



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:50 AM GMT

PDB ID : 4A99
Title : STRUCTURE OF THE TETRACYCLINE DEGRADING MONOOXYGENASE TETX IN COMPLEX WITH MINOCYCLINE
Authors : Volkers, G.; Palm, G.J.; Weiss, M.S.; Hinrichs, W.
Deposited on : 2011-11-25
Resolution : 2.18 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

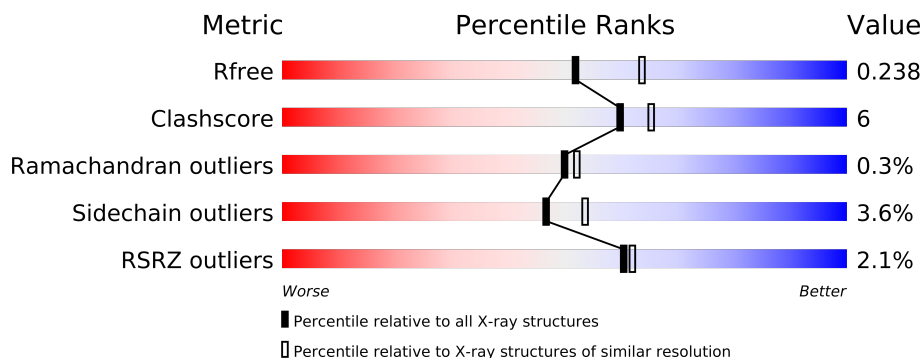
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.18 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	3841 (2.20-2.16)
Clashscore	79885	4835 (2.20-2.16)
Ramachandran outliers	78287	4740 (2.20-2.16)
Sidechain outliers	78261	4741 (2.20-2.16)
RSRZ outliers	66119	3842 (2.20-2.16)

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. 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	398	
1	B	398	
1	C	398	
1	D	398	

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	SO4	A	1383	-	X
4	SO4	B	1384	-	X
4	SO4	B	1385	-	X
4	SO4	C	1383	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	SO4	D	1384	-	X
4	SO4	D	1385	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12662 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 TETX2 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	0	0
			2886	1826	489	559	12			
1	B	368	Total	C	N	O	S	0	0	0
			2883	1826	489	556	12			
1	C	367	Total	C	N	O	S	0	0	0
			2868	1817	485	554	12			
1	D	367	Total	C	N	O	S	0	0	0
			2859	1812	485	550	12			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	EXPRESSION TAG	UNP Q93L51
A	-8	GLY	-	EXPRESSION TAG	UNP Q93L51
A	-7	SER	-	EXPRESSION TAG	UNP Q93L51
A	-6	SER	-	EXPRESSION TAG	UNP Q93L51
A	-5	HIS	-	EXPRESSION TAG	UNP Q93L51
A	-4	HIS	-	EXPRESSION TAG	UNP Q93L51
A	-3	HIS	-	EXPRESSION TAG	UNP Q93L51
A	-2	HIS	-	EXPRESSION TAG	UNP Q93L51
A	-1	HIS	-	EXPRESSION TAG	UNP Q93L51
A	0	HIS	-	EXPRESSION TAG	UNP Q93L51
A	1	SER	-	EXPRESSION TAG	UNP Q93L51
A	2	SER	-	EXPRESSION TAG	UNP Q93L51
A	3	GLY	-	EXPRESSION TAG	UNP Q93L51
A	4	LEU	-	EXPRESSION TAG	UNP Q93L51
A	5	VAL	-	EXPRESSION TAG	UNP Q93L51
A	6	PRO	-	EXPRESSION TAG	UNP Q93L51
A	7	ARG	-	EXPRESSION TAG	UNP Q93L51
A	8	GLY	-	EXPRESSION TAG	UNP Q93L51
A	9	SER	-	EXPRESSION TAG	UNP Q93L51
A	10	HIS	-	EXPRESSION TAG	UNP Q93L51
B	-9	MET	-	EXPRESSION TAG	UNP Q93L51

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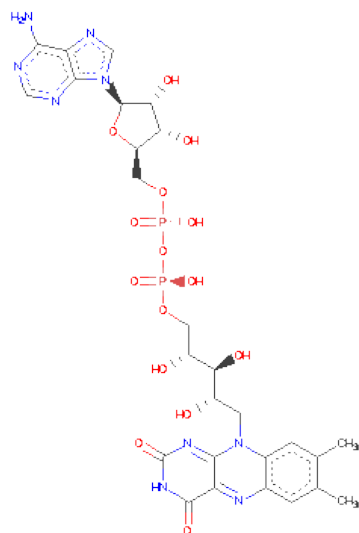
Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	GLY	-	EXPRESSION TAG	UNP Q93L51
B	-7	SER	-	EXPRESSION TAG	UNP Q93L51
B	-6	SER	-	EXPRESSION TAG	UNP Q93L51
B	-5	HIS	-	EXPRESSION TAG	UNP Q93L51
B	-4	HIS	-	EXPRESSION TAG	UNP Q93L51
B	-3	HIS	-	EXPRESSION TAG	UNP Q93L51
B	-2	HIS	-	EXPRESSION TAG	UNP Q93L51
B	-1	HIS	-	EXPRESSION TAG	UNP Q93L51
B	0	HIS	-	EXPRESSION TAG	UNP Q93L51
B	1	SER	-	EXPRESSION TAG	UNP Q93L51
B	2	SER	-	EXPRESSION TAG	UNP Q93L51
B	3	GLY	-	EXPRESSION TAG	UNP Q93L51
B	4	LEU	-	EXPRESSION TAG	UNP Q93L51
B	5	VAL	-	EXPRESSION TAG	UNP Q93L51
B	6	PRO	-	EXPRESSION TAG	UNP Q93L51
B	7	ARG	-	EXPRESSION TAG	UNP Q93L51
B	8	GLY	-	EXPRESSION TAG	UNP Q93L51
B	9	SER	-	EXPRESSION TAG	UNP Q93L51
B	10	HIS	-	EXPRESSION TAG	UNP Q93L51
C	-9	MET	-	EXPRESSION TAG	UNP Q93L51
C	-8	GLY	-	EXPRESSION TAG	UNP Q93L51
C	-7	SER	-	EXPRESSION TAG	UNP Q93L51
C	-6	SER	-	EXPRESSION TAG	UNP Q93L51
C	-5	HIS	-	EXPRESSION TAG	UNP Q93L51
C	-4	HIS	-	EXPRESSION TAG	UNP Q93L51
C	-3	HIS	-	EXPRESSION TAG	UNP Q93L51
C	-2	HIS	-	EXPRESSION TAG	UNP Q93L51
C	-1	HIS	-	EXPRESSION TAG	UNP Q93L51
C	0	HIS	-	EXPRESSION TAG	UNP Q93L51
C	1	SER	-	EXPRESSION TAG	UNP Q93L51
C	2	SER	-	EXPRESSION TAG	UNP Q93L51
C	3	GLY	-	EXPRESSION TAG	UNP Q93L51
C	4	LEU	-	EXPRESSION TAG	UNP Q93L51
C	5	VAL	-	EXPRESSION TAG	UNP Q93L51
C	6	PRO	-	EXPRESSION TAG	UNP Q93L51
C	7	ARG	-	EXPRESSION TAG	UNP Q93L51
C	8	GLY	-	EXPRESSION TAG	UNP Q93L51
C	9	SER	-	EXPRESSION TAG	UNP Q93L51
C	10	HIS	-	EXPRESSION TAG	UNP Q93L51
D	-9	MET	-	EXPRESSION TAG	UNP Q93L51
D	-8	GLY	-	EXPRESSION TAG	UNP Q93L51
D	-7	SER	-	EXPRESSION TAG	UNP Q93L51

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	SER	-	EXPRESSION TAG	UNP Q93L51
D	-5	HIS	-	EXPRESSION TAG	UNP Q93L51
D	-4	HIS	-	EXPRESSION TAG	UNP Q93L51
D	-3	HIS	-	EXPRESSION TAG	UNP Q93L51
D	-2	HIS	-	EXPRESSION TAG	UNP Q93L51
D	-1	HIS	-	EXPRESSION TAG	UNP Q93L51
D	0	HIS	-	EXPRESSION TAG	UNP Q93L51
D	1	SER	-	EXPRESSION TAG	UNP Q93L51
D	2	SER	-	EXPRESSION TAG	UNP Q93L51
D	3	GLY	-	EXPRESSION TAG	UNP Q93L51
D	4	LEU	-	EXPRESSION TAG	UNP Q93L51
D	5	VAL	-	EXPRESSION TAG	UNP Q93L51
D	6	PRO	-	EXPRESSION TAG	UNP Q93L51
D	7	ARG	-	EXPRESSION TAG	UNP Q93L51
D	8	GLY	-	EXPRESSION TAG	UNP Q93L51
D	9	SER	-	EXPRESSION TAG	UNP Q93L51
D	10	HIS	-	EXPRESSION TAG	UNP Q93L51

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



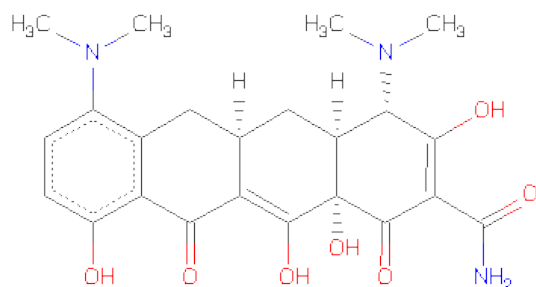
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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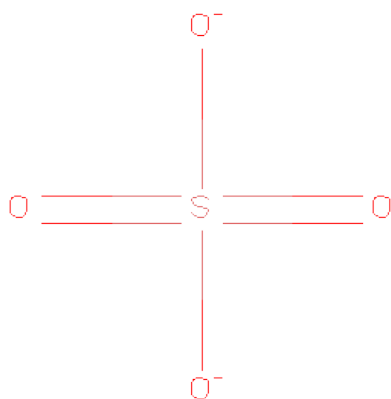
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is (4S,4AS,5AR,12AS)-4,7-BIS(DIMETHYLAMINO)-3,10,12,12A-TETRAHYDROXY-1,11-DIOXO-1,4,4A,5,5A,6,11,12A-OCTAHYDROTETRACENE-2-CARBOXAMIDE (three-letter code: MIY) (formula: C₂₃H₂₇N₃O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			33	23	3	7		
3	A	1	Total	C	N	O	0	0
			33	23	3	7		
3	B	1	Total	C	N	O	0	0
			33	23	3	7		
3	C	1	Total	C	N	O	0	0
			33	23	3	7		
3	C	1	Total	C	N	O	0	0
			33	23	3	7		
3	D	1	Total	C	N	O	0	0
			33	23	3	7		
3	D	1	Total	C	N	O	0	0
			33	23	3	7		
3	D	1	Total	C	N	O	0	0
			33	23	3	7		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	203	Total	O	0	0
			203	203		

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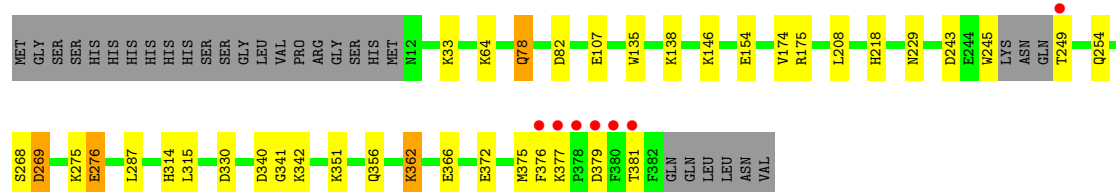
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	189	Total 189	O 189	0	0
5	C	134	Total 134	O 134	0	0
5	D	114	Total 114	O 114	0	0

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.

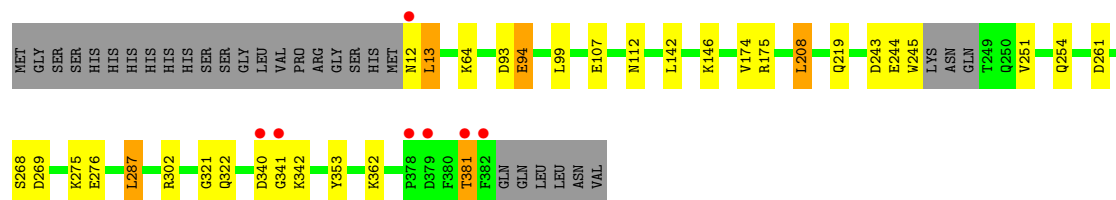
• Molecule 1: TETX2 PROTEIN

Chain A: 



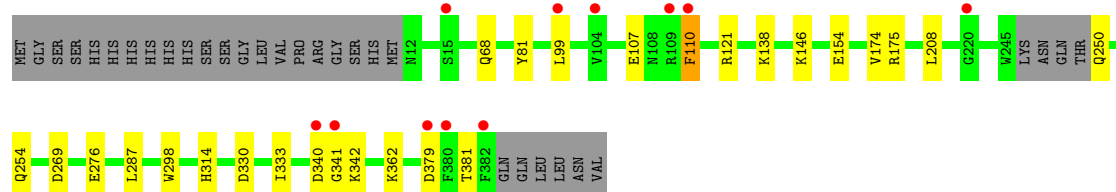
• Molecule 1: TETX2 PROTEIN

Chain B: 



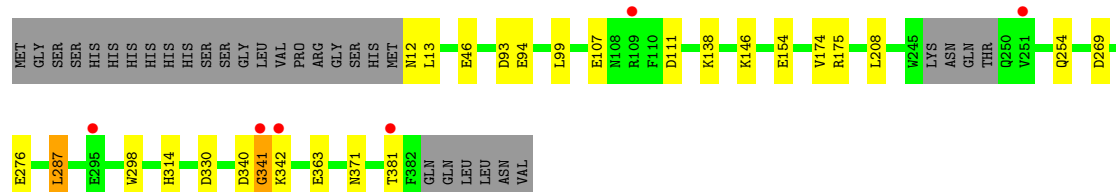
• Molecule 1: TETX2 PROTEIN

Chain C: 



• Molecule 1: TETX2 PROTEIN

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	68.88Å 80.33Å 86.63Å 110.82° 90.27° 93.39°	Depositor
Resolution (Å)	80.94 – 2.18 47.66 – 2.18	Depositor EDS
% Data completeness (in resolution range)	95.5 (80.94-2.18) 81.3 (47.66-2.18)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.6.0116	Depositor
R, R_{free}	0.185 , 0.235 0.189 , 0.238	Depositor DCC
R_{free} test set	4301 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 86442 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12662	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: MIY, SO4, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.90	5/2944 (0.2%)	0.89	3/3988 (0.1%)
1	B	0.92	3/2941 (0.1%)	0.99	10/3983 (0.3%)
1	C	0.79	1/2926 (0.0%)	0.83	4/3965 (0.1%)
1	D	0.82	3/2917 (0.1%)	0.85	6/3954 (0.2%)
All	All	0.86	12/11728 (0.1%)	0.89	23/15890 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	94	GLU	CD-OE2	-9.28	1.15	1.25
1	B	94	GLU	CD-OE1	-6.89	1.18	1.25
1	A	135	TRP	CD2-CE2	5.91	1.48	1.41
1	A	78	GLN	CD-NE2	-5.83	1.18	1.32
1	A	276	GLU	CD-OE1	5.72	1.31	1.25
1	D	371	ASN	CG-ND2	-5.59	1.18	1.32
1	A	245	TRP	CD2-CE2	5.40	1.47	1.41
1	B	276	GLU	CD-OE1	5.22	1.31	1.25
1	C	298	TRP	CD2-CE2	5.17	1.47	1.41
1	D	298	TRP	CD2-CE2	5.17	1.47	1.41
1	A	78	GLN	CD-OE1	-5.06	1.12	1.24
1	D	46	GLU	CD-OE2	5.03	1.31	1.25

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175	ARG	NE-CZ-NH2	-13.46	113.57	120.30
1	A	175	ARG	NE-CZ-NH2	-11.04	114.78	120.30
1	B	94	GLU	OE1-CD-OE2	-10.97	110.13	123.30
1	B	93	ASP	CB-CG-OD2	9.83	127.15	118.30
1	B	175	ARG	NE-CZ-NH1	9.81	125.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	287	LEU	CA-CB-CG	9.75	137.72	115.30
1	A	175	ARG	NE-CZ-NH1	9.72	125.16	120.30
1	B	93	ASP	CB-CG-OD1	8.78	126.20	118.30
1	B	93	ASP	OD1-CG-OD2	-8.77	106.64	123.30
1	D	287	LEU	CA-CB-CG	8.54	134.94	115.30
1	D	175	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	C	175	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	B	208	LEU	CA-CB-CG	6.61	130.50	115.30
1	C	175	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	B	99	LEU	CA-CB-CG	6.03	129.18	115.30
1	A	82	ASP	CB-CG-OD1	5.86	123.58	118.30
1	D	175	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	D	111	ASP	CB-CG-OD2	-5.85	113.04	118.30
1	D	93	ASP	CB-CG-OD1	5.70	123.43	118.30
1	C	121	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	C	99	LEU	CA-CB-CG	5.43	127.80	115.30
1	D	94	GLU	OE1-CD-OE2	-5.36	116.86	123.30
1	B	302	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2886	0	27	18	0
1	B	2883	0	27	17	0
1	C	2868	0	27	9	0
1	D	2859	0	27	9	0
2	A	53	0	31	4	0
2	B	53	0	31	3	0
2	C	53	0	31	1	0
2	D	53	0	31	2	0
3	A	66	0	48	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	33	0	24	2	0
3	C	66	0	49	5	0
3	D	99	0	73	6	0
4	A	5	0	0	0	0
4	B	15	0	0	0	0
4	C	15	0	0	0	0
4	D	15	0	0	0	0
5	A	203	0	0	7	0
5	B	189	0	0	11	0
5	C	134	0	0	1	0
5	D	114	0	0	0	0
All	All	12662	0	426	75	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 6.

All (75) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:269:ASP:CB	5:A:2163:HOH:O	2.02	1.04
1:D:12:ASN:HD21	1:D:341:GLY:CA	1.83	0.92
3:D:392:MIY:O2	3:D:392:MIY:H192	1.70	0.89
1:A:218:HIS:CD2	5:A:2063:HOH:O	2.35	0.79
1:C:250:GLN:N	5:C:2103:HOH:O	2.24	0.70
1:B:322:GLN:OE1	5:B:2176:HOH:O	2.09	0.69
1:B:321:GLY:O	5:B:2174:HOH:O	2.10	0.68
3:D:392:MIY:C19	3:D:392:MIY:O2	2.43	0.65
3:D:393:MIY:C8	3:D:393:MIY:H712	2.30	0.62
2:D:389:FAD:N1	2:D:389:FAD:H2'	2.15	0.60
1:D:12:ASN:ND2	1:D:341:GLY:CA	2.62	0.60
1:B:219:GLN:N	5:B:2140:HOH:O	2.35	0.59
1:C:333:ILE:CD1	3:C:392:MIY:HN73	2.32	0.59
2:B:389:FAD:H2'	2:B:389:FAD:N1	2.19	0.58
1:B:381:THR:CA	5:B:2185:HOH:O	2.51	0.57
2:C:389:FAD:N1	2:C:389:FAD:H2'	2.19	0.56
1:A:229:ASN:ND2	5:A:2028:HOH:O	2.39	0.55
1:B:243:ASP:CB	5:B:2147:HOH:O	2.55	0.55
1:B:64:LYS:NZ	5:B:2037:HOH:O	2.40	0.55
3:C:392:MIY:O5	3:C:392:MIY:O6	2.24	0.54
1:A:64:LYS:NZ	5:A:2039:HOH:O	2.41	0.53
1:A:33:LYS:NZ	5:A:2006:HOH:O	2.41	0.53
1:A:379:ASP:CG	1:A:379:ASP:O	2.47	0.52
1:B:174:VAL:CG2	1:B:174:VAL:O	2.57	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:392:MIY:HN72	3:C:392:MIY:N2	2.26	0.50
3:D:393:MIY:H81	3:D:393:MIY:H712	1.94	0.50
1:D:340:ASP:C	1:D:342:LYS:N	2.66	0.49
1:C:174:VAL:CG2	1:C:174:VAL:O	2.60	0.49
2:A:389:FAD:N1	2:A:389:FAD:H2'	2.28	0.49
1:D:314:HIS:NE2	1:D:330:ASP:OD2	2.45	0.48
1:B:245:TRP:O	5:B:2148:HOH:O	2.20	0.48
1:B:340:ASP:C	1:B:342:LYS:N	2.66	0.48
1:D:12:ASN:CG	1:D:13:LEU:H	2.17	0.48
1:C:340:ASP:C	1:C:342:LYS:N	2.68	0.47
1:A:78:GLN:NE2	3:A:392:MIY:O7	2.47	0.47
1:D:340:ASP:O	1:D:342:LYS:N	2.48	0.47
1:A:356:GLN:NE2	5:A:2192:HOH:O	2.48	0.47
1:A:340:ASP:C	1:A:342:LYS:N	2.68	0.47
1:B:243:ASP:CA	5:B:2147:HOH:O	2.63	0.46
3:D:393:MIY:O6	3:D:393:MIY:O5	2.33	0.45
1:C:138:LYS:NZ	1:C:154:GLU:OE1	2.49	0.45
1:C:314:HIS:NE2	1:C:330:ASP:OD2	2.50	0.45
1:B:112:ASN:ND2	5:B:2069:HOH:O	2.51	0.44
3:C:391:MIY:H5	3:C:391:MIY:H203	1.77	0.44
1:B:340:ASP:O	1:B:342:LYS:N	2.51	0.44
1:B:261:ASP:OD1	5:B:2151:HOH:O	2.21	0.44
2:B:389:FAD:H9	2:B:389:FAD:H1'1	1.75	0.44
1:A:372:GLU:O	1:A:376:PHE:CD2	2.71	0.44
1:A:362:LYS:O	1:A:366:GLU:CG	2.65	0.44
1:A:314:HIS:NE2	1:A:330:ASP:OD2	2.51	0.43
3:B:391:MIY:O6	3:B:391:MIY:O5	2.35	0.43
3:A:391:MIY:O6	3:A:391:MIY:O5	2.35	0.43
1:A:314:HIS:O	1:A:315:LEU:C	2.56	0.43
1:A:138:LYS:NZ	1:A:154:GLU:OE1	2.52	0.43
2:D:389:FAD:H1'1	2:D:389:FAD:H9	1.79	0.43
1:D:138:LYS:NZ	1:D:154:GLU:OE1	2.52	0.43
1:B:244:GLU:CD	1:B:244:GLU:N	2.71	0.43
2:A:389:FAD:H6	3:A:391:MIY:C19	2.48	0.43
3:B:391:MIY:H203	3:B:391:MIY:H5	1.74	0.42
1:B:94:GLU:N	1:B:94:GLU:OE1	2.52	0.42
1:A:340:ASP:O	1:A:342:LYS:N	2.53	0.42
1:B:268:SER:O	1:B:275:LYS:NZ	2.53	0.42
1:C:110:PHE:N	1:C:110:PHE:CD1	2.88	0.42
1:D:174:VAL:CG2	1:D:174:VAL:O	2.67	0.42
1:A:174:VAL:O	1:A:174:VAL:CG2	2.68	0.42
1:D:363:GLU:OE1	3:D:393:MIY:O6	2.37	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:13:LEU:H	1:B:13:LEU:HG	1.72	0.41
1:A:268:SER:O	1:A:275:LYS:NZ	2.54	0.41
1:C:68:GLN:NE2	1:C:81:TYR:OH	2.53	0.41
2:A:389:FAD:H9	5:A:2185:HOH:O	2.21	0.41
1:C:340:ASP:O	1:C:342:LYS:N	2.54	0.41
2:B:389:FAD:H9	5:B:2170:HOH:O	2.21	0.41
3:C:392:MIY:H203	3:C:392:MIY:H5	1.68	0.40
2:A:389:FAD:H9	2:A:389:FAD:H1'1	1.81	0.40
1:A:375:MET:CE	1:A:376:PHE:CE2	3.05	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	364/398 (92%)	352 (97%)	11 (3%)	1 (0%)	50	52
1	B	364/398 (92%)	350 (96%)	12 (3%)	2 (0%)	38	36
1	C	363/398 (91%)	348 (96%)	14 (4%)	1 (0%)	50	52
1	D	363/398 (91%)	348 (96%)	14 (4%)	1 (0%)	50	52
All	All	1454/1592 (91%)	1398 (96%)	51 (4%)	5 (0%)	50	52

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	13	LEU
1	A	341	GLY
1	B	341	GLY
1	D	341	GLY
1	C	341	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	312/345 (90%)	299 (96%)	13 (4%)	40	46
1	B	310/345 (90%)	298 (96%)	12 (4%)	43	50
1	C	307/345 (89%)	296 (96%)	11 (4%)	47	53
1	D	305/345 (88%)	296 (97%)	9 (3%)	53	62
All	All	1234/1380 (89%)	1189 (96%)	45 (4%)	47	53

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	GLU
1	A	146	LYS
1	A	208	LEU
1	A	243	ASP
1	A	249	THR
1	A	254	GLN
1	A	269	ASP
1	A	276	GLU
1	A	287	LEU
1	A	351	LYS
1	A	362	LYS
1	A	377	LYS
1	A	381	THR
1	B	12	ASN
1	B	107	GLU
1	B	142	LEU
1	B	146	LYS
1	B	208	LEU
1	B	251	VAL
1	B	254	GLN
1	B	269	ASP
1	B	287	LEU
1	B	353	TYR
1	B	362	LYS
1	B	381	THR
1	C	107	GLU

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Mol	Chain	Res	Type
1	C	110	PHE
1	C	146	LYS
1	C	208	LEU
1	C	254	GLN
1	C	269	ASP
1	C	276	GLU
1	C	287	LEU
1	C	362	LYS
1	C	379	ASP
1	C	381	THR
1	D	99	LEU
1	D	107	GLU
1	D	146	LYS
1	D	208	LEU
1	D	254	GLN
1	D	269	ASP
1	D	276	GLU
1	D	287	LEU
1	D	381	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	12	ASN
1	D	12	ASN

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 ⓘ

22 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	SO4	A	1383	-	4,4,4	0.57	0	6,6,6	0.31	0
2	FAD	A	389	-	58,58,58	1.26	8 (13%)	85,89,89	2.01	16 (18%)
3	MIY	A	391	-	36,36,36	1.38	4 (11%)	58,58,58	1.92	17 (29%)
3	MIY	A	392	-	36,36,36	1.26	4 (11%)	58,58,58	2.38	19 (32%)
4	SO4	B	1383	-	4,4,4	0.64	0	6,6,6	0.34	0
4	SO4	B	1384	-	4,4,4	0.58	0	6,6,6	0.28	0
4	SO4	B	1385	-	4,4,4	0.65	0	6,6,6	0.16	0
2	FAD	B	389	-	58,58,58	1.45	11 (18%)	85,89,89	2.45	17 (20%)
3	MIY	B	391	-	36,36,36	1.26	3 (8%)	58,58,58	1.93	16 (27%)
4	SO4	C	1383	-	4,4,4	0.81	0	6,6,6	0.27	0
4	SO4	C	1384	-	4,4,4	0.56	0	6,6,6	0.37	0
4	SO4	C	1385	-	4,4,4	0.48	0	6,6,6	0.21	0
2	FAD	C	389	-	58,58,58	1.29	7 (12%)	85,89,89	2.60	19 (22%)
3	MIY	C	391	-	36,36,36	1.10	1 (2%)	58,58,58	2.18	16 (27%)
3	MIY	C	392	-	36,36,36	1.54	7 (19%)	58,58,58	2.76	21 (36%)
4	SO4	D	1383	-	4,4,4	0.90	0	6,6,6	0.23	0
4	SO4	D	1384	-	4,4,4	0.63	0	6,6,6	0.40	0
4	SO4	D	1385	-	4,4,4	0.66	0	6,6,6	0.25	0
2	FAD	D	389	-	58,58,58	1.31	8 (13%)	85,89,89	2.59	18 (21%)
3	MIY	D	391	-	36,36,36	1.08	3 (8%)	58,58,58	2.13	18 (31%)
3	MIY	D	392	-	36,36,36	1.38	5 (13%)	58,58,58	2.77	21 (36%)
3	MIY	D	393	-	36,36,36	1.10	3 (8%)	58,58,58	3.19	22 (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
4	SO4	A	1383	-	-	0/0/0/0	0/0/0/0
2	FAD	A	389	-	-	0/34/50/50	0/1/6/6
3	MIY	A	391	-	-	0/12/70/70	0/0/4/4
3	MIY	A	392	-	-	0/12/70/70	0/0/4/4
4	SO4	B	1383	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1384	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1385	-	-	0/0/0/0	0/0/0/0
2	FAD	B	389	-	-	0/34/50/50	0/1/6/6
3	MIY	B	391	-	-	0/12/70/70	0/0/4/4
4	SO4	C	1383	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1384	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1385	-	-	0/0/0/0	0/0/0/0
2	FAD	C	389	-	-	0/34/50/50	0/1/6/6
3	MIY	C	391	-	-	0/12/70/70	0/0/4/4
3	MIY	C	392	-	-	0/12/70/70	0/0/4/4
4	SO4	D	1383	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1384	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1385	-	-	0/0/0/0	0/0/0/0
2	FAD	D	389	-	-	0/34/50/50	0/1/6/6
3	MIY	D	391	-	-	0/12/70/70	0/0/4/4
3	MIY	D	392	-	-	0/12/70/70	0/0/4/4
3	MIY	D	393	-	-	0/12/70/70	0/0/4/4

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	392	MIY	C18-C5	4.45	1.57	1.53
2	B	389	FAD	C5X-N5	4.23	1.41	1.35
3	A	391	MIY	C18-C5	3.79	1.56	1.53
3	C	392	MIY	C16-C17	-3.67	1.31	1.36
3	C	392	MIY	C18-C5	3.53	1.56	1.53
2	D	389	FAD	O5'-C5'	-3.49	1.30	1.44
2	C	389	FAD	C2A-N1A	3.45	1.40	1.33
2	B	389	FAD	O5'-C5'	-3.41	1.30	1.44
3	A	391	MIY	C6-C5	-3.31	1.48	1.53
2	D	389	FAD	C6-C5X	-3.23	1.37	1.41
2	C	389	FAD	O5'-C5'	-3.18	1.31	1.44
2	D	389	FAD	C10-N1	3.18	1.41	1.35
2	C	389	FAD	C10-N1	3.00	1.41	1.35
3	D	392	MIY	C4-C3	2.96	1.56	1.51
3	D	391	MIY	C18-C5	2.89	1.55	1.53
2	D	389	FAD	C8A-N9A	2.87	1.40	1.36
2	C	389	FAD	C8A-N9A	2.82	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	389	FAD	C2A-N3A	2.82	1.37	1.32
2	B	389	FAD	C4-C4X	-2.81	1.36	1.41
2	A	389	FAD	C1'-N10	2.81	1.51	1.48
3	D	393	MIY	O5-C15	2.78	1.29	1.23
3	D	392	MIY	O7-C18	2.74	1.46	1.42
2	D	389	FAD	C2A-N3A	2.72	1.37	1.32
3	C	392	MIY	C4-C3	2.71	1.56	1.51
2	B	389	FAD	C6-C5X	-2.59	1.38	1.41
2	B	389	FAD	C2B-C1B	-2.58	1.49	1.53
2	A	389	FAD	O5'-C5'	-2.57	1.34	1.44
3	B	391	MIY	C18-C5	2.57	1.55	1.53
2	A	389	FAD	PA-O3P	2.55	1.64	1.59
3	A	392	MIY	C7-C16	2.55	1.54	1.51
2	B	389	FAD	C2A-N1A	2.53	1.38	1.33
3	C	392	MIY	O5-C15	2.52	1.28	1.23
2	B	389	FAD	O4'-C4'	2.51	1.49	1.43
2	A	389	FAD	O4B-C4B	-2.51	1.39	1.45
2	A	389	FAD	C1'-C2'	2.46	1.53	1.51
2	A	389	FAD	C2B-C1B	-2.41	1.50	1.53
3	C	392	MIY	C5-C4	2.40	1.57	1.54
3	D	393	MIY	C14-C9	2.40	1.44	1.40
2	D	389	FAD	C2A-N1A	2.40	1.38	1.33
2	B	389	FAD	C1'-C2'	2.39	1.53	1.51
3	B	391	MIY	C10-C9	2.37	1.43	1.40
3	D	392	MIY	C14-C15	2.35	1.52	1.46
2	A	389	FAD	C2A-N3A	2.32	1.36	1.32
3	D	391	MIY	C6-C5	-2.31	1.49	1.53
3	A	391	MIY	C14-C15	2.31	1.52	1.46
3	B	391	MIY	C5-C4	-2.29	1.51	1.54
2	D	389	FAD	C2-N3	2.27	1.41	1.37
3	A	392	MIY	C14-C15	2.26	1.52	1.46
3	D	392	MIY	C14-C13	-2.26	1.37	1.41
3	C	391	MIY	C2-C21	2.24	1.51	1.47
3	C	392	MIY	C18-C17	2.24	1.54	1.52
2	A	389	FAD	C5X-N5	2.20	1.38	1.35
3	A	392	MIY	O5-C15	2.19	1.28	1.23
3	D	391	MIY	C2-C21	2.17	1.51	1.47
3	C	392	MIY	O7-C18	2.15	1.45	1.42
3	A	391	MIY	C18-C1	-2.13	1.51	1.55
3	D	392	MIY	C18-C1	-2.08	1.51	1.55
2	D	389	FAD	O2'-C2'	-2.04	1.38	1.43
2	B	389	FAD	C10-N1	2.04	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	389	FAD	PA-O3P	2.01	1.63	1.59
3	D	393	MIY	C4-C3	2.01	1.55	1.51
2	C	389	FAD	O2'-C2'	-2.01	1.38	1.43
2	B	389	FAD	C4-N3	2.01	1.40	1.37
2	C	389	FAD	C4X-N5	2.00	1.40	1.36

All (220) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	393	MIY	C9-C10-N7	17.49	129.57	119.06
2	D	389	FAD	N3A-C2A-N1A	-13.80	117.18	128.71
2	D	389	FAD	C5'-C4'-C3'	-13.71	86.19	112.06
2	C	389	FAD	C5'-C4'-C3'	-13.30	86.95	112.06
2	B	389	FAD	C5'-C4'-C3'	-12.95	87.62	112.06
2	A	389	FAD	N3A-C2A-N1A	-12.64	118.14	128.71
2	C	389	FAD	N3A-C2A-N1A	-12.34	118.39	128.71
2	B	389	FAD	N3A-C2A-N1A	-11.92	118.74	128.71
3	D	392	MIY	C5-C4-N1	11.48	130.16	110.45
3	C	392	MIY	O6-C17-C16	-9.74	114.63	123.90
3	A	392	MIY	C5-C4-N1	8.23	124.58	110.45
3	C	392	MIY	C20-N1-C4	-7.01	98.95	114.11
3	C	392	MIY	C5-C18-C17	7.00	113.35	109.80
3	D	391	MIY	C6-C5-C18	-6.42	99.02	109.52
3	C	391	MIY	C6-C5-C18	-6.32	99.18	109.52
3	D	391	MIY	C20-N1-C4	-6.24	100.63	114.11
3	C	391	MIY	C20-N1-C4	-6.14	100.83	114.11
2	C	389	FAD	C8A-N9A-C4A	5.88	111.39	106.90
2	B	389	FAD	C2'-C1'-N10	-5.81	104.75	112.45
3	B	391	MIY	C6-C5-C18	-5.73	100.15	109.52
3	D	392	MIY	C21-C2-C1	-5.70	114.91	121.05
3	D	393	MIY	C11-C10-N7	-5.57	113.70	121.55
3	D	392	MIY	O7-C18-C5	5.52	117.08	110.08
3	C	392	MIY	C6-C5-C18	-5.16	101.09	109.52
3	B	391	MIY	O6-C17-C16	-5.14	119.01	123.90
3	C	392	MIY	C3-C4-N1	-5.12	101.78	113.34
3	A	392	MIY	O7-C18-C5	5.06	116.49	110.08
3	A	392	MIY	C5-C18-C1	-4.99	105.03	111.07
3	D	392	MIY	C18-C5-C4	4.88	118.83	111.80
3	C	392	MIY	O6-C17-C18	4.88	121.47	113.57
3	D	393	MIY	C5-C18-C17	4.83	112.25	109.80
2	A	389	FAD	C5X-C9A-N10	4.82	121.55	116.80
3	D	392	MIY	C20-N1-C4	-4.75	103.85	114.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	391	MIY	O6-C17-C16	-4.74	119.39	123.90
3	A	392	MIY	C7-C6-C5	-4.60	101.64	110.59
3	A	392	MIY	C20-N1-C4	-4.54	104.29	114.11
3	B	391	MIY	C20-N1-C4	-4.54	104.30	114.11
2	C	389	FAD	C2'-C1'-N10	-4.47	106.51	112.45
3	A	391	MIY	C6-C5-C18	-4.46	102.23	109.52
2	C	389	FAD	C5X-C9A-N10	4.46	121.19	116.80
3	C	391	MIY	C5-C4-N1	4.42	118.03	110.45
3	D	393	MIY	C3-C4-N1	-4.39	103.42	113.34
3	D	392	MIY	C6-C5-C4	-4.38	106.97	112.48
3	A	391	MIY	C20-N1-C4	-4.34	104.73	114.11
3	C	392	MIY	C5-C4-N1	4.26	117.76	110.45
3	A	392	MIY	C1-C18-C17	-4.24	104.69	109.79
2	D	389	FAD	C8A-N9A-C4A	4.21	110.11	106.90
3	C	392	MIY	C19-N1-C4	4.16	123.10	114.11
2	D	389	FAD	C2'-C1'-N10	-4.16	106.94	112.45
3	D	392	MIY	C5-C18-C17	-4.07	107.73	109.80
2	D	389	FAD	C5X-C9A-N10	4.05	120.79	116.80
3	D	393	MIY	C20-N1-C4	-3.99	105.49	114.11
3	C	392	MIY	C1-C18-C17	-3.90	105.09	109.79
3	A	391	MIY	C5-C4-N1	3.89	117.13	110.45
3	A	392	MIY	O6-C17-C16	-3.87	120.22	123.90
3	C	391	MIY	C3-C4-N1	-3.81	104.74	113.34
3	D	393	MIY	C5-C4-N1	3.81	116.98	110.45
2	C	389	FAD	C4X-C10-N10	-3.80	118.61	120.51
3	A	391	MIY	C21-C2-C3	3.80	126.68	118.44
2	B	389	FAD	O5'-P-O1P	-3.74	94.74	109.37
3	D	392	MIY	C5-C18-C1	-3.73	106.55	111.07
2	A	389	FAD	C9A-N10-C10	-3.71	118.13	121.77
3	D	393	MIY	C6-C5-C18	-3.70	103.47	109.52
3	D	392	MIY	O8-C21-N2	-3.68	113.63	122.93
3	D	391	MIY	C5-C4-N1	3.63	116.68	110.45
3	D	391	MIY	C6-C5-C4	-3.61	107.94	112.48
3	B	391	MIY	C21-C2-C3	3.57	126.19	118.44
3	D	392	MIY	C8-C7-C16	3.57	114.81	108.94
3	D	391	MIY	O8-C21-N2	-3.57	113.91	122.93
2	A	389	FAD	C2'-C1'-N10	-3.55	107.74	112.45
2	C	389	FAD	N3A-C4A-N9A	3.52	131.78	125.43
3	C	391	MIY	C1-C2-C3	-3.51	114.57	120.41
3	D	392	MIY	C71-N7-C10	-3.48	104.47	115.17
3	D	393	MIY	C8-C7-C16	3.47	114.64	108.94
2	B	389	FAD	N3A-C4A-N9A	3.44	131.65	125.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	391	MIY	O8-C21-N2	-3.44	114.23	122.93
3	D	392	MIY	C11-C12-C13	-3.44	116.75	120.50
3	A	391	MIY	C3-C4-N1	-3.44	105.57	113.34
3	D	391	MIY	O6-C17-C16	-3.44	120.63	123.90
3	C	391	MIY	C21-C2-C3	3.42	125.86	118.44
3	D	393	MIY	C13-C14-C15	-3.39	115.89	121.16
3	D	393	MIY	C1-C2-C3	-3.35	114.83	120.41
3	D	391	MIY	C1-C2-C3	-3.33	114.87	120.41
3	A	392	MIY	C21-C2-C1	-3.32	117.47	121.05
2	A	389	FAD	N3A-C4A-N9A	3.32	131.43	125.43
3	A	392	MIY	C5-C18-C17	3.30	111.47	109.80
3	D	393	MIY	C1-C18-C17	-3.28	105.84	109.79
3	A	392	MIY	C3-C4-N1	-3.26	105.97	113.34
3	C	392	MIY	C9-C10-N7	-3.26	117.11	119.06
3	A	392	MIY	C8-C7-C16	3.26	114.30	108.94
3	D	393	MIY	C13-C14-C9	3.21	122.87	119.11
2	B	389	FAD	C5X-C9A-N10	3.21	119.96	116.80
2	B	389	FAD	C2-N1-C10	3.19	118.19	114.98
3	D	392	MIY	C21-C2-C3	3.19	125.35	118.44
3	C	392	MIY	O2-C3-C2	-3.19	117.67	122.78
3	B	391	MIY	C1-C2-C3	-3.18	115.12	120.41
3	A	391	MIY	C1-C2-C3	-3.16	115.15	120.41
3	D	393	MIY	C11-C10-C9	-3.16	116.61	120.32
3	A	391	MIY	C7-C6-C5	-3.15	104.44	110.59
3	D	391	MIY	C3-C4-N1	-3.15	106.22	113.34
3	D	391	MIY	C21-C2-C3	3.14	125.25	118.44
3	C	391	MIY	C13-C14-C9	3.12	122.77	119.11
2	B	389	FAD	C4X-C10-N10	-3.12	118.95	120.51
2	A	389	FAD	O4B-C1B-N9A	-3.09	105.56	108.44
2	A	389	FAD	C2-N1-C10	3.08	118.08	114.98
3	C	391	MIY	C6-C5-C4	-3.08	108.61	112.48
3	C	391	MIY	O8-C21-N2	-3.07	115.18	122.93
2	D	389	FAD	N3A-C4A-N9A	3.06	130.97	125.43
3	A	392	MIY	C2-C21-N2	3.05	125.09	119.38
2	A	389	FAD	C1'-N10-C9A	3.04	121.83	118.87
3	A	392	MIY	O6-C17-C18	3.04	118.50	113.57
3	D	392	MIY	C5-C4-C3	-2.98	103.93	111.03
3	D	393	MIY	O8-C21-N2	-2.96	115.45	122.93
2	A	389	FAD	C8A-N9A-C4A	2.96	109.16	106.90
2	C	389	FAD	O4'-C4'-C3'	2.96	116.41	109.05
3	D	392	MIY	C1-C18-C17	-2.95	106.24	109.79
3	D	392	MIY	O6-C17-C16	-2.95	121.09	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	391	MIY	C2-C21-N2	2.93	124.87	119.38
3	D	391	MIY	C7-C6-C5	-2.91	104.92	110.59
2	D	389	FAD	C1B-N9A-C4A	-2.91	121.60	126.64
2	C	389	FAD	N7A-C8A-N9A	-2.90	106.15	114.36
3	A	391	MIY	O6-C17-C16	-2.89	121.15	123.90
3	B	391	MIY	O7-C18-C5	2.89	113.74	110.08
2	C	389	FAD	C1B-N9A-C4A	-2.85	121.72	126.64
3	B	391	MIY	O8-C21-N2	-2.80	115.85	122.93
3	A	391	MIY	C21-C2-C1	-2.79	118.05	121.05
3	D	392	MIY	C2-C21-N2	2.78	124.59	119.38
3	D	393	MIY	C21-C2-C3	2.77	124.44	118.44
2	C	389	FAD	C4X-N5-C5X	2.76	119.79	116.69
3	B	391	MIY	C7-C6-C5	-2.74	105.25	110.59
2	D	389	FAD	O3P-P-O5'	2.74	115.64	103.41
3	D	393	MIY	C19-N1-C4	2.71	119.97	114.11
3	C	392	MIY	C8-C9-C14	2.68	123.10	117.80
3	D	392	MIY	O2-C3-C2	-2.68	118.47	122.78
2	B	389	FAD	N7A-C8A-N9A	-2.68	106.77	114.36
2	D	389	FAD	O2B-C2B-C1B	-2.68	103.12	111.23
3	C	391	MIY	C7-C6-C5	-2.67	105.39	110.59
3	C	392	MIY	C6-C5-C4	2.66	115.84	112.48
3	C	391	MIY	C6-C7-C16	-2.63	104.25	109.51
3	A	392	MIY	C6-C5-C18	-2.62	105.24	109.52
2	A	389	FAD	N7A-C8A-N9A	-2.58	107.05	114.36
3	C	392	MIY	C2-C21-N2	2.58	124.20	119.38
2	D	389	FAD	N7A-C8A-N9A	-2.58	107.07	114.36
3	B	391	MIY	C21-C2-C1	-2.57	118.28	121.05
3	A	392	MIY	C21-C2-C3	2.55	123.97	118.44
3	D	393	MIY	C6-C7-C8	2.54	115.21	111.56
3	C	392	MIY	O8-C21-N2	-2.53	116.53	122.93
3	A	391	MIY	C9-C10-N7	-2.53	117.55	119.06
2	B	389	FAD	C8A-N9A-C4A	2.52	108.83	106.90
3	D	393	MIY	C2-C21-N2	2.51	124.07	119.38
3	B	391	MIY	C1-C18-C17	-2.51	106.77	109.79
2	B	389	FAD	C2A-N3A-C4A	2.50	121.14	114.01
3	D	391	MIY	C7-C16-C17	-2.50	119.81	122.50
3	C	392	MIY	C21-C2-C3	2.49	123.84	118.44
3	A	392	MIY	O1-C1-C18	2.49	123.80	118.63
2	C	389	FAD	C2A-N1A-C6A	2.48	123.25	118.77
2	C	389	FAD	O5'-P-O1P	-2.48	99.66	109.37
3	C	391	MIY	C7-C16-C17	-2.47	119.84	122.50
3	C	392	MIY	C7-C16-C17	-2.47	119.84	122.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	391	MIY	C7-C16-C17	-2.46	119.85	122.50
3	B	391	MIY	C71-N7-CN7	-2.46	107.33	115.78
2	C	389	FAD	O2B-C2B-C1B	-2.44	103.84	111.23
3	B	391	MIY	C6-C7-C16	-2.44	104.64	109.51
3	A	392	MIY	O8-C21-N2	-2.43	116.78	122.93
2	A	389	FAD	O4'-C4'-C3'	2.43	115.09	109.05
3	C	391	MIY	O2-C3-C4	-2.39	111.94	115.56
2	A	389	FAD	C1B-N9A-C4A	-2.39	122.50	126.64
2	C	389	FAD	O3B-C3B-C4B	-2.39	104.03	111.08
3	D	392	MIY	O2-C3-C4	-2.39	111.94	115.56
3	D	393	MIY	C15-C16-C17	-2.38	116.77	118.94
2	D	389	FAD	C2A-N3A-C4A	2.35	120.70	114.01
3	C	392	MIY	C5-C18-C1	-2.35	108.23	111.07
2	D	389	FAD	O4'-C4'-C3'	2.34	114.87	109.05
3	A	391	MIY	O7-C18-C17	-2.31	105.44	109.68
3	D	391	MIY	C8-C7-C16	2.30	112.73	108.94
2	A	389	FAD	C4-N3-C2	-2.31	120.66	125.39
2	D	389	FAD	C4-N3-C2	-2.31	120.66	125.39
2	A	389	FAD	C2A-N3A-C4A	2.29	120.54	114.01
3	D	393	MIY	O1-C1-C18	2.29	123.38	118.63
3	D	393	MIY	C12-C11-C10	2.27	124.51	119.34
3	D	391	MIY	O7-C18-C5	2.27	112.95	110.08
2	C	389	FAD	C4-N3-C2	-2.26	120.76	125.39
3	D	391	MIY	O2-C3-C4	-2.24	112.17	115.56
3	B	391	MIY	O6-C17-C18	2.24	117.20	113.57
3	A	391	MIY	O7-C18-C5	2.23	112.91	110.08
3	C	392	MIY	C21-C2-C1	-2.22	118.66	121.05
3	B	391	MIY	C5-C4-N1	2.21	114.24	110.45
3	C	392	MIY	C7-C16-C15	2.20	122.06	118.57
3	A	391	MIY	C6-C7-C16	-2.19	105.15	109.51
2	C	389	FAD	C2-N1-C10	2.18	117.17	114.98
3	C	392	MIY	CN7-N7-C10	-2.17	108.49	115.17
3	D	391	MIY	C5-C4-C3	2.17	116.19	111.03
3	A	391	MIY	C5-C18-C17	2.17	110.90	109.80
3	D	393	MIY	O2-C3-C2	-2.16	119.31	122.78
3	A	391	MIY	C71-N7-CN7	-2.16	108.34	115.78
3	C	391	MIY	C13-C14-C15	-2.16	117.81	121.16
2	D	389	FAD	C9A-N10-C10	-2.16	119.65	121.77
2	D	389	FAD	O4'-C4'-C5'	-2.15	105.69	110.12
2	D	389	FAD	C4X-C10-N10	-2.14	119.44	120.51
3	C	391	MIY	C19-N1-C4	-2.14	109.49	114.11
2	B	389	FAD	O2B-C2B-C1B	-2.13	104.77	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	389	FAD	O2'-C2'-C3'	2.13	114.35	109.05
2	C	389	FAD	O4B-C4B-C3B	2.13	109.48	105.17
2	B	389	FAD	C1B-N9A-C4A	-2.08	123.04	126.64
2	B	389	FAD	O5B-C5B-C4B	-2.07	101.33	108.94
3	D	391	MIY	C6-C7-C16	-2.07	105.38	109.51
2	B	389	FAD	C5A-C4A-N3A	-2.06	121.21	125.70
2	A	389	FAD	C2A-N1A-C6A	2.06	122.49	118.77
3	B	391	MIY	C6-C5-C4	-2.06	109.89	112.48
3	A	392	MIY	C19-N1-C4	2.05	118.55	114.11
2	D	389	FAD	C2-N1-C10	2.05	117.04	114.98
3	D	391	MIY	O7-C18-C17	-2.04	105.93	109.68
3	D	392	MIY	O7-C18-C17	2.04	113.43	109.68
2	C	389	FAD	O3P-P-O5'	2.04	112.52	103.41
2	B	389	FAD	C6-C5X-N5	2.04	121.35	118.97
3	A	391	MIY	C6-C5-C4	-2.02	109.94	112.48
2	B	389	FAD	C4-N3-C2	-2.01	121.26	125.39
2	A	389	FAD	O5'-P-O1P	2.01	117.23	109.37
3	A	392	MIY	C8-C9-C14	2.00	121.76	117.80
3	D	392	MIY	C11-C10-N7	-2.00	118.73	121.55

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, 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	368/398 (92%)	0.09	7 (1%) 64 65	33, 47, 77, 124	0
1	B	368/398 (92%)	0.13	7 (1%) 64 65	32, 48, 80, 124	0
1	C	367/398 (92%)	0.19	11 (2%) 48 50	36, 53, 85, 119	0
1	D	367/398 (92%)	0.15	6 (1%) 68 71	33, 52, 84, 118	0
All	All	1470/1592 (92%)	0.14	31 (2%) 60 62	32, 50, 83, 124	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	378	PRO	6.1
1	B	379	ASP	5.1
1	D	341	GLY	4.6
1	D	109	ARG	4.4
1	A	379	ASP	4.2
1	C	109	ARG	4.1
1	A	377	LYS	3.5
1	C	341	GLY	3.5
1	A	249	THR	3.4
1	C	379	ASP	3.3
1	A	381	THR	3.3
1	B	341	GLY	3.3
1	B	378	PRO	3.1
1	C	382	PHE	3.1
1	D	342	LYS	3.0
1	B	381	THR	2.9
1	A	376	PHE	2.8
1	C	340	ASP	2.8
1	C	110	PHE	2.6
1	D	251	VAL	2.6
1	B	382	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	220	GLY	2.4
1	D	381	THR	2.4
1	B	12	ASN	2.3
1	C	99	LEU	2.2
1	A	380	PHE	2.2
1	C	380	PHE	2.2
1	D	295	GLU	2.1
1	B	340	ASP	2.1
1	C	104	VAL	2.1
1	C	15	SER	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 ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	SO4	D	1385	5/5	0.23	107.00	81,86,93,98	5
4	SO4	B	1385	5/5	0.34	83.00	74,87,92,95	5
4	SO4	D	1384	5/5	0.22	19.65	65,70,80,83	0
4	SO4	B	1384	5/5	0.22	12.55	80,81,83,96	0
4	SO4	C	1383	5/5	0.19	3.08	81,85,105,109	0
4	SO4	A	1383	5/5	0.19	3.02	86,88,91,92	0
4	SO4	D	1383	5/5	0.18	0.64	72,93,95,102	0
2	FAD	A	389	53/53	0.13	0.38	29,38,52,67	0
3	MIY	B	391	33/33	0.15	0.30	32,47,62,71	0
3	MIY	D	392	33/33	0.12	0.25	38,45,54,69	0
2	FAD	C	389	53/53	0.12	-0.10	33,42,60,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	FAD	D	389	53/53	0.11	-0.13	33,42,56,62	0
3	MIY	D	391	33/33	0.11	-0.30	38,55,64,71	0
3	MIY	C	391	33/33	0.12	-0.31	41,50,58,63	0
3	MIY	A	391	33/33	0.12	-0.33	32,43,57,59	0
4	SO4	B	1383	5/5	0.14	-0.39	92,94,101,104	0
3	MIY	C	392	33/33	0.14	-0.40	42,52,55,62	0
2	FAD	B	389	53/53	0.11	-0.51	31,40,55,59	0
3	MIY	A	392	33/33	0.11	-0.52	42,50,55,56	0
4	SO4	C	1384	5/5	0.10	-0.52	79,80,84,87	0
3	MIY	D	393	33/33	0.12	-0.70	42,50,54,60	0
4	SO4	C	1385	5/5	0.14	-0.85	101,102,111,113	0

6.5 Other polymers ⓘ

There are no such residues in this entry.