



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 09:52 PM GMT

PDB ID : 2VYX  
Title : CRYSTAL STRUCTURE OF THE T. THERMOPHILUS DODECIN W38F  
MUTANT  
Authors : Essen, L.-O.; Meissner, B.  
Deposited on : 2008-07-29  
Resolution : 1.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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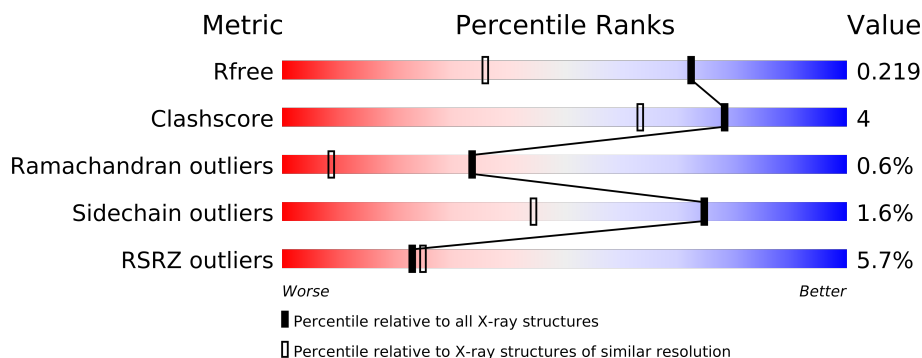
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 1.50 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	1513 (1.50-1.50)
Clashscore	79885	1768 (1.50-1.50)
Ramachandran outliers	78287	1720 (1.50-1.50)
Sidechain outliers	78261	1718 (1.50-1.50)
RSRZ outliers	66119	1514 (1.50-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	69	
1	B	69	
1	C	69	
1	D	69	
1	E	69	
1	F	69	
1	G	69	
1	H	69	
1	I	69	
1	J	69	
1	K	69	
1	L	69	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7888 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 TTHA1431.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	68	Total	C	N	O	0	0	1
			528	336	93	99			
1	B	66	Total	C	N	O	0	0	0
			518	331	91	96			
1	C	68	Total	C	N	O	0	0	0
			535	340	93	102			
1	D	68	Total	C	N	O	0	2	1
			540	344	93	103			
1	E	68	Total	C	N	O	0	2	1
			543	346	95	102			
1	F	68	Total	C	N	O	0	2	1
			534	339	95	100			
1	G	68	Total	C	N	O	0	3	1
			550	351	96	103			
1	H	68	Total	C	N	O	0	0	1
			528	336	93	99			
1	I	68	Total	C	N	O	0	1	1
			534	340	93	101			
1	J	68	Total	C	N	O	0	0	1
			528	336	93	99			
1	K	68	Total	C	N	O	0	2	0
			547	349	94	104			
1	L	66	Total	C	N	O	0	0	0
			518	331	91	96			

There are 12 discrepancies between the modelled and reference sequences:

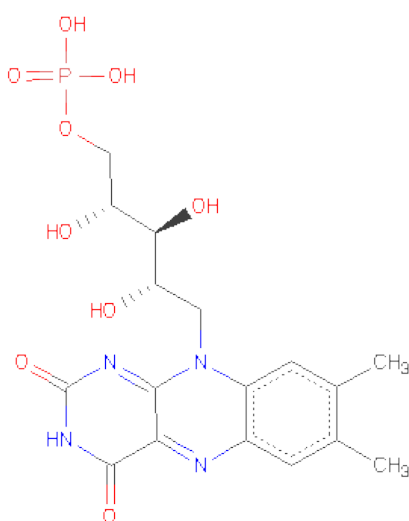
Chain	Residue	Modelled	Actual	Comment	Reference
A	38	PHE	TRP	ENGINEERED MUTATION	UNP Q5SIE3
B	38	PHE	TRP	ENGINEERED MUTATION	UNP Q5SIE3
C	38	PHE	TRP	ENGINEERED MUTATION	UNP Q5SIE3
D	38	PHE	TRP	ENGINEERED MUTATION	UNP Q5SIE3
E	38	PHE	TRP	ENGINEERED MUTATION	UNP Q5SIE3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	38	PHE	TRP	ENGINEERED MUTATION	UNP Q5SIE3
G	38	PHE	TRP	ENGINEERED MUTATION	UNP Q5SIE3
H	38	PHE	TRP	ENGINEERED MUTATION	UNP Q5SIE3
I	38	PHE	TRP	ENGINEERED MUTATION	UNP Q5SIE3
J	38	PHE	TRP	ENGINEERED MUTATION	UNP Q5SIE3
K	38	PHE	TRP	ENGINEERED MUTATION	UNP Q5SIE3
L	38	PHE	TRP	ENGINEERED MUTATION	UNP Q5SIE3

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



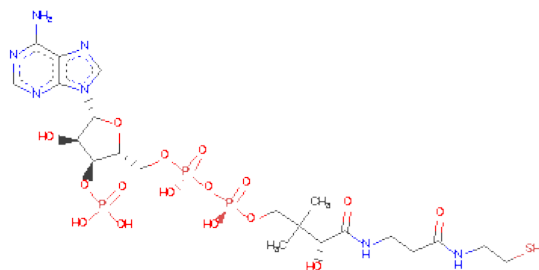
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	F	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	H	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	H	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is COENZYME A (three-letter code: COA) (formula:  $C_{21}H_{36}N_7O_{16}P_3S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
3	A	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
3	B	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
3	C	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
3	D	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
3	E	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
3	F	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	G	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	I	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	J	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	K	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	L	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	1	Total	Na	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	42	Total	O	0	0
			42	42		
6	B	52	Total	O	0	0
			52	52		
6	C	52	Total	O	0	0
			52	52		
6	D	56	Total	O	0	0
			56	56		
6	E	43	Total	O	0	0
			43	43		

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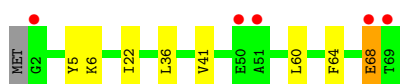
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	52	Total 52	O 52	0	0
6	G	50	Total 50	O 50	0	0
6	H	37	Total 37	O 37	0	0
6	I	43	Total 43	O 43	0	0
6	J	43	Total 43	O 43	0	0
6	K	34	Total 34	O 34	0	0
6	L	28	Total 28	O 28	0	0

### 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.

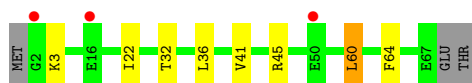
• Molecule 1: TTHA1431

Chain A:



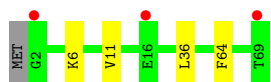
• Molecule 1: TTHA1431

Chain B:



• Molecule 1: TTHA1431

Chain C:



• Molecule 1: TTHA1431

Chain D:



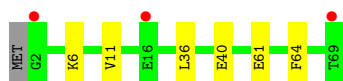
• Molecule 1: TTHA1431

Chain E:



• Molecule 1: TTHA1431

Chain F:

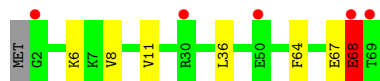




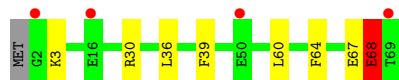
## ● Molecule 1: TTHA1431

Chain G: 

## ● Molecule 1: TTHA1431

Chain H: 

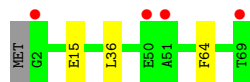
## ● Molecule 1: TTHA1431

Chain I: 

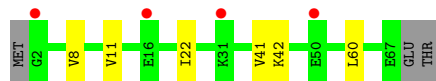
## ● Molecule 1: TTHA1431

Chain J: 

## ● Molecule 1: TTHA1431

Chain K: 

## ● Molecule 1: TTHA1431

Chain L: 

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.63Å 98.55Å 139.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	9.99 – 1.50 9.97 – 1.50	Depositor EDS
% Data completeness (in resolution range)	97.5 (9.99-1.50) 97.6 (9.97-1.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.05 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.218 , 0.250 0.226 , 0.219	Depositor DCC
$R_{free}$ test set	7305 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.3	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.49 , 59.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 145584 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7888	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: COA, FMN, CL, NA

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	0.45	0/533	0.65	0/713
1	B	0.52	0/523	0.75	1/699 (0.1%)
1	C	0.48	0/540	0.69	0/721
1	D	0.52	0/551	0.70	0/737
1	E	0.50	0/551	0.65	0/736
1	F	0.64	0/538	0.76	0/719
1	G	0.56	0/558	0.74	1/746 (0.1%)
1	H	0.50	0/533	0.65	0/713
1	I	0.51	0/542	0.72	0/725
1	J	0.50	0/533	0.69	0/713
1	K	0.45	0/558	0.62	0/744
1	L	0.43	0/523	0.59	0/699
All	All	0.51	0/6483	0.69	2/8665 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	60	LEU	CA-CB-CG	5.86	128.77	115.30
1	G	28	ARG	NE-CZ-NH1	5.56	123.08	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	528	0	544	7	0
1	B	518	0	538	6	0
1	C	535	0	551	3	0
1	D	540	0	556	3	0
1	E	543	0	562	4	0
1	F	534	0	546	5	0
1	G	550	0	570	3	0
1	H	528	0	544	5	0
1	I	534	0	550	4	0
1	J	528	0	544	6	0
1	K	547	0	570	2	0
1	L	518	0	538	4	0
2	A	62	0	38	1	0
2	B	62	0	38	2	0
2	C	62	0	38	1	0
2	D	62	0	38	2	0
2	F	62	0	38	1	0
2	H	62	0	38	1	0
3	A	96	0	64	2	0
3	B	48	0	32	4	0
3	C	48	0	32	0	0
3	D	48	0	32	0	0
3	E	48	0	32	1	0
3	F	48	0	32	0	0
3	G	48	0	32	3	0
3	I	48	0	32	0	0
3	J	48	0	32	1	0
3	K	48	0	32	1	0
3	L	48	0	32	0	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	F	1	0	0	0	0
6	A	42	0	0	0	0
6	B	52	0	0	1	0
6	C	52	0	0	0	0
6	D	56	0	0	0	0
6	E	43	0	0	0	0
6	F	52	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	50	0	0	1	0
6	H	37	0	0	0	0
6	I	43	0	0	0	0
6	J	43	0	0	0	0
6	K	34	0	0	1	0
6	L	28	0	0	0	0
All	All	7888	0	7225	53	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 4.

All (53) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:1071:COA:O9P	3:A:1071:COA:H141	1.90	0.69
1:K:15:GLU:OE1	6:K:2003:HOH:O	2.13	0.66
1:F:6:LYS:HE3	1:G:8[A]:VAL:HG13	1.80	0.64
1:C:36:LEU:HD23	1:C:64:PHE:HB3	1.81	0.62
1:J:42:LYS:HE3	1:J:61:GLU:HG3	1.85	0.58
1:I:36:LEU:HD23	1:I:64:PHE:HB3	1.85	0.58
1:F:40:GLU:OE1	1:F:61:GLU:OE1	2.23	0.57
2:B:1070:FMN:HM71	1:C:11:VAL:HG11	1.87	0.56
2:B:1068:FMN:HM71	1:F:11:VAL:HG11	1.89	0.54
2:D:1072:FMN:HM72	1:E:45:ARG:HD3	1.89	0.54
1:G:67:GLU:O	1:G:68:GLU:HB3	2.07	0.53
1:A:22:ILE:HG23	1:A:60:LEU:HD11	1.91	0.53
3:K:1070:COA:O9P	3:K:1070:COA:H141	2.08	0.53
1:A:36:LEU:HD23	1:A:64:PHE:HB3	1.93	0.51
2:A:1072:FMN:HM72	1:B:45:ARG:HD3	1.93	0.51
1:H:6:LYS:HE3	1:L:8:VAL:HG13	1.92	0.51
1:A:68:GLU:O	1:A:68:GLU:CG	2.58	0.50
1:H:36:LEU:HD23	1:H:64:PHE:HB3	1.95	0.49
1:K:36:LEU:HD23	1:K:64:PHE:HB3	1.95	0.48
1:D:11:VAL:HG11	2:F:1072:FMN:HM71	1.96	0.48
3:A:1071:COA:O9P	3:A:1071:COA:CEP	2.61	0.48
1:J:39:PHE:CD1	1:J:60:LEU:HD11	2.49	0.47
1:L:41:VAL:HG22	1:L:60:LEU:CD2	2.43	0.47
1:B:41:VAL:HG22	1:B:60:LEU:HD23	1.95	0.47
1:C:6:LYS:HE3	1:J:8:VAL:HG13	1.97	0.46
1:I:67:GLU:O	1:I:68:GLU:HB2	2.16	0.46
1:G:32:THR:O	3:G:1070:COA:H8A	2.15	0.46
1:L:22:ILE:HG23	1:L:60:LEU:HD11	1.98	0.46
1:B:22:ILE:HG23	1:B:60:LEU:HD11	1.96	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:36:LEU:HD23	1:B:64:PHE:HB3	1.97	0.46
1:I:39:PHE:CD1	1:I:60:LEU:HD11	2.51	0.46
1:A:68:GLU:HG3	1:A:68:GLU:O	2.15	0.45
1:E:36:LEU:HD23	1:E:64:PHE:HB3	1.98	0.45
3:B:1069:COA:H61	3:G:1070:COA:H10	2.00	0.44
2:C:1070:FMN:HM72	1:J:45:ARG:HD3	2.00	0.44
1:F:36:LEU:HD23	1:F:64:PHE:HB3	2.00	0.44
1:B:41:VAL:HG22	1:B:60:LEU:CD2	2.48	0.43
1:H:67:GLU:O	1:H:68:GLU:O	2.36	0.43
3:B:1069:COA:O2A	6:B:2047:HOH:O	2.21	0.42
1:D:3:LYS:NZ	2:D:1070:FMN:O1P	2.38	0.42
1:A:41:VAL:HG22	1:A:60:LEU:CD2	2.50	0.41
1:B:32:THR:O	3:B:1069:COA:H8A	2.20	0.41
1:J:13:THR:HG22	1:J:57:GLN:HG2	2.02	0.41
3:B:1069:COA:C6P	3:G:1070:COA:H10	2.50	0.41
1:D:45:ARG:NH1	1:F:40:GLU:HG2	2.36	0.41
3:J:1070:COA:O9P	3:J:1070:COA:H141	2.21	0.41
1:E:32:THR:O	3:E:1070:COA:H8A	2.20	0.41
2:H:1070:FMN:HM71	1:L:11:VAL:HG11	2.03	0.41
1:E:9:GLU:OE2	1:E:42[B]:LYS:NZ	2.46	0.41
6:G:2032:HOH:O	1:I:30:ARG:HD2	2.20	0.41
1:A:5:TYR:HB2	1:H:11:VAL:HB	2.02	0.41
1:J:36:LEU:HD23	1:J:64:PHE:HB3	2.03	0.40
1:A:6:LYS:HE3	1:H:8:VAL:HG13	2.04	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	66/69 (96%)	65 (98%)	1 (2%)	0	100	100
1	B	64/69 (93%)	64 (100%)	0	0	100	100
1	C	66/69 (96%)	66 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	68/69 (99%)	67 (98%)	1 (2%)	0	100	100
1	E	68/69 (99%)	67 (98%)	0	1 (2%)	15	2
1	F	67/69 (97%)	67 (100%)	0	0	100	100
1	G	69/69 (100%)	68 (99%)	0	1 (1%)	16	2
1	H	66/69 (96%)	65 (98%)	0	1 (2%)	15	2
1	I	67/69 (97%)	65 (97%)	1 (2%)	1 (2%)	15	2
1	J	66/69 (96%)	62 (94%)	3 (4%)	1 (2%)	15	2
1	K	68/69 (99%)	67 (98%)	1 (2%)	0	100	100
1	L	64/69 (93%)	62 (97%)	2 (3%)	0	100	100
All	All	799/828 (96%)	785 (98%)	9 (1%)	5 (1%)	33	9

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	68	GLU
1	H	68	GLU
1	I	68	GLU
1	J	68	GLU
1	G	68	GLU

### 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	53/55 (96%)	52 (98%)	1 (2%)	69	35
1	B	52/55 (94%)	51 (98%)	1 (2%)	69	35
1	C	54/55 (98%)	54 (100%)	0	100	100
1	D	55/55 (100%)	55 (100%)	0	100	100
1	E	55/55 (100%)	53 (96%)	2 (4%)	47	12
1	F	53/55 (96%)	53 (100%)	0	100	100
1	G	56/55 (102%)	55 (98%)	1 (2%)	71	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	53/55 (96%)	52 (98%)	1 (2%)	69	35
1	I	54/55 (98%)	52 (96%)	2 (4%)	45	11
1	J	53/55 (96%)	52 (98%)	1 (2%)	69	35
1	K	56/55 (102%)	56 (100%)	0	100	100
1	L	52/55 (94%)	51 (98%)	1 (2%)	69	35
All	All	646/660 (98%)	636 (98%)	10 (2%)	75	47

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

Mol	Chain	Res	Type
1	A	68	GLU
1	B	3	LYS
1	E	3	LYS
1	E	68	GLU
1	G	68	GLU
1	H	68	GLU
1	I	3	LYS
1	I	68	GLU
1	J	68	GLU
1	L	42	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 5.6 Ligand geometry

Of 29 ligands modelled in this entry, 5 are monoatomic - leaving 24 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$
2	FMN	A	1070	-	33,33,33	1.02	2 (6%)	46,50,50	1.43	7 (15%)
3	COA	A	1071	-	50,50,50	1.54	3 (6%)	75,75,75	1.74	10 (13%)
2	FMN	A	1072	-	33,33,33	1.03	2 (6%)	46,50,50	1.33	6 (13%)
3	COA	A	1073	-	50,50,50	1.53	4 (8%)	75,75,75	1.55	7 (9%)
2	FMN	B	1068	-	33,33,33	0.99	2 (6%)	46,50,50	1.33	8 (17%)
3	COA	B	1069	-	50,50,50	1.45	4 (8%)	75,75,75	1.56	9 (12%)
2	FMN	B	1070	-	33,33,33	0.98	4 (12%)	46,50,50	1.42	7 (15%)
2	FMN	C	1070	-	33,33,33	1.03	2 (6%)	46,50,50	1.57	7 (15%)
3	COA	C	1071	-	50,50,50	1.45	3 (6%)	75,75,75	1.73	7 (9%)
2	FMN	C	1072	-	33,33,33	0.97	2 (6%)	46,50,50	1.53	5 (10%)
2	FMN	D	1070	-	33,33,33	1.06	3 (9%)	46,50,50	1.51	6 (13%)
3	COA	D	1071	-	50,50,50	1.45	4 (8%)	75,75,75	1.73	9 (12%)
2	FMN	D	1072	-	33,33,33	0.98	1 (3%)	46,50,50	1.52	6 (13%)
3	COA	E	1070	-	50,50,50	1.48	4 (8%)	75,75,75	1.49	7 (9%)
2	FMN	F	1070	-	33,33,33	0.93	1 (3%)	46,50,50	1.35	8 (17%)
3	COA	F	1071	-	50,50,50	1.45	3 (6%)	75,75,75	1.78	7 (9%)
2	FMN	F	1072	-	33,33,33	1.08	3 (9%)	46,50,50	1.61	9 (19%)
3	COA	G	1070	-	50,50,50	1.52	3 (6%)	75,75,75	1.87	13 (17%)
2	FMN	H	1070	-	33,33,33	0.96	2 (6%)	46,50,50	1.52	7 (15%)
2	FMN	H	1071	-	33,33,33	0.94	1 (3%)	46,50,50	1.53	8 (17%)
3	COA	I	1070	-	50,50,50	1.44	4 (8%)	75,75,75	1.73	5 (6%)
3	COA	J	1070	-	50,50,50	1.46	3 (6%)	75,75,75	1.64	6 (8%)
3	COA	K	1070	-	50,50,50	1.48	2 (4%)	75,75,75	1.77	10 (13%)
3	COA	L	1068	-	50,50,50	1.48	4 (8%)	75,75,75	1.69	8 (10%)

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
2	FMN	A	1070	-	-	0/18/18/18	0/0/3/3
3	COA	A	1071	-	1/1/11/13	0/48/64/64	0/1/3/3
2	FMN	A	1072	-	-	0/18/18/18	0/0/3/3
3	COA	A	1073	-	-	0/48/64/64	0/1/3/3
2	FMN	B	1068	-	-	0/18/18/18	0/0/3/3
3	COA	B	1069	-	-	0/48/64/64	0/1/3/3
2	FMN	B	1070	-	-	0/18/18/18	0/0/3/3
2	FMN	C	1070	-	-	0/18/18/18	0/0/3/3
3	COA	C	1071	-	-	0/48/64/64	0/1/3/3
2	FMN	C	1072	-	-	0/18/18/18	0/0/3/3
2	FMN	D	1070	-	-	0/18/18/18	0/0/3/3
3	COA	D	1071	-	-	0/48/64/64	0/1/3/3
2	FMN	D	1072	-	-	0/18/18/18	0/0/3/3
3	COA	E	1070	-	-	0/48/64/64	0/1/3/3
2	FMN	F	1070	-	-	0/18/18/18	0/0/3/3
3	COA	F	1071	-	-	0/48/64/64	0/1/3/3
2	FMN	F	1072	-	-	0/18/18/18	0/0/3/3
3	COA	G	1070	-	-	0/48/64/64	0/1/3/3
2	FMN	H	1070	-	-	0/18/18/18	0/0/3/3
2	FMN	H	1071	-	-	0/18/18/18	0/0/3/3
3	COA	I	1070	-	-	0/48/64/64	0/1/3/3
3	COA	J	1070	-	-	0/48/64/64	0/1/3/3
3	COA	K	1070	-	1/1/11/13	0/48/64/64	0/1/3/3
3	COA	L	1068	-	-	0/48/64/64	0/1/3/3

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1071	COA	O9P-C9P	9.12	1.41	1.23
3	K	1070	COA	O9P-C9P	8.95	1.41	1.23
3	G	1070	COA	O9P-C9P	8.89	1.41	1.23
3	F	1071	COA	O9P-C9P	8.61	1.40	1.23
3	E	1070	COA	O9P-C9P	8.61	1.40	1.23
3	A	1073	COA	O9P-C9P	8.59	1.40	1.23
3	L	1068	COA	O9P-C9P	8.49	1.40	1.23
3	J	1070	COA	O9P-C9P	8.36	1.40	1.23
3	D	1071	COA	O9P-C9P	8.31	1.39	1.23
3	C	1071	COA	O9P-C9P	8.25	1.39	1.23
3	I	1070	COA	O9P-C9P	8.09	1.39	1.23
3	B	1069	COA	O9P-C9P	8.01	1.39	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1073	COA	C2A-N3A	3.29	1.38	1.32
2	F	1072	FMN	C1'-N10	3.24	1.51	1.48
3	A	1071	COA	C2A-N3A	3.24	1.38	1.32
3	D	1071	COA	C2A-N3A	3.21	1.38	1.32
2	C	1070	FMN	C1'-N10	3.17	1.51	1.48
3	I	1070	COA	C2A-N3A	3.14	1.38	1.32
2	A	1072	FMN	C1'-N10	3.07	1.51	1.48
3	J	1070	COA	C2A-N3A	2.88	1.37	1.32
3	L	1068	COA	C2A-N3A	2.85	1.37	1.32
3	F	1071	COA	C2A-N3A	2.85	1.37	1.32
3	C	1071	COA	C2A-N3A	2.85	1.37	1.32
3	E	1070	COA	C2A-N3A	2.81	1.37	1.32
2	H	1070	FMN	C1'-N10	2.69	1.51	1.48
2	D	1070	FMN	C1'-N10	2.64	1.51	1.48
2	F	1072	FMN	C6-C5A	-2.62	1.38	1.41
3	K	1070	COA	C2A-N3A	2.58	1.37	1.32
3	B	1069	COA	C2A-N3A	2.58	1.37	1.32
2	D	1070	FMN	C6-C5A	-2.57	1.38	1.41
3	B	1069	COA	CBP-CAP	-2.56	1.52	1.55
3	C	1071	COA	C2A-N1A	2.51	1.38	1.33
3	A	1073	COA	CBP-CAP	-2.49	1.53	1.55
2	B	1070	FMN	C1'-N10	2.48	1.51	1.48
3	D	1071	COA	C2A-N1A	2.47	1.38	1.33
2	A	1070	FMN	C1'-N10	2.41	1.50	1.48
3	L	1068	COA	CBP-CAP	-2.38	1.53	1.55
3	E	1070	COA	CBP-CAP	-2.38	1.53	1.55
3	G	1070	COA	C2A-N3A	2.38	1.36	1.32
2	C	1072	FMN	C5A-N5	2.35	1.38	1.35
3	L	1068	COA	C2A-N1A	2.35	1.38	1.33
2	F	1070	FMN	C6-C5A	-2.34	1.38	1.41
2	B	1068	FMN	C1'-N10	2.33	1.50	1.48
2	C	1070	FMN	C6-C5A	-2.33	1.39	1.41
2	A	1070	FMN	C5A-N5	2.30	1.38	1.35
2	B	1070	FMN	C6-C5A	-2.29	1.39	1.41
2	C	1072	FMN	C1'-N10	2.29	1.50	1.48
3	A	1071	COA	C2A-N1A	2.29	1.38	1.33
3	J	1070	COA	C2A-N1A	2.25	1.38	1.33
3	A	1073	COA	C2A-N1A	2.25	1.38	1.33
3	D	1071	COA	CBP-CAP	-2.24	1.53	1.55
2	D	1072	FMN	C1'-N10	2.23	1.50	1.48
3	I	1070	COA	C2A-N1A	2.21	1.38	1.33
2	H	1071	FMN	C1'-N10	2.20	1.50	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1070	COA	CBP-CAP	-2.19	1.53	1.55
2	A	1072	FMN	C5A-N5	2.16	1.38	1.35
3	F	1071	COA	C2A-N1A	2.15	1.38	1.33
3	B	1069	COA	C2A-N1A	2.13	1.38	1.33
3	E	1070	COA	C2A-N1A	2.11	1.38	1.33
2	H	1070	FMN	C5A-N5	2.10	1.38	1.35
2	B	1070	FMN	C1'-C2'	2.09	1.53	1.51
2	D	1070	FMN	C1'-C2'	2.05	1.53	1.51
2	B	1068	FMN	C5A-N5	2.04	1.38	1.35
2	F	1072	FMN	C1'-C2'	2.04	1.53	1.51
2	B	1070	FMN	C5A-N5	2.01	1.38	1.35
3	I	1070	COA	O4B-C4B	-2.00	1.40	1.45

All (182) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	1070	COA	N3A-C2A-N1A	-12.00	118.68	128.71
3	C	1071	COA	N3A-C2A-N1A	-11.69	118.93	128.71
3	F	1071	COA	N3A-C2A-N1A	-11.69	118.94	128.71
3	G	1070	COA	N3A-C2A-N1A	-11.51	119.09	128.71
3	J	1070	COA	N3A-C2A-N1A	-10.99	119.52	128.71
3	L	1068	COA	N3A-C2A-N1A	-10.83	119.66	128.71
3	K	1070	COA	N3A-C2A-N1A	-10.76	119.71	128.71
3	A	1071	COA	N3A-C2A-N1A	-10.73	119.74	128.71
3	D	1071	COA	N3A-C2A-N1A	-10.69	119.77	128.71
3	A	1073	COA	N3A-C2A-N1A	-10.04	120.31	128.71
3	E	1070	COA	N3A-C2A-N1A	-9.21	121.01	128.71
3	B	1069	COA	N3A-C2A-N1A	-9.14	121.07	128.71
2	C	1072	FMN	C2-N1-C10	5.66	120.69	114.98
2	F	1072	FMN	C2-N1-C10	5.56	120.59	114.98
2	D	1072	FMN	C2-N1-C10	5.39	120.41	114.98
2	H	1070	FMN	C2-N1-C10	5.38	120.40	114.98
2	C	1070	FMN	C2-N1-C10	5.24	120.26	114.98
2	D	1070	FMN	C2-N1-C10	4.92	119.94	114.98
2	B	1068	FMN	C2-N1-C10	4.68	119.69	114.98
2	H	1070	FMN	C4A-N5-C5A	4.48	121.73	116.69
2	A	1070	FMN	C2-N1-C10	4.37	119.38	114.98
2	A	1072	FMN	C2-N1-C10	4.37	119.38	114.98
2	H	1071	FMN	C4A-N5-C5A	4.27	121.49	116.69
2	C	1070	FMN	C4A-N5-C5A	4.22	121.43	116.69
2	H	1071	FMN	C2-N1-C10	4.19	119.20	114.98
2	C	1072	FMN	C4A-N5-C5A	4.12	121.32	116.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	1068	COA	P2A-O3A-P1A	-4.09	119.68	131.68
2	B	1070	FMN	C2-N1-C10	4.06	119.07	114.98
2	B	1070	FMN	C1'-N10-C9A	4.06	122.82	118.87
3	F	1071	COA	P2A-O3A-P1A	-4.04	119.85	131.68
3	K	1070	COA	O4B-C1B-N9A	3.93	112.09	108.44
2	A	1070	FMN	C1'-N10-C9A	3.87	122.64	118.87
2	C	1070	FMN	C4A-C10-N1	-3.86	118.88	122.73
2	D	1070	FMN	C4A-N5-C5A	3.82	120.98	116.69
2	F	1072	FMN	C4A-N5-C5A	3.81	120.97	116.69
2	D	1072	FMN	C4A-N5-C5A	3.80	120.96	116.69
2	D	1072	FMN	C4A-C10-N1	-3.75	118.99	122.73
3	G	1070	COA	O4B-C1B-N9A	-3.74	104.96	108.44
3	C	1071	COA	N3A-C4A-N9A	3.72	132.16	125.43
3	D	1071	COA	N3A-C4A-N9A	3.67	132.05	125.43
3	G	1070	COA	N3A-C4A-N9A	3.66	132.05	125.43
3	L	1068	COA	N3A-C4A-N9A	3.65	132.01	125.43
2	A	1072	FMN	C1'-N10-C9A	3.62	122.39	118.87
3	K	1070	COA	CEP-CBP-CAP	3.60	115.07	108.82
3	B	1069	COA	N3A-C4A-N9A	3.55	131.85	125.43
3	L	1068	COA	O4B-C1B-N9A	3.56	111.75	108.44
2	F	1070	FMN	C2-N1-C10	3.49	118.50	114.98
3	A	1071	COA	N3A-C4A-N9A	3.43	131.63	125.43
2	C	1072	FMN	C4A-C10-N1	-3.41	119.32	122.73
3	A	1071	COA	CEP-CBP-CAP	3.37	114.67	108.82
3	J	1070	COA	P2A-O3A-P1A	-3.35	121.85	131.68
3	E	1070	COA	N3A-C4A-N9A	3.32	131.43	125.43
3	D	1071	COA	O4B-C1B-N9A	3.27	111.48	108.44
2	F	1072	FMN	C4A-C10-N1	-3.27	119.47	122.73
3	E	1070	COA	C4A-C5A-N7A	-3.27	106.72	109.52
3	A	1073	COA	N3A-C4A-N9A	3.26	131.32	125.43
2	F	1070	FMN	C4A-N5-C5A	3.23	120.31	116.69
3	K	1070	COA	CBP-CAP-C9P	3.20	115.83	112.73
3	K	1070	COA	N3A-C4A-N9A	3.17	131.16	125.43
3	D	1071	COA	P2A-O3A-P1A	-3.13	122.49	131.68
3	I	1070	COA	N3A-C4A-N9A	3.13	131.09	125.43
3	A	1073	COA	P2A-O3A-P1A	-3.11	122.56	131.68
2	F	1072	FMN	C4-N3-C2	-3.11	119.01	125.39
2	F	1072	FMN	C5A-C9A-N10	3.08	119.84	116.80
2	A	1070	FMN	C2'-C1'-N10	-3.08	108.37	112.45
2	C	1070	FMN	C1'-N10-C9A	3.07	121.86	118.87
2	D	1070	FMN	C4A-C10-N1	-3.02	119.71	122.73
2	H	1071	FMN	C4A-C10-N1	-3.01	119.72	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1071	COA	P3B-O3B-C3B	3.01	128.29	121.96
2	D	1070	FMN	C1'-N10-C9A	2.99	121.78	118.87
3	C	1071	COA	P2A-O3A-P1A	-2.99	122.92	131.68
2	C	1072	FMN	C4-N3-C2	-2.95	119.33	125.39
3	G	1070	COA	C8A-N9A-C4A	2.94	109.14	106.90
3	A	1071	COA	P2A-O3A-P1A	-2.93	123.09	131.68
2	B	1070	FMN	C4A-N5-C5A	2.91	119.96	116.69
3	G	1070	COA	C4A-C5A-N7A	-2.89	107.05	109.52
2	H	1071	FMN	C2'-C1'-N10	-2.88	108.63	112.45
2	D	1070	FMN	C4-N3-C2	-2.88	119.49	125.39
3	A	1071	COA	O4B-C1B-N9A	2.87	111.11	108.44
3	F	1071	COA	N3A-C4A-N9A	2.84	130.56	125.43
2	F	1070	FMN	C4A-C10-N1	-2.84	119.89	122.73
3	G	1070	COA	N7A-C8A-N9A	-2.83	106.34	114.36
2	B	1068	FMN	C4A-N5-C5A	2.83	119.87	116.69
2	H	1070	FMN	C4A-C10-N1	-2.82	119.91	122.73
3	F	1071	COA	O4B-C1B-N9A	2.80	111.04	108.44
2	A	1072	FMN	C4A-N5-C5A	2.79	119.83	116.69
3	J	1070	COA	N3A-C4A-N9A	2.79	130.48	125.43
2	B	1070	FMN	C5A-C9A-N10	2.79	119.55	116.80
2	C	1070	FMN	C4-N3-C2	-2.78	119.68	125.39
2	F	1070	FMN	C4-C4A-C10	2.76	121.41	116.95
2	B	1068	FMN	C4A-C10-N1	-2.75	119.98	122.73
3	A	1071	COA	CBP-CAP-C9P	2.74	115.39	112.73
2	A	1070	FMN	C4-N3-C2	-2.73	119.78	125.39
2	D	1072	FMN	C2'-C1'-N10	-2.70	108.87	112.45
3	B	1069	COA	C4A-C5A-N7A	-2.68	107.23	109.52
2	F	1070	FMN	C1'-N10-C9A	2.67	121.47	118.87
2	A	1072	FMN	C4-N3-C2	-2.64	119.97	125.39
2	H	1071	FMN	C5A-C9A-N10	2.62	119.38	116.80
2	B	1070	FMN	C4A-C10-N1	-2.61	120.12	122.73
3	J	1070	COA	C4A-C5A-N7A	-2.61	107.29	109.52
2	D	1072	FMN	C4-N3-C2	-2.60	120.05	125.39
2	C	1072	FMN	C1'-N10-C9A	2.61	121.41	118.87
2	A	1072	FMN	C5A-C9A-N10	2.60	119.36	116.80
3	B	1069	COA	N7A-C8A-N9A	-2.59	107.05	114.36
2	H	1070	FMN	C5A-C9A-N10	2.58	119.34	116.80
3	K	1070	COA	C4A-C5A-N7A	-2.57	107.32	109.52
2	B	1070	FMN	C9A-N10-C10	-2.56	119.25	121.77
2	A	1070	FMN	C4A-N5-C5A	2.56	119.56	116.69
3	B	1069	COA	O4B-C1B-N9A	2.54	110.80	108.44
2	B	1070	FMN	C4-N3-C2	-2.53	120.19	125.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1068	FMN	C4-N3-C2	-2.52	120.22	125.39
2	H	1071	FMN	C1'-N10-C9A	2.50	121.31	118.87
2	H	1070	FMN	C1'-N10-C9A	2.49	121.30	118.87
2	H	1071	FMN	C4-C4A-C10	2.47	120.94	116.95
3	G	1070	COA	C2A-N3A-C4A	2.46	121.00	114.01
2	H	1071	FMN	C4-N3-C2	-2.45	120.35	125.39
3	A	1071	COA	C4A-C5A-N7A	-2.44	107.43	109.52
2	F	1070	FMN	C4-N3-C2	-2.42	120.43	125.39
2	B	1068	FMN	C1'-N10-C9A	2.42	121.22	118.87
2	H	1070	FMN	C4-N3-C2	-2.41	120.45	125.39
2	B	1068	FMN	C2'-C1'-N10	-2.40	109.27	112.45
3	F	1071	COA	CBP-CAP-C9P	2.39	115.04	112.73
2	A	1070	FMN	C4A-C10-N1	-2.38	120.35	122.73
3	G	1070	COA	C6P-C7P-N8P	-2.36	106.79	111.87
3	L	1068	COA	N7A-C8A-N9A	-2.36	107.69	114.36
2	D	1070	FMN	C5A-C9A-N10	2.36	119.12	116.80
3	K	1070	COA	N7A-C8A-N9A	-2.35	107.71	114.36
3	B	1069	COA	C8A-N9A-C4A	2.34	108.69	106.90
3	C	1071	COA	N7A-C8A-N9A	-2.32	107.78	114.36
2	A	1070	FMN	C5A-C9A-N10	2.31	119.08	116.80
3	D	1071	COA	C5A-C4A-N3A	-2.30	120.68	125.70
2	F	1072	FMN	C4A-C10-N10	-2.28	119.37	120.51
3	G	1070	COA	O6A-CCP-CBP	-2.28	106.75	110.57
3	L	1068	COA	C5A-C4A-N3A	-2.27	120.76	125.70
3	E	1070	COA	C5A-C4A-N3A	-2.26	120.78	125.70
3	A	1071	COA	C5A-C4A-N3A	-2.26	120.79	125.70
3	L	1068	COA	C4A-C5A-N7A	-2.25	107.59	109.52
3	A	1071	COA	N7A-C8A-N9A	-2.24	108.01	114.36
3	E	1070	COA	P2A-O3A-P1A	-2.23	125.16	131.68
2	C	1070	FMN	C4-C4A-C10	2.22	120.54	116.95
3	A	1073	COA	N7A-C8A-N9A	-2.22	108.09	114.36
3	G	1070	COA	C8A-N7A-C5A	2.21	110.45	103.58
3	D	1071	COA	C3B-C2B-C1B	2.21	105.23	99.98
3	I	1070	COA	C2A-N1A-C6A	2.21	122.76	118.77
3	J	1070	COA	N7A-C8A-N9A	-2.21	108.12	114.36
2	B	1068	FMN	C5A-C9A-N10	2.19	118.96	116.80
3	G	1070	COA	C5A-C4A-N3A	-2.19	120.94	125.70
3	J	1070	COA	O6A-CCP-CBP	-2.18	106.92	110.57
3	G	1070	COA	CDP-CBP-CCP	2.15	111.86	108.76
3	L	1068	COA	C2A-N3A-C4A	2.14	120.11	114.01
3	C	1071	COA	C2A-N3A-C4A	2.13	120.08	114.01
2	D	1072	FMN	C4-C4A-C10	2.12	120.38	116.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1073	COA	C1B-N9A-C4A	-2.12	122.97	126.64
3	B	1069	COA	C7P-N8P-C9P	-2.12	118.23	122.57
3	K	1070	COA	C5A-C4A-N3A	-2.11	121.10	125.70
3	D	1071	COA	N7A-C8A-N9A	-2.11	108.39	114.36
3	C	1071	COA	O4B-C1B-N9A	2.11	110.40	108.44
3	I	1070	COA	P2A-O3A-P1A	-2.11	125.51	131.68
3	G	1070	COA	P2A-O3A-P1A	-2.09	125.54	131.68
3	B	1069	COA	C8A-N7A-C5A	2.09	110.05	103.58
3	I	1070	COA	N7A-C8A-N9A	-2.09	108.45	114.36
2	F	1072	FMN	C4A-C4-N3	2.08	121.49	115.39
3	B	1069	COA	C5A-C4A-N3A	-2.08	121.17	125.70
3	E	1070	COA	N7A-C8A-N9A	-2.08	108.47	114.36
3	C	1071	COA	C5A-C4A-N3A	-2.08	121.18	125.70
2	C	1070	FMN	C2'-C1'-N10	-2.07	109.70	112.45
3	F	1071	COA	C2A-N1A-C6A	2.07	122.51	118.77
3	D	1071	COA	C2A-N3A-C4A	2.07	119.91	114.01
3	F	1071	COA	N7A-C8A-N9A	-2.07	108.51	114.36
3	A	1073	COA	C5A-C4A-N3A	-2.06	121.21	125.70
3	A	1071	COA	C2A-N3A-C4A	2.05	119.86	114.01
2	B	1068	FMN	C4-C4A-C10	2.04	120.25	116.95
3	A	1073	COA	C4A-C5A-N7A	-2.03	107.78	109.52
2	H	1070	FMN	C9A-C5A-N5	-2.03	119.26	122.37
3	K	1070	COA	P2A-O3A-P1A	-2.03	125.74	131.68
3	E	1070	COA	O5A-P2A-O3A	2.02	114.73	105.14
2	F	1070	FMN	C4A-C10-N10	2.02	121.52	120.51
2	A	1072	FMN	C4A-C10-N1	-2.01	120.72	122.73
2	F	1072	FMN	C1'-N10-C9A	2.01	120.83	118.87
3	K	1070	COA	C8A-N7A-C5A	2.01	109.80	103.58
2	F	1072	FMN	C2'-C1'-N10	-2.00	109.80	112.45
2	F	1070	FMN	C2'-C1'-N10	-2.00	109.80	112.45

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	K	1070	COA	CAP
3	A	1071	COA	CAP

There are no torsion outliers.

There are no ring outliers.



## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	68/69 (98%)	0.58	5 (7%) 14 16	18, 24, 36, 42	0
1	B	66/69 (95%)	0.20	3 (4%) 32 35	13, 19, 29, 36	0
1	C	68/69 (98%)	0.14	3 (4%) 33 36	14, 21, 29, 31	0
1	D	68/69 (98%)	0.31	3 (4%) 33 36	12, 20, 30, 37	0
1	E	68/69 (98%)	0.37	5 (7%) 14 16	14, 19, 30, 36	0
1	F	68/69 (98%)	0.10	3 (4%) 33 36	10, 17, 26, 33	0
1	G	68/69 (98%)	0.15	4 (5%) 22 23	11, 18, 27, 34	0
1	H	68/69 (98%)	0.64	5 (7%) 14 16	15, 23, 36, 45	0
1	I	68/69 (98%)	0.33	4 (5%) 22 23	11, 18, 28, 33	0
1	J	68/69 (98%)	0.45	5 (7%) 14 16	16, 23, 32, 39	0
1	K	68/69 (98%)	0.51	4 (5%) 22 23	16, 23, 31, 35	0
1	L	66/69 (95%)	0.67	4 (6%) 21 22	19, 25, 35, 37	0
All	All	812/828 (98%)	0.37	48 (5%) 23 23	10, 21, 33, 45	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	69	THR	11.8
1	H	69	THR	10.7
1	E	69	THR	6.4
1	L	2	GLY	6.1
1	A	69	THR	5.7
1	J	69	THR	5.7
1	H	2	GLY	5.6
1	D	69	THR	5.0
1	F	69[A]	THR	4.6
1	J	2	GLY	4.4
1	G	2	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
1	K	50	GLU	3.9
1	K	2	GLY	3.8
1	A	68	GLU	3.8
1	E	50	GLU	3.6
1	I	2	GLY	3.6
1	H	68	GLU	3.6
1	E	2	GLY	3.4
1	K	51	ALA	3.4
1	L	50	GLU	3.3
1	J	68	GLU	3.3
1	E	68	GLU	3.2
1	B	50	GLU	2.9
1	K	69	THR	2.9
1	E	16	GLU	2.8
1	A	50	GLU	2.8
1	C	69	THR	2.7
1	C	2	GLY	2.7
1	J	50	GLU	2.7
1	D	2	GLY	2.6
1	A	51	ALA	2.6
1	C	16	GLU	2.5
1	D	16	GLU	2.4
1	A	2	GLY	2.4
1	I	16	GLU	2.4
1	L	16	GLU	2.4
1	G	50	GLU	2.3
1	H	30	ARG	2.2
1	J	16	GLU	2.2
1	F	2	GLY	2.2
1	F	16	GLU	2.2
1	L	31	LYS	2.2
1	B	2	GLY	2.2
1	I	50	GLU	2.2
1	G	69	THR	2.1
1	B	16	GLU	2.1
1	G	68	GLU	2.0
1	H	50	GLU	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	FMN	B	1068	31/31	0.14	1.53	25,27,32,34	0
3	COA	F	1071	48/48	0.10	1.24	15,23,34,35	0
3	COA	D	1071	48/48	0.11	1.15	20,26,44,45	0
2	FMN	B	1070	31/31	0.13	0.79	25,26,37,38	0
3	COA	L	1068	48/48	0.14	0.71	30,38,43,44	0
3	COA	A	1073	48/48	0.14	0.37	31,37,47,48	0
3	COA	B	1069	48/48	0.09	0.36	16,24,33,34	0
3	COA	K	1070	48/48	0.11	0.35	18,28,36,37	0
3	COA	A	1071	48/48	0.13	0.17	27,36,45,46	0
3	COA	G	1070	48/48	0.09	0.05	15,24,33,34	0
3	COA	I	1070	48/48	0.09	-0.08	16,24,32,34	0
3	COA	C	1071	48/48	0.09	-0.13	19,25,35,37	0
2	FMN	D	1070	31/31	0.09	-0.16	17,19,29,32	0
2	FMN	H	1070	31/31	0.10	-0.18	20,21,41,42	0
2	FMN	C	1070	31/31	0.10	-0.18	19,20,29,32	0
3	COA	J	1070	48/48	0.10	-0.18	19,27,37,39	0
3	COA	E	1070	48/48	0.09	-0.19	15,24,30,35	0
2	FMN	F	1070	31/31	0.07	-0.25	11,14,21,24	0
2	FMN	H	1071	31/31	0.09	-0.27	20,22,35,36	0
5	NA	F	1073	1/1	0.08	-0.38	33,33,33,33	0
2	FMN	F	1072	31/31	0.07	-0.49	12,14,23,25	0
2	FMN	A	1072	31/31	0.08	-0.54	17,18,25,26	0
2	FMN	A	1070	31/31	0.07	-0.75	19,20,29,30	0
2	FMN	C	1072	31/31	0.09	-0.85	20,21,32,33	0
2	FMN	D	1072	31/31	0.07	-0.94	18,19,27,28	0
4	CL	A	1074	1/1	0.03	-3.81	30,30,30,30	0
4	CL	B	1071	1/1	0.03	-4.17	15,15,15,15	0
4	CL	D	1073	1/1	0.03	-4.81	20,20,20,20	0
4	CL	C	1073	1/1	0.02	-4.86	21,21,21,21	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.