



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 06:35 AM GMT

PDB ID : 1O27  
Title : Crystal structure of Thymidylate Synthase Complementing Protein (TM0449) from *Thermotoga maritima* with FAD and BrdUMP at 2.3 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 : 2.30 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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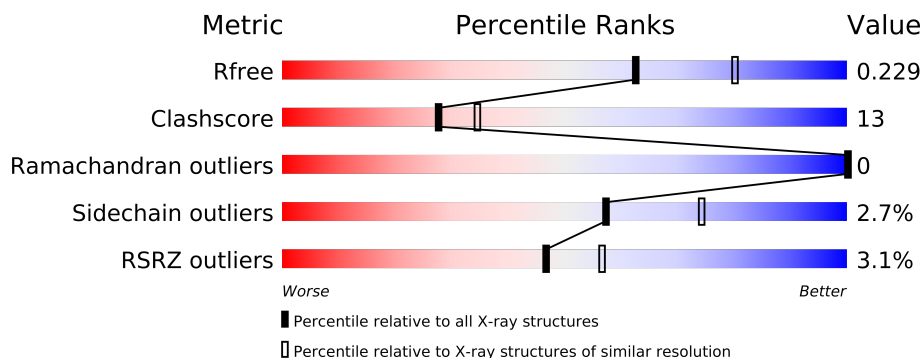
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.30 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	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7718 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	216	Total	C	N	O	S	0	0	0
			1793	1167	308	312	6			
1	B	217	Total	C	N	O	S	0	0	0
			1812	1179	310	317	6			
1	C	216	Total	C	N	O	S	0	0	0
			1813	1180	310	318	5			
1	D	215	Total	C	N	O	S	0	0	0
			1803	1173	307	317	6			

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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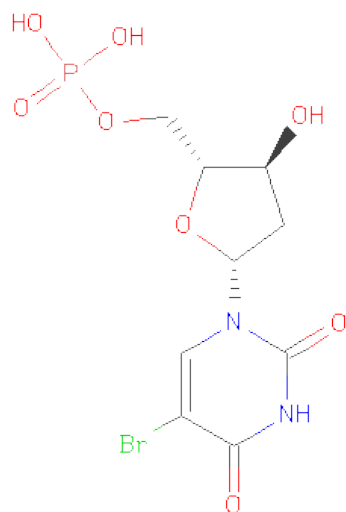
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
B	-1	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
B	0	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
C	-11	MET	-	LEADER SEQUENCE	UNP Q9WYT0
C	-10	GLY	-	LEADER SEQUENCE	UNP Q9WYT0
C	-9	SER	-	LEADER SEQUENCE	UNP Q9WYT0
C	-8	ASP	-	LEADER SEQUENCE	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 5-BROMO-2'-DEOXYURIDINE-5'-MONOPHOSPHATE (three-letter code: BRU) (formula:  $C_9H_{12}BrN_2O_8P$ ).

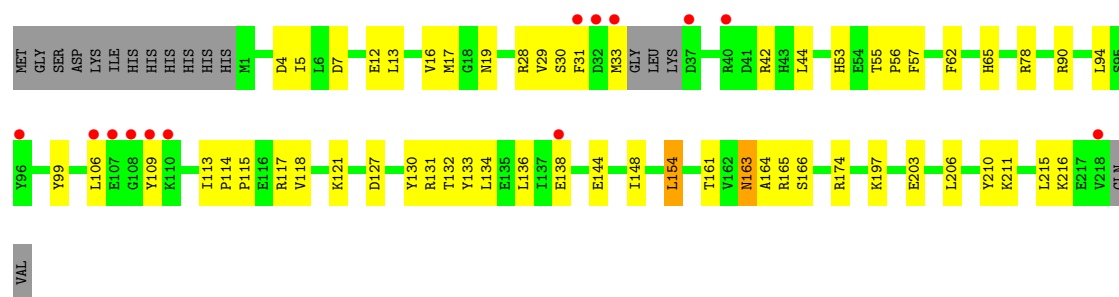


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 21	Br 1	C 9	N 2	O 8	P 1	0	0
3	B	1	Total 21	Br 1	C 9	N 2	O 8	P 1	0	0
3	C	1	Total 21	Br 1	C 9	N 2	O 8	P 1	0	0
3	D	1	Total 21	Br 1	C 9	N 2	O 8	P 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	55	Total 55	O 55	0	0
4	B	52	Total 52	O 52	0	0
4	C	53	Total 53	O 53	0	0
4	D	41	Total 41	O 41	0	0







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.35Å 116.43Å 140.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 46.48 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.2 (20.00-2.30) 97.8 (46.48-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.46 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.188 , 0.230 0.187 , 0.229	Depositor DCC
$R_{free}$ test set	1986 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.5	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 37.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 39615 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7718	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.50% 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: BRU, 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	0.35	0/1842	0.58	0/2490
1	B	0.35	0/1860	0.59	0/2513
1	C	0.36	0/1861	0.59	0/2514
1	D	0.36	0/1851	0.58	0/2502
All	All	0.36	0/7414	0.58	0/10019

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	1793	0	1785	59	0
1	B	1812	0	1806	64	0
1	C	1813	0	1811	44	0
1	D	1803	0	1794	50	0
2	A	53	0	30	1	0
2	B	53	0	30	0	0
2	C	53	0	30	1	0
2	D	53	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	21	0	10	3	0
3	B	21	0	10	2	0
3	C	21	0	10	3	0
3	D	21	0	10	2	0
4	A	55	0	0	0	0
4	B	52	0	0	0	0
4	C	53	0	0	0	0
4	D	41	0	0	3	0
All	All	7718	0	7356	191	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 13.

All (191) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:125:ILE:HG13	1:C:132:THR:HG21	1.37	1.06
1:B:174:ARG:HH12	3:C:613:BRU:HN3	1.10	0.98
1:A:174:ARG:HH12	3:D:618:BRU:HN3	1.08	0.94
3:B:608:BRU:HN3	1:C:174:ARG:HH12	1.11	0.91
1:C:17:MET:HB2	1:D:17:MET:HB2	1.51	0.89
1:A:17:MET:HB2	1:B:17:MET:HB2	1.52	0.89
1:C:94:LEU:HD13	1:C:154:LEU:HD21	1.56	0.88
1:B:149:VAL:HB	1:C:125:ILE:HD13	1.54	0.87
1:A:116:GLU:O	1:A:120:GLU:HG2	1.77	0.84
1:B:125:ILE:CG1	1:C:132:THR:HG21	2.09	0.82
1:C:87:LEU:HA	1:D:30:SER:HA	1.61	0.81
3:A:603:BRU:HN3	1:D:174:ARG:HH12	1.25	0.80
1:D:113:ILE:HD13	1:D:121:LYS:HE3	1.67	0.76
1:D:106:LEU:HD22	1:D:115:PRO:HA	1.71	0.72
1:A:116:GLU:CD	1:A:116:GLU:H	1.94	0.71
1:A:55:THR:OG1	1:A:56:PRO:HD3	1.94	0.68
1:A:29:VAL:HG21	1:B:159:PHE:CE1	2.29	0.67
1:C:128:LYS:O	1:C:132:THR:HG22	1.95	0.67
1:B:54:GLU:HB3	1:B:165:ARG:HG3	1.78	0.66
1:D:94:LEU:HD13	1:D:154:LEU:HD11	1.78	0.65
1:C:129:ALA:O	1:C:132:THR:HG23	1.96	0.65
1:D:28:ARG:HD2	1:D:33:MET:HG3	1.79	0.63
1:B:125:ILE:HG21	1:C:149:VAL:HB	1.80	0.63
1:B:192:ARG:HH12	1:B:220:VAL:HG11	1.63	0.63
1:A:180:GLN:O	1:A:183:ILE:HG22	2.00	0.62
1:B:128:LYS:NZ	1:C:128:LYS:HD3	2.15	0.62
1:B:199:PRO:O	1:B:203:GLU:HG2	1.98	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:90:ARG:HD3	3:C:613:BRU:BR	2.54	0.62
1:D:113:ILE:HG22	1:D:117:ARG:HB3	1.81	0.61
1:B:5:ILE:HG22	1:B:6:LEU:HG	1.83	0.60
1:A:94:LEU:HD13	1:A:154:LEU:HD21	1.83	0.60
1:C:124:GLU:HG2	1:C:128:LYS:HE3	1.83	0.60
1:A:159:PHE:CD1	1:B:29:VAL:HG21	2.37	0.60
1:B:24:VAL:O	1:B:28:ARG:HG2	2.02	0.59
1:B:50:LYS:HB3	1:B:208:TYR:CD2	2.37	0.59
1:B:127:ASP:O	1:B:131:ARG:HG3	2.03	0.58
1:C:159:PHE:CE1	1:D:29:VAL:HG21	2.39	0.58
1:A:57:PHE:O	1:A:164:ALA:HB3	2.03	0.58
1:C:151:PRO:HB2	1:C:153:ASN:OD1	2.05	0.57
1:B:129:ALA:HA	1:C:125:ILE:HD12	1.87	0.57
1:C:87:LEU:HD23	1:D:29:VAL:C	2.25	0.57
1:A:2:LYS:HE3	1:A:4:ASP:OD1	2.03	0.57
1:B:174:ARG:NH1	3:C:613:BRU:HN3	1.93	0.57
1:B:42:ARG:HG3	1:B:42:ARG:HH11	1.69	0.56
1:C:116:GLU:CD	1:C:116:GLU:H	2.09	0.56
1:D:132:THR:O	1:D:136:LEU:HG	2.06	0.56
1:A:145:VAL:O	1:A:148:ILE:HG12	2.04	0.56
1:D:163:ASN:ND2	1:D:166:SER:H	2.03	0.56
1:B:129:ALA:HA	1:C:125:ILE:CD1	2.35	0.56
1:C:130:TYR:CE2	1:C:134:LEU:HD11	2.39	0.56
1:B:87:LEU:HD13	1:B:88:SER:N	2.21	0.55
1:B:127:ASP:HB3	1:B:131:ARG:NH1	2.22	0.55
1:A:163:ASN:HD22	1:A:163:ASN:C	2.11	0.55
1:B:57:PHE:O	1:B:164:ALA:HB3	2.07	0.54
1:D:117:ARG:HG3	1:D:117:ARG:HH11	1.72	0.54
1:D:57:PHE:O	1:D:164:ALA:HB3	2.08	0.54
1:D:12:GLU:HG3	1:D:65:HIS:HB3	1.89	0.54
1:D:117:ARG:HH12	1:D:121:LYS:NZ	2.04	0.54
1:C:30:SER:O	1:C:31:PHE:HB2	2.08	0.54
1:B:145:VAL:O	1:B:148:ILE:HG12	2.07	0.53
1:D:42:ARG:NH2	1:D:203:GLU:OE2	2.42	0.53
1:B:132:THR:O	1:B:136:LEU:HG	2.08	0.53
1:A:142:PRO:HG3	1:D:109:TYR:CE2	2.44	0.53
1:A:5:ILE:HD11	1:A:189:ALA:HB2	1.91	0.53
1:A:44:LEU:HD22	1:A:48:LEU:HG	1.89	0.53
1:A:134:LEU:O	1:A:138:GLU:HG3	2.08	0.53
1:A:171:LEU:O	1:A:175:ALA:HB3	2.08	0.53
1:D:163:ASN:C	1:D:163:ASN:HD22	2.13	0.52
1:D:127:ASP:OD1	1:D:131:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:210:TYR:CE2	1:A:215:LEU:HB2	2.44	0.52
1:C:40:ARG:HG3	1:C:40:ARG:HH11	1.74	0.52
1:D:12:GLU:CG	1:D:65:HIS:HB3	2.40	0.51
1:A:2:LYS:C	1:A:2:LYS:HD2	2.31	0.51
1:C:62:PHE:O	1:C:161:THR:HA	2.11	0.51
1:D:29:VAL:O	1:D:29:VAL:HG12	2.11	0.50
1:B:128:LYS:HZ1	1:C:128:LYS:HD3	1.74	0.50
1:B:28:ARG:HG3	1:B:34:GLY:O	2.10	0.50
1:D:4:ASP:O	1:D:5:ILE:HD13	2.11	0.50
1:C:143:ARG:HG2	1:C:143:ARG:HH11	1.77	0.50
1:A:122:ILE:O	1:A:125:ILE:HG22	2.12	0.50
1:B:117:ARG:NH1	1:B:121:LYS:NZ	2.60	0.50
1:D:31:PHE:HB2	1:D:33:MET:HG2	1.93	0.50
1:C:94:LEU:HD13	1:C:154:LEU:CD2	2.36	0.49
1:D:206:LEU:O	1:D:216:LYS:HE3	2.12	0.49
1:D:55:THR:OG1	1:D:56:PRO:HD3	2.12	0.49
1:D:28:ARG:HB3	1:D:33:MET:HB2	1.94	0.49
1:A:174:ARG:HD2	1:A:183:ILE:HG12	1.95	0.49
1:C:94:LEU:HD12	1:C:150:LEU:HD12	1.95	0.49
1:A:62:PHE:O	1:A:161:THR:HA	2.13	0.49
1:B:13:LEU:HD11	1:B:16:VAL:HG22	1.94	0.49
1:D:106:LEU:HD21	1:D:118:VAL:HG21	1.95	0.48
1:B:106:LEU:HD11	1:B:118:VAL:HG11	1.94	0.48
1:B:127:ASP:HB3	1:B:131:ARG:HH12	1.78	0.48
1:D:113:ILE:CG2	1:D:117:ARG:HB3	2.42	0.48
1:B:117:ARG:NH1	1:B:121:LYS:HZ2	2.12	0.48
1:B:94:LEU:HD13	1:B:154:LEU:HD21	1.94	0.48
1:A:146:ALA:O	1:A:149:VAL:HG22	2.14	0.48
1:D:130:TYR:CE2	1:D:134:LEU:HD11	2.49	0.48
1:A:5:ILE:HG22	1:A:6:LEU:HG	1.96	0.47
1:B:128:LYS:HZ1	1:C:128:LYS:HB3	1.79	0.47
1:D:197:LYS:NZ	4:D:436:HOH:O	2.48	0.47
1:B:31:PHE:O	1:B:33:MET:HG3	2.15	0.47
1:B:42:ARG:HD3	1:B:42:ARG:O	2.16	0.46
1:A:86:GLU:HB2	1:A:158:PHE:HB3	1.97	0.46
1:B:13:LEU:HD21	1:B:16:VAL:HG21	1.96	0.46
1:A:2:LYS:HD2	1:A:3:ILE:N	2.31	0.46
1:B:167:LEU:O	1:B:167:LEU:HD23	2.16	0.46
1:A:29:VAL:HG21	1:B:159:PHE:CD1	2.50	0.46
1:C:94:LEU:HD12	1:C:150:LEU:CD1	2.46	0.46
1:D:62:PHE:O	1:D:161:THR:HA	2.15	0.46
1:A:175:ALA:HA	1:A:214:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:7:ASP:OD1	1:D:99:TYR:HD2	1.99	0.46
1:D:106:LEU:N	1:D:106:LEU:HD12	2.30	0.46
1:D:134:LEU:O	1:D:138:GLU:HG3	2.16	0.46
1:B:7:ASP:CG	1:B:8:LYS:HD2	2.36	0.46
1:C:134:LEU:O	1:C:138:GLU:HG3	2.15	0.46
1:A:192:ARG:C	1:A:192:ARG:HD3	2.36	0.45
1:A:210:TYR:CZ	1:A:215:LEU:HB2	2.51	0.45
1:A:120:GLU:O	1:A:124:GLU:HG3	2.16	0.45
1:B:147:ARG:HD2	1:B:148:ILE:N	2.32	0.45
1:D:210:TYR:CZ	1:D:215:LEU:HB2	2.52	0.45
1:A:163:ASN:ND2	1:A:166:SER:H	2.15	0.45
1:A:13:LEU:CD2	1:A:197:LYS:HE3	2.47	0.45
1:B:13:LEU:HD21	1:B:16:VAL:CG2	2.47	0.45
1:B:139:SER:O	1:C:111:THR:HA	2.17	0.44
1:B:117:ARG:HH11	1:B:121:LYS:NZ	2.14	0.44
1:B:54:GLU:OE1	1:B:165:ARG:HD3	2.17	0.44
1:B:42:ARG:NH1	1:B:42:ARG:HG3	2.32	0.44
1:B:90:ARG:HD3	3:B:608:BRU:BR	2.72	0.44
1:B:5:ILE:HD11	1:B:189:ALA:HB2	1.99	0.44
1:B:167:LEU:HD23	1:B:167:LEU:C	2.38	0.44
1:B:143:ARG:O	1:B:147:ARG:HG3	2.17	0.44
1:D:130:TYR:O	1:D:133:TYR:HB3	2.18	0.44
1:A:176:ASP:OD2	1:A:178:HIS:HD2	2.01	0.44
1:B:46:GLU:O	1:B:50:LYS:HG2	2.18	0.44
3:A:603:BRU:H1'	1:D:78:ARG:NH1	2.32	0.43
1:B:62:PHE:O	1:B:161:THR:HA	2.18	0.43
1:A:31:PHE:HA	1:B:92:SER:OG	2.18	0.43
1:C:216:LYS:NZ	1:C:216:LYS:HB2	2.34	0.43
1:C:106:LEU:HD11	1:C:118:VAL:HG11	2.00	0.43
1:B:210:TYR:CE2	1:B:215:LEU:HB2	2.53	0.43
1:D:28:ARG:HG3	4:D:352:HOH:O	2.19	0.43
1:C:220:VAL:OXT	1:C:220:VAL:HG23	2.19	0.43
1:D:19:ASN:HB2	4:D:498:HOH:O	2.17	0.43
1:A:113:ILE:HD12	1:A:117:ARG:HB3	2.00	0.43
1:B:55:THR:OG1	1:B:56:PRO:HD3	2.19	0.43
1:D:117:ARG:HH12	1:D:121:LYS:HZ3	1.66	0.43
1:A:59:HIS:CD2	1:B:85:ASN:HD22	2.37	0.43
1:B:148:ILE:HB	1:C:153:ASN:HB3	2.00	0.42
1:A:25:ARG:O	1:A:29:VAL:HG23	2.19	0.42
1:A:176:ASP:OD2	1:A:178:HIS:CD2	2.72	0.42
1:A:9:GLY:O	1:A:10:PHE:HB3	2.18	0.42
1:A:86:GLU:CG	1:A:87:LEU:N	2.83	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:87:LEU:HD23	1:D:30:SER:N	2.35	0.42
1:D:114:PRO:HA	1:D:115:PRO:HD3	1.97	0.42
1:B:28:ARG:HB3	1:B:33:MET:O	2.20	0.42
1:A:104:GLU:HA	1:A:107:GLU:HG3	2.01	0.42
1:B:220:VAL:HG23	1:B:220:VAL:OXT	2.20	0.42
1:A:117:ARG:O	1:A:121:LYS:HG3	2.20	0.42
1:B:96:TYR:HB2	1:B:130:TYR:CE2	2.55	0.42
1:A:44:LEU:O	1:A:47:TYR:HB3	2.20	0.41
1:D:211:LYS:HB3	1:D:211:LYS:HE2	1.87	0.41
1:D:210:TYR:CE2	1:D:215:LEU:HB2	2.55	0.41
1:A:167:LEU:HD23	1:A:167:LEU:C	2.40	0.41
1:C:150:LEU:HA	1:C:151:PRO:HD3	1.77	0.41
1:A:90:ARG:HD3	3:A:603:BRU:BR	2.75	0.41
1:A:147:ARG:HD2	1:A:148:ILE:N	2.35	0.41
1:D:163:ASN:HD21	1:D:166:SER:H	1.65	0.41
1:C:114:PRO:HA	1:C:115:PRO:HD3	1.98	0.41
1:C:127:ASP:OD2	1:C:131:ARG:NH1	2.48	0.41
1:A:173:LEU:HD13	2:A:615:FAD:O4'	2.20	0.41
1:A:181:TRP:O	1:A:185:GLN:HG2	2.21	0.41
1:A:153:ASN:HB3	1:D:148:ILE:HB	2.01	0.41
1:A:14:VAL:CG1	1:B:25:ARG:HH11	2.34	0.41
1:C:188:LEU:O	1:C:192:ARG:HG3	2.19	0.41
1:D:90:ARG:CB	1:D:144:GLU:HB3	2.51	0.41
1:A:78:ARG:NH1	3:D:618:BRU:H1'	2.35	0.41
1:A:163:ASN:HD21	2:C:605:FAD:H2A	1.86	0.41
1:A:202:PHE:O	1:A:205:PHE:HB3	2.20	0.41
1:B:219:GLN:O	1:B:220:VAL:OXT	2.39	0.41
1:A:143:ARG:O	1:A:147:ARG:HG3	2.20	0.41
1:B:112:THR:HB	1:C:139:SER:HB2	2.02	0.41
1:A:50:LYS:HE3	1:A:208:TYR:CE1	2.56	0.41
1:D:117:ARG:NH1	1:D:121:LYS:HE2	2.36	0.41
1:C:98:PHE:HE2	1:C:151:PRO:HD2	1.86	0.40
1:D:13:LEU:HD11	1:D:16:VAL:CG2	2.52	0.40
1:C:150:LEU:HA	1:C:150:LEU:HD23	1.91	0.40
1:A:167:LEU:O	1:A:170:PHE:HB3	2.21	0.40
1:C:162:VAL:CG2	1:C:166:SER:HB3	2.51	0.40
1:A:210:TYR:CE1	1:A:215:LEU:HD12	2.56	0.40
1:B:50:LYS:HB3	1:B:208:TYR:CG	2.56	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	214/232 (92%)	208 (97%)	6 (3%)	0	100	100
1	B	213/232 (92%)	209 (98%)	4 (2%)	0	100	100
1	C	212/232 (91%)	205 (97%)	7 (3%)	0	100	100
1	D	211/232 (91%)	203 (96%)	8 (4%)	0	100	100
All	All	850/928 (92%)	825 (97%)	25 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	189/207 (91%)	183 (97%)	6 (3%)	51	67
1	B	192/207 (93%)	187 (97%)	5 (3%)	59	76
1	C	193/207 (93%)	188 (97%)	5 (3%)	59	76
1	D	192/207 (93%)	187 (97%)	5 (3%)	59	76
All	All	766/828 (92%)	745 (97%)	21 (3%)	57	74

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	87	LEU
1	A	96	TYR
1	A	147	ARG
1	A	163	ASN

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Mol	Chain	Res	Type
1	A	192	ARG
1	B	42	ARG
1	B	44	LEU
1	B	117	ARG
1	B	147	ARG
1	B	192	ARG
1	C	92	SER
1	C	117	ARG
1	C	132	THR
1	C	147	ARG
1	C	216	LYS
1	D	44	LEU
1	D	53	HIS
1	D	154	LEU
1	D	163	ASN
1	D	165	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	ASN
1	A	178	HIS
1	A	185	GLN
1	B	85	ASN
1	C	51	HIS
1	D	163	ASN
1	D	178	HIS

### 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

8 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
3	BRU	A	603	-	22,22,22	2.86	11 (50%)	28,33,33	4.18	10 (35%)
2	FAD	A	615	-	58,58,58	2.99	27 (46%)	85,89,89	2.73	22 (25%)
3	BRU	B	608	-	22,22,22	2.67	10 (45%)	28,33,33	4.28	10 (35%)
2	FAD	B	610	-	58,58,58	2.83	27 (46%)	85,89,89	2.78	22 (25%)
2	FAD	C	605	-	58,58,58	2.75	27 (46%)	85,89,89	2.77	24 (28%)
3	BRU	C	613	-	22,22,22	2.84	10 (45%)	28,33,33	4.37	10 (35%)
2	FAD	D	600	-	58,58,58	2.83	28 (48%)	85,89,89	2.79	22 (25%)
3	BRU	D	618	-	22,22,22	2.88	9 (40%)	28,33,33	4.05	10 (35%)

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
3	BRU	A	603	-	-	0/7/22/22	0/2/2/2
2	FAD	A	615	-	1/1/9/9	0/34/50/50	0/1/6/6
3	BRU	B	608	-	-	0/7/22/22	0/2/2/2
2	FAD	B	610	-	1/1/9/9	0/34/50/50	0/1/6/6
2	FAD	C	605	-	1/1/9/9	0/34/50/50	0/1/6/6
3	BRU	C	613	-	-	0/7/22/22	0/2/2/2
2	FAD	D	600	-	1/1/9/9	0/34/50/50	0/1/6/6
3	BRU	D	618	-	-	0/7/22/22	0/2/2/2

All (149) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	618	BRU	C2-N1	9.23	1.48	1.38
3	A	603	BRU	C2-N1	9.21	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	613	BRU	C2-N1	8.42	1.47	1.38
3	B	608	BRU	C2-N1	8.11	1.47	1.38
2	B	610	FAD	C1'-C2'	6.65	1.57	1.51
2	A	615	FAD	C1'-C2'	6.64	1.57	1.51
2	A	615	FAD	C4A-N3A	6.40	1.45	1.35
2	A	615	FAD	C2B-C1B	6.36	1.62	1.53
2	B	610	FAD	C2B-C1B	6.35	1.62	1.53
2	D	600	FAD	C1'-C2'	6.13	1.57	1.51
2	D	600	FAD	C4A-N3A	6.09	1.44	1.35
2	C	605	FAD	C1'-C2'	6.07	1.57	1.51
2	B	610	FAD	C4A-N3A	5.89	1.44	1.35
2	A	615	FAD	C4-C4X	5.78	1.50	1.41
2	C	605	FAD	C4A-N3A	5.69	1.44	1.35
2	D	600	FAD	C2B-C1B	5.50	1.61	1.53
2	C	605	FAD	C2B-C1B	5.40	1.61	1.53
2	A	615	FAD	C4X-C10	5.35	1.50	1.40
2	B	610	FAD	C4-C4X	5.03	1.49	1.41
2	D	600	FAD	C6-C5X	5.02	1.47	1.41
2	C	605	FAD	C9A-C5X	4.94	1.52	1.42
2	A	615	FAD	C9A-C5X	4.91	1.52	1.42
2	B	610	FAD	C4X-C10	4.85	1.49	1.40
2	D	600	FAD	C4-C4X	4.84	1.49	1.41
2	A	615	FAD	C5X-N5	4.83	1.42	1.35
2	B	610	FAD	C8A-N7A	-4.75	1.25	1.34
2	D	600	FAD	C8A-N7A	-4.75	1.25	1.34
2	C	605	FAD	C4-C4X	4.71	1.48	1.41
2	B	610	FAD	C9A-C5X	4.67	1.52	1.42
2	A	615	FAD	C8A-N7A	-4.66	1.25	1.34
2	C	605	FAD	C4X-C10	4.59	1.48	1.40
2	A	615	FAD	C9-C9A	4.58	1.49	1.40
2	D	600	FAD	C4X-C10	4.57	1.48	1.40
2	C	605	FAD	C8A-N7A	-4.56	1.25	1.34
2	D	600	FAD	C9A-C5X	4.50	1.51	1.42
2	A	615	FAD	C6-C5X	4.47	1.47	1.41
2	B	610	FAD	C6-C5X	4.47	1.47	1.41
2	A	615	FAD	C4-N3	4.45	1.44	1.37
2	B	610	FAD	C4-N3	4.43	1.44	1.37
3	C	613	BRU	C6-N1	4.38	1.45	1.34
2	D	600	FAD	C4-N3	4.36	1.44	1.37
2	D	600	FAD	C9-C9A	4.35	1.49	1.40
2	C	605	FAD	C4-N3	4.32	1.44	1.37
3	D	618	BRU	C6-N1	4.28	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	610	FAD	C5X-N5	4.27	1.41	1.35
2	C	605	FAD	C6-C5X	4.22	1.46	1.41
2	B	610	FAD	C9-C9A	4.19	1.49	1.40
3	A	603	BRU	C6-N1	4.19	1.44	1.34
2	C	605	FAD	C9-C9A	4.18	1.49	1.40
3	B	608	BRU	C6-N1	4.07	1.44	1.34
2	D	600	FAD	C5X-N5	4.03	1.41	1.35
3	C	613	BRU	C4-C5	3.99	1.46	1.39
3	D	618	BRU	C4-C5	3.97	1.46	1.39
2	D	600	FAD	C8-C7	3.97	1.52	1.40
2	C	605	FAD	C8-C7	3.96	1.52	1.40
2	A	615	FAD	C8-C7	3.95	1.52	1.40
2	A	615	FAD	C6-C7	3.88	1.48	1.37
2	B	610	FAD	C8-C7	3.88	1.52	1.40
3	C	613	BRU	O4'-C1'	3.88	1.51	1.42
3	C	613	BRU	C4-N3	3.83	1.43	1.37
2	A	615	FAD	C10-N1	3.80	1.42	1.35
3	D	618	BRU	C4-N3	3.78	1.43	1.37
2	C	605	FAD	C5X-N5	3.77	1.41	1.35
3	B	608	BRU	C4-N3	3.74	1.43	1.37
2	B	610	FAD	C6-C7	3.74	1.48	1.37
3	A	603	BRU	C4-N3	3.72	1.43	1.37
2	C	605	FAD	C10-N1	3.67	1.42	1.35
2	D	600	FAD	C10-N1	3.67	1.42	1.35
2	A	615	FAD	C2-N3	3.65	1.44	1.37
3	B	608	BRU	O4'-C1'	3.64	1.51	1.42
2	D	600	FAD	C2A-N3A	3.62	1.39	1.32
2	A	615	FAD	C2A-N3A	3.58	1.39	1.32
3	A	603	BRU	C4-C5	3.57	1.46	1.39
2	B	610	FAD	C2-N3	3.57	1.44	1.37
3	A	603	BRU	O4'-C1'	3.57	1.50	1.42
2	D	600	FAD	O4B-C1B	3.55	1.46	1.41
2	D	600	FAD	P-O3P	-3.54	1.53	1.59
2	D	600	FAD	C6-C7	3.51	1.47	1.37
3	D	618	BRU	O4'-C1'	3.48	1.50	1.42
2	B	610	FAD	C10-N1	3.45	1.41	1.35
2	C	605	FAD	C2A-N3A	3.39	1.38	1.32
2	A	615	FAD	P-O3P	-3.39	1.53	1.59
2	C	605	FAD	O4B-C1B	3.39	1.46	1.41
2	D	600	FAD	PA-O3P	-3.36	1.53	1.59
2	B	610	FAD	C10-N10	3.36	1.46	1.38
2	A	615	FAD	C10-N10	3.35	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	615	FAD	C2A-N1A	3.35	1.40	1.33
2	D	600	FAD	C2A-N1A	3.34	1.40	1.33
2	C	605	FAD	C6-C7	3.31	1.46	1.37
2	C	605	FAD	C10-N10	3.28	1.45	1.38
2	A	615	FAD	C4X-N5	3.26	1.43	1.36
2	A	615	FAD	C8A-N9A	3.25	1.41	1.36
2	C	605	FAD	C2A-N1A	3.24	1.40	1.33
2	D	600	FAD	C2-N3	3.22	1.43	1.37
2	D	600	FAD	C10-N10	3.20	1.45	1.38
2	B	610	FAD	C2A-N1A	3.13	1.40	1.33
2	A	615	FAD	C5A-C4A	3.07	1.47	1.40
2	D	600	FAD	C8A-N9A	3.05	1.41	1.36
2	C	605	FAD	C5A-C4A	2.98	1.47	1.40
3	B	608	BRU	C4-C5	2.96	1.44	1.39
2	B	610	FAD	C2A-N3A	2.96	1.38	1.32
3	C	613	BRU	C2-N3	2.93	1.43	1.37
2	A	615	FAD	PA-O3P	-2.92	1.54	1.59
2	B	610	FAD	P-O3P	-2.90	1.54	1.59
2	A	615	FAD	O4B-C1B	2.88	1.45	1.41
2	C	605	FAD	C8A-N9A	2.86	1.40	1.36
2	C	605	FAD	C2-N3	2.85	1.42	1.37
2	C	605	FAD	P-O3P	-2.84	1.54	1.59
2	D	600	FAD	C5A-C4A	2.83	1.46	1.40
2	B	610	FAD	C8A-N9A	2.72	1.40	1.36
2	D	600	FAD	C9-C8	2.71	1.45	1.37
2	B	610	FAD	O4B-C1B	2.71	1.45	1.41
2	B	610	FAD	C9-C8	2.69	1.45	1.37
2	B	610	FAD	C5A-C4A	2.69	1.46	1.40
2	C	605	FAD	C4X-N5	2.68	1.41	1.36
2	C	605	FAD	C9-C8	2.66	1.45	1.37
3	B	608	BRU	C2-N3	2.63	1.42	1.37
2	C	605	FAD	C1B-N9A	-2.63	1.40	1.48
2	B	610	FAD	C4X-N5	2.62	1.41	1.36
3	D	618	BRU	C2-N3	2.57	1.42	1.37
3	C	613	BRU	O4'-C4'	2.56	1.51	1.45
2	A	615	FAD	C9-C8	2.53	1.44	1.37
2	B	610	FAD	PA-O3P	-2.52	1.55	1.59
3	A	603	BRU	O4'-C4'	2.52	1.50	1.45
3	D	618	BRU	O4'-C4'	2.50	1.50	1.45
2	D	600	FAD	C4X-N5	2.46	1.41	1.36
2	B	610	FAD	C1B-N9A	-2.43	1.41	1.48
3	C	613	BRU	C2'-C1'	2.42	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	FAD	C1B-N9A	-2.38	1.41	1.48
3	B	608	BRU	O4'-C4'	2.38	1.50	1.45
3	B	608	BRU	C2'-C1'	2.35	1.59	1.52
2	D	600	FAD	C5B-C4B	2.30	1.59	1.51
3	B	608	BRU	C2'-C3'	2.29	1.59	1.52
3	A	603	BRU	C2'-C1'	2.28	1.58	1.52
3	A	603	BRU	P-OP2	-2.26	1.46	1.54
3	C	613	BRU	P-OP2	-2.25	1.46	1.54
2	C	605	FAD	PA-O3P	-2.24	1.55	1.59
3	D	618	BRU	C2'-C1'	2.22	1.58	1.52
2	A	615	FAD	C1B-N9A	-2.20	1.41	1.48
3	D	618	BRU	P-OP2	-2.20	1.46	1.54
3	A	603	BRU	C2-N3	2.15	1.41	1.37
2	C	605	FAD	O5B-C5B	2.13	1.53	1.44
3	A	603	BRU	C2'-C3'	2.13	1.58	1.52
3	C	613	BRU	C2'-C3'	2.10	1.58	1.52
2	D	600	FAD	O5B-C5B	2.10	1.53	1.44
2	A	615	FAD	C5B-C4B	2.08	1.58	1.51
2	B	610	FAD	C5B-C4B	2.08	1.58	1.51
3	B	608	BRU	P-OP2	-2.07	1.47	1.54
3	A	603	BRU	P-OP3	-2.01	1.47	1.54

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	613	BRU	C6-N1-C2	-17.17	117.53	122.41
3	B	608	BRU	C6-N1-C2	-16.95	117.59	122.41
3	A	603	BRU	C6-N1-C2	-16.32	117.77	122.41
3	D	618	BRU	C6-N1-C2	-15.71	117.94	122.41
3	C	613	BRU	C5-C6-N1	10.70	126.72	119.67
3	B	608	BRU	C5-C6-N1	10.42	126.53	119.67
3	A	603	BRU	C5-C6-N1	9.89	126.19	119.67
3	D	618	BRU	C5-C6-N1	9.83	126.14	119.67
2	A	615	FAD	C2B-C1B-N9A	9.40	137.41	113.27
2	B	610	FAD	C2B-C1B-N9A	9.38	137.35	113.27
2	B	610	FAD	C4B-O4B-C1B	-9.37	99.57	109.75
2	D	600	FAD	C4B-O4B-C1B	-9.34	99.60	109.75
2	C	605	FAD	C2B-C1B-N9A	9.23	136.96	113.27
2	D	600	FAD	C2B-C1B-N9A	9.19	136.87	113.27
2	C	605	FAD	C4B-O4B-C1B	-9.09	99.87	109.75
2	D	600	FAD	O4B-C1B-N9A	9.03	116.84	108.44
2	C	605	FAD	O4B-C1B-N9A	8.84	116.67	108.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	615	FAD	C4B-O4B-C1B	-8.79	100.20	109.75
2	A	615	FAD	O4B-C1B-N9A	8.57	116.42	108.44
2	B	610	FAD	O4B-C1B-N9A	8.41	116.27	108.44
2	D	600	FAD	C3B-C2B-C1B	-7.96	88.45	100.91
2	B	610	FAD	C3B-C2B-C1B	-7.93	88.50	100.91
2	A	615	FAD	C3B-C2B-C1B	-7.92	88.51	100.91
2	C	605	FAD	C3B-C2B-C1B	-7.84	88.64	100.91
2	B	610	FAD	C2-N1-C10	6.80	121.83	114.98
2	A	615	FAD	C2-N1-C10	6.77	121.80	114.98
2	D	600	FAD	C2-N1-C10	6.71	121.74	114.98
2	B	610	FAD	N3A-C2A-N1A	-6.70	123.10	128.71
2	C	605	FAD	C2-N1-C10	6.69	121.72	114.98
2	D	600	FAD	N3A-C2A-N1A	-6.66	123.14	128.71
2	A	615	FAD	N3A-C2A-N1A	-6.43	123.33	128.71
3	A	603	BRU	C2'-C1'-N1	-6.42	97.41	114.08
3	C	613	BRU	C2'-C1'-N1	-6.40	97.45	114.08
2	C	605	FAD	N3A-C2A-N1A	-6.38	123.37	128.71
3	D	618	BRU	C2'-C1'-N1	-6.19	98.01	114.08
3	B	608	BRU	C2'-C1'-N1	-5.86	98.85	114.08
2	A	615	FAD	O2B-C2B-C1B	5.85	128.91	111.23
2	B	610	FAD	O2B-C2B-C1B	5.83	128.86	111.23
2	D	600	FAD	O2B-C2B-C1B	5.61	128.21	111.23
2	C	605	FAD	O2B-C2B-C1B	5.56	128.06	111.23
3	C	613	BRU	O4'-C1'-N1	5.30	117.63	107.68
3	A	603	BRU	O4'-C1'-N1	5.16	117.38	107.68
3	B	608	BRU	O4'-C1'-N1	5.15	117.35	107.68
2	D	600	FAD	C4X-C10-N10	-4.95	118.04	120.51
2	C	605	FAD	C2'-C1'-N10	-4.90	105.95	112.45
2	C	605	FAD	C4X-C10-N10	-4.87	118.08	120.51
3	D	618	BRU	O4'-C1'-N1	4.85	116.79	107.68
2	B	610	FAD	C2'-C1'-N10	-4.78	106.11	112.45
2	A	615	FAD	C2'-C1'-N10	-4.76	106.14	112.45
2	B	610	FAD	C4X-C10-N10	-4.71	118.16	120.51
2	D	600	FAD	C2'-C1'-N10	-4.43	106.57	112.45
2	A	615	FAD	C4X-C10-N10	-4.32	118.36	120.51
2	C	605	FAD	C1'-N10-C9A	4.06	122.83	118.87
2	C	605	FAD	C4A-C5A-N7A	-4.03	106.07	109.52
2	A	615	FAD	C4A-C5A-N7A	-3.98	106.11	109.52
2	B	610	FAD	P-O3P-PA	3.92	143.17	131.68
2	B	610	FAD	C4A-C5A-N7A	-3.88	106.19	109.52
2	B	610	FAD	C1'-N10-C9A	3.84	122.61	118.87
2	D	600	FAD	C1'-N10-C9A	3.84	122.61	118.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	600	FAD	C4A-C5A-N7A	-3.77	106.29	109.52
2	C	605	FAD	P-O3P-PA	3.74	142.64	131.68
2	D	600	FAD	P-O3P-PA	3.72	142.59	131.68
2	D	600	FAD	C4X-N5-C5X	3.70	120.85	116.69
2	B	610	FAD	C4X-N5-C5X	3.69	120.84	116.69
2	A	615	FAD	C1'-N10-C9A	3.66	122.44	118.87
2	C	605	FAD	C4X-N5-C5X	3.66	120.80	116.69
2	A	615	FAD	P-O3P-PA	3.64	142.36	131.68
3	A	603	BRU	BR-C5-C6	3.55	125.01	117.98
2	C	605	FAD	C1'-N10-C10	-3.44	114.29	119.17
3	B	608	BRU	BR-C5-C6	3.40	124.72	117.98
3	D	618	BRU	BR-C5-C6	3.40	124.71	117.98
2	D	600	FAD	C1'-N10-C10	-3.36	114.40	119.17
3	C	613	BRU	BR-C5-C6	3.34	124.59	117.98
2	A	615	FAD	C4X-N5-C5X	3.33	120.44	116.69
2	B	610	FAD	C1'-N10-C10	-3.33	114.44	119.17
2	A	615	FAD	C1'-N10-C10	-3.30	114.49	119.17
2	A	615	FAD	N3A-C4A-N9A	3.03	130.91	125.43
2	D	600	FAD	N3A-C4A-N9A	3.02	130.88	125.43
3	C	613	BRU	P-O5'-C5'	2.97	126.78	118.19
3	D	618	BRU	N3-C2-N1	-2.92	113.53	115.97
2	B	610	FAD	N3A-C4A-N9A	2.90	130.66	125.43
3	B	608	BRU	N3-C2-N1	-2.84	113.61	115.97
2	C	605	FAD	N3A-C4A-N9A	2.82	130.52	125.43
3	D	618	BRU	P-O5'-C5'	2.79	126.25	118.19
2	B	610	FAD	C8A-N7A-C5A	2.78	112.19	103.58
3	A	603	BRU	P-O5'-C5'	2.77	126.20	118.19
2	A	615	FAD	O3B-C3B-C4B	2.77	119.23	111.08
3	A	603	BRU	N3-C2-N1	-2.76	113.67	115.97
2	D	600	FAD	C8A-N7A-C5A	2.76	112.14	103.58
2	B	610	FAD	O3B-C3B-C4B	2.75	119.17	111.08
2	A	615	FAD	C8A-N7A-C5A	2.73	112.05	103.58
2	C	605	FAD	O3B-C3B-C4B	2.71	119.06	111.08
2	C	605	FAD	C8A-N7A-C5A	2.71	111.98	103.58
2	B	610	FAD	O4B-C4B-C3B	2.71	110.66	105.17
3	B	608	BRU	P-O5'-C5'	2.70	126.00	118.19
3	C	613	BRU	N3-C2-N1	-2.66	113.75	115.97
2	D	600	FAD	O3B-C3B-C4B	2.65	118.88	111.08
2	B	610	FAD	C5B-C4B-C3B	-2.63	104.66	115.21
2	D	600	FAD	C5B-C4B-C3B	-2.58	104.88	115.21
2	C	605	FAD	C5B-C4B-C3B	-2.57	104.91	115.21
2	A	615	FAD	O4B-C4B-C3B	2.56	110.36	105.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	605	FAD	O4B-C4B-C3B	2.56	110.36	105.17
2	D	600	FAD	O4B-C4B-C3B	2.54	110.31	105.17
2	D	600	FAD	C5A-C4A-N9A	-2.47	103.60	107.16
2	A	615	FAD	C5B-C4B-C3B	-2.45	105.40	115.21
2	D	600	FAD	P-O5'-C5'	2.43	139.47	122.03
2	A	615	FAD	P-O5'-C5'	2.36	138.98	122.03
2	C	605	FAD	P-O5'-C5'	2.36	138.99	122.03
2	B	610	FAD	C5A-C4A-N9A	-2.36	103.76	107.16
2	A	615	FAD	C5A-C4A-N9A	-2.35	103.77	107.16
3	B	608	BRU	O4'-C4'-C3'	-2.29	99.87	105.66
2	C	605	FAD	C5A-C4A-N9A	-2.28	103.88	107.16
3	A	603	BRU	C4'-O4'-C1'	2.25	115.15	109.44
3	C	613	BRU	O4'-C4'-C3'	-2.24	99.97	105.66
2	D	600	FAD	C8A-N9A-C4A	2.24	108.61	106.90
3	C	613	BRU	C4'-O4'-C1'	2.21	115.04	109.44
2	C	605	FAD	C8A-N9A-C4A	2.19	108.57	106.90
2	B	610	FAD	P-O5'-C5'	2.16	137.59	122.03
2	B	610	FAD	C2A-N1A-C6A	2.14	122.64	118.77
3	A	603	BRU	O4'-C4'-C3'	-2.13	100.26	105.66
3	A	603	BRU	BR-C5-C4	-2.08	116.33	120.11
3	D	618	BRU	C4'-O4'-C1'	2.08	114.70	109.44
2	C	605	FAD	C9-C9A-N10	2.07	126.05	121.59
3	C	613	BRU	OP3-P-O5'	2.07	112.35	106.65
3	D	618	BRU	O4'-C4'-C3'	-2.04	100.50	105.66
3	B	608	BRU	C4'-O4'-C1'	2.03	114.59	109.44
2	C	605	FAD	C2A-N1A-C6A	2.03	122.44	118.77
2	A	615	FAD	C2A-N1A-C6A	2.02	122.42	118.77
3	D	618	BRU	BR-C5-C4	-2.01	116.45	120.11
3	B	608	BRU	BR-C5-C4	-2.00	116.47	120.11

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	615	FAD	C1B
2	C	605	FAD	C1B
2	D	600	FAD	C1B
2	B	610	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	216/232 (93%)	0.06	7 (3%) 45 55	18, 31, 50, 56	0
1	B	217/232 (93%)	0.04	3 (1%) 72 80	19, 32, 52, 65	0
1	C	216/232 (93%)	-0.10	4 (1%) 64 73	19, 29, 50, 60	0
1	D	215/232 (92%)	0.15	13 (6%) 21 30	19, 31, 56, 65	0
All	All	864/928 (93%)	0.04	27 (3%) 47 56	18, 30, 53, 65	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	33	MET	4.9
1	C	220	VAL	4.5
1	D	32	ASP	4.2
1	C	219	GLN	3.5
1	D	106	LEU	3.1
1	B	220	VAL	3.0
1	D	108	GLY	2.9
1	D	107	GLU	2.8
1	D	40	ARG	2.8
1	A	112	THR	2.7
1	D	218	VAL	2.7
1	B	112	THR	2.6
1	D	96	TYR	2.5
1	D	109	TYR	2.5
1	C	94	LEU	2.4
1	D	31	PHE	2.4
1	A	47	TYR	2.3
1	A	36	LYS	2.3
1	A	40	ARG	2.3
1	C	40	ARG	2.2
1	A	81	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	37	ASP	2.1
1	D	138	GLU	2.0
1	A	31	PHE	2.0
1	D	110	LYS	2.0
1	A	107	GLU	2.0
1	B	107	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	FAD	B	610	53/53	0.16	0.16	20,29,32,34	0
2	FAD	C	605	53/53	0.16	0.08	22,26,28,33	0
2	FAD	D	600	53/53	0.15	0.06	20,27,30,31	0
2	FAD	A	615	53/53	0.15	-0.13	24,34,40,41	0
3	BRU	B	608	21/21	0.11	-0.42	23,24,26,29	0
3	BRU	A	603	21/21	0.10	-0.55	25,28,30,33	0
3	BRU	C	613	21/21	0.11	-0.57	24,28,31,35	0
3	BRU	D	618	21/21	0.11	-0.63	29,33,38,43	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.