



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:49 AM GMT

PDB ID : 3G5M  
Title : Synthesis of Casimiroin and Optimization of Its Quinone Reductase 2 and Aromatase Inhibitory activity  
Authors : Maiti, A.; Sturdy, M.; Marler, L.; Pegan, S.D.; Mesecar, A.D.; Pezzuto, J.M.; Cushman, M.  
Deposited on : 2009-02-05  
Resolution : 1.84 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

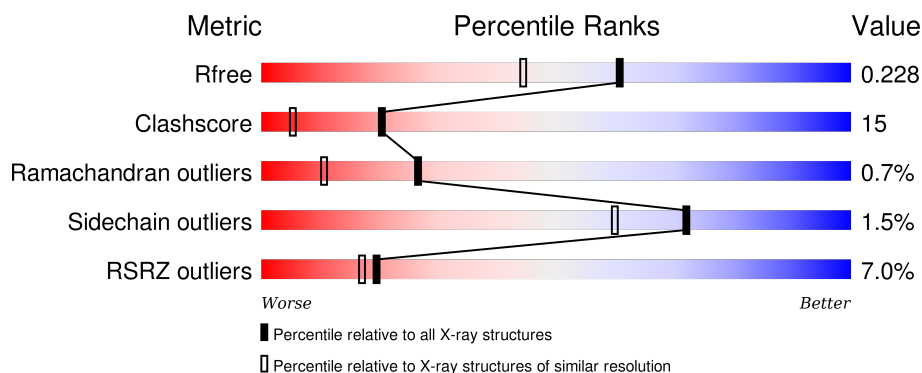
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.84 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	2634 (1.86-1.82)
Clashscore	102246	2862 (1.86-1.82)
Ramachandran outliers	100387	2831 (1.86-1.82)
Sidechain outliers	100360	2832 (1.86-1.82)
RSRZ outliers	91569	2639 (1.86-1.82)

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	231	<div> <div>9%</div> <div>76%</div> <div>22%</div> </div>
1	B	231	<div> <div>5%</div> <div>85%</div> <div>13%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	XM5	A	233[B]	-	-	X	-
3	XM5	A	234[A]	-	-	X	-
4	FAD	B	233	X	-	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4287 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.

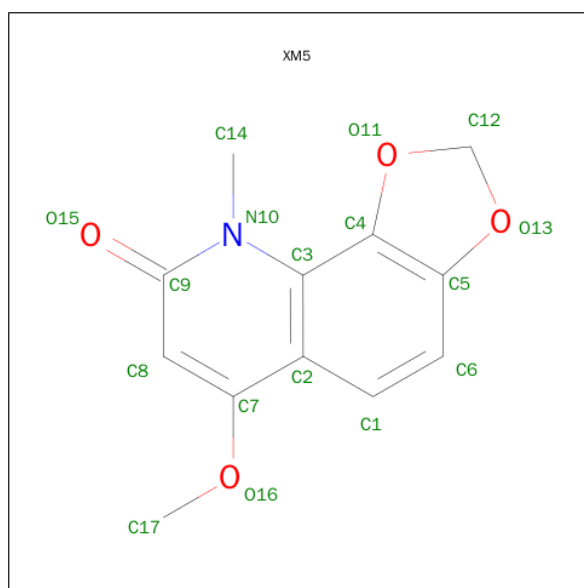
- Molecule 1 is a protein called Ribosyldihydronicotinamide dehydrogenase [quinone].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	6	0
			1869	1204	311	345	9			
1	B	230	Total	C	N	O	S	0	3	0
			1846	1187	306	344	9			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

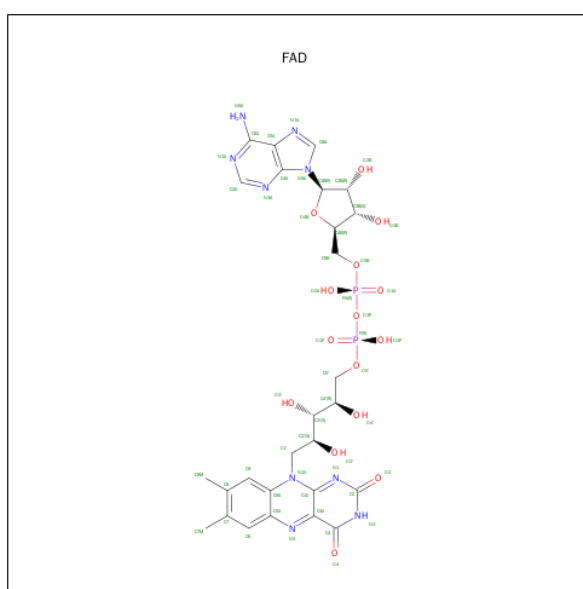
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 6-METHOXY-9-METHYL[1,3]DIOXOLO[4,5-H]QUINOLIN-8(9H)-ONE (three-letter code: XM5) (formula: C<sub>12</sub>H<sub>11</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			17	12	1	4		
3	A	1	Total	C	N	O	0	1
			17	12	1	4		
3	A	1	Total	C	N	O	0	1
			17	12	1	4		
3	B	1	Total	C	N	O	0	1
			17	12	1	4		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



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

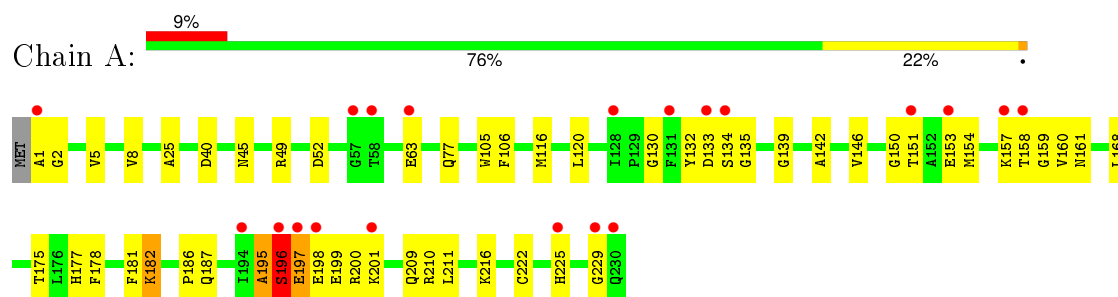
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	176	Total	O	0	0
			176	176		
5	B	220	Total	O	0	0
			220	220		

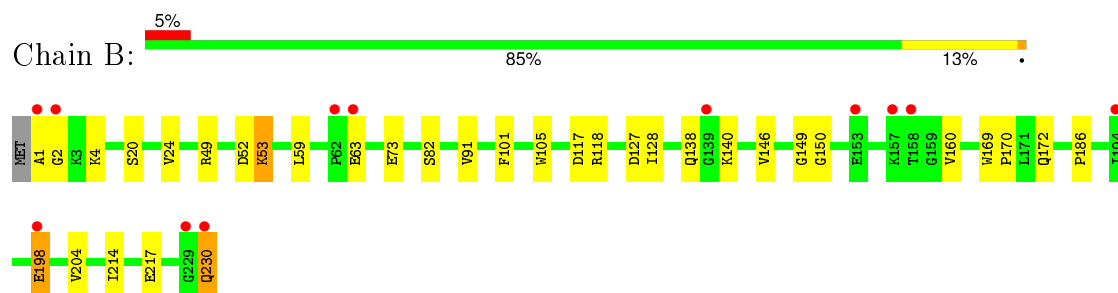
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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: Ribosyldihydronicotinamide dehydrogenase [quinone]



- Molecule 1: Ribosyldihydronicotinamide dehydrogenase [quinone]



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.73 Å 84.23 Å 106.31 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.08 – 1.84 19.91 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.1 (66.08-1.84) 99.2 (19.91-1.84)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.27 (at 1.84 Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.182 , 0.242 0.176 , 0.228	Depositor DCC
$R_{free}$ test set	2256 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.5	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 56.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 44742 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4287	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: XM5, ZN, 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	1.15	3/1923 (0.2%)	0.98	4/2608 (0.2%)
1	B	1.13	1/1899 (0.1%)	0.98	7/2575 (0.3%)
All	All	1.14	4/3822 (0.1%)	0.98	11/5183 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	5	VAL	CB-CG2	5.69	1.64	1.52
1	B	91	VAL	CB-CG2	5.47	1.64	1.52
1	A	222	CYS	CB-SG	5.45	1.91	1.82
1	A	8	VAL	CB-CG1	5.16	1.63	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	49	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	A	52	ASP	CB-CG-OD1	6.81	124.43	118.30
1	A	49	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	B	49	ARG	NE-CZ-NH2	-6.15	117.23	120.30
1	B	117	ASP	CB-CG-OD2	-5.85	113.04	118.30
1	A	146	VAL	CB-CA-C	-5.50	100.95	111.40
1	B	118	ARG	NE-CZ-NH2	-5.10	117.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	118	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	B	127[A]	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	B	127[B]	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	A	40	ASP	CB-CG-OD1	5.02	122.82	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	195[A]	ALA	Peptide
1	A	195[B]	ALA	Peptide
1	A	196	SER	Peptide

## 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	1869	0	1820	64	0
1	B	1846	0	1796	40	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	51	0	28	22	0
3	B	17	0	8	1	0
4	A	53	0	31	3	0
4	B	53	0	30	3	0
5	A	176	0	0	29	0
5	B	220	0	0	27	0
All	All	4287	0	3713	111	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 15.

All (111) 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:216:LYS:HE2	5:A:388:HOH:O	1.27	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:HIS:N	5:A:391:HOH:O	1.60	1.27
1:A:135:GLY:N	5:A:394:HOH:O	1.69	1.21
1:B:138:GLN:CD	5:B:390:HOH:O	1.81	1.18
1:B:2:GLY:HA3	5:B:381:HOH:O	1.43	1.14
1:A:197:GLU:HA	1:A:197:GLU:OE1	1.45	1.12
1:A:198:GLU:HG2	5:A:327:HOH:O	1.51	1.09
1:B:63:GLU:HB2	5:B:384:HOH:O	1.54	1.07
1:A:177:HIS:CA	5:A:391:HOH:O	1.89	1.07
1:B:138:GLN:NE2	5:B:390:HOH:O	1.88	1.03
1:B:63:GLU:CB	5:B:384:HOH:O	2.07	1.02
4:B:233:FAD:H2B	5:B:256:HOH:O	1.61	1.00
1:B:2:GLY:CA	5:B:381:HOH:O	2.00	0.99
1:B:1:ALA:HB1	5:B:373:HOH:O	1.63	0.97
3:A:232[A]:XM5:C17	5:A:387:HOH:O	2.18	0.89
1:B:1:ALA:HB3	5:B:370:HOH:O	1.72	0.89
1:A:182:LYS:HE2	5:A:371:HOH:O	1.73	0.88
1:A:196:SER:O	1:A:198:GLU:O	1.92	0.87
1:A:178:PHE:CD1	3:A:234[A]:XM5:H17B	2.10	0.86
1:A:133:ASP:C	5:A:394:HOH:O	2.14	0.85
1:A:116[B]:MET:HG3	1:A:120:LEU:HD12	1.56	0.84
1:A:200:ARG:NH1	4:A:235:FAD:N3A	2.26	0.84
1:B:1:ALA:CB	5:B:373:HOH:O	2.23	0.83
1:B:2:GLY:N	5:B:381:HOH:O	2.10	0.81
1:A:178:PHE:CE1	3:A:234[A]:XM5:H17B	2.19	0.78
1:A:63:GLU:O	5:A:292:HOH:O	2.01	0.78
3:A:234[A]:XM5:H14	3:A:234[A]:XM5:O11	1.84	0.77
1:A:178:PHE:CG	3:A:234[A]:XM5:H17B	2.19	0.76
1:A:157:LYS:HG3	1:A:158:THR:HG23	1.68	0.76
1:B:1:ALA:HA	5:B:285:HOH:O	1.86	0.75
1:B:63:GLU:CA	5:B:384:HOH:O	2.29	0.75
1:A:187:GLN:HE21	1:A:210:ARG:HH11	1.34	0.75
1:A:45[A]:ASN:ND2	5:A:306:HOH:O	2.18	0.70
1:B:73[B]:GLU:HG2	5:B:427:HOH:O	1.91	0.69
1:A:209:GLN:OE1	5:A:360:HOH:O	2.10	0.68
1:A:187:GLN:NE2	1:A:210:ARG:HH11	1.91	0.68
1:B:63:GLU:HA	5:B:384:HOH:O	1.91	0.68
1:A:178:PHE:CD2	3:A:234[A]:XM5:H17B	2.29	0.67
1:A:160:VAL:N	5:A:366:HOH:O	1.78	0.66
3:A:234[A]:XM5:H14A	1:B:150:GLY:N	2.10	0.66
1:A:150:GLY:CA	3:A:233[B]:XM5:H14A	2.25	0.66
1:A:63:GLU:HB3	5:A:395:HOH:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:SER:CA	5:A:394:HOH:O	2.42	0.66
1:A:151:THR:HG23	1:A:154:MET:HE3	1.78	0.66
1:A:177:HIS:HB2	5:A:391:HOH:O	1.97	0.64
1:A:198:GLU:O	1:A:199:GLU:HB2	1.95	0.64
1:B:169:TRP:HB3	1:B:170:PRO:HD3	1.81	0.63
1:A:116[B]:MET:HG2	1:A:175:THR:HG21	1.80	0.63
1:B:230:GLN:HA	1:B:230:GLN:HE21	1.64	0.63
1:A:178:PHE:CZ	3:A:234[A]:XM5:H17B	2.35	0.62
1:A:77[A]:GLN:HG2	5:A:386:HOH:O	1.99	0.62
1:A:105:TRP:CZ3	3:A:232[A]:XM5:H12A	2.37	0.60
1:A:106[B]:PHE:CZ	3:A:233[B]:XM5:H8	2.38	0.59
1:B:149:GLY:N	4:B:233:FAD:H2'	2.18	0.58
1:A:160:VAL:HG22	5:A:366:HOH:O	2.03	0.58
1:B:1:ALA:CA	5:B:285:HOH:O	2.48	0.58
1:A:159:GLY:CA	5:A:366:HOH:O	2.51	0.58
1:B:172:GLN:HE22	1:B:186:PRO:HD3	1.69	0.57
1:B:4:LYS:HD2	5:B:283:HOH:O	2.05	0.57
1:A:178:PHE:CE2	3:A:234[A]:XM5:H17B	2.39	0.57
1:A:225:HIS:HD2	1:A:229:GLY:HA3	1.71	0.56
1:B:198:GLU:H	1:B:198:GLU:CD	2.09	0.56
1:A:150:GLY:N	3:A:233[B]:XM5:H14A	2.21	0.56
1:B:2:GLY:N	5:B:262:HOH:O	2.39	0.55
3:A:234[A]:XM5:H14A	1:B:149:GLY:C	2.27	0.55
1:A:182:LYS:HG3	5:A:371:HOH:O	2.05	0.54
1:A:198:GLU:HG3	5:A:374:HOH:O	2.07	0.54
1:B:20:SER:O	1:B:24:VAL:HG13	2.09	0.53
1:A:187:GLN:HE21	1:A:210:ARG:NH1	2.04	0.53
1:A:151:THR:HG23	1:A:154:MET:CE	2.37	0.53
1:B:52:ASP:OD1	1:B:53:LYS:HE2	2.10	0.52
1:B:24:VAL:HG11	1:B:204:VAL:CG1	2.40	0.52
1:A:116[B]:MET:HG3	1:A:120:LEU:CD1	2.34	0.51
1:B:82:SER:HB2	5:B:249:HOH:O	2.10	0.51
1:A:177:HIS:CB	5:A:391:HOH:O	2.35	0.50
1:A:106[B]:PHE:HZ	3:A:233[B]:XM5:H8	1.76	0.50
1:A:134:SER:C	5:A:394:HOH:O	2.22	0.50
1:A:178:PHE:CD2	3:A:234[A]:XM5:C17	2.95	0.49
1:A:196:SER:C	1:A:198:GLU:O	2.51	0.48
1:B:1:ALA:C	5:B:285:HOH:O	2.52	0.47
1:A:157:LYS:HB3	5:A:304:HOH:O	2.14	0.46
1:A:197:GLU:O	1:A:201:LYS:HG2	2.15	0.46
1:B:230:GLN:CA	1:B:230:GLN:HE21	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:232[A]:XM5:H17B	5:A:387:HOH:O	1.99	0.46
1:B:73[B]:GLU:CG	5:B:427:HOH:O	2.59	0.46
1:A:105:TRP:CH2	3:A:232[A]:XM5:H12A	2.52	0.45
1:B:1:ALA:O	5:B:450:HOH:O	2.21	0.45
1:A:139:GLY:N	5:A:371:HOH:O	2.23	0.45
1:A:1:ALA:HA	1:A:2:GLY:HA2	1.65	0.44
1:B:138:GLN:OE1	5:B:390:HOH:O	2.12	0.44
1:A:168:LEU:HD13	1:A:186:PRO:HG3	1.99	0.44
3:A:233[B]:XM5:O11	3:A:233[B]:XM5:H14	2.18	0.43
1:A:142:ALA:HB2	1:A:181:PHE:CD1	2.53	0.43
1:B:1:ALA:HB1	5:B:262:HOH:O	2.18	0.43
1:A:178:PHE:CG	3:A:234[A]:XM5:C17	2.98	0.43
3:A:232[A]:XM5:H17B	1:B:128:ILE:HG21	2.01	0.43
1:A:195[A]:ALA:HB3	1:A:200:ARG:HG3	2.00	0.43
1:A:177:HIS:HA	5:A:391:HOH:O	1.81	0.42
1:A:77[A]:GLN:CG	5:A:386:HOH:O	2.64	0.42
4:B:233:FAD:H1'2	4:B:233:FAD:H9	1.71	0.42
1:B:101:PHE:CZ	1:B:146:VAL:HG22	2.54	0.42
4:A:235:FAD:HM72	5:B:276:HOH:O	2.19	0.42
1:B:105:TRP:CZ3	3:B:232[B]:XM5:H12A	2.55	0.42
1:A:25:ALA:HA	1:A:211:LEU:HD13	2.02	0.41
1:B:59:LEU:HD13	5:B:385:HOH:O	2.21	0.41
1:A:161:ASN:ND2	3:A:233[B]:XM5:O15	2.30	0.41
1:B:214:ILE:HD12	1:B:217:GLU:OE2	2.21	0.41
1:A:153:GLU:HG3	5:A:373:HOH:O	2.20	0.41
1:A:200:ARG:NH1	4:A:235:FAD:H1B	2.35	0.40
1:A:182:LYS:CG	5:A:371:HOH:O	2.68	0.40
1:B:140:LYS:HE2	5:B:443:HOH:O	2.20	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	234/231 (101%)	219 (94%)	12 (5%)	3 (1%)	15	4
1	B	231/231 (100%)	224 (97%)	7 (3%)	0	100	100
All	All	465/462 (101%)	443 (95%)	19 (4%)	3 (1%)	26	14

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	SER
1	A	132	TYR
1	A	130	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	199/195 (102%)	197 (99%)	2 (1%)	82	75
1	B	197/195 (101%)	193 (98%)	4 (2%)	63	47
All	All	396/390 (102%)	390 (98%)	6 (2%)	72	60

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	LYS
1	A	197	GLU
1	B	53	LYS
1	B	160	VAL
1	B	198	GLU
1	B	230	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
1	A	172	GLN

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Mol	Chain	Res	Type
1	A	187	GLN
1	A	212	GLN
1	B	138	GLN
1	B	172	GLN
1	B	187	GLN
1	B	230	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	XM5	A	232[A]	-	17,19,19	1.32	2 (11%)	23,28,28	2.14	9 (39%)
3	XM5	A	233[B]	-	17,19,19	1.24	1 (5%)	23,28,28	2.18	8 (34%)
3	XM5	A	234[A]	-	17,19,19	1.48	3 (17%)	23,28,28	4.31	8 (34%)
4	FAD	A	235	-	48,58,58	1.42	9 (18%)	54,89,89	2.55	13 (24%)
3	XM5	B	232[B]	-	17,19,19	1.46	3 (17%)	23,28,28	2.59	8 (34%)
4	FAD	B	233	-	48,58,58	1.35	6 (12%)	54,89,89	4.21	17 (31%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	XM5	A	232[A]	-	-	0/2/8/8	0/3/3/3
3	XM5	A	233[B]	-	-	0/2/8/8	0/3/3/3
3	XM5	A	234[A]	-	-	0/2/8/8	0/3/3/3
4	FAD	A	235	-	-	0/30/50/50	0/6/6/6
3	XM5	B	232[B]	-	-	0/2/8/8	0/3/3/3
4	FAD	B	233	-	4/4/9/9	0/30/50/50	0/6/6/6

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	233	FAD	C1'-N10	-3.04	1.45	1.48
4	A	235	FAD	C8-C7	2.04	1.46	1.41
4	A	235	FAD	C9-C8	2.05	1.43	1.37
4	B	233	FAD	C4-C4X	2.05	1.45	1.41
4	A	235	FAD	O4B-C1B	2.07	1.43	1.41
4	B	233	FAD	C2A-N3A	2.13	1.36	1.32
4	B	233	FAD	C8-C7	2.22	1.46	1.41
4	A	235	FAD	C10-N1	2.30	1.39	1.35
3	A	234[A]	XM5	C2-C3	2.31	1.48	1.42
3	A	233[B]	XM5	C2-C3	2.37	1.48	1.42
3	B	232[B]	XM5	C7-C2	2.40	1.49	1.42
3	A	232[A]	XM5	C9-N10	2.41	1.41	1.38
3	B	232[B]	XM5	C2-C3	2.51	1.48	1.42
4	A	235	FAD	C4-N3	2.56	1.37	1.33
4	A	235	FAD	C4-C4X	2.65	1.46	1.41
4	B	233	FAD	C5A-C4A	2.70	1.46	1.40
3	A	232[A]	XM5	C2-C3	2.86	1.49	1.42
3	A	234[A]	XM5	C7-C2	2.90	1.50	1.42
3	A	234[A]	XM5	C1-C6	2.99	1.42	1.36
4	A	235	FAD	C9A-C5X	3.19	1.49	1.42
4	B	233	FAD	C4-N3	3.21	1.39	1.33
4	A	235	FAD	C5A-C4A	3.33	1.48	1.40
3	B	232[B]	XM5	C9-N10	3.47	1.43	1.38
4	A	235	FAD	C9A-N10	3.75	1.43	1.38

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	233	FAD	C4B-O4B-C1B	-23.72	83.65	109.72
4	A	235	FAD	C4-C4X-C10	-8.42	114.55	119.94
4	A	235	FAD	N3A-C2A-N1A	-8.26	122.57	128.89
3	A	234[A]	XM5	O16-C7-C8	-7.83	111.22	123.60
4	B	233	FAD	N3A-C2A-N1A	-6.79	123.69	128.89
4	B	233	FAD	C4-C4X-C10	-6.48	115.80	119.94
4	B	233	FAD	C2B-C3B-C4B	-6.18	89.91	102.61
4	B	233	FAD	O5B-C5B-C4B	-5.75	87.90	109.12
4	A	235	FAD	C1B-N9A-C4A	-4.48	120.18	126.94
3	A	234[A]	XM5	O13-C5-C4	-4.33	105.49	109.73
4	A	235	FAD	P-O3P-PA	-3.93	121.68	132.73
4	A	235	FAD	O3B-C3B-C4B	-3.57	100.34	111.05
4	A	235	FAD	O3P-PA-O5B	-3.21	94.42	102.94
3	B	232[B]	XM5	O16-C7-C8	-3.19	118.55	123.60
3	B	232[B]	XM5	C9-N10-C3	-3.15	118.83	121.75
4	A	235	FAD	C4X-C10-N10	-3.08	118.70	120.52
4	B	233	FAD	C4X-C4-N3	-2.83	119.72	123.59
3	A	232[A]	XM5	C9-N10-C3	-2.68	119.26	121.75
3	B	232[B]	XM5	O13-C5-C4	-2.55	107.22	109.73
4	A	235	FAD	C4X-C4-N3	-2.55	120.11	123.59
3	A	233[B]	XM5	O13-C5-C4	-2.40	107.38	109.73
3	A	232[A]	XM5	C4-C3-C2	-2.38	114.22	118.46
3	A	233[B]	XM5	C9-N10-C3	-2.16	119.75	121.75
4	B	233	FAD	P-O3P-PA	-2.13	126.74	132.73
4	B	233	FAD	O3P-PA-O5B	-2.09	97.38	102.94
3	A	233[B]	XM5	C4-C3-C2	-2.02	114.86	118.46
3	B	232[B]	XM5	C9-C8-C7	2.15	120.98	117.09
3	B	232[B]	XM5	C1-C2-C3	2.17	121.34	117.00
3	A	232[A]	XM5	C1-C2-C3	2.21	121.41	117.00
3	A	234[A]	XM5	C14-N10-C3	2.24	121.16	118.11
3	A	232[A]	XM5	C12-O13-C5	2.43	108.85	105.35
3	B	232[B]	XM5	C12-O13-C5	2.43	108.85	105.35
3	A	232[A]	XM5	C12-O11-C4	2.52	108.44	105.08
3	A	232[A]	XM5	C9-C8-C7	2.52	121.64	117.09
4	A	235	FAD	C2A-N1A-C6A	2.59	123.39	118.77
3	A	232[A]	XM5	C17-O16-C7	2.61	121.59	117.77
3	A	233[B]	XM5	C1-C2-C3	2.63	122.25	117.00
4	A	235	FAD	O2A-PA-O3P	2.64	117.05	105.09
3	A	233[B]	XM5	C14-N10-C3	2.64	121.71	118.11
4	B	233	FAD	N6A-C6A-N1A	2.82	125.26	119.20
4	B	233	FAD	O3'-C3'-C4'	2.87	115.98	108.75
3	A	233[B]	XM5	C12-O13-C5	2.91	109.54	105.35
3	A	232[A]	XM5	C14-N10-C3	2.91	122.08	118.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	233	FAD	C4X-N5-C5X	2.91	120.11	116.76
4	B	233	FAD	O4B-C1B-N9A	3.04	114.47	108.10
3	A	233[B]	XM5	C9-C8-C7	3.12	122.73	117.09
3	A	234[A]	XM5	O13-C5-C6	3.14	132.97	127.96
3	A	234[A]	XM5	C12-O13-C5	3.28	110.06	105.35
4	B	233	FAD	O2'-C2'-C1'	3.34	118.16	109.94
3	B	232[B]	XM5	C14-N10-C3	3.53	122.93	118.11
4	B	233	FAD	C4-C4X-N5	3.62	123.11	118.72
4	B	233	FAD	C1B-N9A-C4A	3.90	132.83	126.94
3	A	234[A]	XM5	C9-C8-C7	3.96	124.25	117.09
4	A	235	FAD	C4-C4X-N5	4.04	123.63	118.72
3	A	234[A]	XM5	C17-O16-C7	4.36	124.16	117.77
4	A	235	FAD	C4X-N5-C5X	4.58	122.03	116.76
3	A	232[A]	XM5	O16-C7-C2	5.92	119.53	114.43
3	A	233[B]	XM5	O16-C7-C2	6.59	120.11	114.43
4	A	235	FAD	C4-N3-C2	6.65	120.99	115.25
4	B	233	FAD	C4-N3-C2	6.75	121.08	115.25
4	B	233	FAD	C2B-C1B-N9A	7.89	126.34	114.29
3	B	232[B]	XM5	O16-C7-C2	8.84	122.05	114.43
3	A	234[A]	XM5	O16-C7-C2	16.42	128.57	114.43

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	233	FAD	C1B
4	B	233	FAD	C4B
4	B	233	FAD	C2'
4	B	233	FAD	C3'

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	232[A]	XM5	5	0
3	A	233[B]	XM5	6	0
3	A	234[A]	XM5	11	0
4	A	235	FAD	3	0
3	B	232[B]	XM5	1	0
4	B	233	FAD	3	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	230/231 (99%)	0.34	20 (8%) 13 11	7, 22, 42, 56	0
1	B	230/231 (99%)	-0.07	12 (5%) 31 28	7, 17, 36, 49	0
All	All	460/462 (99%)	0.13	32 (6%) 19 17	7, 18, 40, 56	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	ALA	10.4
1	A	1	ALA	10.2
1	A	230	GLN	8.2
1	B	230	GLN	6.9
1	A	229	GLY	5.0
1	A	158	THR	4.6
1	B	2	GLY	4.5
1	A	157	LYS	3.9
1	A	57	GLY	3.8
1	A	63	GLU	3.6
1	B	63	GLU	3.4
1	B	198	GLU	3.4
1	A	196	SER	3.4
1	A	198	GLU	3.3
1	A	225	HIS	3.3
1	A	128	ILE	3.2
1	B	158	THR	3.1
1	A	197	GLU	3.0
1	A	134	SER	2.7
1	A	58	THR	2.7
1	B	153	GLU	2.5
1	A	133	ASP	2.5
1	A	153	GLU	2.5
1	A	131	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	229	GLY	2.4
1	A	201	LYS	2.4
1	A	151	THR	2.3
1	B	194	ILE	2.2
1	B	157	LYS	2.1
1	B	62	PRO	2.1
1	A	194	ILE	2.0
1	B	139	GLY	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	XM5	A	233[B]	17/17	0.93	0.14	0.96	20,24,26,26	17
3	XM5	A	234[A]	17/17	0.92	0.14	0.65	16,22,27,28	17
3	XM5	A	232[A]	17/17	0.92	0.13	0.33	15,19,22,22	17
3	XM5	B	232[B]	17/17	0.90	0.13	0.09	18,23,25,26	17
4	FAD	B	233	53/53	0.95	0.10	-0.23	13,19,31,33	0
4	FAD	A	235	53/53	0.96	0.09	-0.58	10,17,40,42	0
2	ZN	A	231	1/1	0.98	0.04	-2.63	28,28,28,28	0
2	ZN	B	231	1/1	0.99	0.04	-	20,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.