



# Full wwPDB X-ray Structure Validation Report i

Feb 28, 2014 – 12:59 AM GMT

PDB ID : 1O2A  
Title : Crystal structure of Thymidylate Synthase Complementing Protein (TM0449) from *Thermotoga maritima* with FAD at 1.8 Å resolution  
Authors : Mathews, I.I.; Deacon, A.M.; Canaves, J.M.; McMullan, D.; Lesley, S.A.; Agarwalla, S.; Kuhn, P.; Joint Center for Structural Genomics (JCSG)  
Deposited on : 2003-02-18  
Resolution : 1.80 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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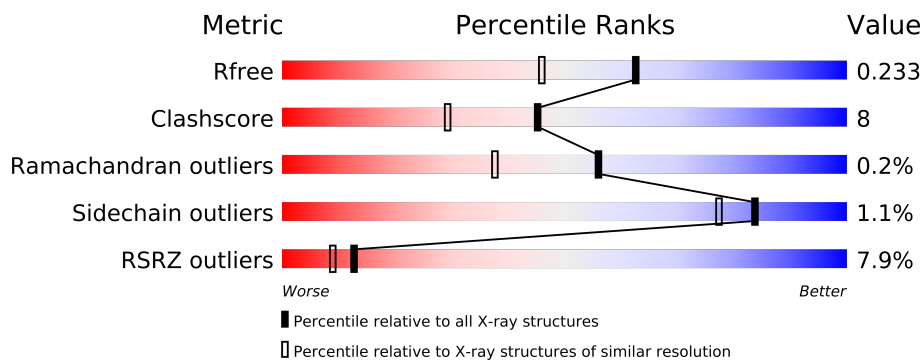
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.80 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	3513 (1.80-1.80)
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (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  $\geq 3$ , 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	232	
1	B	232	
1	C	232	
1	D	232	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	FAD	B	710	-	X
2	FAD	C	705	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7668 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 Thymidylate synthase thyX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1764	1148	304	307	5			
1	B	214	Total	C	N	O	S	0	0	0
			1786	1164	307	310	5			
1	C	214	Total	C	N	O	S	0	0	0
			1783	1157	306	315	5			
1	D	213	Total	C	N	O	S	0	5	0
			1815	1179	312	319	5			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	LEADER SEQUENCE	UNP Q9WYT0
A	-10	GLY	-	LEADER SEQUENCE	UNP Q9WYT0
A	-9	SER	-	LEADER SEQUENCE	UNP Q9WYT0
A	-8	ASP	-	LEADER SEQUENCE	UNP Q9WYT0
A	-7	LYS	-	LEADER SEQUENCE	UNP Q9WYT0
A	-6	ILE	-	LEADER SEQUENCE	UNP Q9WYT0
A	-5	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
A	-4	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
A	-3	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
A	-2	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
A	-1	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
A	0	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
B	-11	MET	-	LEADER SEQUENCE	UNP Q9WYT0
B	-10	GLY	-	LEADER SEQUENCE	UNP Q9WYT0
B	-9	SER	-	LEADER SEQUENCE	UNP Q9WYT0
B	-8	ASP	-	LEADER SEQUENCE	UNP Q9WYT0
B	-7	LYS	-	LEADER SEQUENCE	UNP Q9WYT0
B	-6	ILE	-	LEADER SEQUENCE	UNP Q9WYT0
B	-5	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
B	-4	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
B	-3	HIS	-	LEADER SEQUENCE	UNP Q9WYT0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
B	-1	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
B	0	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
C	-11	MET	-	LEADER SEQUENCE	UNP Q9WYT0
C	-10	GLY	-	LEADER SEQUENCE	UNP Q9WYT0
C	-9	SER	-	LEADER SEQUENCE	UNP Q9WYT0
C	-8	ASP	-	LEADER SEQUENCE	UNP Q9WYT0
C	-7	LYS	-	LEADER SEQUENCE	UNP Q9WYT0
C	-6	ILE	-	LEADER SEQUENCE	UNP Q9WYT0
C	-5	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
C	-4	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
C	-3	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
C	-2	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
C	-1	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
C	0	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
D	-11	MET	-	LEADER SEQUENCE	UNP Q9WYT0
D	-10	GLY	-	LEADER SEQUENCE	UNP Q9WYT0
D	-9	SER	-	LEADER SEQUENCE	UNP Q9WYT0
D	-8	ASP	-	LEADER SEQUENCE	UNP Q9WYT0
D	-7	LYS	-	LEADER SEQUENCE	UNP Q9WYT0
D	-6	ILE	-	LEADER SEQUENCE	UNP Q9WYT0
D	-5	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
D	-4	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
D	-3	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
D	-2	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
D	-1	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
D	0	HIS	-	LEADER SEQUENCE	UNP Q9WYT0

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

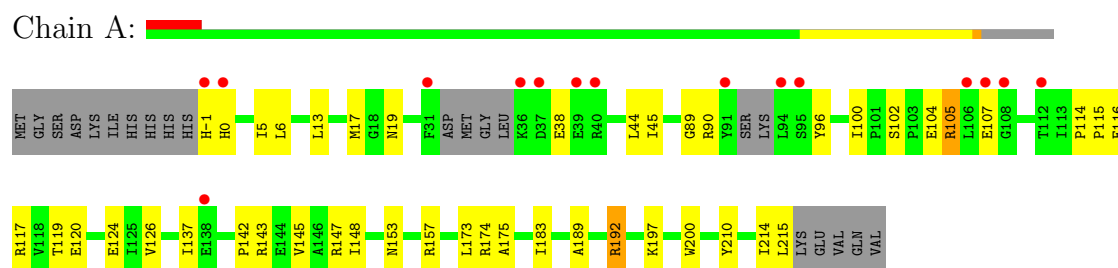
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	82	Total	O	0	0
			82	82		
3	B	80	Total	O	0	0
			80	80		
3	C	72	Total	O	0	0
			72	72		
3	D	74	Total	O	0	0
			74	74		

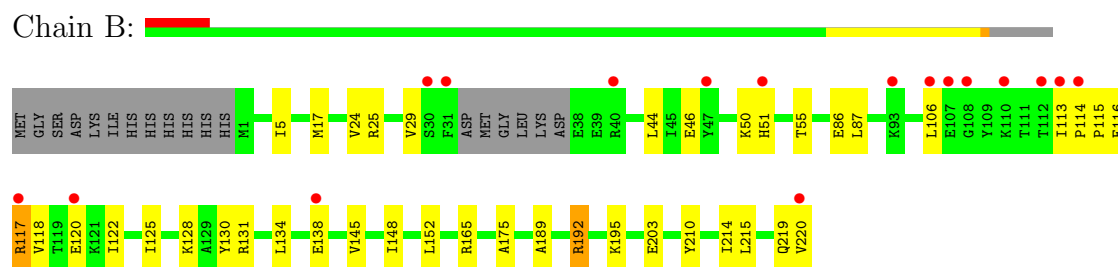
### 3 Residue-property plots

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.

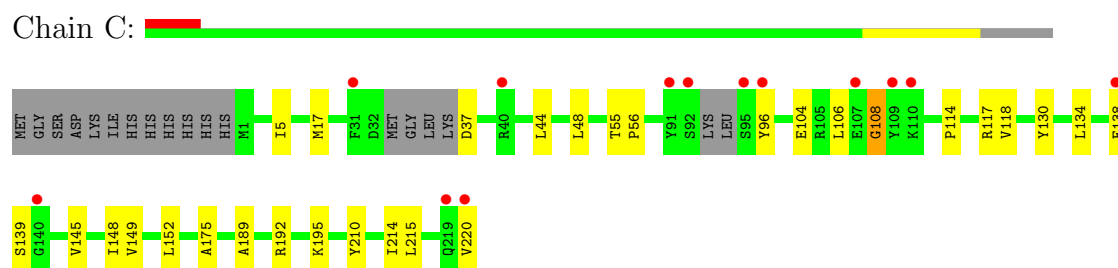
#### • Molecule 1: Thymidylate synthase thyX



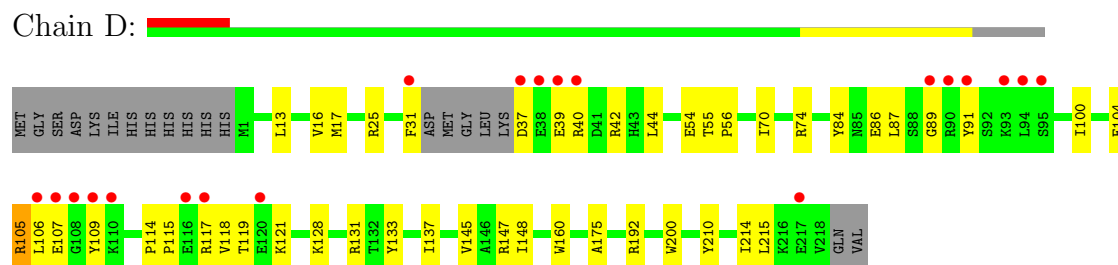
#### • Molecule 1: Thymidylate synthase thyX



#### • Molecule 1: Thymidylate synthase thyX



#### • Molecule 1: Thymidylate synthase thyX



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.50Å 116.95Å 141.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 36.73 – 1.71	Depositor EDS
% Data completeness (in resolution range)	91.7 (20.00-1.80) 88.6 (36.73-1.71)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.03	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.74 (at 1.71Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.203 , 0.230 0.207 , 0.233	Depositor DCC
$R_{free}$ test set	3918 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.1	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 47.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 87308 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7668	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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: 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	0.32	0/1812	0.56	0/2448
1	B	0.32	0/1834	0.56	0/2478
1	C	0.33	0/1829	0.58	0/2470
1	D	0.31	0/1863	0.55	0/2519
All	All	0.32	0/7338	0.56	0/9915

There are no bond length outliers.

There are no bond angle outliers.

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	1764	0	1741	34	0
1	B	1786	0	1784	37	0
1	C	1783	0	1766	25	0
1	D	1815	0	1798	34	0
2	A	53	0	30	1	0
2	B	53	0	30	0	0
2	C	53	0	30	0	0
2	D	53	0	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	82	0	0	2	0
3	B	80	0	0	5	0
3	C	72	0	0	1	0
3	D	74	0	0	3	0
All	All	7668	0	7209	123	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 8.

All (123) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:55:THR:HA	3:B:544:HOH:O	1.64	0.97
1:B:165:ARG:HD2	3:B:544:HOH:O	1.66	0.96
1:A:17:MET:HB2	1:B:17:MET:HB2	1.48	0.94
1:C:17:MET:HB2	1:D:17:MET:HB2	1.56	0.86
1:B:134:LEU:O	1:B:138:GLU:HG2	1.79	0.82
1:B:192:ARG:HG2	1:B:220:VAL:HG12	1.63	0.80
1:B:219:GLN:HG3	1:B:220:VAL:HG23	1.63	0.79
1:B:24:VAL:HG13	1:B:44:LEU:HD23	1.65	0.79
1:C:106:LEU:HD21	1:C:118:VAL:HG11	1.68	0.75
1:D:106:LEU:HD21	1:D:118:VAL:HG11	1.72	0.70
1:B:116:GLU:O	1:B:120:GLU:HG3	1.96	0.66
1:C:37:ASP:N	3:C:327:HOH:O	2.30	0.65
1:A:104:GLU:O	1:A:107:GLU:HG3	1.97	0.65
1:B:195:LYS:NZ	1:B:220:VAL:HG22	2.13	0.64
1:D:25:ARG:HH21	1:D:31:PHE:C	2.01	0.62
1:B:50:LYS:HG3	1:B:51:HIS:ND1	2.15	0.62
1:A:105:ARG:HD2	1:A:105:ARG:O	2.00	0.61
1:B:114:PRO:HD2	1:B:117:ARG:HG3	1.83	0.60
1:A:102:SER:HB3	3:A:573:HOH:O	2.01	0.60
1:A:192:ARG:HH11	1:A:192:ARG:HG2	1.65	0.60
1:B:116:GLU:H	1:B:116:GLU:CD	2.04	0.59
1:B:128:LYS:HG2	1:B:131:ARG:HH21	1.67	0.59
1:D:128:LYS:HG2	1:D:131:ARG:HH21	1.69	0.58
1:D:42:ARG:HG2	1:D:200:TRP:CD2	2.39	0.57
1:C:134:LEU:O	1:C:138:GLU:HG3	2.05	0.57
1:D:74:ARG:HD3	3:D:313:HOH:O	2.05	0.56
1:D:86:GLU:HG2	1:D:87[B]:LEU:N	2.21	0.55
1:D:37:ASP:HB3	1:D:40:ARG:HB2	1.87	0.55
1:C:195:LYS:HE2	1:C:220:VAL:HG12	1.88	0.55
1:A:5:ILE:HD11	1:A:189:ALA:HB2	1.88	0.55
1:A:38:GLU:HG3	1:A:200:TRP:CH2	2.42	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:192:ARG:HH11	1:A:192:ARG:CG	2.20	0.54
1:A:174:ARG:HD2	1:A:183:ILE:HD13	1.89	0.53
1:A:19:ASN:HB2	3:A:400:HOH:O	2.08	0.53
1:A:38:GLU:HG3	1:A:200:TRP:CZ2	2.44	0.52
1:D:105:ARG:HD2	1:D:105:ARG:O	2.09	0.52
1:A:5:ILE:HG22	1:A:6:LEU:HG	1.91	0.52
1:D:192:ARG:HG3	1:D:192:ARG:HH11	1.74	0.51
1:B:25:ARG:HD2	3:B:578:HOH:O	2.10	0.51
1:B:122:ILE:O	1:B:125:ILE:HG22	2.10	0.51
1:B:5:ILE:HD11	1:B:189:ALA:HB2	1.92	0.51
1:A:117:ARG:HD3	1:A:120:GLU:OE2	2.11	0.50
1:B:113:ILE:HG12	1:C:139:SER:OG	2.10	0.50
1:B:195:LYS:HZ2	1:B:220:VAL:HG22	1.75	0.50
1:A:89:GLY:HA3	1:A:147:ARG:NE	2.27	0.50
1:D:175:ALA:HA	1:D:214:ILE:HD11	1.92	0.49
1:B:175:ALA:HA	1:B:214:ILE:HD11	1.93	0.49
1:A:120:GLU:O	1:A:124:GLU:HG3	2.12	0.49
1:D:86:GLU:CG	1:D:87[B]:LEU:N	2.76	0.49
1:B:165:ARG:NH1	3:B:544:HOH:O	2.46	0.49
1:A:210:TYR:CE2	1:A:215:LEU:HB2	2.48	0.48
1:D:145:VAL:O	1:D:148:ILE:HG12	2.13	0.48
1:A:175:ALA:HA	1:A:214:ILE:HD11	1.94	0.48
1:C:195:LYS:CE	1:C:220:VAL:HG12	2.44	0.47
1:C:192:ARG:HH12	1:C:220:VAL:HG21	1.79	0.47
1:C:220:VAL:HG23	1:C:220:VAL:OXT	2.15	0.47
1:A:104:GLU:HB3	1:A:107:GLU:OE2	2.14	0.47
1:B:195:LYS:HZ3	1:B:220:VAL:HG22	1.80	0.47
1:C:96:TYR:HB3	1:C:130:TYR:CE1	2.50	0.46
1:A:90:ARG:HH12	2:D:700:FAD:HM72	1.80	0.46
1:A:137:ILE:HD11	1:A:143:ARG:HA	1.97	0.46
1:D:106:LEU:HD12	1:D:106:LEU:N	2.31	0.46
1:C:55:THR:OG1	1:C:56:PRO:HD3	2.16	0.46
1:B:29:VAL:O	1:B:29:VAL:HG12	2.16	0.46
1:B:192:ARG:NE	1:B:220:VAL:HG11	2.30	0.46
1:B:145:VAL:O	1:B:148:ILE:HG12	2.16	0.46
1:D:133:TYR:CE1	1:D:137:ILE:HD11	2.50	0.45
1:D:86:GLU:HG2	1:D:87[A]:LEU:N	2.31	0.45
1:A:45:ILE:HD12	1:A:200:TRP:HE3	1.81	0.45
1:C:192:ARG:NH2	1:C:220:VAL:HG23	2.31	0.45
1:D:40:ARG:HH11	1:D:40:ARG:HG2	1.82	0.45
1:D:210:TYR:CE2	1:D:215:LEU:HB2	2.51	0.45
1:D:91[A]:TYR:HB2	3:D:539:HOH:O	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:70:ILE:O	1:D:74:ARG:HG3	2.16	0.45
1:B:114:PRO:O	1:B:117:ARG:HB2	2.17	0.44
1:D:37:ASP:OD1	1:D:39:GLU:HG2	2.17	0.44
1:C:145:VAL:O	1:C:148:ILE:HG12	2.17	0.44
1:A:104:GLU:OE1	1:A:104:GLU:N	2.50	0.44
1:B:46:GLU:O	1:B:50:LYS:HG2	2.17	0.44
1:A:142:PRO:HG3	1:D:109:TYR:CE2	2.52	0.44
1:D:133:TYR:O	1:D:137:ILE:HD13	2.18	0.44
1:A:-1:HIS:O	1:A:0:HIS:HB2	2.18	0.43
1:C:44:LEU:O	1:C:48:LEU:HG	2.19	0.43
1:C:104:GLU:H	1:C:104:GLU:CD	2.22	0.43
1:D:104:GLU:HA	1:D:107:GLU:HG3	2.00	0.43
1:D:25:ARG:HD3	3:D:587:HOH:O	2.18	0.43
1:A:100:ILE:HG22	1:A:119:THR:HG23	1.99	0.42
1:D:55:THR:OG1	1:D:56:PRO:HD3	2.18	0.42
1:D:13:LEU:HD11	1:D:16:VAL:CG2	2.50	0.42
1:B:210:TYR:CE2	1:B:215:LEU:HB2	2.54	0.42
1:D:89[B]:GLY:O	1:D:147:ARG:HD2	2.20	0.42
1:B:106:LEU:HD21	1:B:118:VAL:HG11	2.01	0.42
1:C:175:ALA:HA	1:C:214:ILE:HD11	2.02	0.42
1:B:203:GLU:HG2	3:B:603:HOH:O	2.19	0.42
1:A:157:ARG:NH1	1:B:29:VAL:O	2.48	0.42
1:B:130:TYR:O	1:B:134:LEU:HG	2.20	0.42
1:C:210:TYR:CE2	1:C:215:LEU:HB2	2.55	0.42
1:A:173:LEU:HD13	2:A:715:FAD:O3'	2.20	0.42
1:A:192:ARG:NH1	1:A:192:ARG:CG	2.79	0.41
1:D:86:GLU:CG	1:D:87[A]:LEU:N	2.83	0.41
1:C:5:ILE:HD11	1:C:189:ALA:HB2	2.01	0.41
1:A:145:VAL:O	1:A:148:ILE:HG12	2.20	0.41
1:A:116:GLU:O	1:A:120:GLU:HG3	2.20	0.41
1:B:106:LEU:HD12	1:B:106:LEU:N	2.35	0.41
1:C:106:LEU:N	1:C:106:LEU:HD12	2.35	0.41
1:D:117:ARG:NH2	1:D:121:LYS:HZ3	2.18	0.41
1:C:192:ARG:HH22	1:C:220:VAL:HG23	1.86	0.41
1:B:125:ILE:HG21	1:C:149:VAL:HB	2.01	0.41
1:A:116:GLU:CD	1:A:116:GLU:H	2.24	0.41
1:A:114:PRO:HA	1:A:115:PRO:HD3	1.98	0.41
1:C:106:LEU:CD2	1:C:118:VAL:HG21	2.50	0.41
1:A:126:VAL:HG21	1:A:153:ASN:HD21	1.86	0.41
1:C:106:LEU:O	1:C:108:GLY:N	2.50	0.41
1:B:152:LEU:HD23	1:C:152:LEU:HD23	2.03	0.41
1:B:86:GLU:CG	1:B:87:LEU:N	2.84	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:114:PRO:HA	1:B:115:PRO:HD3	1.98	0.40
1:D:100:ILE:HG22	1:D:119:THR:HG23	2.04	0.40
1:D:84:TYR:CE2	1:D:160:TRP:CD1	3.09	0.40
1:B:115:PRO:HD2	1:B:116:GLU:OE2	2.20	0.40
1:D:42:ARG:HG2	1:D:200:TRP:CE3	2.57	0.40
1:C:114:PRO:HD2	1:C:117:ARG:HG3	2.03	0.40
1:A:13:LEU:CD2	1:A:197:LYS:HE3	2.52	0.40
1:D:114:PRO:HA	1:D:115:PRO:HD3	1.97	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	205/232 (88%)	198 (97%)	6 (3%)	1 (0%)	38	19
1	B	210/232 (90%)	205 (98%)	5 (2%)	0	100	100
1	C	208/232 (90%)	198 (95%)	9 (4%)	1 (0%)	38	19
1	D	214/232 (92%)	209 (98%)	5 (2%)	0	100	100
All	All	837/928 (90%)	810 (97%)	25 (3%)	2 (0%)	56	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	TYR
1	C	108	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	185/207 (89%)	182 (98%)	3 (2%)	75	63
1	B	189/207 (91%)	187 (99%)	2 (1%)	84	77
1	C	189/207 (91%)	189 (100%)	0	100	100
1	D	191/207 (92%)	188 (98%)	3 (2%)	75	63
All	All	754/828 (91%)	746 (99%)	8 (1%)	84	77

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	105	ARG
1	A	192	ARG
1	B	117	ARG
1	B	192	ARG
1	D	44	LEU
1	D	54	GLU
1	D	105	ARG

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	185	GLN
1	D	75	GLN

### 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

4 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$
2	FAD	A	715	-	58,58,58	2.88	28 (48%)	85,89,89	2.71	23 (27%)
2	FAD	B	710	-	58,58,58	2.88	28 (48%)	85,89,89	2.71	22 (25%)
2	FAD	C	705	-	58,58,58	2.87	28 (48%)	85,89,89	2.69	22 (25%)
2	FAD	D	700	-	58,58,58	2.84	28 (48%)	85,89,89	2.74	24 (28%)

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	FAD	A	715	-	1/1/9/9	0/34/50/50	0/1/6/6
2	FAD	B	710	-	1/1/9/9	0/34/50/50	0/1/6/6
2	FAD	C	705	-	1/1/9/9	0/34/50/50	0/1/6/6
2	FAD	D	700	-	1/1/9/9	0/34/50/50	0/1/6/6

All (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	700	FAD	C4A-N3A	6.49	1.45	1.35
2	B	710	FAD	C4A-N3A	6.42	1.45	1.35
2	C	705	FAD	C4A-N3A	6.39	1.45	1.35
2	A	715	FAD	C4A-N3A	6.31	1.45	1.35
2	A	715	FAD	C2B-C1B	6.20	1.62	1.53
2	B	710	FAD	C2B-C1B	6.19	1.62	1.53
2	C	705	FAD	C2B-C1B	6.09	1.62	1.53
2	D	700	FAD	C2B-C1B	5.79	1.61	1.53
2	A	715	FAD	C4-C4X	5.68	1.50	1.41
2	C	705	FAD	C4-C4X	5.64	1.50	1.41
2	B	710	FAD	C4-C4X	5.58	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	700	FAD	C4-C4X	5.53	1.50	1.41
2	C	705	FAD	C4X-C10	5.10	1.49	1.40
2	A	715	FAD	C4X-C10	5.09	1.49	1.40
2	B	710	FAD	C4X-C10	5.02	1.49	1.40
2	D	700	FAD	C4X-C10	4.96	1.49	1.40
2	A	715	FAD	C1'-C2'	4.96	1.56	1.51
2	A	715	FAD	C9A-C5X	4.91	1.52	1.42
2	B	710	FAD	C9A-C5X	4.91	1.52	1.42
2	C	705	FAD	C9A-C5X	4.86	1.52	1.42
2	D	700	FAD	C6-C5X	4.78	1.47	1.41
2	A	715	FAD	C6-C5X	4.77	1.47	1.41
2	C	705	FAD	C6-C5X	4.75	1.47	1.41
2	D	700	FAD	C9A-C5X	4.74	1.52	1.42
2	C	705	FAD	C4-N3	4.69	1.45	1.37
2	A	715	FAD	C4-N3	4.63	1.45	1.37
2	C	705	FAD	C1'-C2'	4.62	1.56	1.51
2	B	710	FAD	C4-N3	4.62	1.44	1.37
2	D	700	FAD	C4-N3	4.60	1.44	1.37
2	C	705	FAD	C5X-N5	4.58	1.42	1.35
2	D	700	FAD	C8A-N7A	-4.57	1.25	1.34
2	B	710	FAD	C1'-C2'	4.56	1.55	1.51
2	B	710	FAD	C5X-N5	4.55	1.42	1.35
2	A	715	FAD	C5X-N5	4.54	1.42	1.35
2	D	700	FAD	C9-C9A	4.50	1.49	1.40
2	B	710	FAD	C8A-N7A	-4.50	1.25	1.34
2	B	710	FAD	C6-C5X	4.49	1.47	1.41
2	B	710	FAD	C9-C9A	4.44	1.49	1.40
2	D	700	FAD	C5X-N5	4.39	1.42	1.35
2	D	700	FAD	C1'-C2'	4.36	1.55	1.51
2	C	705	FAD	C8A-N7A	-4.34	1.26	1.34
2	A	715	FAD	C9-C9A	4.34	1.49	1.40
2	A	715	FAD	C8A-N7A	-4.29	1.26	1.34
2	C	705	FAD	C9-C9A	4.26	1.49	1.40
2	D	700	FAD	C10-N1	3.99	1.42	1.35
2	C	705	FAD	C6-C7	3.96	1.48	1.37
2	D	700	FAD	C6-C7	3.96	1.48	1.37
2	B	710	FAD	C6-C7	3.96	1.48	1.37
2	A	715	FAD	C6-C7	3.94	1.48	1.37
2	B	710	FAD	C10-N1	3.86	1.42	1.35
2	A	715	FAD	C8-C7	3.83	1.51	1.40
2	C	705	FAD	C8-C7	3.83	1.51	1.40
2	B	710	FAD	C8-C7	3.81	1.51	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	715	FAD	C10-N1	3.76	1.42	1.35
2	D	700	FAD	C8-C7	3.75	1.51	1.40
2	C	705	FAD	C10-N1	3.75	1.42	1.35
2	C	705	FAD	C2-N3	3.63	1.44	1.37
2	B	710	FAD	C2-N3	3.59	1.44	1.37
2	A	715	FAD	C2-N3	3.58	1.44	1.37
2	B	710	FAD	C2A-N1A	3.54	1.40	1.33
2	A	715	FAD	C10-N10	3.49	1.46	1.38
2	B	710	FAD	C2A-N3A	3.43	1.38	1.32
2	D	700	FAD	C2-N3	3.40	1.43	1.37
2	C	705	FAD	C2A-N1A	3.40	1.40	1.33
2	B	710	FAD	C10-N10	3.39	1.46	1.38
2	D	700	FAD	C2A-N3A	3.37	1.38	1.32
2	A	715	FAD	C2A-N3A	3.36	1.38	1.32
2	C	705	FAD	C10-N10	3.36	1.46	1.38
2	C	705	FAD	C2A-N3A	3.32	1.38	1.32
2	D	700	FAD	C2A-N1A	3.30	1.40	1.33
2	C	705	FAD	C8A-N9A	3.26	1.41	1.36
2	A	715	FAD	C8A-N9A	3.25	1.41	1.36
2	D	700	FAD	C8A-N9A	3.23	1.41	1.36
2	D	700	FAD	C10-N10	3.21	1.45	1.38
2	A	715	FAD	C2A-N1A	3.20	1.40	1.33
2	D	700	FAD	C4X-N5	3.19	1.42	1.36
2	A	715	FAD	C4X-N5	3.19	1.42	1.36
2	D	700	FAD	O4B-C1B	3.18	1.46	1.41
2	B	710	FAD	C4X-N5	3.16	1.42	1.36
2	C	705	FAD	C4X-N5	3.14	1.42	1.36
2	B	710	FAD	C8A-N9A	3.12	1.41	1.36
2	A	715	FAD	C5A-C4A	3.11	1.47	1.40
2	C	705	FAD	C5A-C4A	3.10	1.47	1.40
2	B	710	FAD	P-O3P	-3.09	1.54	1.59
2	B	710	FAD	C5A-C4A	3.08	1.47	1.40
2	B	710	FAD	O4B-C1B	3.02	1.46	1.41
2	D	700	FAD	P-O3P	-3.02	1.54	1.59
2	A	715	FAD	O4B-C1B	3.00	1.45	1.41
2	D	700	FAD	C5A-C4A	2.96	1.47	1.40
2	C	705	FAD	P-O3P	-2.94	1.54	1.59
2	A	715	FAD	P-O3P	-2.94	1.54	1.59
2	C	705	FAD	O4B-C1B	2.83	1.45	1.41
2	A	715	FAD	C9-C8	2.62	1.45	1.37
2	B	710	FAD	C9-C8	2.61	1.45	1.37
2	B	710	FAD	PA-O3P	-2.60	1.55	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	705	FAD	C9-C8	2.58	1.44	1.37
2	D	700	FAD	PA-O3P	-2.55	1.55	1.59
2	D	700	FAD	C9-C8	2.54	1.44	1.37
2	C	705	FAD	PA-O3P	-2.49	1.55	1.59
2	A	715	FAD	PA-O3P	-2.41	1.55	1.59
2	D	700	FAD	C1B-N9A	-2.36	1.41	1.48
2	B	710	FAD	C1B-N9A	-2.19	1.41	1.48
2	D	700	FAD	P-O5'	-2.18	1.49	1.59
2	C	705	FAD	P-O5'	-2.18	1.49	1.59
2	A	715	FAD	P-O5'	-2.16	1.49	1.59
2	B	710	FAD	P-O5'	-2.13	1.49	1.59
2	C	705	FAD	C5B-C4B	2.13	1.58	1.51
2	A	715	FAD	C1B-N9A	-2.12	1.42	1.48
2	C	705	FAD	C1B-N9A	-2.11	1.42	1.48
2	D	700	FAD	C5B-C4B	2.05	1.58	1.51
2	A	715	FAD	PA-O5B	-2.05	1.49	1.59
2	B	710	FAD	C5B-C4B	2.05	1.58	1.51

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	705	FAD	C2B-C1B-N9A	9.64	138.03	113.27
2	B	710	FAD	C2B-C1B-N9A	9.49	137.62	113.27
2	A	715	FAD	C2B-C1B-N9A	9.43	137.46	113.27
2	D	700	FAD	C2B-C1B-N9A	9.37	137.33	113.27
2	D	700	FAD	C4B-O4B-C1B	-8.93	100.05	109.75
2	A	715	FAD	C4B-O4B-C1B	-8.81	100.18	109.75
2	A	715	FAD	O4B-C1B-N9A	8.80	116.63	108.44
2	B	710	FAD	C4B-O4B-C1B	-8.77	100.22	109.75
2	D	700	FAD	O4B-C1B-N9A	8.74	116.57	108.44
2	B	710	FAD	O4B-C1B-N9A	8.63	116.47	108.44
2	C	705	FAD	C4B-O4B-C1B	-8.49	100.52	109.75
2	C	705	FAD	O4B-C1B-N9A	8.48	116.33	108.44
2	B	710	FAD	C3B-C2B-C1B	-7.65	88.93	100.91
2	D	700	FAD	C3B-C2B-C1B	-7.64	88.95	100.91
2	A	715	FAD	C3B-C2B-C1B	-7.61	89.00	100.91
2	C	705	FAD	C3B-C2B-C1B	-7.56	89.07	100.91
2	A	715	FAD	C2-N1-C10	6.96	122.00	114.98
2	C	705	FAD	C2-N1-C10	6.94	121.97	114.98
2	B	710	FAD	C2-N1-C10	6.87	121.90	114.98
2	D	700	FAD	C2-N1-C10	6.81	121.84	114.98
2	D	700	FAD	N3A-C2A-N1A	-6.67	123.14	128.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	705	FAD	N3A-C2A-N1A	-6.63	123.16	128.71
2	B	710	FAD	N3A-C2A-N1A	-6.58	123.20	128.71
2	A	715	FAD	N3A-C2A-N1A	-6.58	123.21	128.71
2	D	700	FAD	O2B-C2B-C1B	5.69	128.44	111.23
2	B	710	FAD	O2B-C2B-C1B	5.65	128.32	111.23
2	A	715	FAD	O2B-C2B-C1B	5.61	128.21	111.23
2	C	705	FAD	O2B-C2B-C1B	5.58	128.11	111.23
2	D	700	FAD	C4X-C10-N10	-4.81	118.11	120.51
2	B	710	FAD	C4X-C10-N10	-4.57	118.23	120.51
2	A	715	FAD	C4X-C10-N10	-4.55	118.24	120.51
2	C	705	FAD	C4X-C10-N10	-4.54	118.25	120.51
2	A	715	FAD	C4A-C5A-N7A	-4.01	106.09	109.52
2	C	705	FAD	C4A-C5A-N7A	-3.95	106.14	109.52
2	B	710	FAD	P-O3P-PA	3.92	143.19	131.68
2	D	700	FAD	C4A-C5A-N7A	-3.89	106.19	109.52
2	B	710	FAD	C4A-C5A-N7A	-3.86	106.21	109.52
2	C	705	FAD	P-O3P-PA	3.84	142.93	131.68
2	D	700	FAD	C1'-N10-C9A	3.79	122.56	118.87
2	D	700	FAD	P-O3P-PA	3.71	142.55	131.68
2	A	715	FAD	P-O3P-PA	3.68	142.47	131.68
2	B	710	FAD	C1'-N10-C9A	3.58	122.35	118.87
2	D	700	FAD	C1'-N10-C10	-3.45	114.27	119.17
2	D	700	FAD	C4X-N5-C5X	3.36	120.47	116.69
2	A	715	FAD	C1'-N10-C9A	3.35	122.13	118.87
2	C	705	FAD	C1'-N10-C9A	3.33	122.12	118.87
2	C	705	FAD	C4X-N5-C5X	3.28	120.37	116.69
2	A	715	FAD	C4X-N5-C5X	3.27	120.37	116.69
2	B	710	FAD	C4X-N5-C5X	3.27	120.36	116.69
2	B	710	FAD	C1'-N10-C10	-3.20	114.62	119.17
2	A	715	FAD	C1'-N10-C10	-3.01	114.89	119.17
2	C	705	FAD	C1'-N10-C10	-3.01	114.89	119.17
2	A	715	FAD	C2'-C1'-N10	-2.96	108.53	112.45
2	B	710	FAD	N3A-C4A-N9A	2.91	130.69	125.43
2	D	700	FAD	N3A-C4A-N9A	2.88	130.63	125.43
2	C	705	FAD	N3A-C4A-N9A	2.86	130.59	125.43
2	A	715	FAD	O3B-C3B-C4B	2.80	119.33	111.08
2	D	700	FAD	O3B-C3B-C4B	2.79	119.29	111.08
2	A	715	FAD	N3A-C4A-N9A	2.79	130.46	125.43
2	D	700	FAD	C2'-C1'-N10	-2.76	108.79	112.45
2	B	710	FAD	O3B-C3B-C4B	2.76	119.22	111.08
2	B	710	FAD	C5B-C4B-C3B	-2.75	104.21	115.21
2	A	715	FAD	C5B-C4B-C3B	-2.74	104.22	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	715	FAD	O4B-C4B-C3B	2.74	110.73	105.17
2	C	705	FAD	C5B-C4B-C3B	-2.73	104.27	115.21
2	C	705	FAD	O3B-C3B-C4B	2.73	119.13	111.08
2	B	710	FAD	O4B-C4B-C3B	2.73	110.70	105.17
2	B	710	FAD	C8A-N7A-C5A	2.71	111.97	103.58
2	D	700	FAD	O4B-C4B-C3B	2.70	110.64	105.17
2	C	705	FAD	C8A-N7A-C5A	2.70	111.94	103.58
2	D	700	FAD	C5B-C4B-C3B	-2.69	104.43	115.21
2	C	705	FAD	O4B-C4B-C3B	2.69	110.62	105.17
2	D	700	FAD	C8A-N7A-C5A	2.69	111.91	103.58
2	A	715	FAD	C8A-N7A-C5A	2.68	111.88	103.58
2	B	710	FAD	C2'-C1'-N10	-2.64	108.95	112.45
2	C	705	FAD	C2'-C1'-N10	-2.39	109.28	112.45
2	D	700	FAD	C1'-C2'-C3'	-2.36	103.07	109.82
2	B	710	FAD	C5A-C4A-N9A	-2.34	103.78	107.16
2	D	700	FAD	C5A-C4A-N9A	-2.30	103.84	107.16
2	D	700	FAD	C8A-N9A-C4A	2.26	108.62	106.90
2	C	705	FAD	C1'-C2'-C3'	-2.24	103.40	109.82
2	C	705	FAD	C5A-C4A-N9A	-2.23	103.94	107.16
2	B	710	FAD	C1'-C2'-C3'	-2.23	103.45	109.82
2	A	715	FAD	C2A-N1A-C6A	2.21	122.77	118.77
2	D	700	FAD	C2A-N1A-C6A	2.19	122.73	118.77
2	A	715	FAD	C5A-C4A-N9A	-2.18	104.01	107.16
2	C	705	FAD	C2A-N1A-C6A	2.13	122.62	118.77
2	A	715	FAD	P-O5'-C5'	2.12	137.29	122.03
2	A	715	FAD	C8A-N9A-C4A	2.11	108.51	106.90
2	B	710	FAD	C2A-N1A-C6A	2.08	122.52	118.77
2	D	700	FAD	P-O5'-C5'	2.03	136.66	122.03

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	700	FAD	C1B
2	C	705	FAD	C1B
2	A	715	FAD	C1B
2	B	710	FAD	C1B

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	211/232 (90%)	0.27	15 (7%) 16 11	15, 26, 50, 61	0
1	B	214/232 (92%)	0.35	17 (7%) 13 9	16, 28, 53, 58	0
1	C	214/232 (92%)	0.17	13 (6%) 21 15	15, 25, 47, 55	0
1	D	213/232 (91%)	0.42	20 (9%) 9 6	16, 29, 55, 65	0
All	All	852/928 (91%)	0.30	65 (7%) 13 10	15, 27, 52, 65	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	220	VAL	7.5
1	A	31	PHE	6.8
1	A	91	TYR	5.1
1	B	107	GLU	5.0
1	D	109	TYR	4.8
1	D	116	GLU	4.8
1	C	31	PHE	4.6
1	B	31	PHE	4.4
1	A	107	GLU	4.2
1	B	40	ARG	4.2
1	C	107	GLU	4.0
1	C	220	VAL	4.0
1	D	39	GLU	3.7
1	D	91[A]	TYR	3.7
1	A	37	ASP	3.7
1	A	0	HIS	3.6
1	D	93	LYS	3.5
1	B	113	ILE	3.5
1	D	40	ARG	3.4
1	D	107	GLU	3.2
1	D	108	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	112	THR	3.1
1	D	90[A]	ARG	3.1
1	B	114	PRO	3.1
1	C	138	GLU	3.0
1	C	109	TYR	3.0
1	C	95	SER	3.0
1	D	37	ASP	3.0
1	C	92	SER	3.0
1	A	40	ARG	3.0
1	A	36	LYS	2.9
1	C	96	TYR	2.9
1	B	110	LYS	2.9
1	B	93	LYS	2.9
1	D	94	LEU	2.9
1	C	219	GLN	2.8
1	A	95	SER	2.8
1	D	38	GLU	2.8
1	D	106	LEU	2.7
1	B	120	GLU	2.7
1	D	110	LYS	2.6
1	A	94	LEU	2.6
1	B	51	HIS	2.5
1	A	-1	HIS	2.5
1	D	31	PHE	2.5
1	D	120	GLU	2.5
1	B	47	TYR	2.5
1	B	106	LEU	2.4
1	A	112	THR	2.4
1	C	110	LYS	2.3
1	B	30	SER	2.3
1	B	108	GLY	2.3
1	C	40	ARG	2.3
1	A	39	GLU	2.2
1	B	138	GLU	2.2
1	A	106	LEU	2.2
1	D	95	SER	2.1
1	C	140	GLY	2.1
1	D	217	GLU	2.1
1	A	138	GLU	2.1
1	B	117	ARG	2.0
1	D	89[A]	GLY	2.0
1	C	91	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	108	GLY	2.0
1	D	117	ARG	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	FAD	B	710	53/53	0.28	5.89	35,52,65,65	0
2	FAD	C	705	53/53	0.24	4.19	33,50,69,69	0
2	FAD	D	700	53/53	0.18	1.49	25,39,50,50	0
2	FAD	A	715	53/53	0.22	1.08	34,48,68,69	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.