



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:43 AM GMT

PDB ID : 2Y3S
Title : STRUCTURE OF THE TIRANDAMYCINE-BOUND FAD-DEPENDENT
TIRANDAMYCIN OXIDASE TAML IN C2 SPACE GROUP
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Sherman, D.H.
Deposited on : 2010-12-23
Resolution : 1.67 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (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

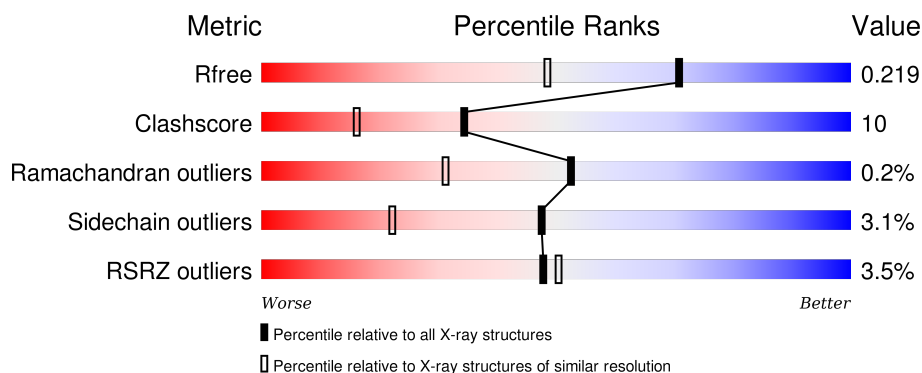
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.67 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	4802 (1.70-1.66)
Clashscore	102246	5317 (1.70-1.66)
Ramachandran outliers	100387	5225 (1.70-1.66)
Sidechain outliers	100360	5224 (1.70-1.66)
RSRZ outliers	91569	4813 (1.70-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	530	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>16%</div> <div>• 6%</div> </div> </div>
1	B	530	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>15%</div> <div>• 7%</div> </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
5	GOL	A	1501	-	-	X	X
5	GOL	A	1502	-	-	X	X
5	GOL	A	1503	-	-	X	X
5	GOL	B	1501	-	-	-	X
5	GOL	B	1503	-	-	X	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8851 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 TAML.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	23	0
			3943	2489	698	746	10			
1	B	493	Total	C	N	O	S	0	7	0
			3819	2410	687	713	9			

There are 60 discrepancies between the modelled and reference sequences:

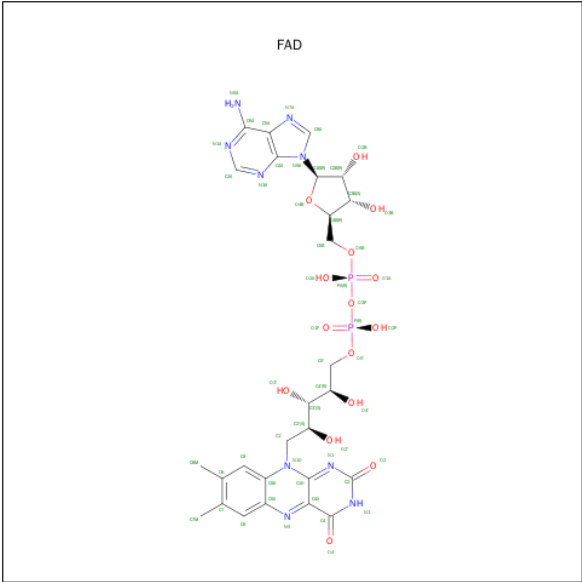
Chain	Residue	Modelled	Actual	Comment	Reference
A	-29	MET	-	EXPRESSION TAG	UNP D3Y1I2
A	-28	GLY	-	EXPRESSION TAG	UNP D3Y1I2
A	-27	SER	-	EXPRESSION TAG	UNP D3Y1I2
A	-26	HIS	-	EXPRESSION TAG	UNP D3Y1I2
A	-25	HIS	-	EXPRESSION TAG	UNP D3Y1I2
A	-24	HIS	-	EXPRESSION TAG	UNP D3Y1I2
A	-23	HIS	-	EXPRESSION TAG	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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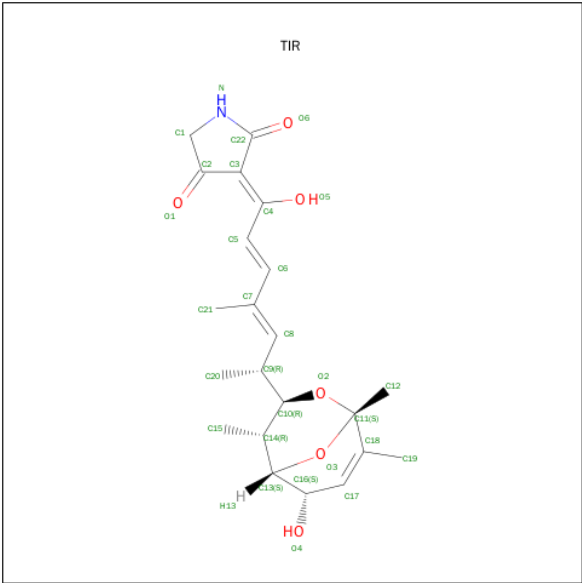
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLN	-	EXPRESSION TAG	UNP D3Y1I2
A	-3	GLY	-	EXPRESSION TAG	UNP D3Y1I2
A	-2	SER	-	EXPRESSION TAG	UNP D3Y1I2
A	-1	GLU	-	EXPRESSION TAG	UNP D3Y1I2
A	0	PHE	-	EXPRESSION TAG	UNP D3Y1I2
B	-29	MET	-	EXPRESSION TAG	UNP D3Y1I2
B	-28	GLY	-	EXPRESSION TAG	UNP 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: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 3 is TIRANDAMYCIN E (three-letter code: TIR) (formula: C₂₂H₂₉NO₆).

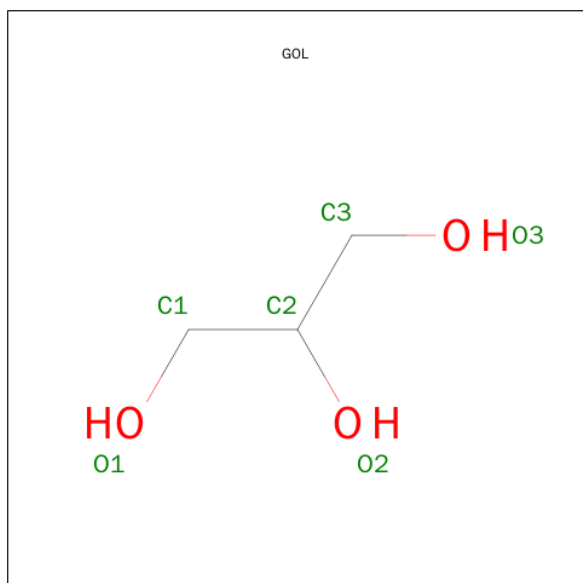


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			29	22	1	6		
3	B	1	Total	C	N	O	0	0
			29	22	1	6		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	3	Total Cl 3 3	0	0
6	A	2	Total Cl 2 2	0	0

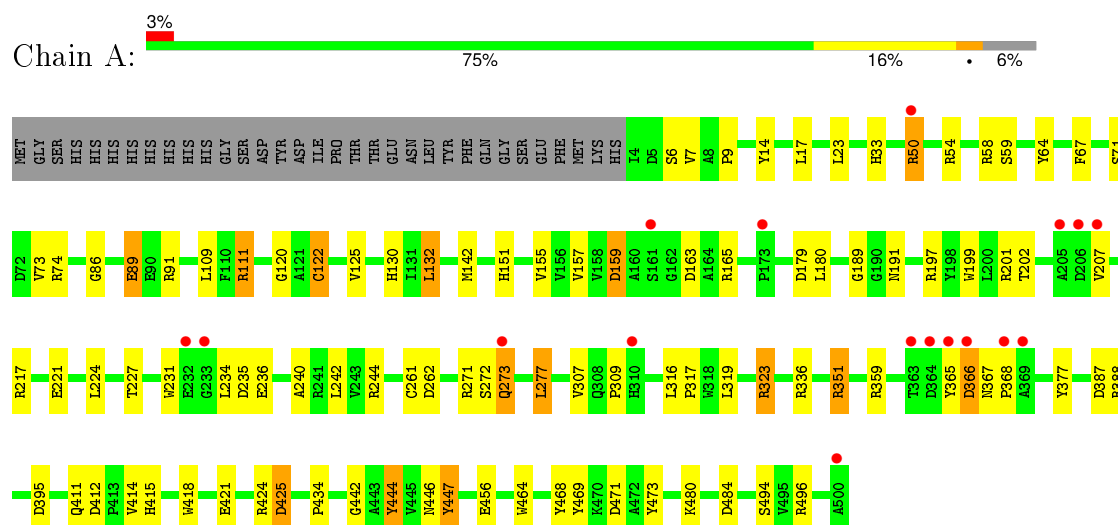
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	456	Total 456	O 456	0	0
7	B	432	Total 432	O 432	0	0

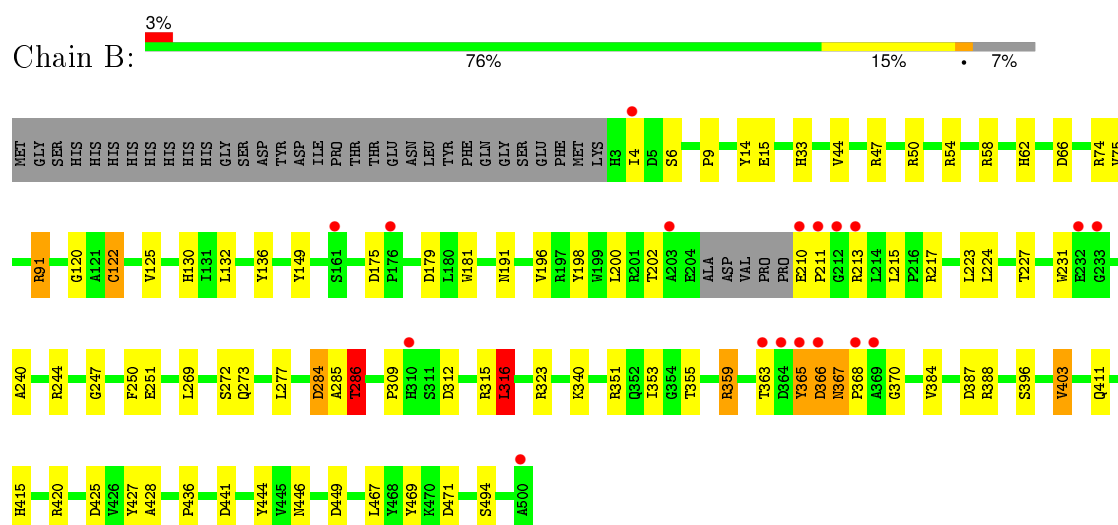
3 Residue-property plots [i](#)

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 ($RSRZ > 2$). 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



• Molecule 1: TAML



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.05Å 105.79Å 70.97Å 90.00° 110.67° 90.00°	Depositor
Resolution (Å)	86.76 – 1.67 66.40 – 1.67	Depositor EDS
% Data completeness (in resolution range)	92.8 (86.76-1.67) 92.8 (66.40-1.67)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 1.67Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.161 , 0.220 0.160 , 0.219	Depositor DCC
R_{free} test set	6026 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	16.8	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 120163 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8851	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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: GOL, MG, FAD, TIR, 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	1.26	12/4089 (0.3%)	1.07	24/5587 (0.4%)
1	B	1.27	11/3940 (0.3%)	1.07	25/5380 (0.5%)
All	All	1.26	23/8029 (0.3%)	1.07	49/10967 (0.4%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	198	TYR	CD2-CE2	7.09	1.50	1.39
1	B	427	TYR	CD1-CE1	7.04	1.50	1.39
1	B	286	THR	CB-CG2	-6.74	1.30	1.52
1	A	468	TYR	CE2-CZ	6.53	1.47	1.38
1	A	447	TYR	CD1-CE1	6.18	1.48	1.39
1	A	64	TYR	CD2-CE2	6.15	1.48	1.39
1	A	377	TYR	CE1-CZ	6.06	1.46	1.38
1	B	428	ALA	CA-CB	5.96	1.65	1.52
1	A	73	VAL	CB-CG1	5.80	1.65	1.52
1	A	67	PHE	CE2-CZ	5.71	1.48	1.37
1	B	14	TYR	CE2-CZ	5.70	1.46	1.38
1	B	181	TRP	CE3-CZ3	5.70	1.48	1.38
1	A	469	TYR	CE2-CZ	5.60	1.45	1.38
1	B	196	VAL	CB-CG2	5.57	1.64	1.52
1	A	473	TYR	CE1-CZ	5.50	1.45	1.38
1	B	15	GLU	CB-CG	5.35	1.62	1.52
1	B	469	TYR	CE2-CZ	5.28	1.45	1.38
1	B	250	PHE	CD2-CE2	5.25	1.49	1.39
1	A	89	GLU	CG-CD	-5.19	1.44	1.51
1	A	240	ALA	CA-CB	5.12	1.63	1.52
1	B	396	SER	CB-OG	5.08	1.48	1.42
1	A	444	TYR	CD2-CE2	5.06	1.47	1.39
1	A	464	TRP	CG-CD1	5.05	1.43	1.36

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	74	ARG	NE-CZ-NH2	-11.75	114.43	120.30
1	A	351	ARG	NE-CZ-NH2	-11.45	114.58	120.30
1	B	74	ARG	NE-CZ-NH1	10.63	125.61	120.30
1	A	351	ARG	NE-CZ-NH1	9.80	125.20	120.30
1	B	312	ASP	CB-CG-OD1	7.90	125.41	118.30
1	A	54	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	A	163	ASP	CB-CG-OD1	6.91	124.52	118.30
1	A	217	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	A	50	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	B	359	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	A	395	ASP	CB-CG-OD1	6.69	124.32	118.30
1	B	323	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	B	58	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	B	403	VAL	CG1-CB-CG2	6.44	121.20	110.90
1	A	425	ASP	CB-CG-OD1	6.31	123.98	118.30
1	B	471	ASP	CB-CG-OD1	6.26	123.93	118.30
1	A	54	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	B	316	LEU	CA-CB-CG	6.16	129.47	115.30
1	B	323	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	B	47	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	A	471	ASP	CB-CG-OD1	6.04	123.74	118.30
1	A	271	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	A	277	LEU	CA-CB-CG	5.97	129.04	115.30
1	B	387	ASP	CB-CG-OD1	5.70	123.43	118.30
1	B	449	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	B	312	ASP	CB-CG-OD2	-5.55	113.30	118.30
1	A	271	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	A	336	ARG	NE-CZ-NH1	-5.48	117.56	120.30
1	B	441	ASP	CB-CG-OD2	5.46	123.22	118.30
1	A	235	ASP	CB-CG-OD1	5.44	123.19	118.30
1	B	175	ASP	CB-CG-OD1	5.41	123.17	118.30
1	B	315	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	B	66	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	323	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	B	471	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	B	179	ASP	CB-CG-OD1	5.31	123.08	118.30
1	B	370	GLY	N-CA-C	-5.31	99.83	113.10
1	B	284	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	B	449	ASP	CB-CG-OD1	5.15	122.94	118.30
1	A	58	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	109	LEU	CB-CG-CD1	-5.12	102.30	111.00
1	A	197	ARG	NE-CZ-NH1	5.08	122.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	244	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	B	122	CYS	N-CA-CB	-5.06	101.49	110.60
1	A	111	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	388	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	425	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	A	412	ASP	CB-CG-OD1	5.02	122.82	118.30
1	A	122	CYS	N-CA-CB	-5.01	101.57	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3943	0	3801	80	0
1	B	3819	0	3700	68	0
2	A	53	0	29	5	0
2	B	53	0	29	9	0
3	A	29	0	28	5	0
3	B	29	0	28	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	18	0	23	16	0
5	B	12	0	16	8	0
6	A	2	0	0	0	0
6	B	3	0	0	0	0
7	A	456	0	0	20	0
7	B	432	0	0	5	0
All	All	8851	0	7654	156	0

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

All (156) 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:273:GLN:NE2	1:A:368:PRO:HA	1.48	1.27
1:A:273:GLN:NE2	1:A:368:PRO:CA	2.11	1.13
2:A:600:FAD:N5	3:A:700:TIR:H16	1.65	1.12
1:B:367:ASN:N	1:B:367:ASN:HD22	1.51	1.07
1:A:366:ASP:O	1:A:368:PRO:HD3	1.52	1.06
1:B:366:ASP:C	1:B:367:ASN:HD22	1.57	1.05
1:B:273:GLN:HE22	1:B:368:PRO:N	1.55	1.03
2:B:600:FAD:N5	3:B:700:TIR:H16	1.73	1.02
1:A:273:GLN:HE22	1:A:368:PRO:CA	1.71	1.01
1:B:202[B]:THR:HG21	7:B:2186:HOH:O	1.60	1.00
1:A:201:ARG:NH1	1:A:202:THR:O	1.97	0.98
1:A:273:GLN:HE21	1:A:368:PRO:HA	1.17	0.90
1:A:414[A]:VAL:HG23	7:A:2361:HOH:O	1.72	0.88
1:B:273:GLN:NE2	1:B:368:PRO:HA	1.86	0.88
1:B:273:GLN:NE2	1:B:368:PRO:CA	2.39	0.85
1:A:244:ARG:HG2	7:A:2128:HOH:O	1.79	0.83
1:B:91:ARG:HG2	1:B:91:ARG:HH11	1.42	0.83
1:B:273:GLN:HG3	7:B:2221:HOH:O	1.77	0.83
1:B:284:ASP:OD1	1:B:286:THR:HG22	1.78	0.82
1:B:367:ASN:N	1:B:367:ASN:ND2	2.24	0.82
1:A:50:ARG:HG3	7:A:2161:HOH:O	1.80	0.81
2:A:600:FAD:C4X	3:A:700:TIR:H16	2.11	0.81
1:A:273:GLN:HG3	7:A:2236:HOH:O	1.80	0.80
1:B:75:VAL:CG1	5:B:1503:GOL:H32	2.11	0.80
1:A:366:ASP:O	1:A:368:PRO:CD	2.30	0.79
1:A:323:ARG:HG3	5:A:1501:GOL:H31	1.66	0.78
1:B:273:GLN:NE2	1:B:368:PRO:N	2.32	0.78
1:A:273:GLN:NE2	1:A:368:PRO:CB	2.46	0.78
1:B:62:HIS:CE1	2:B:600:FAD:C8M	2.67	0.77
1:B:273:GLN:HE21	1:B:368:PRO:HA	1.49	0.76
1:A:151:HIS:HD2	7:A:2149:HOH:O	1.68	0.76
1:B:75:VAL:HG13	5:B:1503:GOL:H32	1.66	0.76
1:A:273:GLN:NE2	1:A:368:PRO:HB3	2.02	0.74
1:A:111:ARG:HH21	5:A:1501:GOL:H11	1.52	0.74
1:B:62:HIS:ND1	2:B:600:FAD:HM81	1.96	0.74
1:B:363:THR:C	1:B:365:TYR:H	1.92	0.72
1:A:71[B]:SER:HB3	7:A:2080:HOH:O	1.90	0.72
1:A:273:GLN:HE22	1:A:368:PRO:CB	2.03	0.71
1:A:234:LEU:HD12	1:A:307:VAL:HG21	1.72	0.71
1:B:366:ASP:CA	1:B:367:ASN:HD22	2.04	0.71
1:B:366:ASP:C	1:B:367:ASN:ND2	2.40	0.70
1:A:236[B]:GLU:OE2	7:A:2214:HOH:O	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:600:FAD:C4X	3:B:700:TIR:H16	2.23	0.68
1:B:223[B]:LEU:HD22	1:B:285:ALA:HB2	1.76	0.67
1:A:111:ARG:NH2	5:A:1501:GOL:H11	2.10	0.66
1:B:273:GLN:HE22	1:B:367:ASN:C	1.99	0.66
1:B:284:ASP:OD1	1:B:286:THR:CG2	2.44	0.65
1:A:155[B]:VAL:HG21	1:A:180:LEU:HD21	1.77	0.65
1:B:411:GLN:O	1:B:415:HIS:HD2	1.80	0.63
1:A:59[B]:SER:OG	2:A:600:FAD:O2P	2.16	0.63
1:B:351:ARG:NH2	7:B:2288:HOH:O	2.27	0.63
1:B:62:HIS:CG	2:B:600:FAD:C8M	2.74	0.63
1:B:91:ARG:CG	1:B:91:ARG:HH11	2.10	0.63
1:A:359:ARG:NH2	1:A:425:ASP:OD2	2.30	0.62
1:A:86:GLY:HA3	5:A:1502:GOL:C3	2.30	0.61
1:A:273:GLN:HE22	1:A:368:PRO:N	1.99	0.61
1:B:273:GLN:HE22	1:B:368:PRO:CA	2.07	0.61
1:B:33:HIS:HE1	5:B:1503:GOL:O3	1.84	0.60
1:A:421[A]:GLU:HG3	1:A:424:ARG:NH2	2.16	0.60
1:A:142[A]:MET:CE	5:A:1503:GOL:O2	2.50	0.60
1:B:62:HIS:ND1	2:B:600:FAD:C8	2.62	0.59
1:B:444:TYR:CZ	1:B:446:ASN:HB2	2.37	0.59
1:B:33:HIS:CE1	5:B:1503:GOL:H11	2.38	0.58
1:B:227:THR:HG23	1:B:309:PRO:HB2	1.83	0.58
1:A:33:HIS:HE1	7:A:2039:HOH:O	1.85	0.58
1:A:415:HIS:HE1	7:A:2324:HOH:O	1.87	0.58
1:A:273:GLN:CG	7:A:2236:HOH:O	2.47	0.58
1:A:33:HIS:HD2	7:A:2002:HOH:O	1.87	0.57
1:A:122:CYS:HB2	1:A:125:VAL:HG23	1.88	0.56
1:A:74:ARG:HD3	7:A:2030:HOH:O	2.05	0.56
1:A:142[A]:MET:HE3	1:A:262:ASP:HA	1.88	0.55
1:A:359:ARG:HD2	7:A:2321:HOH:O	2.05	0.55
1:A:86:GLY:HA3	5:A:1502:GOL:H31	1.89	0.55
1:A:120:GLY:H	1:A:130:HIS:CE1	2.26	0.54
1:A:155[B]:VAL:HG23	1:A:157:VAL:HG13	1.89	0.54
1:A:142[A]:MET:HE3	5:A:1503:GOL:O2	2.08	0.54
5:A:1501:GOL:H2	7:B:2017:HOH:O	2.08	0.53
1:A:319:LEU:HG	5:A:1501:GOL:H12	1.91	0.53
1:B:44:VAL:HG13	5:B:1503:GOL:H2	1.89	0.53
1:A:86:GLY:CA	5:A:1502:GOL:H31	2.40	0.52
1:A:142[B]:MET:SD	5:A:1503:GOL:O2	2.66	0.52
1:B:366:ASP:CA	1:B:367:ASN:ND2	2.72	0.52
1:B:351:ARG:HH11	1:B:351:ARG:HB3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:ARG:NE	7:A:2317:HOH:O	2.43	0.52
1:B:91:ARG:NH1	1:B:91:ARG:CG	2.72	0.52
1:A:234:LEU:CD1	1:A:307:VAL:HG21	2.40	0.52
1:B:384:VAL:HG13	1:B:388:ARG:HD2	1.91	0.51
1:B:75:VAL:HG11	5:B:1503:GOL:H32	1.92	0.51
1:B:120:GLY:HA2	1:B:136:TYR:O	2.10	0.51
1:B:436:PRO:HD3	1:B:467:LEU:HD23	1.92	0.51
1:B:363:THR:C	1:B:365:TYR:N	2.60	0.51
1:A:86:GLY:HA3	5:A:1502:GOL:H32	1.92	0.50
1:A:142[A]:MET:HE1	5:A:1503:GOL:O2	2.12	0.50
1:A:191:ASN:HD21	1:A:494:SER:HA	1.77	0.50
1:A:434:PRO:O	1:A:442:GLY:HA2	2.11	0.50
3:B:700:TIR:H121	3:B:700:TIR:H315	1.94	0.50
1:A:142[A]:MET:CE	5:A:1503:GOL:HO2	2.23	0.50
1:A:244:ARG:CG	7:A:2128:HOH:O	2.47	0.49
1:B:223[B]:LEU:HD22	1:B:285:ALA:CB	2.42	0.49
1:A:480:LYS:HD2	1:A:484:ASP:HB3	1.93	0.49
1:A:179[B]:ASP:OD2	7:A:2189:HOH:O	2.19	0.49
2:A:600:FAD:C4X	3:A:700:TIR:C16	2.88	0.49
1:A:71[A]:SER:HB2	7:A:2080:HOH:O	2.13	0.49
1:A:130:HIS:HD2	2:A:600:FAD:O2'	1.96	0.49
1:A:261:CYS:O	5:A:1503:GOL:H12	2.13	0.48
1:A:273:GLN:HE21	1:A:368:PRO:CA	1.97	0.47
1:B:149:TYR:HE2	1:B:202[B]:THR:HG22	1.78	0.47
1:B:33:HIS:HE1	5:B:1503:GOL:C3	2.26	0.47
1:B:191:ASN:HD21	1:B:494:SER:HA	1.78	0.47
1:B:247:GLY:O	1:B:251:GLU:HG3	2.15	0.47
1:A:365[A]:TYR:CD1	1:A:418:TRP:HD1	2.33	0.47
1:A:496:ARG:NE	7:A:2438:HOH:O	2.48	0.47
1:A:132:LEU:HD13	1:A:189:GLY:HA2	1.95	0.47
1:A:227:THR:HG23	1:A:309:PRO:HB2	1.97	0.47
1:A:224:LEU:CD1	1:A:316:LEU:HD12	2.45	0.46
2:B:600:FAD:C4X	3:B:700:TIR:C16	2.93	0.46
1:A:91:ARG:HD2	1:A:199:TRP:CE2	2.51	0.46
1:A:411:GLN:O	1:A:415:HIS:HD2	1.99	0.45
1:B:50:ARG:NH2	7:B:2050:HOH:O	2.49	0.45
1:B:130:HIS:HD2	2:B:600:FAD:O2'	1.99	0.45
1:A:444:TYR:CZ	1:A:446:ASN:HB2	2.52	0.45
1:B:273:GLN:HB2	1:B:273:GLN:HE21	1.50	0.45
1:A:447:TYR:HH	3:A:700:TIR:HO4	1.62	0.45
1:B:273:GLN:HE21	1:B:368:PRO:CA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:LEU:HD12	1:B:316:LEU:HD22	2.00	0.44
1:B:120:GLY:H	1:B:130:HIS:CE1	2.36	0.44
1:A:151:HIS:CD2	7:A:2149:HOH:O	2.54	0.44
1:B:231:TRP:CD1	1:B:272:SER:HA	2.51	0.44
1:A:351:ARG:NH2	7:A:2313:HOH:O	2.49	0.44
1:B:367:ASN:HA	1:B:368:PRO:HD2	1.79	0.43
1:B:340:LYS:HE3	1:B:420:ARG:HA	1.99	0.43
1:A:231:TRP:CD1	1:A:272:SER:HA	2.54	0.43
1:A:159[B]:ASP:HB3	1:A:165:ARG:NH1	2.33	0.43
1:B:33:HIS:NE2	5:B:1503:GOL:H11	2.33	0.43
1:A:421[A]:GLU:OE2	1:A:424:ARG:CZ	2.66	0.43
1:A:221:GLU:HG2	1:A:317:PRO:HA	2.01	0.43
1:A:421[A]:GLU:OE2	1:A:424:ARG:NH2	2.52	0.42
1:B:62:HIS:HB3	2:B:600:FAD:HM81	2.01	0.42
3:A:700:TIR:H315	3:A:700:TIR:H121	2.01	0.42
1:B:210:GLU:HA	1:B:211:PRO:HD2	1.95	0.42
1:A:224:LEU:HD12	1:A:316:LEU:HD12	2.01	0.41
1:B:269:LEU:HA	1:B:277:LEU:HD22	2.02	0.41
1:B:202[B]:THR:HG23	1:B:215:LEU:HA	2.02	0.41
1:B:149:TYR:O	1:B:200:LEU:HA	2.21	0.41
1:B:122:CYS:HB2	1:B:125:VAL:HG23	2.01	0.41
1:A:242:LEU:C	1:A:242:LEU:HD23	2.41	0.41
1:B:240:ALA:HA	1:B:353:ILE:HG21	2.03	0.41
1:A:7:VAL:HG21	1:A:17:LEU:HD12	2.03	0.41
1:B:355:THR:O	1:B:359:ARG:HG3	2.21	0.41
1:A:421[A]:GLU:OE2	1:A:424:ARG:NH1	2.54	0.40
1:A:111:ARG:HH21	5:A:1501:GOL:C1	2.29	0.40
1:A:23:LEU:HD11	1:B:316:LEU:HD11	2.03	0.40
1:B:149:TYR:CE2	1:B:202[B]:THR:HG22	2.57	0.40
1:A:9:PRO:HG3	1:A:14:TYR:CZ	2.57	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	518/530 (98%)	504 (97%)	12 (2%)	2 (0%)	39	19
1	B	496/530 (94%)	486 (98%)	10 (2%)	0	100	100
All	All	1014/1060 (96%)	990 (98%)	22 (2%)	2 (0%)	52	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	367	ASN
1	A	366	ASP

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	408/421 (97%)	396 (97%)	12 (3%)	50	25
1	B	390/421 (93%)	375 (96%)	15 (4%)	40	15
All	All	798/842 (95%)	771 (97%)	27 (3%)	47	19

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6[A]	SER
1	A	6[B]	SER
1	A	89	GLU
1	A	132	LEU
1	A	159[A]	ASP
1	A	159[B]	ASP
1	A	207	VAL
1	A	273	GLN
1	A	277	LEU
1	A	387[A]	ASP
1	A	387[B]	ASP

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Mol	Chain	Res	Type
1	A	456	GLU
1	B	4	ILE
1	B	6	SER
1	B	9	PRO
1	B	54	ARG
1	B	91	ARG
1	B	132	LEU
1	B	213	ARG
1	B	217	ARG
1	B	286	THR
1	B	316	LEU
1	B	365	TYR
1	B	366	ASP
1	B	367	ASN
1	B	403	VAL
1	B	425	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	43	GLN
1	A	130	HIS
1	A	151	HIS
1	A	191	ASN
1	A	225	ASN
1	A	273	GLN
1	A	415	HIS
1	B	33	HIS
1	B	130	HIS
1	B	177	ASN
1	B	191	ASN
1	B	225	ASN
1	B	273	GLN
1	B	367	ASN
1	B	415	HIS

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 ⓘ

Of 16 ligands modelled in this entry, 7 are monoatomic - leaving 9 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$
5	GOL	A	1501	-	5,5,5	0.42	0	5,5,5	0.68	0
5	GOL	A	1502	-	5,5,5	0.27	0	5,5,5	0.43	0
5	GOL	A	1503	-	5,5,5	0.68	0	5,5,5	2.44	3 (60%)
2	FAD	A	600	1	48,58,58	1.51	9 (18%)	54,89,89	2.42	17 (31%)
3	TIR	A	700	4	28,31,31	1.92	7 (25%)	32,47,47	2.33	11 (34%)
5	GOL	B	1501	-	5,5,5	0.81	0	5,5,5	1.40	1 (20%)
5	GOL	B	1503	-	5,5,5	0.73	0	5,5,5	0.88	0
2	FAD	B	600	1	48,58,58	1.15	5 (10%)	54,89,89	2.08	10 (18%)
3	TIR	B	700	4	28,31,31	1.76	8 (28%)	32,47,47	2.15	12 (37%)

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
5	GOL	A	1501	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1502	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1503	-	-	0/4/4/4	0/0/0/0
2	FAD	A	600	1	-	0/30/50/50	0/6/6/6
3	TIR	A	700	4	-	0/17/62/62	0/1/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	1501	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1503	-	-	0/4/4/4	0/0/0/0
2	FAD	B	600	1	-	0/30/50/50	0/6/6/6
3	TIR	B	700	4	-	0/17/62/62	0/1/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	C10-N10	-3.97	1.34	1.39
2	A	600	FAD	C6-C5X	-3.46	1.36	1.41
2	B	600	FAD	C10-N10	-3.37	1.35	1.39
3	B	700	TIR	C1-C2	-3.31	1.48	1.52
3	B	700	TIR	O4-C16	-2.37	1.38	1.43
2	A	600	FAD	C9A-N10	-2.26	1.35	1.38
2	B	600	FAD	C10-N1	-2.21	1.32	1.35
3	A	700	TIR	C1-C2	-2.14	1.50	1.52
2	B	600	FAD	O4B-C1B	-2.13	1.38	1.41
2	A	600	FAD	O4'-C4'	2.09	1.48	1.43
3	B	700	TIR	C3-C4	2.17	1.46	1.40
2	A	600	FAD	C4-N3	2.27	1.37	1.33
3	B	700	TIR	C5-C4	2.31	1.48	1.45
3	B	700	TIR	C22-N	2.34	1.38	1.35
2	A	600	FAD	O3B-C3B	2.37	1.48	1.43
3	A	700	TIR	C3-C4	2.52	1.47	1.40
2	B	600	FAD	O4-C4	2.59	1.30	1.24
2	A	600	FAD	C7M-C7	2.60	1.56	1.51
2	B	600	FAD	C2A-N3A	2.90	1.37	1.32
3	B	700	TIR	O6-C22	2.91	1.29	1.23
2	A	600	FAD	C4X-N5	3.24	1.38	1.33
3	B	700	TIR	O1-C2	3.35	1.30	1.23
3	A	700	TIR	O6-C22	3.59	1.30	1.23
3	A	700	TIR	C1-N	3.64	1.49	1.45
3	A	700	TIR	C13-C16	3.78	1.57	1.51
3	A	700	TIR	O1-C2	3.80	1.31	1.23
3	B	700	TIR	C17-C18	4.38	1.38	1.33
2	A	600	FAD	C1'-N10	4.49	1.53	1.48
3	A	700	TIR	C17-C18	4.53	1.38	1.33

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	FAD	N3A-C2A-N1A	-7.58	123.09	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	FAD	N3A-C2A-N1A	-6.08	124.24	128.89
3	A	700	TIR	O2-C11-O3	-5.98	105.76	110.95
3	B	700	TIR	O2-C11-O3	-5.34	106.32	110.95
3	A	700	TIR	C5-C4-C3	-5.22	119.15	124.36
2	B	600	FAD	C4A-C5A-N7A	-5.06	104.82	109.48
3	A	700	TIR	O1-C2-C3	-4.39	121.43	128.81
3	A	700	TIR	O3-C13-C16	-3.85	103.53	108.56
3	B	700	TIR	C1-N-C22	-3.83	108.77	113.29
2	A	600	FAD	C4X-C4-N3	-3.75	118.46	123.59
2	B	600	FAD	C4X-C4-N3	-3.75	118.46	123.59
3	B	700	TIR	O1-C2-C3	-3.53	122.88	128.81
2	A	600	FAD	C5X-C9A-N10	-3.17	115.21	117.62
3	B	700	TIR	O3-C13-C16	-2.98	104.67	108.56
3	A	700	TIR	C1-N-C22	-2.97	109.78	113.29
3	A	700	TIR	C9-C10-C14	-2.79	110.93	115.69
3	B	700	TIR	C5-C4-C3	-2.69	121.68	124.36
3	A	700	TIR	O6-C22-C3	-2.62	120.18	129.33
3	B	700	TIR	C5-C6-C7	-2.61	122.23	126.22
3	B	700	TIR	O6-C22-N	-2.54	122.50	125.44
2	B	600	FAD	O2'-C2'-C1'	-2.39	104.08	109.94
3	A	700	TIR	C5-C6-C7	-2.34	122.64	126.22
5	A	1503	GOL	O2-C2-C3	-2.31	98.06	108.65
2	A	600	FAD	C4A-C5A-N7A	-2.29	107.37	109.48
3	A	700	TIR	C19-C18-C17	-2.22	116.66	121.77
5	A	1503	GOL	O1-C1-C2	-2.20	99.50	110.18
2	A	600	FAD	C4-C4X-C10	-2.19	118.54	119.94
2	A	600	FAD	C6-C7-C8	-2.18	115.88	120.04
2	A	600	FAD	O3B-C3B-C2B	-2.13	104.89	111.83
2	A	600	FAD	O3B-C3B-C4B	-2.11	104.73	111.05
3	B	700	TIR	C6-C5-C4	-2.09	119.61	122.46
3	B	700	TIR	O6-C22-C3	-2.05	122.15	129.33
2	A	600	FAD	C7M-C7-C8	2.15	125.46	120.73
2	A	600	FAD	O2A-PA-O3P	2.20	115.09	105.09
3	B	700	TIR	C13-C16-C17	2.25	117.22	111.13
2	A	600	FAD	O2B-C2B-C3B	2.34	119.44	111.83
2	B	600	FAD	O2A-PA-O3P	2.44	116.16	105.09
2	A	600	FAD	C6-C5X-N5	2.45	122.11	118.96
3	A	700	TIR	O2-C11-C12	2.53	112.25	107.16
5	B	1501	GOL	C3-C2-C1	2.69	121.67	111.12
2	B	600	FAD	C1'-N10-C9A	2.75	121.95	118.86
3	B	700	TIR	C20-C9-C10	2.84	116.50	111.08
2	A	600	FAD	O4B-C1B-N9A	3.23	114.85	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	FAD	C4B-O4B-C1B	3.39	113.44	109.72
2	A	600	FAD	C7-C6-C5X	3.47	126.59	120.92
5	A	1503	GOL	C3-C2-C1	3.57	125.10	111.12
2	B	600	FAD	C4-C4X-N5	3.65	123.15	118.72
3	A	700	TIR	O5-C4-C5	4.14	120.97	115.63
2	B	600	FAD	C4X-N5-C5X	4.61	122.06	116.76
3	B	700	TIR	O5-C4-C5	4.81	121.84	115.63
2	A	600	FAD	C4X-N5-C5X	6.28	123.99	116.76
2	A	600	FAD	C4-C4X-N5	6.79	126.96	118.72
2	A	600	FAD	C4-N3-C2	7.12	121.40	115.25
2	B	600	FAD	C4-N3-C2	7.14	121.42	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1501	GOL	6	0
5	A	1502	GOL	4	0
5	A	1503	GOL	6	0
2	A	600	FAD	5	0
3	A	700	TIR	5	0
5	B	1503	GOL	8	0
2	B	600	FAD	9	0
3	B	700	TIR	4	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	497/530 (93%)	0.10	17 (3%)	49	51	9, 14, 30, 45	0
1	B	493/530 (93%)	0.04	18 (3%)	45	48	9, 14, 30, 47	0
All	All	990/1060 (93%)	0.07	35 (3%)	48	50	9, 14, 30, 47	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	365[A]	TYR	7.7
1	A	500	ALA	7.7
1	B	364	ASP	7.6
1	A	206	ASP	7.5
1	A	368	PRO	7.3
1	A	205	ALA	6.9
1	B	500	ALA	6.7
1	B	365	TYR	5.5
1	B	369	ALA	5.3
1	A	233	GLY	5.1
1	A	369	ALA	5.1
1	B	363	THR	4.6
1	B	203	ALA	4.2
1	B	233	GLY	4.1
1	B	368	PRO	4.0
1	A	207	VAL	3.9
1	A	364	ASP	3.9
1	A	363	THR	3.9
1	B	210	GLU	3.7
1	B	212	GLY	3.2
1	B	213	ARG	3.0
1	B	366	ASP	3.0
1	A	161[A]	SER	3.0
1	A	366	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	50	ARG	2.7
1	B	4	ILE	2.5
1	B	211	PRO	2.5
1	B	176	PRO	2.5
1	A	310	HIS	2.4
1	A	232	GLU	2.4
1	B	310	HIS	2.3
1	A	273	GLN	2.2
1	B	161	SER	2.1
1	A	173	PRO	2.1
1	B	232	GLU	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	GOL	A	1502	6/6	0.89	0.23	15.93	35,38,40,42	0
5	GOL	B	1503	6/6	0.88	0.21	4.61	25,30,30,36	0
5	GOL	A	1501	6/6	0.94	0.15	2.57	26,34,35,36	0
5	GOL	B	1501	6/6	0.87	0.13	2.28	20,20,24,31	0
5	GOL	A	1503	6/6	0.90	0.13	2.14	17,25,28,33	0
3	TIR	B	700	29/29	0.90	0.11	1.89	13,17,19,22	0
3	TIR	A	700	29/29	0.90	0.11	1.09	14,16,19,20	0
6	CL	B	1505	1/1	1.00	0.09	0.38	19,19,19,19	0
2	FAD	B	600	53/53	0.97	0.09	0.34	8,10,12,14	0
2	FAD	A	600	53/53	0.97	0.08	-0.47	7,10,12,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	CL	B	1502	1/1	0.97	0.04	-2.20	47,47,47,47	0
4	MG	B	800	1/1	1.00	0.05	-	18,18,18,18	0
6	CL	B	1504	1/1	0.96	0.14	-	60,60,60,60	0
6	CL	A	1505	1/1	1.00	0.07	-	17,17,17,17	0
6	CL	A	1504	1/1	1.00	0.04	-	31,31,31,31	0
4	MG	A	800	1/1	1.00	0.06	-	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.