



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:43 AM GMT

PDB ID : 2Y3R
Title : STRUCTURE OF THE TIRANDAMYCIN-BOUND FAD-DEPENDENT
TIRANDAMYCIN OXIDASE TAML IN P21 SPACE GROUP
Authors : Carlson, J.C.; Li, S.; Gunatilleke, S.S.; Anzai, Y.; Burr, D.A.; Podust, L.M.;
Sherman, D.H.
Deposited on : 2010-12-22
Resolution : 1.79 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

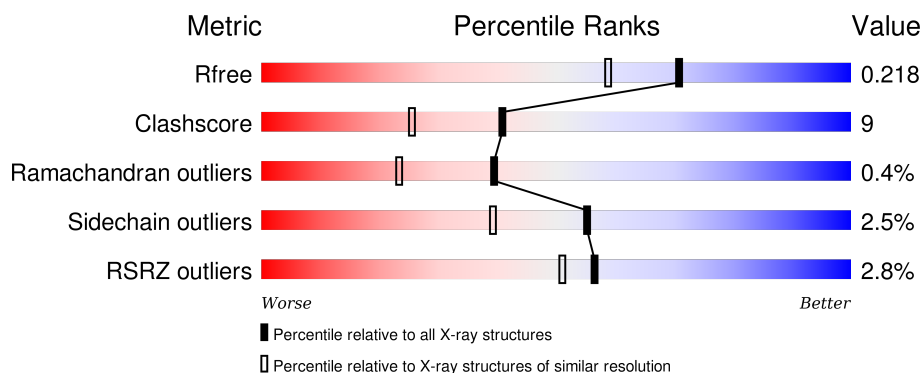
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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>78% 13% • 7%</div> </div>
1	B	530	<div> <div>2%</div> <div>78% 12% • 8%</div> </div>
1	C	530	<div> <div>2%</div> <div>81% 10% •• 7%</div> </div>
1	D	530	<div> <div>3%</div> <div>78% 13% • 7%</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	1500	-	-	-	X
5	GOL	B	1500	-	-	-	X
5	GOL	B	1501	-	-	X	X
5	GOL	C	1501	-	-	-	X
5	GOL	C	1502	-	-	X	X
5	GOL	D	1501	-	-	-	X
5	GOL	D	1502	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 17755 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	492	Total	C	N	O	S	0	20	0
			3936	2473	716	739	8			
1	B	487	Total	C	N	O	S	0	8	0
			3768	2381	678	700	9			
1	C	492	Total	C	N	O	S	0	10	0
			3852	2424	704	716	8			
1	D	491	Total	C	N	O	S	0	7	0
			3819	2402	704	705	8			

There are 120 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
C	-29	MET	-	EXPRESSION TAG	UNP D3Y1I2
C	-28	GLY	-	EXPRESSION TAG	UNP D3Y1I2
C	-27	SER	-	EXPRESSION TAG	UNP D3Y1I2

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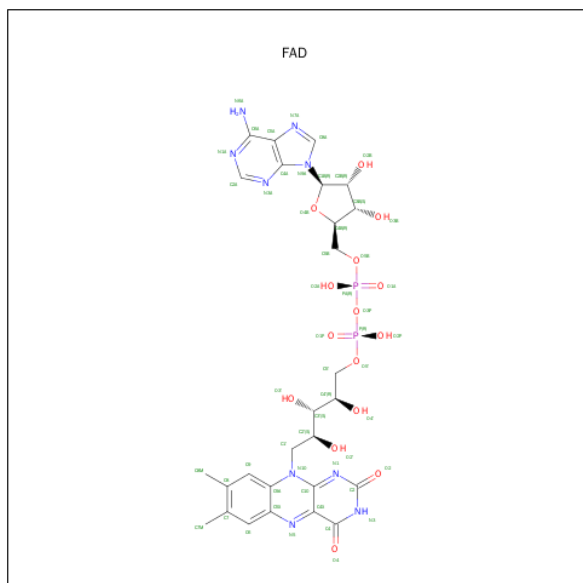
Chain	Residue	Modelled	Actual	Comment	Reference
C	-26	HIS	-	EXPRESSION TAG	UNP D3Y1I2
C	-25	HIS	-	EXPRESSION TAG	UNP D3Y1I2
C	-24	HIS	-	EXPRESSION TAG	UNP D3Y1I2
C	-23	HIS	-	EXPRESSION TAG	UNP D3Y1I2
C	-22	HIS	-	EXPRESSION TAG	UNP D3Y1I2
C	-21	HIS	-	EXPRESSION TAG	UNP D3Y1I2
C	-20	HIS	-	EXPRESSION TAG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

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-14	ASP	-	EXPRESSION TAG	UNP D3Y1I2
D	-13	ILE	-	EXPRESSION TAG	UNP D3Y1I2
D	-12	PRO	-	EXPRESSION TAG	UNP D3Y1I2
D	-11	THR	-	EXPRESSION TAG	UNP D3Y1I2
D	-10	THR	-	EXPRESSION TAG	UNP D3Y1I2
D	-9	GLU	-	EXPRESSION TAG	UNP D3Y1I2
D	-8	ASN	-	EXPRESSION TAG	UNP D3Y1I2
D	-7	LEU	-	EXPRESSION TAG	UNP D3Y1I2
D	-6	TYR	-	EXPRESSION TAG	UNP D3Y1I2
D	-5	PHE	-	EXPRESSION TAG	UNP D3Y1I2
D	-4	GLN	-	EXPRESSION TAG	UNP D3Y1I2
D	-3	GLY	-	EXPRESSION TAG	UNP D3Y1I2
D	-2	SER	-	EXPRESSION TAG	UNP D3Y1I2
D	-1	GLU	-	EXPRESSION TAG	UNP D3Y1I2
D	0	PHE	-	EXPRESSION TAG	UNP D3Y1I2

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



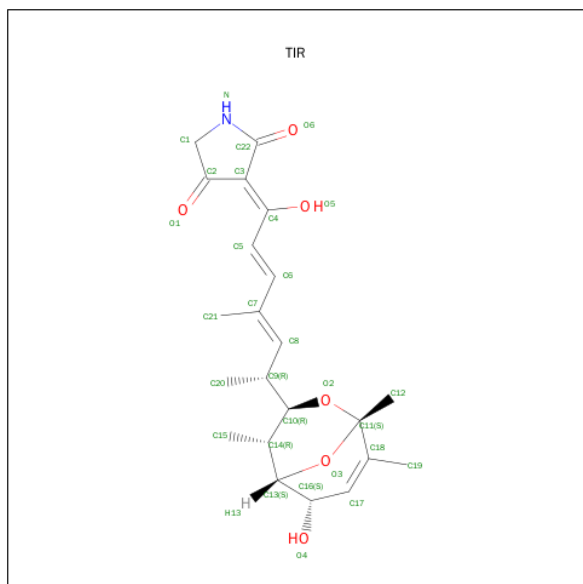
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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

- Molecule 3 is TIRANDAMYCIN E (three-letter code: TIR) (formula: $C_{22}H_{29}NO_6$).

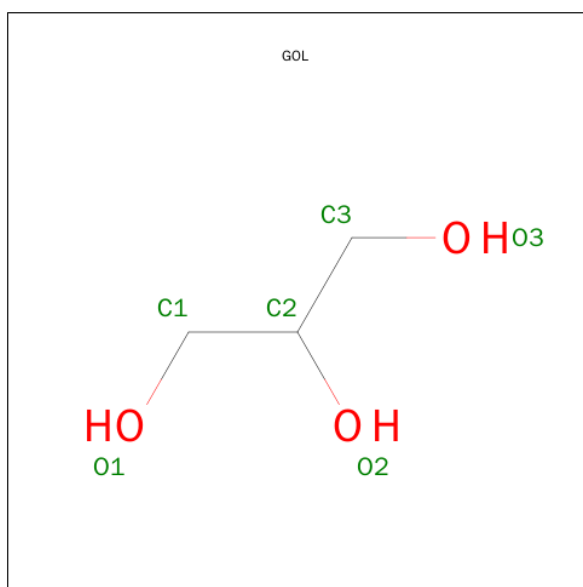


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			29	22	1	6		
3	C	1	Total	C	N	O	0	0
			29	22	1	6		

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

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

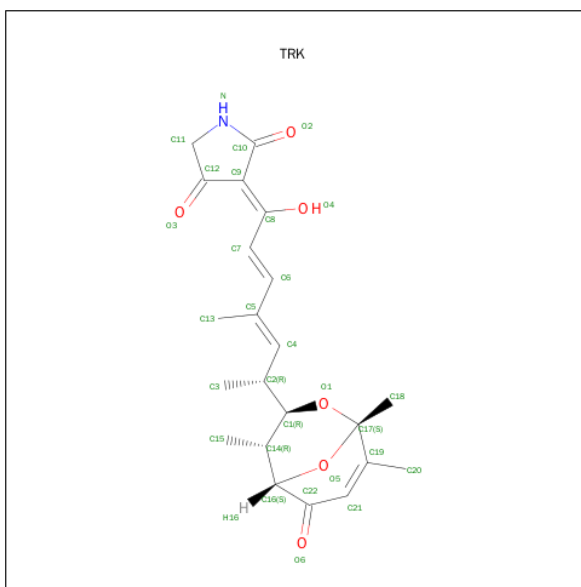


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		
6	A	1	Total	Cl	0	0
			1	1		
6	D	2	Total	Cl	0	0
			2	2		
6	C	2	Total	Cl	0	0
			2	2		

- Molecule 7 is TIRANDAMYCIN D (three-letter code: TRK) (formula: C₂₂H₂₇NO₆).



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

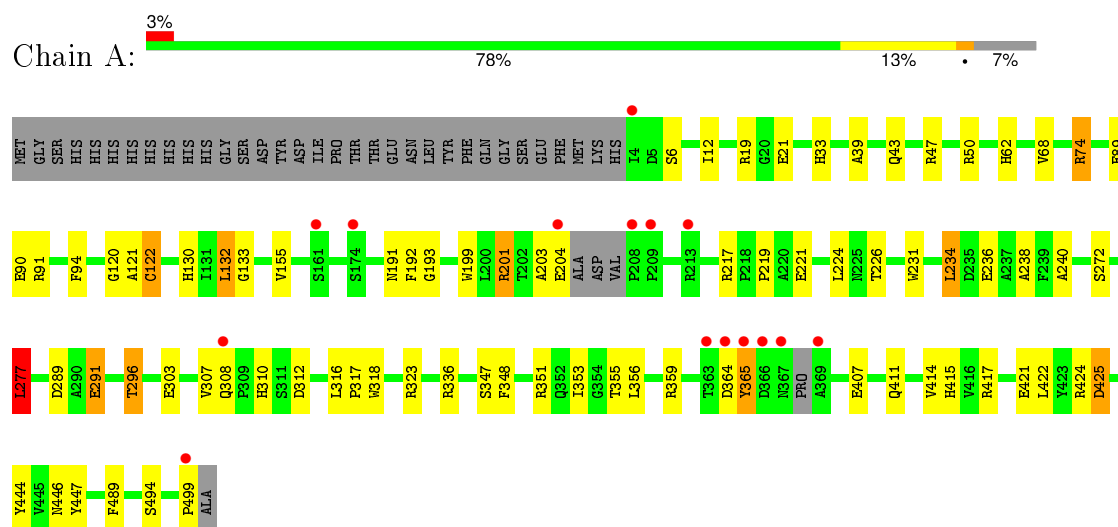
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	499	Total O 499 499	0	0
8	B	495	Total O 495 495	0	0
8	C	535	Total O 535 535	0	0
8	D	471	Total O 471 471	0	0

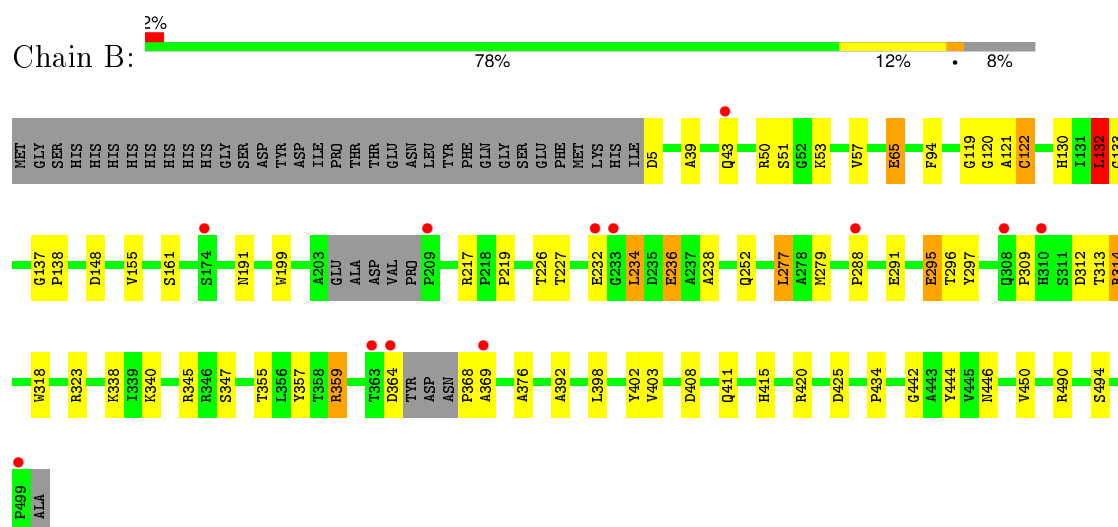
3 Residue-property plots [i](#)

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.

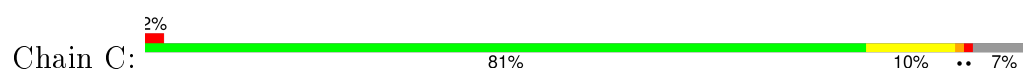
• Molecule 1: TAML

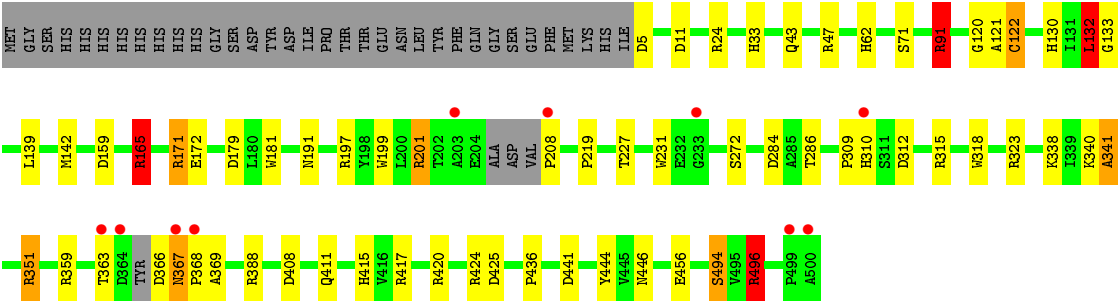


• Molecule 1: TAML

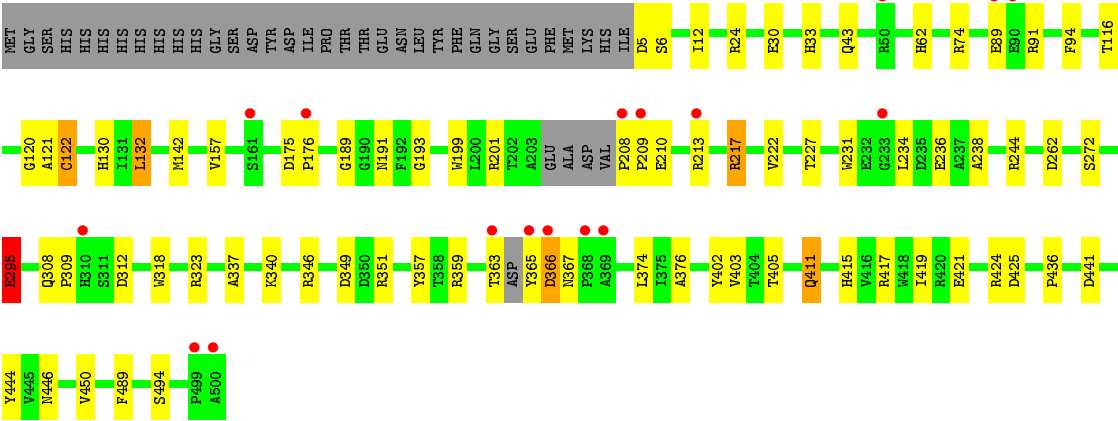
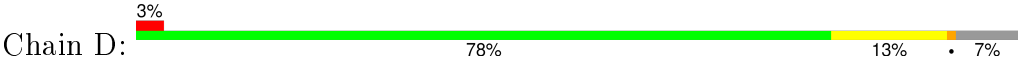


• Molecule 1: TAML





• Molecule 1: TAML



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.09 Å 106.17 Å 151.17 Å 90.00° 94.63° 90.00°	Depositor
Resolution (Å)	150.68 – 1.79 19.82 – 1.79	Depositor EDS
% Data completeness (in resolution range)	76.5 (150.68-1.79) 76.5 (19.82-1.79)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 1.79 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.146 , 0.219 0.146 , 0.218	Depositor DCC
R_{free} test set	8138 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	16.6	Xtriage
Anisotropy	0.436	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	6 of 160766 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	17755	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.20 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.3666e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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: GOL, MG, CL, TRK, TIR, 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	1.14	6/4037 (0.1%)	0.99	12/5512 (0.2%)
1	B	1.15	7/3867 (0.2%)	0.99	12/5284 (0.2%)
1	C	1.14	5/3952 (0.1%)	1.00	19/5397 (0.4%)
1	D	1.13	6/3918 (0.2%)	0.97	6/5348 (0.1%)
All	All	1.14	24/15774 (0.2%)	0.99	49/21541 (0.2%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	201	ARG	CB-CG	-6.92	1.33	1.52
1	D	295	GLU	CB-CG	-6.48	1.39	1.52
1	A	21	GLU	CG-CD	6.40	1.61	1.51
1	B	347	SER	CB-OG	6.26	1.50	1.42
1	B	402	TYR	CD2-CE2	6.15	1.48	1.39
1	C	494	SER	CB-OG	6.14	1.50	1.42
1	A	348	PHE	CE2-CZ	6.11	1.49	1.37
1	B	65	GLU	CB-CG	5.96	1.63	1.52
1	C	341	ALA	CA-CB	5.91	1.64	1.52
1	B	392	ALA	CA-CB	5.86	1.64	1.52
1	B	295	GLU	CB-CG	-5.85	1.41	1.52
1	B	347	SER	CA-CB	5.77	1.61	1.52
1	C	179	ASP	CB-CG	5.72	1.63	1.51
1	D	157	VAL	CB-CG2	5.52	1.64	1.52
1	B	402	TYR	CD1-CE1	5.38	1.47	1.39
1	A	201	ARG	CB-CG	-5.26	1.38	1.52
1	A	407	GLU	CB-CG	-5.24	1.42	1.52
1	D	402	TYR	CD1-CE1	5.23	1.47	1.39
1	A	68	VAL	CB-CG2	5.16	1.63	1.52
1	A	192	PHE	CE2-CZ	5.13	1.47	1.37
1	D	89	GLU	CG-CD	5.12	1.59	1.51
1	D	222	VAL	CB-CG2	5.08	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	351	ARG	CZ-NH1	5.07	1.39	1.33
1	D	376	ALA	CA-CB	5.01	1.62	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	351	ARG	NE-CZ-NH2	-8.70	115.95	120.30
1	A	19	ARG	NE-CZ-NH2	-8.63	115.99	120.30
1	C	312	ASP	CB-CG-OD1	7.95	125.46	118.30
1	B	323	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	A	74	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	B	277	LEU	CA-CB-CG	7.63	132.85	115.30
1	A	277	LEU	CA-CB-CG	7.09	131.60	115.30
1	C	315	ARG	NE-CZ-NH2	-6.93	116.84	120.30
1	A	336	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	B	132[A]	LEU	CB-CG-CD2	-6.46	100.02	111.00
1	B	132[B]	LEU	CB-CG-CD2	-6.46	100.02	111.00
1	B	347	SER	N-CA-CB	6.43	120.15	110.50
1	D	208	PRO	N-CA-CB	6.36	110.94	103.30
1	B	277	LEU	CB-CG-CD2	-6.22	100.43	111.00
1	C	351	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	D	24	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	D	24	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	C	408	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	336	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	C	165[A]	ARG	NE-CZ-NH1	-5.73	117.44	120.30
1	C	165[B]	ARG	NE-CZ-NH1	-5.73	117.44	120.30
1	B	403	VAL	CB-CA-C	-5.72	100.53	111.40
1	C	179	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	201	ARG	CG-CD-NE	-5.70	99.82	111.80
1	B	345	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	C	165[A]	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	C	165[B]	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	C	323	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	C	417	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	B	408	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	C	91	ARG	CG-CD-NE	-5.52	100.21	111.80
1	A	289	ASP	CB-CG-OD1	5.44	123.20	118.30
1	B	345	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	C	197	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	D	312	ASP	CB-CG-OD1	5.34	123.11	118.30
1	D	323	ARG	NE-CZ-NH2	-5.33	117.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	11	ASP	CB-CG-OD1	5.27	123.05	118.30
1	A	91	ARG	CG-CD-NE	-5.23	100.81	111.80
1	B	408	ASP	CB-CG-OD1	5.23	123.00	118.30
1	C	132[A]	LEU	CB-CG-CD2	-5.21	102.14	111.00
1	C	132[B]	LEU	CB-CG-CD2	-5.21	102.14	111.00
1	C	91	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	A	291	GLU	OE1-CD-OE2	-5.18	117.09	123.30
1	C	496	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	91	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	323	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	A	19	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	D	91	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	B	148	ASP	CB-CG-OD2	5.01	122.81	118.30

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	3936	0	3761	65	0
1	B	3768	0	3615	56	0
1	C	3852	0	3705	65	0
1	D	3819	0	3671	60	0
2	A	53	0	30	9	0
2	B	53	0	29	1	0
2	C	53	0	29	9	0
2	D	53	0	29	6	0
3	A	29	0	28	5	0
3	C	29	0	28	5	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	6	0	8	1	0
5	B	12	0	15	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	12	0	15	11	0
5	D	12	0	15	2	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	2	0	0	0	0
6	D	2	0	0	0	0
7	B	29	0	26	3	0
7	D	29	0	26	2	0
8	A	499	0	0	17	0
8	B	495	0	0	13	1
8	C	535	0	0	17	0
8	D	471	0	0	16	0
All	All	17755	0	15030	261	1

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 (261) 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:62:HIS:ND1	2:A:600:FAD:HM83	0.95	1.27
1:A:62:HIS:CE1	2:A:600:FAD:HM83	1.71	1.24
1:D:121:ALA:O	1:D:122:CYS:CB	1.86	1.20
1:C:121:ALA:O	1:C:122:CYS:CB	1.82	1.19
1:A:121:ALA:O	1:A:122:CYS:CB	1.87	1.19
1:B:121:ALA:O	1:B:122:CYS:CB	1.89	1.17
1:C:286:THR:HG22	8:C:2259:HOH:O	1.45	1.15
1:C:338:LYS:HE2	5:C:1502:GOL:H31	1.24	1.09
2:C:600:FAD:N5	3:C:700:TIR:H16	1.68	1.09
1:D:346[B]:ARG:HG3	1:D:346[B]:ARG:HH11	1.08	1.08
1:C:338:LYS:CE	5:C:1502:GOL:H31	1.82	1.08
1:C:24:ARG:HH22	5:C:1502:GOL:H12	1.13	1.06
1:D:5:ASP:N	8:D:2002:HOH:O	1.89	1.04
1:C:208:PRO:HD3	8:C:2250:HOH:O	1.56	1.04
1:D:210:GLU:CB	1:D:213:ARG:HH21	1.70	1.03
1:A:499:PRO:C	8:A:2492:HOH:O	1.95	1.03
1:C:71:SER:HB2	8:C:2043:HOH:O	1.60	1.01
2:A:600:FAD:N5	3:A:700:TIR:H16	1.76	0.99
1:B:368:PRO:CD	8:B:2358:HOH:O	2.09	0.99
1:C:165[A]:ARG:HG3	1:C:165[A]:ARG:HH11	1.24	0.98
1:A:121:ALA:O	1:A:122:CYS:HB2	1.16	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:ALA:O	1:D:122:CYS:HB2	1.12	0.96
1:B:121:ALA:O	1:B:122:CYS:HB2	1.14	0.95
1:C:165[A]:ARG:CG	1:C:165[A]:ARG:HH11	1.76	0.95
1:A:365:TYR:OH	1:A:421[A]:GLU:OE1	1.87	0.93
1:C:24:ARG:HH22	5:C:1502:GOL:C1	1.82	0.91
1:C:165[A]:ARG:HG3	1:C:165[A]:ARG:NH1	1.82	0.90
1:A:414[A]:VAL:HG23	8:A:2403:HOH:O	1.71	0.90
1:D:213:ARG:HG2	8:D:2205:HOH:O	1.74	0.88
1:C:121:ALA:O	1:C:122:CYS:HB2	1.04	0.88
1:C:24:ARG:NH2	5:C:1502:GOL:H12	1.89	0.87
1:A:74:ARG:HD3	8:A:2110:HOH:O	1.73	0.87
1:C:284:ASP:OD1	1:C:286:THR:HG23	1.75	0.87
1:D:346[B]:ARG:NH1	1:D:346[B]:ARG:HG3	1.82	0.84
1:A:89[B]:GLU:N	1:A:89[B]:GLU:OE1	2.09	0.84
1:A:89[B]:GLU:CD	1:A:89[B]:GLU:H	1.76	0.83
1:C:62:HIS:ND1	2:C:600:FAD:HM81	1.94	0.82
1:D:359:ARG:NH1	1:D:425:ASP:OD2	2.13	0.81
1:D:421[B]:GLU:OE1	1:D:424:ARG:NH2	2.13	0.80
1:C:62:HIS:CE1	2:C:600:FAD:C8M	2.64	0.80
1:D:244[B]:ARG:NH2	1:D:349:ASP:HA	1.96	0.80
1:C:338:LYS:HE2	5:C:1502:GOL:C3	2.09	0.79
1:C:159:ASP:OD1	1:C:165[A]:ARG:NH1	2.16	0.79
1:B:359:ARG:NH1	1:B:425:ASP:OD2	2.17	0.78
1:C:359:ARG:NH1	1:C:425:ASP:OD2	2.17	0.77
1:D:244[B]:ARG:HH21	1:D:349:ASP:HA	1.50	0.77
1:A:421[B]:GLU:OE1	1:A:424:ARG:NH2	2.17	0.77
1:A:132[A]:LEU:C	1:A:132[A]:LEU:HD23	2.04	0.77
1:D:62:HIS:CE1	2:D:600:FAD:C8M	2.67	0.76
1:C:366:ASP:O	1:C:368:PRO:HD3	1.86	0.75
1:B:279[B]:MET:CE	1:B:297:TYR:OH	2.34	0.74
1:B:39:ALA:O	1:B:43[A]:GLN:HG2	1.87	0.74
2:C:600:FAD:C4X	3:C:700:TIR:H16	2.17	0.73
2:A:600:FAD:C4X	3:A:700:TIR:H16	2.18	0.73
1:D:346[B]:ARG:NH1	1:D:346[B]:ARG:CG	2.50	0.72
1:A:62:HIS:ND1	2:A:600:FAD:HM81	1.97	0.72
1:C:369:ALA:O	8:C:2396:HOH:O	2.07	0.71
1:D:365:TYR:CB	8:D:2364:HOH:O	2.38	0.70
1:A:33:HIS:HE1	8:A:2043:HOH:O	1.73	0.70
1:C:5:ASP:CB	8:D:2131:HOH:O	2.40	0.69
1:B:279[B]:MET:HE2	1:B:297:TYR:OH	1.91	0.69
1:D:417[B]:ARG:HG2	8:D:2372:HOH:O	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ALA:O	1:A:43[A]:GLN:HG2	1.91	0.68
1:B:368:PRO:CG	8:B:2358:HOH:O	2.40	0.68
1:B:217:ARG:NH2	8:B:2230:HOH:O	2.18	0.68
1:B:65:GLU:OE1	5:B:1501:GOL:H31	1.94	0.68
1:D:308:GLN:O	8:D:2274:HOH:O	2.11	0.68
1:D:62:HIS:ND1	2:D:600:FAD:HM81	1.98	0.67
1:B:227:THR:HG23	1:B:309:PRO:HB2	1.75	0.67
1:A:355:THR:HG21	1:A:425[A]:ASP:HB3	1.77	0.67
1:B:132[A]:LEU:HD23	1:B:132[A]:LEU:C	2.12	0.67
1:B:338:LYS:NZ	5:B:1501:GOL:H2	2.10	0.66
1:A:236:GLU:OE2	8:A:2259:HOH:O	2.12	0.66
1:A:234:LEU:HD23	1:A:307:VAL:HG21	1.77	0.65
1:A:310[B]:HIS:HD2	8:A:2250:HOH:O	1.80	0.64
1:B:369:ALA:HA	8:B:2164:HOH:O	1.98	0.64
1:D:374:LEU:N	1:D:374:LEU:HD12	2.13	0.63
1:A:132[A]:LEU:HD23	1:A:133:GLY:N	2.14	0.63
1:C:91:ARG:HD2	1:C:199:TRP:CE2	2.34	0.63
1:B:313:THR:C	1:B:314[B]:ARG:HG2	2.17	0.63
1:D:411:GLN:O	1:D:415:HIS:HD2	1.80	0.62
1:C:62:HIS:ND1	2:C:600:FAD:C8	2.59	0.62
1:B:279[B]:MET:HE1	1:B:297:TYR:OH	1.99	0.62
1:B:291:GLU:O	1:B:295:GLU:HG2	1.99	0.62
1:A:296:THR:HG21	8:A:2046:HOH:O	2.00	0.62
1:B:252:GLN:CG	8:B:2254:HOH:O	2.48	0.61
1:A:351[A]:ARG:NH1	8:A:2362:HOH:O	2.20	0.61
1:A:62:HIS:ND1	2:A:600:FAD:C8	2.59	0.61
1:C:310:HIS:HD2	8:C:2262:HOH:O	1.83	0.61
1:C:33:HIS:HE1	8:C:2054:HOH:O	1.83	0.61
1:C:227:THR:HG23	1:C:309:PRO:HB2	1.81	0.60
1:D:142:MET:HE2	1:D:262:ASP:HA	1.83	0.60
1:D:62:HIS:CG	2:D:600:FAD:C8M	2.76	0.59
1:C:132[A]:LEU:H	1:C:132[A]:LEU:HD22	1.67	0.59
1:D:130:HIS:HD2	2:D:600:FAD:O2'	1.85	0.59
1:A:130:HIS:HD2	2:A:600:FAD:O2'	1.85	0.59
1:D:244[B]:ARG:NH2	8:D:2225:HOH:O	2.11	0.59
5:C:1502:GOL:O1	8:C:2535:HOH:O	2.16	0.59
1:B:132[A]:LEU:N	1:B:132[A]:LEU:CD2	2.63	0.58
1:C:132[A]:LEU:N	1:C:132[A]:LEU:CD2	2.66	0.57
1:C:456:GLU:OE1	8:C:2469:HOH:O	2.17	0.57
1:C:366:ASP:O	1:C:368:PRO:CD	2.52	0.57
1:C:91:ARG:NE	8:C:2150:HOH:O	2.26	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:GLU:HG3	1:D:357:TYR:CG	2.38	0.57
1:D:210:GLU:CB	1:D:213:ARG:NH2	2.55	0.57
1:C:132[A]:LEU:HD23	1:C:132[A]:LEU:C	2.26	0.57
1:A:414[A]:VAL:CG2	8:A:2403:HOH:O	2.43	0.56
7:B:700:TRK:C7	5:B:1500:GOL:H31	2.34	0.56
1:C:338:LYS:HD3	5:C:1502:GOL:H11	1.87	0.56
1:A:411[A]:GLN:O	1:A:415:HIS:HD2	1.89	0.56
1:B:236:GLU:HG2	1:B:357:TYR:CG	2.41	0.55
1:A:234:LEU:HD22	1:A:238:ALA:HB3	1.89	0.55
7:D:700:TRK:H132	7:D:700:TRK:H14	1.89	0.55
1:C:341:ALA:HB3	8:C:2456:HOH:O	2.07	0.54
1:A:411[B]:GLN:O	1:A:415:HIS:HD2	1.91	0.54
1:A:308:GLN:O	8:A:2318:HOH:O	2.18	0.54
1:D:295:GLU:HG2	8:D:2261:HOH:O	2.08	0.54
1:B:368:PRO:HD3	8:B:2358:HOH:O	1.89	0.54
1:A:120:GLY:H	1:A:130:HIS:CE1	2.26	0.53
1:D:120:GLY:H	1:D:130:HIS:CE1	2.26	0.53
1:B:132[A]:LEU:HD23	1:B:132[A]:LEU:N	2.15	0.53
3:A:700:TIR:H121	3:A:700:TIR:H315	1.91	0.53
1:B:132[A]:LEU:H	1:B:132[A]:LEU:CD2	2.21	0.53
1:C:444:TYR:CZ	1:C:446:ASN:HB2	2.43	0.53
1:B:368:PRO:HD2	8:B:2358:HOH:O	1.94	0.53
1:A:204:GLU:C	8:A:2237:HOH:O	2.46	0.53
1:B:234:LEU:HD22	1:B:238:ALA:HB3	1.91	0.53
1:A:444:TYR:CZ	1:A:446:ASN:HB2	2.44	0.53
7:B:700:TRK:H132	7:B:700:TRK:H14	1.90	0.53
1:D:244[B]:ARG:HH21	1:D:349:ASP:CA	2.22	0.53
1:D:217:ARG:NH2	8:D:2209:HOH:O	2.21	0.53
3:C:700:TIR:H121	3:C:700:TIR:H315	1.91	0.53
1:B:338:LYS:HZ3	5:B:1501:GOL:H2	1.74	0.53
1:C:132[A]:LEU:H	1:C:132[A]:LEU:CD2	2.22	0.53
1:A:193:GLY:HA2	1:A:489:PHE:CE2	2.44	0.53
7:B:700:TRK:C6	5:B:1500:GOL:H31	2.40	0.52
1:D:444:TYR:CZ	1:D:446:ASN:HB2	2.44	0.52
1:A:231:TRP:CE2	1:A:277:LEU:HD13	2.44	0.52
1:B:450:VAL:CG2	5:B:1501:GOL:H32	2.39	0.52
1:D:227:THR:HG23	1:D:309:PRO:HB2	1.92	0.52
1:C:120:GLY:H	1:C:130:HIS:CE1	2.27	0.52
1:B:130:HIS:HD2	2:B:600:FAD:O2'	1.93	0.52
1:A:221:GLU:HG2	1:A:317:PRO:HA	1.91	0.52
1:A:47:ARG:HG2	1:A:50[B]:ARG:NH2	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:LYS:CD	5:C:1502:GOL:H31	2.38	0.51
1:B:411:GLN:O	1:B:415:HIS:HD2	1.93	0.51
1:B:191:ASN:HD21	1:B:494:SER:HA	1.75	0.51
1:B:444:TYR:CZ	1:B:446:ASN:HB2	2.45	0.51
1:B:288:PRO:HD2	8:B:2283:HOH:O	2.10	0.51
1:A:217:ARG:NH2	8:A:2243:HOH:O	2.35	0.51
1:C:191:ASN:HD21	1:C:494:SER:HA	1.75	0.51
1:B:132[A]:LEU:HD22	1:B:132[A]:LEU:H	1.75	0.51
1:A:296:THR:CG2	8:A:2046:HOH:O	2.59	0.51
1:A:231:TRP:CD1	1:A:272:SER:HA	2.46	0.51
1:B:132[A]:LEU:HD23	1:B:133:GLY:N	2.25	0.51
1:D:337:ALA:HB2	1:D:405:THR:HG22	1.91	0.51
1:C:231:TRP:CD1	1:C:272:SER:HA	2.47	0.50
1:A:226[A]:THR:HG23	1:A:226[A]:THR:O	2.11	0.50
1:B:5:ASP:HA	8:B:2004:HOH:O	2.10	0.50
1:B:119:GLY:O	1:B:137:GLY:HA3	2.12	0.49
1:D:62:HIS:ND1	2:D:600:FAD:C8	2.66	0.49
1:A:365:TYR:HE1	1:A:417:ARG:HG2	1.76	0.49
1:C:132[A]:LEU:HD23	1:C:132[A]:LEU:N	2.27	0.49
1:D:231:TRP:CD1	1:D:272:SER:HA	2.47	0.49
1:A:355:THR:HG21	1:A:425[B]:ASP:CG	2.33	0.49
1:D:417[B]:ARG:HG3	8:D:2367:HOH:O	2.12	0.49
1:A:191:ASN:HD21	1:A:494:SER:HA	1.78	0.49
1:B:120:GLY:H	1:B:130:HIS:CE1	2.30	0.48
1:A:356:LEU:HD23	1:A:422:LEU:HD11	1.95	0.48
1:C:132[A]:LEU:HD23	1:C:133:GLY:N	2.28	0.48
1:A:62:HIS:CG	2:A:600:FAD:C8M	2.82	0.48
1:B:57[B]:VAL:HG12	8:B:2486:HOH:O	2.13	0.48
1:C:436:PRO:HA	1:C:441:ASP:HA	1.96	0.48
1:D:33:HIS:HD2	8:D:2001:HOH:O	1.96	0.48
1:C:388:ARG:HG2	1:C:388:ARG:O	2.14	0.47
1:D:236:GLU:HG2	1:D:236:GLU:O	2.15	0.47
1:C:411:GLN:O	1:C:415:HIS:HD2	1.97	0.47
1:B:234:LEU:HD22	1:B:238:ALA:CB	2.44	0.47
1:A:291:GLU:HG2	8:A:2144:HOH:O	2.14	0.47
1:A:359:ARG:NH2	1:A:425[A]:ASP:OD2	2.40	0.47
1:C:130:HIS:HD2	2:C:600:FAD:O2'	1.98	0.47
1:B:338:LYS:HZ2	5:B:1501:GOL:H2	1.76	0.47
1:A:90:GLU:OE2	1:C:47:ARG:NH1	2.48	0.47
1:A:234:LEU:HD22	1:A:238:ALA:CB	2.45	0.47
1:D:193:GLY:HA2	1:D:489:PHE:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:VAL:HG22	5:B:1501:GOL:H32	1.95	0.47
1:A:310[A]:HIS:CE1	8:A:2319:HOH:O	2.68	0.46
1:C:91:ARG:NH2	8:C:2150:HOH:O	2.46	0.46
1:B:313:THR:O	1:B:314[B]:ARG:HG2	2.15	0.46
1:D:234:LEU:HD12	1:D:238:ALA:HB3	1.96	0.46
1:A:121:ALA:O	1:A:122:CYS:SG	2.70	0.46
1:A:231:TRP:NE1	1:A:277:LEU:HD13	2.31	0.46
1:D:351[A]:ARG:NH2	8:D:2324:HOH:O	2.27	0.46
1:A:203:ALA:O	1:A:204:GLU:C	2.54	0.46
1:A:224:LEU:CD1	1:A:316:LEU:HD12	2.46	0.45
1:D:94:PHE:O	1:D:199:TRP:HA	2.16	0.45
1:D:30:GLU:OE2	1:D:74:ARG:HD2	2.16	0.45
1:A:347:SER:HB2	8:A:2360:HOH:O	2.15	0.45
7:D:700:TRK:H182	5:D:1501:GOL:H11	1.97	0.45
1:A:219:PRO:O	1:A:318:TRP:HB2	2.17	0.44
1:A:89[B]:GLU:OE1	1:C:43:GLN:OE1	2.35	0.44
1:B:450:VAL:HG22	5:B:1501:GOL:C3	2.47	0.44
3:A:700:TIR:C21	3:A:700:TIR:H14	2.48	0.44
1:A:364:ASP:O	1:A:365:TYR:HB2	2.18	0.44
1:D:351[B]:ARG:NH1	8:D:2324:HOH:O	2.50	0.44
1:D:121:ALA:O	1:D:122:CYS:SG	2.74	0.44
1:A:447:TYR:HH	3:A:700:TIR:HO4	1.57	0.43
1:C:62:HIS:CG	2:C:600:FAD:C8M	2.84	0.43
8:C:2173:HOH:O	1:D:5:ASP:CB	2.65	0.43
1:B:368:PRO:HG3	8:B:2358:HOH:O	2.13	0.43
5:C:1501:GOL:H31	8:C:2357:HOH:O	2.19	0.43
1:A:417:ARG:NH1	1:A:421[A]:GLU:OE2	2.48	0.43
1:A:94:PHE:O	1:A:199:TRP:HA	2.18	0.43
1:D:116:THR:HG1	1:D:318:TRP:HH2	1.65	0.43
1:C:424:ARG:NH1	8:C:2439:HOH:O	2.04	0.43
1:B:51:SER:HB3	1:B:53:LYS:HG3	2.00	0.43
1:D:436:PRO:HA	1:D:441:ASP:HA	2.00	0.43
1:D:417[A]:ARG:HD3	8:D:2373:HOH:O	2.19	0.43
1:C:171[B]:ARG:O	1:C:171[B]:ARG:HG2	2.18	0.43
1:A:226[A]:THR:HG22	1:A:312:ASP:HB3	2.01	0.43
2:C:600:FAD:C4X	3:C:700:TIR:C16	2.93	0.42
1:C:338:LYS:NZ	5:C:1502:GOL:H31	2.31	0.42
1:A:414[B]:VAL:HG13	8:A:2403:HOH:O	2.18	0.42
1:D:236:GLU:HG3	1:D:357:TYR:CD2	2.54	0.42
1:D:191:ASN:HD21	1:D:494:SER:HA	1.85	0.42
1:D:351[A]:ARG:NE	8:D:2324:HOH:O	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:340:LYS:HE3	1:C:420:ARG:HA	2.00	0.42
1:D:363:THR:HA	1:D:366:ASP:OD1	2.19	0.42
2:A:600:FAD:HM72	5:A:1500:GOL:O3	2.19	0.42
2:D:600:FAD:H1'2	2:D:600:FAD:H9	1.83	0.42
1:C:219:PRO:O	1:C:318:TRP:HB2	2.19	0.42
1:D:450:VAL:HG22	5:D:1502:GOL:H2	2.02	0.42
1:D:340:LYS:HD2	1:D:419:ILE:HG12	2.03	0.41
1:C:496:ARG:HD2	8:C:2522:HOH:O	2.20	0.41
1:D:351[A]:ARG:NH1	8:D:2321:HOH:O	2.53	0.41
1:C:496:ARG:HD2	8:C:2523:HOH:O	2.20	0.41
1:A:240:ALA:HA	1:A:353:ILE:HG21	2.03	0.41
2:C:600:FAD:C5X	3:C:700:TIR:H16	2.47	0.41
1:C:351:ARG:NE	8:C:2384:HOH:O	2.53	0.41
1:D:175:ASP:OD1	1:D:176:PRO:HD2	2.21	0.41
1:C:121:ALA:O	1:C:122:CYS:SG	2.77	0.41
1:B:121:ALA:O	1:B:122:CYS:SG	2.77	0.41
1:B:364:ASP:C	8:B:2355:HOH:O	2.58	0.41
1:D:142:MET:HB2	1:D:142:MET:HE2	1.89	0.41
1:D:12:ILE:HG21	1:D:12:ILE:HD13	1.79	0.41
1:B:490:ARG:HD2	8:B:2467:HOH:O	2.21	0.41
1:D:132:LEU:HD13	1:D:189:GLY:HA2	2.02	0.41
1:C:139:LEU:HD22	1:C:142:MET:HE3	2.03	0.41
1:A:12:ILE:HG21	1:A:12:ILE:HD13	1.72	0.40
1:B:161:SER:HB2	1:D:43[B]:GLN:HE22	1.86	0.40
1:B:434:PRO:O	1:B:442:GLY:HA2	2.20	0.40
1:B:376:ALA:HA	1:B:398:LEU:HD23	2.02	0.40
1:C:367:ASN:H	1:C:367:ASN:HD22	1.69	0.40
1:C:171[A]:ARG:HB3	1:C:181:TRP:CE2	2.56	0.40
1:B:219:PRO:O	1:B:318:TRP:HB2	2.22	0.40
1:B:355:THR:O	1:B:359:ARG:HG3	2.22	0.40
1:B:94:PHE:O	1:B:199:TRP:HA	2.21	0.40
1:B:226[A]:THR:HG23	1:B:226[A]:THR:O	2.22	0.40
1:B:340:LYS:HE3	1:B:420:ARG:HA	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:2285:HOH:O	8:B:2431:HOH:O[2_556]	2.13	0.07

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	506/530 (96%)	491 (97%)	13 (3%)	2 (0%)	39	23
1	B	489/530 (92%)	477 (98%)	11 (2%)	1 (0%)	52	35
1	C	496/530 (94%)	485 (98%)	9 (2%)	2 (0%)	39	23
1	D	492/530 (93%)	481 (98%)	8 (2%)	3 (1%)	30	14
All	All	1983/2120 (94%)	1934 (98%)	41 (2%)	8 (0%)	39	23

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	CYS
1	B	122	CYS
1	C	122	CYS
1	C	367	ASN
1	D	122	CYS
1	A	365	TYR
1	D	366	ASP
1	D	209	PRO

5.3.2 Protein sidechains [i](#)

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	400/421 (95%)	388 (97%)	12 (3%)	48	31
1	B	378/421 (90%)	363 (96%)	15 (4%)	38	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	389/421 (92%)	377 (97%)	12 (3%)	47	30
1	D	382/421 (91%)	374 (98%)	8 (2%)	61	47
All	All	1549/1684 (92%)	1502 (97%)	47 (3%)	55	31

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	132[A]	LEU
1	A	132[B]	LEU
1	A	155[A]	VAL
1	A	155[B]	VAL
1	A	201	ARG
1	A	234	LEU
1	A	277	LEU
1	A	296	THR
1	A	303	GLU
1	A	425[A]	ASP
1	A	425[B]	ASP
1	B	50	ARG
1	B	132[A]	LEU
1	B	132[B]	LEU
1	B	138	PRO
1	B	155[A]	VAL
1	B	155[B]	VAL
1	B	232	GLU
1	B	234	LEU
1	B	236	GLU
1	B	277	LEU
1	B	296	THR
1	B	312	ASP
1	B	314[A]	ARG
1	B	314[B]	ARG
1	B	359	ARG
1	C	91	ARG
1	C	132[A]	LEU
1	C	132[B]	LEU
1	C	165[A]	ARG
1	C	165[B]	ARG
1	C	171[A]	ARG
1	C	171[B]	ARG

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Mol	Chain	Res	Type
1	C	172[A]	GLU
1	C	172[B]	GLU
1	C	201	ARG
1	C	363	THR
1	C	496	ARG
1	D	6	SER
1	D	132	LEU
1	D	201	ARG
1	D	217	ARG
1	D	295	GLU
1	D	367	ASN
1	D	403	VAL
1	D	411	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	130	HIS
1	A	177	ASN
1	A	191	ASN
1	A	225	ASN
1	A	415	HIS
1	B	130	HIS
1	B	177	ASN
1	B	191	ASN
1	B	225	ASN
1	B	415	HIS
1	C	33	HIS
1	C	43	GLN
1	C	130	HIS
1	C	177	ASN
1	C	191	ASN
1	C	225	ASN
1	C	252	GLN
1	C	310	HIS
1	C	415	HIS
1	D	130	HIS
1	D	151	HIS
1	D	177	ASN
1	D	191	ASN
1	D	225	ASN

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Mol	Chain	Res	Type
1	D	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 25 ligands modelled in this entry, 10 are monoatomic - leaving 15 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	1500	-	5,5,5	0.89	0	5,5,5	1.27	1 (20%)
2	FAD	A	600	1	48,58,58	1.28	7 (14%)	54,89,89	2.67	12 (22%)
3	TIR	A	700	4	28,31,31	1.60	5 (17%)	32,47,47	2.08	10 (31%)
5	GOL	B	1500	-	5,5,5	0.76	0	5,5,5	0.83	0
5	GOL	B	1501	-	5,5,5	1.26	1 (20%)	5,5,5	1.40	1 (20%)
2	FAD	B	600	1	48,58,58	1.27	4 (8%)	54,89,89	2.30	14 (25%)
7	TRK	B	700	4	28,31,31	1.36	3 (10%)	28,47,47	2.31	11 (39%)
5	GOL	C	1501	-	5,5,5	0.69	0	5,5,5	0.28	0
5	GOL	C	1502	-	5,5,5	1.09	0	5,5,5	1.81	2 (40%)
2	FAD	C	600	1	48,58,58	1.12	4 (8%)	54,89,89	2.11	14 (25%)
3	TIR	C	700	4	28,31,31	1.69	8 (28%)	32,47,47	2.13	10 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	D	1501	-	5,5,5	0.92	0	5,5,5	1.03	0
5	GOL	D	1502	-	5,5,5	1.47	1 (20%)	5,5,5	1.85	2 (40%)
2	FAD	D	600	1	48,58,58	0.98	3 (6%)	54,89,89	2.41	11 (20%)
7	TRK	D	700	4	28,31,31	1.61	6 (21%)	28,47,47	2.41	7 (25%)

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	1500	-	-	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
5	GOL	B	1500	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1501	-	-	0/4/4/4	0/0/0/0
2	FAD	B	600	1	-	0/30/50/50	0/6/6/6
7	TRK	B	700	4	-	0/17/62/62	0/1/3/3
5	GOL	C	1501	-	-	0/4/4/4	0/0/0/0
5	GOL	C	1502	-	-	0/4/4/4	0/0/0/0
2	FAD	C	600	1	-	0/30/50/50	0/6/6/6
3	TIR	C	700	4	-	0/17/62/62	0/1/3/3
5	GOL	D	1501	-	-	0/4/4/4	0/0/0/0
5	GOL	D	1502	-	-	0/4/4/4	0/0/0/0
2	FAD	D	600	1	-	0/30/50/50	0/6/6/6
7	TRK	D	700	4	-	0/17/62/62	0/1/3/3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	FAD	C10-N10	-4.00	1.34	1.39
3	C	700	TIR	C1-C2	-3.30	1.48	1.52
5	D	1502	GOL	O2-C2	-3.01	1.34	1.43
2	C	600	FAD	C9A-N10	-2.67	1.35	1.38
5	B	1501	GOL	O2-C2	-2.46	1.36	1.43
2	D	600	FAD	C6-C5X	-2.21	1.38	1.41
2	A	600	FAD	C10-N10	-2.19	1.36	1.39
2	A	600	FAD	C9A-N10	-2.13	1.35	1.38
7	B	700	TRK	O5-C16	2.03	1.46	1.43
2	A	600	FAD	C8M-C8	2.04	1.55	1.51
2	D	600	FAD	C5'-C4'	2.04	1.54	1.51
7	D	700	TRK	C21-C22	2.08	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	O3'-C3'	2.12	1.48	1.43
2	B	600	FAD	C5'-C4'	2.22	1.55	1.51
7	D	700	TRK	C13-C5	2.31	1.55	1.50
7	D	700	TRK	C9-C8	2.31	1.47	1.40
2	D	600	FAD	C4X-N5	2.34	1.37	1.33
3	C	700	TIR	C3-C4	2.39	1.47	1.40
3	A	700	TIR	C1-N	2.41	1.48	1.45
3	C	700	TIR	O1-C2	2.50	1.28	1.23
3	A	700	TIR	O6-C22	2.55	1.28	1.23
7	D	700	TRK	C7-C8	2.61	1.48	1.45
3	C	700	TIR	C13-C16	2.63	1.55	1.51
2	C	600	FAD	C4X-N5	2.70	1.37	1.33
3	C	700	TIR	C16-C17	2.70	1.53	1.50
3	A	700	TIR	O1-C2	2.74	1.29	1.23
3	C	700	TIR	O6-C22	2.82	1.29	1.23
7	B	700	TRK	C9-C8	2.95	1.49	1.40
2	A	600	FAD	O4-C4	3.00	1.31	1.24
2	C	600	FAD	C2A-N3A	3.03	1.37	1.32
3	C	700	TIR	C17-C18	3.05	1.36	1.33
2	B	600	FAD	C4X-N5	3.06	1.38	1.33
3	A	700	TIR	C16-C17	3.13	1.54	1.50
2	A	600	FAD	O4B-C1B	3.17	1.45	1.41
2	C	600	FAD	C5X-N5	3.18	1.40	1.35
7	B	700	TRK	O3-C12	3.32	1.30	1.23
2	B	600	FAD	O3'-C3'	3.49	1.51	1.43
2	A	600	FAD	C4X-N5	3.60	1.39	1.33
7	D	700	TRK	O3-C12	3.68	1.31	1.23
7	D	700	TRK	C21-C19	3.73	1.38	1.33
3	C	700	TIR	C1-N	3.82	1.50	1.45
3	A	700	TIR	C17-C18	4.60	1.38	1.33

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	600	FAD	N3A-C2A-N1A	-12.37	119.42	128.89
2	B	600	FAD	N3A-C2A-N1A	-9.42	121.68	128.89
2	A	600	FAD	N3A-C2A-N1A	-9.26	121.80	128.89
2	C	600	FAD	N3A-C2A-N1A	-9.13	121.90	128.89
2	A	600	FAD	C4X-C4-N3	-6.26	115.03	123.59
7	D	700	TRK	C19-C21-C22	-5.95	117.42	123.81
7	B	700	TRK	C19-C21-C22	-5.42	117.99	123.81
3	C	700	TIR	C5-C4-C3	-4.91	119.47	124.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	700	TIR	O1-C2-C3	-4.66	120.98	128.81
2	D	600	FAD	C2B-C1B-N9A	-4.56	107.33	114.29
2	B	600	FAD	C2B-C1B-N9A	-4.50	107.42	114.29
7	B	700	TRK	C7-C6-C5	-4.48	119.39	126.22
2	B	600	FAD	C4X-C4-N3	-4.41	117.56	123.59
3	A	700	TIR	C5-C6-C7	-4.40	119.51	126.22
2	A	600	FAD	C2B-C1B-N9A	-4.35	107.65	114.29
7	B	700	TRK	O5-C17-O1	-4.33	107.19	110.95
3	C	700	TIR	C5-C6-C7	-4.29	119.68	126.22
7	D	700	TRK	C7-C6-C5	-4.22	119.78	126.22
2	D	600	FAD	C4X-C4-N3	-4.22	117.82	123.59
7	D	700	TRK	O3-C12-C9	-3.96	122.16	128.81
3	C	700	TIR	O3-C13-C16	-3.84	103.54	108.56
2	A	600	FAD	O2'-C2'-C1'	-3.59	101.12	109.94
3	C	700	TIR	O1-C2-C3	-3.50	122.93	128.81
7	D	700	TRK	C7-C8-C9	-3.49	120.88	124.36
3	A	700	TIR	C5-C4-C3	-3.48	120.89	124.36
3	A	700	TIR	C1-N-C22	-3.38	109.29	113.29
7	B	700	TRK	C11-N-C10	-3.36	109.32	113.29
2	C	600	FAD	O2'-C2'-C1'	-3.30	101.83	109.94
3	C	700	TIR	C6-C5-C4	-3.29	117.96	122.46
7	D	700	TRK	C11-N-C10	-3.23	109.47	113.29
2	C	600	FAD	C4A-C5A-N7A	-3.18	106.55	109.48
2	A	600	FAD	C4A-C5A-N7A	-3.17	106.56	109.48
5	C	1502	GOL	O3-C3-C2	-3.16	94.85	110.18
7	B	700	TRK	O3-C12-C9	-3.07	123.65	128.81
2	C	600	FAD	C1B-N9A-C4A	-3.03	122.37	126.94
7	B	700	TRK	C7-C8-C9	-3.02	121.35	124.36
2	C	600	FAD	C2B-C1B-N9A	-3.02	109.69	114.29
2	B	600	FAD	O2'-C2'-C1'	-2.95	102.69	109.94
3	C	700	TIR	C1-N-C22	-2.89	109.88	113.29
2	B	600	FAD	C1B-N9A-C4A	-2.83	122.67	126.94
3	C	700	TIR	O2-C11-O3	-2.74	108.58	110.95
7	D	700	TRK	O2-C10-C9	-2.72	119.83	129.33
2	C	600	FAD	C4X-C4-N3	-2.71	119.89	123.59
3	A	700	TIR	O2-C11-O3	-2.69	108.62	110.95
2	D	600	FAD	C4A-C5A-N7A	-2.54	107.15	109.48
5	D	1502	GOL	O2-C2-C3	-2.51	97.12	108.65
5	C	1502	GOL	O1-C1-C2	-2.48	98.17	110.18
3	A	700	TIR	O6-C22-C3	-2.46	120.73	129.33
7	B	700	TRK	O2-C10-N	-2.44	122.61	125.44
3	C	700	TIR	O6-C22-N	-2.37	122.69	125.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	700	TRK	C3-C2-C4	-2.36	105.76	110.03
2	D	600	FAD	O3B-C3B-C2B	-2.35	104.19	111.83
7	B	700	TRK	O2-C10-C9	-2.26	121.42	129.33
5	A	1500	GOL	O2-C2-C3	-2.23	98.42	108.65
3	A	700	TIR	C20-C9-C10	-2.22	106.84	111.08
2	B	600	FAD	C6-C7-C8	-2.06	116.11	120.04
2	A	600	FAD	O4B-C1B-N9A	2.01	112.31	108.10
3	C	700	TIR	O2-C11-C12	2.05	111.29	107.16
3	A	700	TIR	C11-O2-C10	2.05	118.99	114.33
2	D	600	FAD	C2A-N1A-C6A	2.09	122.50	118.77
2	D	600	FAD	O2'-C2'-C3'	2.10	114.29	109.02
2	D	600	FAD	C7M-C7-C8	2.11	125.37	120.73
2	C	600	FAD	C7-C6-C5X	2.13	124.40	120.92
2	B	600	FAD	C7-C6-C5X	2.31	124.70	120.92
2	D	600	FAD	O2P-P-O3P	2.32	115.61	105.09
5	B	1501	GOL	O3-C3-C2	2.36	121.64	110.18
3	A	700	TIR	O4-C16-C17	2.37	114.96	109.45
2	D	600	FAD	C4X-C10-N10	2.38	121.92	120.52
2	B	600	FAD	C2A-N1A-C6A	2.40	123.06	118.77
2	A	600	FAD	C7M-C7-C8	2.49	126.20	120.73
2	B	600	FAD	O4'-C4'-C3'	2.51	115.33	109.02
5	D	1502	GOL	C3-C2-C1	2.53	121.03	111.12
2	C	600	FAD	O2P-P-O3P	2.54	116.61	105.09
2	A	600	FAD	C4X-C10-N10	2.57	122.04	120.52
2	B	600	FAD	C1'-N10-C9A	2.59	121.77	118.86
2	C	600	FAD	C4X-N5-C5X	2.62	119.77	116.76
2	B	600	FAD	C4X-N5-C5X	2.62	119.78	116.76
7	B	700	TRK	C15-C14-C16	2.72	115.59	111.33
7	B	700	TRK	O4-C8-C7	2.75	119.18	115.63
2	C	600	FAD	O2A-PA-O3P	2.85	118.04	105.09
2	A	600	FAD	O2'-C2'-C3'	3.05	116.68	109.02
2	C	600	FAD	C4X-C10-N10	3.15	122.38	120.52
2	B	600	FAD	C4-C4X-N5	3.48	122.94	118.72
2	C	600	FAD	C4-C4X-N5	3.49	122.96	118.72
2	C	600	FAD	C4-N3-C2	3.78	118.52	115.25
2	C	600	FAD	C1'-N10-C9A	4.18	123.56	118.86
3	A	700	TIR	O5-C4-C5	4.31	121.19	115.63
3	C	700	TIR	O5-C4-C5	4.31	121.19	115.63
2	B	600	FAD	C4X-C10-N10	4.45	123.14	120.52
2	A	600	FAD	C4-C4X-N5	4.57	124.27	118.72
2	A	600	FAD	C4X-N5-C5X	5.19	122.73	116.76
2	B	600	FAD	C4-N3-C2	5.71	120.19	115.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	700	TRK	O4-C8-C7	6.28	123.74	115.63
2	D	600	FAD	C4-N3-C2	6.64	120.98	115.25
2	A	600	FAD	C4-N3-C2	10.25	124.11	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1500	GOL	1	0
2	A	600	FAD	9	0
3	A	700	TIR	5	0
5	B	1500	GOL	2	0
5	B	1501	GOL	7	0
2	B	600	FAD	1	0
7	B	700	TRK	3	0
5	C	1501	GOL	1	0
5	C	1502	GOL	10	0
2	C	600	FAD	9	0
3	C	700	TIR	5	0
5	D	1501	GOL	1	0
5	D	1502	GOL	1	0
2	D	600	FAD	6	0
7	D	700	TRK	2	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	492/530 (92%)	-0.21	15 (3%) 54 48	8, 15, 31, 45	0
1	B	487/530 (91%)	-0.24	12 (2%) 61 56	7, 15, 29, 50	0
1	C	492/530 (92%)	-0.21	10 (2%) 68 64	7, 14, 31, 42	0
1	D	491/530 (92%)	-0.18	17 (3%) 48 42	7, 15, 32, 45	0
All	All	1962/2120 (92%)	-0.21	54 (2%) 56 51	7, 15, 31, 50	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	365	TYR	10.0
1	D	500	ALA	8.2
1	C	500	ALA	7.8
1	D	208	PRO	7.1
1	C	368	PRO	7.1
1	A	208	PRO	6.5
1	B	363	THR	5.3
1	A	364	ASP	5.0
1	D	209	PRO	4.9
1	B	369	ALA	4.7
1	D	368	PRO	4.4
1	A	209	PRO	4.1
1	B	364	ASP	3.9
1	A	204	GLU	3.9
1	C	363	THR	3.9
1	C	499	PRO	3.8
1	C	208	PRO	3.8
1	C	203	ALA	3.6
1	A	363	THR	3.6
1	D	50	ARG	3.6
1	D	90	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	89	GLU	3.4
1	C	364	ASP	3.4
1	D	233	GLY	3.4
1	D	365	TYR	3.4
1	D	369	ALA	3.3
1	B	233	GLY	3.3
1	D	366	ASP	3.2
1	D	161	SER	3.1
1	A	499	PRO	3.1
1	B	310	HIS	3.0
1	B	232	GLU	3.0
1	A	4	ILE	3.0
1	A	369	ALA	3.0
1	C	233	GLY	3.0
1	A	366	ASP	2.9
1	A	367	ASN	2.9
1	D	499	PRO	2.7
1	B	499	PRO	2.7
1	A	161[A]	SER	2.7
1	B	209	PRO	2.7
1	D	363	THR	2.6
1	D	213	ARG	2.6
1	B	288	PRO	2.6
1	D	310	HIS	2.4
1	C	310	HIS	2.4
1	A	213	ARG	2.4
1	C	367	ASN	2.2
1	A	308	GLN	2.2
1	B	43[A]	GLN	2.2
1	A	174	SER	2.1
1	B	174	SER	2.1
1	D	176	PRO	2.0
1	B	308	GLN	2.0

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 [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	D	1502	6/6	0.87	0.16	12.02	27,29,30,30	0
5	GOL	D	1501	6/6	0.91	0.13	6.28	29,33,36,38	0
5	GOL	C	1502	6/6	0.97	0.16	3.77	23,28,31,35	0
5	GOL	B	1501	6/6	0.90	0.11	3.74	28,30,31,33	0
5	GOL	B	1500	6/6	0.91	0.12	3.20	31,33,35,35	0
5	GOL	C	1501	6/6	0.93	0.11	3.08	31,35,37,40	0
5	GOL	A	1500	6/6	0.95	0.10	2.35	30,33,34,38	0
7	TRK	B	700	29/29	0.96	0.08	1.65	14,18,20,20	0
3	TIR	C	700	29/29	0.96	0.08	1.40	12,15,18,21	0
7	TRK	D	700	29/29	0.96	0.07	0.82	12,16,20,21	0
3	TIR	A	700	29/29	0.97	0.07	0.50	12,15,20,21	0
2	FAD	D	600	53/53	0.98	0.06	-0.16	7,9,11,11	0
2	FAD	A	600	53/53	0.98	0.06	-0.31	6,9,11,16	0
2	FAD	B	600	53/53	0.98	0.07	-0.34	6,9,11,14	0
2	FAD	C	600	53/53	0.98	0.06	-0.52	5,8,11,13	0
6	CL	B	1502	1/1	1.00	0.03	-2.07	18,18,18,18	0
6	CL	C	1503	1/1	1.00	0.04	-2.82	24,24,24,24	0
4	MG	C	800	1/1	1.00	0.05	-	19,19,19,19	0
6	CL	C	1504	1/1	1.00	0.03	-	16,16,16,16	0
4	MG	A	800	1/1	1.00	0.03	-	19,19,19,19	0
6	CL	A	1501	1/1	0.99	0.04	-	19,19,19,19	0
6	CL	D	1503	1/1	1.00	0.04	-	19,19,19,19	0
6	CL	D	1504	1/1	0.95	0.07	-	54,54,54,54	0
4	MG	B	800	1/1	0.99	0.09	-	21,21,21,21	0
4	MG	D	800	1/1	0.98	0.05	-	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.