	138	ALA	2.4
1	B	196	GLY	2.4
1	A	178	TYR	2.4
1	B	100	LYS	2.3
1	B	183	ALA	2.3
1	B	212	LEU	2.2
1	B	313	ARG	2.2
1	A	62	PRO	2.2
1	B	139	THR	2.2
1	A	104	ARG	2.2
1	B	156	LEU	2.1
1	B	190	GLN	2.1
1	A	85	GLY	2.1
1	B	661	ASP	2.0
1	B	148	ASN	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( $\text{\AA}^2$ )	Q<0.9
2	FMN	B	701	31/31	0.87	0.24	0.59	60,70,74,74	0
3	FAD	B	702	53/53	0.98	0.12	0.10	20,24,32,33	0
4	NAP	A	703	31/48	0.98	0.10	-0.39	22,24,36,46	0
2	FMN	A	701	31/31	0.94	0.14	-0.57	32,38,41,43	0
3	FAD	A	702	53/53	0.98	0.11	-0.61	21,25,32,37	0
4	NAP	B	703	31/48	0.97	0.10	-0.62	21,25,42,50	0
5	PO4	B	704	5/5	0.76	0.23	-	106,106,107,107	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.