



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 08:15 AM GMT

PDB ID : 2Y08  
Title : STRUCTURE OF THE SUBSTRATE-FREE FAD-DEPENDENT TIRANDAMYCIN OXIDASE TAML  
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Deposited on : 2010-11-30  
Resolution : 1.70 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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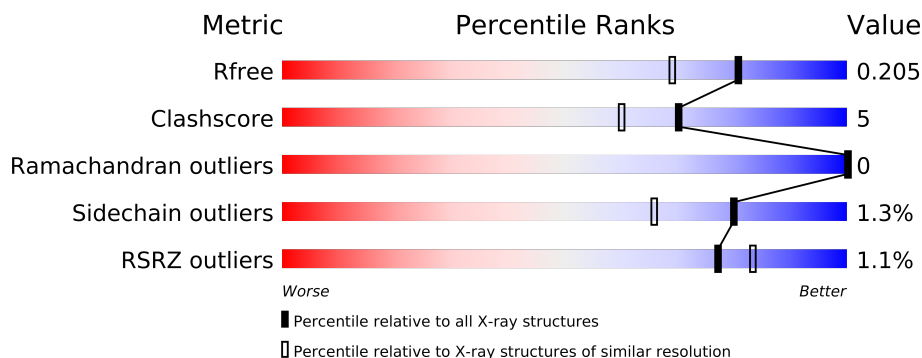
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.70 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))
$R_{free}$	66092	2456 (1.70-1.70)
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (1.70-1.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	530	
1	B	530	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	GOL	A	1504	-	X
4	GOL	A	1505	-	X
4	GOL	A	1506	-	X
4	GOL	A	1507	-	X
4	GOL	A	1508	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9191 atoms, of which 0 are hydrogen and 0 are deuterium.

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 TAML.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	17	0
			3946	2486	706	745	9			
1	B	500	Total	C	N	O	S	0	15	0
			3954	2488	723	735	8			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-29	MET	-	EXPRESSION TAG	UNP D3Y1I2
A	-28	GLY	-	EXPRESSION TAG	UNP D3Y1I2
A	-27	SER	-	EXPRESSION TAG	UNP D3Y1I2
A	-26	HIS	-	EXPRESSION TAG	UNP D3Y1I2
A	-25	HIS	-	EXPRESSION TAG	UNP D3Y1I2
A	-24	HIS	-	EXPRESSION TAG	UNP D3Y1I2
A	-23	HIS	-	EXPRESSION TAG	UNP D3Y1I2
A	-22	HIS	-	EXPRESSION TAG	UNP D3Y1I2
A	-21	HIS	-	EXPRESSION TAG	UNP D3Y1I2
A	-20	HIS	-	EXPRESSION TAG	UNP D3Y1I2
A	-19	HIS	-	EXPRESSION TAG	UNP D3Y1I2
A	-18	GLY	-	EXPRESSION TAG	UNP D3Y1I2
A	-17	SER	-	EXPRESSION TAG	UNP D3Y1I2
A	-16	ASP	-	EXPRESSION TAG	UNP D3Y1I2
A	-15	TYR	-	EXPRESSION TAG	UNP D3Y1I2
A	-14	ASP	-	EXPRESSION TAG	UNP D3Y1I2
A	-13	ILE	-	EXPRESSION TAG	UNP D3Y1I2
A	-12	PRO	-	EXPRESSION TAG	UNP D3Y1I2
A	-11	THR	-	EXPRESSION TAG	UNP D3Y1I2
A	-10	THR	-	EXPRESSION TAG	UNP D3Y1I2
A	-9	GLU	-	EXPRESSION TAG	UNP D3Y1I2
A	-8	ASN	-	EXPRESSION TAG	UNP D3Y1I2
A	-7	LEU	-	EXPRESSION TAG	UNP D3Y1I2
A	-6	TYR	-	EXPRESSION TAG	UNP D3Y1I2
A	-5	PHE	-	EXPRESSION TAG	UNP D3Y1I2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLN	-	EXPRESSION TAG	UNP D3Y1I2
A	-3	GLY	-	EXPRESSION TAG	UNP D3Y1I2
A	-2	SER	-	EXPRESSION TAG	UNP D3Y1I2
A	-1	GLU	-	EXPRESSION TAG	UNP D3Y1I2
A	0	PHE	-	EXPRESSION TAG	UNP D3Y1I2
B	-29	MET	-	EXPRESSION TAG	UNP D3Y1I2
B	-28	GLY	-	EXPRESSION TAG	UNP D3Y1I2
B	-27	SER	-	EXPRESSION TAG	UNP D3Y1I2
B	-26	HIS	-	EXPRESSION TAG	UNP D3Y1I2
B	-25	HIS	-	EXPRESSION TAG	UNP D3Y1I2
B	-24	HIS	-	EXPRESSION TAG	UNP D3Y1I2
B	-23	HIS	-	EXPRESSION TAG	UNP D3Y1I2
B	-22	HIS	-	EXPRESSION TAG	UNP D3Y1I2
B	-21	HIS	-	EXPRESSION TAG	UNP D3Y1I2
B	-20	HIS	-	EXPRESSION TAG	UNP D3Y1I2
B	-19	HIS	-	EXPRESSION TAG	UNP D3Y1I2
B	-18	GLY	-	EXPRESSION TAG	UNP D3Y1I2
B	-17	SER	-	EXPRESSION TAG	UNP D3Y1I2
B	-16	ASP	-	EXPRESSION TAG	UNP D3Y1I2
B	-15	TYR	-	EXPRESSION TAG	UNP D3Y1I2
B	-14	ASP	-	EXPRESSION TAG	UNP D3Y1I2
B	-13	ILE	-	EXPRESSION TAG	UNP D3Y1I2
B	-12	PRO	-	EXPRESSION TAG	UNP D3Y1I2
B	-11	THR	-	EXPRESSION TAG	UNP D3Y1I2
B	-10	THR	-	EXPRESSION TAG	UNP D3Y1I2
B	-9	GLU	-	EXPRESSION TAG	UNP D3Y1I2
B	-8	ASN	-	EXPRESSION TAG	UNP D3Y1I2
B	-7	LEU	-	EXPRESSION TAG	UNP D3Y1I2
B	-6	TYR	-	EXPRESSION TAG	UNP D3Y1I2
B	-5	PHE	-	EXPRESSION TAG	UNP D3Y1I2
B	-4	GLN	-	EXPRESSION TAG	UNP D3Y1I2
B	-3	GLY	-	EXPRESSION TAG	UNP D3Y1I2
B	-2	SER	-	EXPRESSION TAG	UNP D3Y1I2
B	-1	GLU	-	EXPRESSION TAG	UNP D3Y1I2
B	0	PHE	-	EXPRESSION TAG	UNP D3Y1I2

- Molecule 2 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
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Cl	0	0
			2	2		

- Molecule 6 is water.

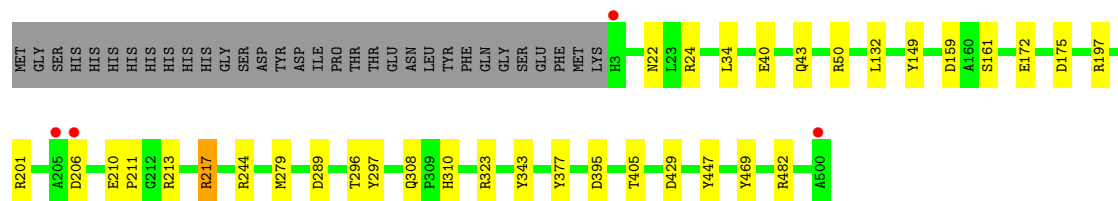
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	555	Total 555	O 555	0	0
6	B	578	Total 578	O 578	0	0

### 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.

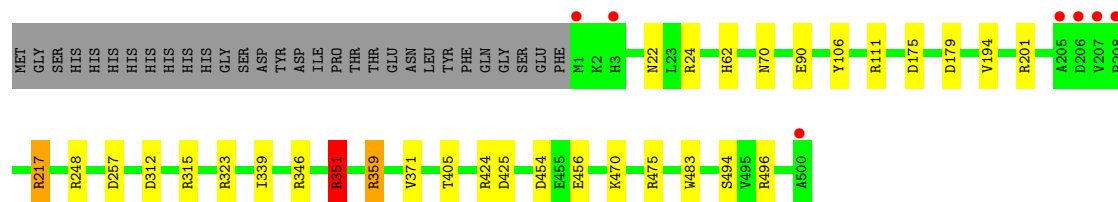
- Molecule 1: TAML

Chain A: 



- Molecule 1: TAML

Chain B: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.38Å 129.56Å 134.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	134.59 – 1.70 67.29 – 1.70	Depositor EDS
% Data completeness (in resolution range)	92.7 (134.59-1.70) 92.7 (67.29-1.70)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.141 , 0.205 0.141 , 0.205	Depositor DCC
$R_{free}$ test set	5763 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.4	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 47.4	EDS
Estimated twinning fraction	0.007 for -h,l,k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 115265 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9191	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, FAD, CL

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	1.20	7/4049 (0.2%)	0.97	11/5539 (0.2%)
1	B	1.17	4/4059 (0.1%)	0.97	14/5547 (0.3%)
All	All	1.18	11/8108 (0.1%)	0.97	25/11086 (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	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	90	GLU	CD-OE2	9.04	1.35	1.25
1	A	149	TYR	CG-CD1	5.83	1.46	1.39
1	B	194	VAL	CB-CG1	5.68	1.64	1.52
1	A	343	TYR	CE2-CZ	5.39	1.45	1.38
1	B	483	TRP	CG-CD1	5.37	1.44	1.36
1	A	469	TYR	CG-CD1	5.28	1.46	1.39
1	A	447	TYR	CG-CD2	-5.26	1.32	1.39
1	A	172	GLU	CD-OE2	5.19	1.31	1.25
1	A	469	TYR	CE1-CZ	5.19	1.45	1.38
1	B	106	TYR	CD2-CE2	5.14	1.47	1.39
1	A	377	TYR	CE1-CZ	5.04	1.45	1.38

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	351	ARG	NE-CZ-NH2	-10.49	115.06	120.30
1	B	323	ARG	NE-CZ-NH2	-10.21	115.20	120.30
1	B	351	ARG	NE-CZ-NH1	9.24	124.92	120.30
1	B	217	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	A	323	ARG	NE-CZ-NH2	-7.45	116.57	120.30
1	A	217	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	B	323	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	A	323	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	A	217	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	175	ASP	CB-CG-OD1	6.35	124.02	118.30
1	B	24	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	B	454	ASP	CB-CG-OD1	6.14	123.83	118.30
1	B	217	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	B	175	ASP	CB-CG-OD1	5.84	123.56	118.30
1	A	395	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	A	482	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	A	24	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	B	111	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	34	LEU	CA-CB-CG	-5.25	103.22	115.30
1	B	371[A]	VAL	CB-CA-C	-5.22	101.48	111.40
1	B	371[B]	VAL	CB-CA-C	-5.22	101.48	111.40
1	B	248	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	248	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	429	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	A	197	ARG	NE-CZ-NH1	5.12	122.86	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	206	ASP	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3946	0	0	16	0
1	B	3954	0	0	19	0
2	A	53	0	0	0	0
2	B	53	0	0	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	36	0	0	2	0
4	B	12	0	0	0	0
5	A	2	0	0	0	0
6	A	555	0	0	12	0
6	B	578	0	0	12	0
All	All	9191	0	0	36	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (36) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:279[B]:MET:CE	1:A:297:TYR:OH	2.19	0.89
1:B:351:ARG:NH2	1:B:425:ASP:O	2.07	0.87
1:B:359:ARG:NH1	1:B:425:ASP:OD2	2.08	0.86
1:B:62:HIS:CE1	2:B:600:FAD:C8M	2.62	0.82
1:B:257:ASP:OD1	6:B:2334:HOH:O	2.02	0.76
1:A:43[A]:GLN:NE2	4:A:1506:GOL:O1	2.20	0.74
1:B:496[B]:ARG:CD	6:B:2524:HOH:O	2.37	0.73
1:A:289:ASP:CB	6:A:2178:HOH:O	2.38	0.71
1:B:405[B]:THR:CG2	6:B:2472:HOH:O	2.38	0.71
1:A:289:ASP:CB	6:A:2346:HOH:O	2.40	0.68
4:A:1507:GOL:O3	6:A:2555:HOH:O	2.13	0.66
1:A:40:GLU:OE1	6:A:2083:HOH:O	2.15	0.65
1:A:210[B]:GLU:OE2	6:A:2287:HOH:O	2.14	0.65
1:B:62:HIS:ND1	2:B:600:FAD:C8	2.58	0.64
1:A:310:HIS:N	1:A:310:HIS:CD2	2.65	0.63
1:B:346[A]:ARG:NH2	6:B:2419:HOH:O	2.32	0.62
1:A:22:ASN:ND2	6:A:2053:HOH:O	2.32	0.61
1:B:217:ARG:NH2	6:B:2289:HOH:O	2.33	0.61
1:A:244:ARG:NH2	6:A:2313:HOH:O	2.33	0.59
1:A:210[A]:GLU:OE1	1:A:213:ARG:NH1	2.40	0.55
1:A:210[B]:GLU:CG	6:A:2288:HOH:O	2.58	0.52
1:B:494:SER:N	1:B:496[B]:ARG:NH2	2.58	0.51
1:B:315:ARG:NH1	6:B:2387:HOH:O	2.44	0.51
1:A:50:ARG:CB	6:A:2095:HOH:O	2.60	0.48
1:B:201[A]:ARG:NH1	6:B:2281:HOH:O	2.47	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:405[A]:THR:CG2	6:A:2444:HOH:O	2.61	0.48
1:B:179[B]:ASP:OD2	1:B:475:ARG:NE	2.48	0.47
1:B:22:ASN:ND2	6:B:2045:HOH:O	2.49	0.45
1:B:496[B]:ARG:NH1	6:B:2570:HOH:O	2.50	0.45
1:B:494:SER:O	1:B:496[B]:ARG:CZ	2.65	0.45
1:A:308:GLN:O	6:A:2360:HOH:O	2.21	0.45
1:A:159[A]:ASP:OD1	1:A:161:SER:OG	2.34	0.45
1:B:470:LYS:NZ	6:B:2533:HOH:O	2.49	0.44
1:B:496[A]:ARG:NH2	6:B:2567:HOH:O	2.52	0.43
1:B:424:ARG:NH1	6:B:2490:HOH:O	2.53	0.41
1:A:201:ARG:NH2	6:A:2284:HOH:O	2.54	0.41

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	513/530 (97%)	501 (98%)	12 (2%)	0	100	100
1	B	513/530 (97%)	501 (98%)	12 (2%)	0	100	100
All	All	1026/1060 (97%)	1002 (98%)	24 (2%)	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	401/421 (95%)	397 (99%)	4 (1%)	85	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	398/421 (94%)	392 (98%)	6 (2%)	76	60
All	All	799/842 (95%)	789 (99%)	10 (1%)	80	66

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	LEU
1	A	211	PRO
1	A	217	ARG
1	A	296	THR
1	B	70	ASN
1	B	312	ASP
1	B	339	ILE
1	B	351	ARG
1	B	359	ARG
1	B	456	GLU

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 chains 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 ⓘ

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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	$\# Z  > 2$
4	GOL	A	1501	-	5,5,5	0.36	0	5,5,5	0.75	0
4	GOL	A	1504	-	5,5,5	0.94	0	5,5,5	1.19	0
4	GOL	A	1505	-	5,5,5	0.62	0	5,5,5	1.34	1 (20%)
4	GOL	A	1506	-	5,5,5	0.26	0	5,5,5	0.48	0
4	GOL	A	1507	-	5,5,5	0.44	0	5,5,5	1.09	0
4	GOL	A	1508	-	5,5,5	0.77	0	5,5,5	0.51	0
2	FAD	A	600	1	58,58,58	1.16	4 (6%)	85,89,89	2.12	23 (27%)
4	GOL	B	1501	-	5,5,5	0.30	0	5,5,5	0.66	0
4	GOL	B	1502	-	5,5,5	0.33	0	5,5,5	0.68	0
2	FAD	B	600	1	58,58,58	1.21	7 (12%)	85,89,89	1.67	17 (20%)

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
4	GOL	A	1501	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1504	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1505	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1506	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1507	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1508	-	-	0/4/4/4	0/0/0/0
2	FAD	A	600	1	-	0/34/50/50	0/1/6/6
4	GOL	B	1501	-	-	0/4/4/4	0/0/0/0
4	GOL	B	1502	-	-	0/4/4/4	0/0/0/0
2	FAD	B	600	1	-	0/34/50/50	0/1/6/6

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	C8A-N9A	3.03	1.41	1.36
2	B	600	FAD	C8A-N9A	3.00	1.41	1.36
2	B	600	FAD	C4A-N9A	-2.88	1.33	1.37
2	A	600	FAD	C6-C5X	-2.74	1.38	1.41
2	A	600	FAD	C7M-C7	2.64	1.56	1.51
2	B	600	FAD	C5X-N5	2.64	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	FAD	O3B-C3B	2.25	1.48	1.43
2	B	600	FAD	C6-C5X	-2.22	1.39	1.41
2	A	600	FAD	C2A-N3A	2.14	1.36	1.32
2	B	600	FAD	C9-C8	2.10	1.43	1.37
2	B	600	FAD	C7M-C7	2.08	1.55	1.51

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	FAD	N3A-C2A-N1A	-11.23	119.32	128.71
2	B	600	FAD	N3A-C2A-N1A	-7.86	122.14	128.71
2	A	600	FAD	O4B-C1B-N9A	5.35	113.42	108.44
2	A	600	FAD	N3A-C4A-N9A	4.27	133.14	125.43
2	A	600	FAD	C4X-C10-N1	-4.22	118.51	122.73
2	B	600	FAD	N3A-C4A-N9A	4.10	132.84	125.43
2	A	600	FAD	C2-N1-C10	4.10	119.11	114.98
2	A	600	FAD	C5A-C4A-N3A	-3.32	118.47	125.70
2	A	600	FAD	C4B-O4B-C1B	3.17	113.19	109.75
2	B	600	FAD	C5A-C4A-N3A	-3.13	118.88	125.70
2	A	600	FAD	C4-N3-C2	-3.01	119.20	125.39
2	A	600	FAD	N7A-C8A-N9A	-2.99	105.90	114.36
2	A	600	FAD	C2A-N3A-C4A	2.99	122.51	114.01
2	B	600	FAD	C4A-C5A-N7A	-2.90	107.04	109.52
2	A	600	FAD	C5'-C4'-C3'	-2.84	106.69	112.06
2	B	600	FAD	C2-N1-C10	2.75	117.75	114.98
2	B	600	FAD	N7A-C8A-N9A	-2.67	106.82	114.36
2	B	600	FAD	C2A-N3A-C4A	2.65	121.55	114.01
2	A	600	FAD	C4X-N5-C5X	2.65	119.67	116.69
2	A	600	FAD	O3B-C3B-C2B	-2.61	103.35	111.83
2	B	600	FAD	C4X-C10-N1	-2.59	120.14	122.73
2	A	600	FAD	C4-C4X-C10	2.57	121.11	116.95
2	B	600	FAD	O2P-P-O3P	2.54	117.19	105.14
2	B	600	FAD	C4-N3-C2	-2.47	120.32	125.39
2	B	600	FAD	C7-C6-C5X	2.41	124.95	120.91
2	A	600	FAD	C2'-C1'-N10	2.41	115.65	112.45
2	A	600	FAD	C4A-C5A-N7A	-2.41	107.46	109.52
2	B	600	FAD	O4B-C1B-N9A	2.34	110.62	108.44
2	B	600	FAD	O2'-C2'-C1'	-2.31	103.96	109.71
4	A	1505	GOL	C3-C2-C1	2.30	121.42	111.26
2	A	600	FAD	C8A-N9A-C4A	2.30	108.65	106.90
2	A	600	FAD	C3B-C2B-C1B	2.28	104.48	100.91
2	A	600	FAD	O2A-PA-O3P	2.24	115.78	105.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	FAD	O2B-C2B-C3B	2.24	119.11	111.83
2	B	600	FAD	C6-C7-C8	-2.23	116.30	119.88
2	B	600	FAD	C8M-C8-C7	-2.23	115.59	120.74
2	B	600	FAD	C1'-N10-C9A	2.17	120.99	118.87
2	A	600	FAD	C1B-N9A-C4A	-2.17	122.89	126.64
2	B	600	FAD	O2A-PA-O3P	2.07	114.96	105.14
2	A	600	FAD	C7-C6-C5X	2.03	124.32	120.91
2	A	600	FAD	C8A-N7A-C5A	2.03	109.88	103.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	498/530 (93%)	-0.57	4 (0%) 83 88	11, 20, 39, 47	0
1	B	500/530 (94%)	-0.60	7 (1%) 72 78	12, 20, 37, 48	0
All	All	998/1060 (94%)	-0.59	11 (1%) 77 83	11, 20, 38, 48	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	500	ALA	6.4
1	A	206	ASP	4.6
1	B	207	VAL	3.3
1	A	500	ALA	3.1
1	B	206	ASP	3.0
1	A	205	ALA	3.0
1	A	3	HIS	3.0
1	B	3	HIS	2.6
1	B	1	MET	2.6
1	B	205	ALA	2.6
1	B	208	PRO	2.1

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	A	1505	6/6	0.18	13.17	47,50,51,55	0
4	GOL	A	1507	6/6	0.16	12.05	25,36,39,42	0
4	GOL	A	1504	6/6	0.15	10.51	36,43,45,47	0
4	GOL	A	1506	6/6	0.27	6.97	41,45,46,50	0
4	GOL	A	1508	6/6	0.21	3.80	23,36,39,43	0
3	MG	B	700	1/1	0.12	1.76	35,35,35,35	0
4	GOL	B	1501	6/6	0.06	1.59	26,31,33,33	0
4	GOL	B	1502	6/6	0.06	0.82	24,25,26,28	0
2	FAD	B	600	53/53	0.06	0.02	8,13,16,18	0
2	FAD	A	600	53/53	0.05	-0.57	9,12,16,18	0
4	GOL	A	1501	6/6	0.05	-1.96	22,22,24,25	0
5	CL	A	1502	1/1	0.04	-2.07	26,26,26,26	0
3	MG	A	700	1/1	0.04	-2.08	31,31,31,31	0
5	CL	A	1503	1/1	0.03	-2.42	26,26,26,26	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.