



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 12:53 AM GMT

PDB ID : 1O26
Title : Crystal structure of Thymidylate Synthase Complementing Protein (TM0449) from *Thermotoga maritima* with FAD and dUMP at 1.6 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 : 1.60 Å(reported)

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

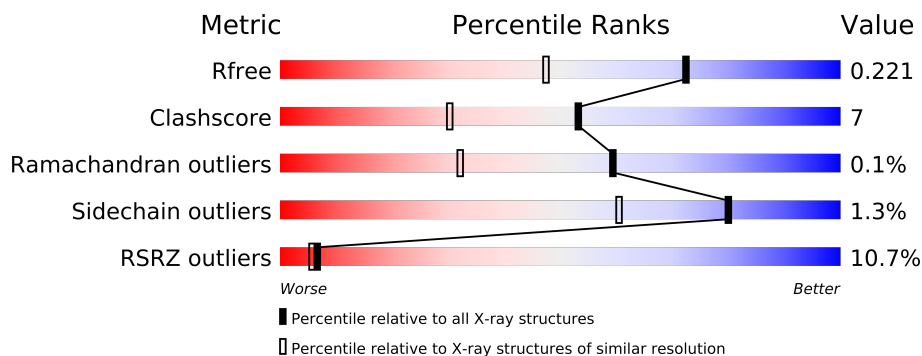
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 1.60 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	1872 (1.60-1.60)
Clashscore	79885	2199 (1.60-1.60)
Ramachandran outliers	78287	2126 (1.60-1.60)
Sidechain outliers	78261	2125 (1.60-1.60)
RSRZ outliers	66119	1872 (1.60-1.60)

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

Mol	Chain	Length	Quality of chain
1	A	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
4	PGE	A	635	-	X
4	PGE	B	630	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7940 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	219	Total	C	N	O	S	0	0	0
			1831	1190	314	321	6			
1	B	221	Total	C	N	O	S	0	0	0
			1851	1203	317	325	6			
1	C	218	Total	C	N	O	S	0	0	0
			1824	1187	311	320	6			
1	D	218	Total	C	N	O	S	0	0	0
			1824	1187	311	320	6			

There are 48 discrepancies between the modelled and reference sequences:

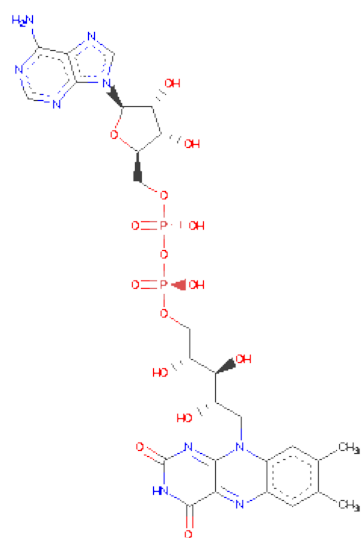
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	LEADER SEQUENCE	UNP Q9WYT0
A	-10	GLY	-	LEADER SEQUENCE	UNP Q9WYT0
A	-9	SER	-	LEADER SEQUENCE	UNP Q9WYT0
A	-8	ASP	-	LEADER SEQUENCE	UNP Q9WYT0
A	-7	LYS	-	LEADER SEQUENCE	UNP Q9WYT0
A	-6	ILE	-	LEADER SEQUENCE	UNP Q9WYT0
A	-5	HIS	-	LEADER SEQUENCE	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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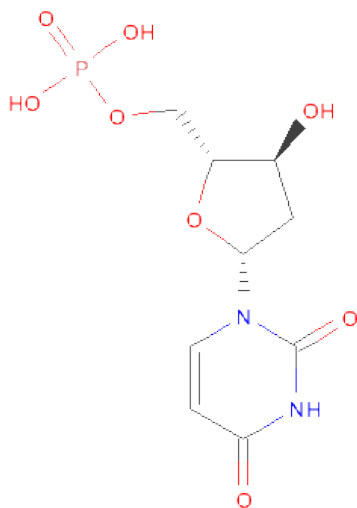
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
B	-1	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
B	0	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
C	-11	MET	-	LEADER SEQUENCE	UNP Q9WYT0
C	-10	GLY	-	LEADER SEQUENCE	UNP Q9WYT0
C	-9	SER	-	LEADER SEQUENCE	UNP Q9WYT0
C	-8	ASP	-	LEADER SEQUENCE	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: $C_{27}H_{33}N_9O_{15}P_2$).



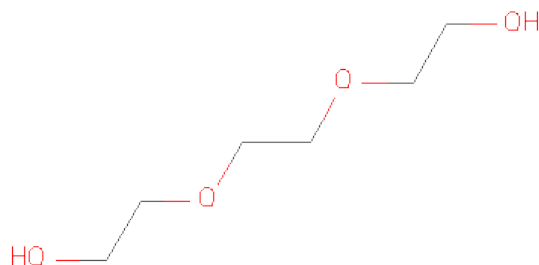
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: $C_9H_{13}N_2O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
3	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
3	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
3	D	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			10	6	4		
4	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	68	Total	O	0	0
			68	68		

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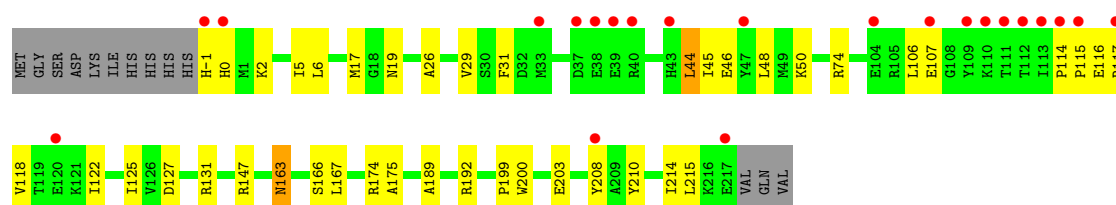
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	52	Total 52	O 52	0	0
5	C	82	Total 82	O 82	0	0
5	D	66	Total 66	O 66	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

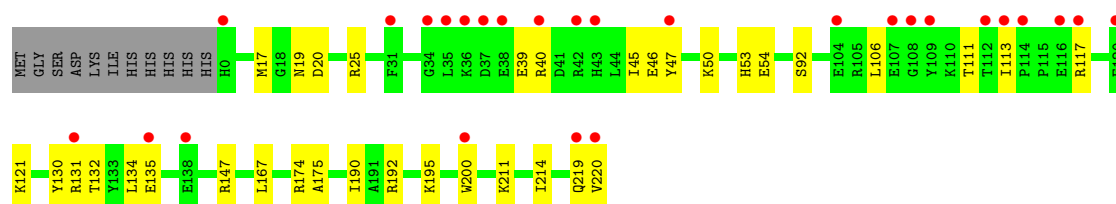
• Molecule 1: Thymidylate synthase thyX

Chain A: 



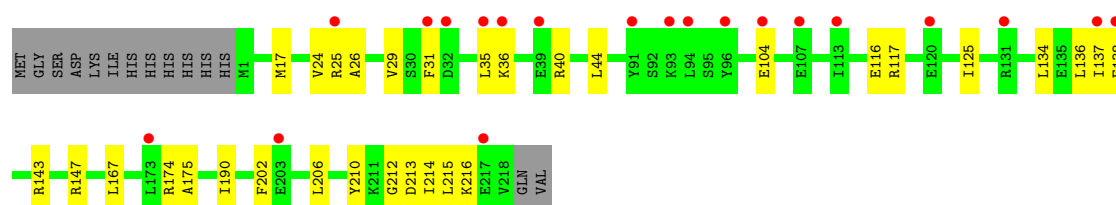
• Molecule 1: Thymidylate synthase thyX

Chain B: 



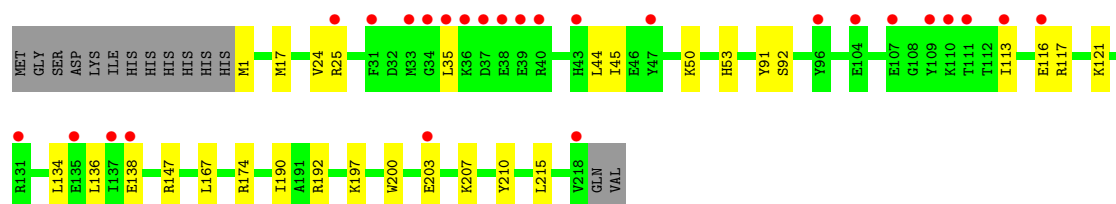
• Molecule 1: Thymidylate synthase thyX

Chain C: 



• Molecule 1: Thymidylate synthase thyX

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.56Å 117.73Å 141.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.60 50.25 – 1.60	Depositor EDS
% Data completeness (in resolution range)	98.1 (20.00-1.60) 98.8 (50.25-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 1.60Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.203 , 0.218 0.205 , 0.221	Depositor DCC
R_{free} test set	6155 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 60.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 121887 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7940	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, UMP, 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	0.38	0/1881	0.61	0/2542
1	B	0.36	0/1901	0.60	0/2569
1	C	0.38	0/1873	0.62	0/2532
1	D	0.38	0/1873	0.61	0/2532
All	All	0.38	0/7528	0.61	0/10175

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	1831	0	1821	33	0
1	B	1851	0	1846	31	0
1	C	1824	0	1822	30	0
1	D	1824	0	1822	23	0
2	A	53	0	30	0	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	20	0	11	1	0
3	B	20	0	11	1	0
3	C	20	0	11	1	0
3	D	20	0	11	1	0
4	A	10	0	14	1	0
4	B	20	0	28	2	0
4	D	20	0	28	1	0
5	A	68	0	0	1	0
5	B	52	0	0	1	0
5	C	82	0	0	0	0
5	D	66	0	0	1	0
All	All	7940	0	7545	107	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 7.

All (107) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:132:THR:HG21	1:C:125:ILE:HD11	1.42	1.01
3:A:603:UMP:HN3	1:D:174:ARG:HH12	1.10	0.99
1:B:174:ARG:HH12	3:C:613:UMP:HN3	1.16	0.93
3:B:608:UMP:HN3	1:C:174:ARG:HH12	1.14	0.93
1:A:174:ARG:HH12	3:D:618:UMP:HN3	1.14	0.91
1:B:132:THR:CG2	1:C:125:ILE:HD11	2.07	0.85
1:C:17:MET:HB2	1:D:17:MET:HB2	1.64	0.79
1:B:53:HIS:HA	4:B:630:PGE:H3	1.66	0.78
1:A:17:MET:HB2	1:B:17:MET:HB2	1.65	0.77
1:B:111:THR:HG22	1:B:113:ILE:H	1.54	0.72
1:D:117:ARG:HG3	1:D:121:LYS:HE2	1.71	0.72
1:C:25:ARG:HG2	1:C:35:LEU:HD21	1.71	0.72
1:B:132:THR:CB	1:C:125:ILE:HD11	2.21	0.70
1:D:203:GLU:HG2	1:D:207:LYS:HE2	1.76	0.67
1:D:167:LEU:HD11	1:D:190:ILE:HG21	1.80	0.62
1:B:132:THR:HG21	1:C:125:ILE:CD1	2.25	0.62
1:C:25:ARG:HG3	1:C:35:LEU:HD11	1.81	0.62
1:A:116:GLU:CD	1:A:116:GLU:H	2.04	0.60
1:C:167:LEU:HD11	1:C:190:ILE:HG21	1.82	0.60
1:C:117:ARG:HH11	1:C:117:ARG:HG3	1.67	0.59
1:B:167:LEU:HD11	1:B:190:ILE:HG21	1.84	0.59
1:B:47:TYR:HA	1:B:50:LYS:HE2	1.84	0.59
1:A:50:LYS:HE3	1:A:208:TYR:CE2	2.38	0.58
1:D:113:ILE:HD13	1:D:121:LYS:HE3	1.86	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:192:ARG:HG3	1:D:192:ARG:HH11	1.69	0.56
1:A:210:TYR:CE2	1:A:215:LEU:HB2	2.40	0.56
1:A:192:ARG:HH11	1:A:192:ARG:HG2	1.71	0.56
1:C:31:PHE:HA	1:D:92:SER:OG	2.06	0.56
1:A:127:ASP:O	1:A:131:ARG:HG3	2.06	0.55
1:A:45:ILE:HD12	1:A:200:TRP:HE3	1.72	0.55
1:A:175:ALA:HA	1:A:214:ILE:HD11	1.89	0.55
1:B:175:ALA:HA	1:B:214:ILE:HD11	1.89	0.55
1:C:104:GLU:HG2	1:C:104:GLU:O	2.06	0.54
1:D:167:LEU:HD11	1:D:190:ILE:CG2	2.37	0.54
1:B:25:ARG:HH11	1:B:25:ARG:HG3	1.73	0.53
1:B:131:ARG:O	1:B:135:GLU:HG3	2.07	0.53
1:A:31:PHE:HA	1:B:92:SER:OG	2.08	0.53
1:B:113:ILE:HB	1:B:117:ARG:HD3	1.91	0.53
1:D:203:GLU:CG	1:D:207:LYS:HE2	2.39	0.53
1:C:167:LEU:HD11	1:C:190:ILE:CG2	2.38	0.53
1:C:202:PHE:CE2	1:C:206:LEU:HD11	2.44	0.52
1:B:106:LEU:HD12	1:B:106:LEU:N	2.24	0.52
4:A:635:PGE:H22	2:C:605:FAD:H2'	1.92	0.52
1:B:167:LEU:HD11	1:B:190:ILE:CG2	2.40	0.52
1:A:114:PRO:HD2	1:A:117:ARG:HG3	1.92	0.52
1:D:50:LYS:HE3	5:D:314:HOH:O	2.10	0.51
1:C:35:LEU:HD22	1:C:35:LEU:N	2.25	0.51
1:B:46:GLU:O	1:B:50:LYS:HG2	2.10	0.51
1:D:134:LEU:O	1:D:138:GLU:HG3	2.11	0.51
1:C:137:ILE:HD11	1:C:143:ARG:HA	1.92	0.51
1:B:121:LYS:HD2	1:C:136:LEU:HD21	1.94	0.50
1:A:163:ASN:HD22	1:A:163:ASN:C	2.15	0.50
1:A:5:ILE:HD11	1:A:189:ALA:HB2	1.94	0.49
1:B:20:ASP:HB3	1:B:45:ILE:HD11	1.93	0.49
1:D:24:VAL:HG13	1:D:44:LEU:HD23	1.95	0.49
1:C:24:VAL:HG13	1:C:44:LEU:HD23	1.94	0.49
1:D:117:ARG:O	1:D:121:LYS:HG3	2.12	0.49
1:A:26:ALA:O	1:A:29:VAL:HG12	2.13	0.49
1:A:106:LEU:HD12	1:A:106:LEU:N	2.28	0.48
1:D:210:TYR:CE2	1:D:215:LEU:HB2	2.48	0.48
1:C:212:GLY:O	1:C:216:LYS:NZ	2.47	0.48
1:C:213:ASP:HA	1:C:216:LYS:NZ	2.28	0.48
1:C:134:LEU:O	1:C:138:GLU:HG3	2.14	0.48
1:A:199:PRO:O	1:A:203:GLU:HG2	2.14	0.48
1:D:116:GLU:H	1:D:116:GLU:CD	2.17	0.47
1:A:-1:HIS:O	1:A:0:HIS:ND1	2.46	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:116:GLU:CD	1:C:116:GLU:H	2.16	0.47
1:B:195:LYS:HD3	1:B:220:VAL:HG12	1.97	0.47
1:A:46:GLU:HB3	1:A:50:LYS:NZ	2.31	0.46
1:B:20:ASP:HB3	1:B:45:ILE:CD1	2.44	0.46
1:A:114:PRO:HB3	1:A:116:GLU:OE1	2.16	0.46
1:A:44:LEU:O	1:A:48:LEU:HG	2.16	0.45
1:D:45:ILE:HD12	1:D:200:TRP:HE3	1.80	0.45
1:B:220:VAL:OXT	1:B:220:VAL:HG23	2.17	0.45
1:D:25:ARG:HG3	1:D:35:LEU:HD21	1.99	0.45
1:A:167:LEU:HD23	1:A:167:LEU:C	2.37	0.45
1:B:19:ASN:HB2	5:B:492:HOH:O	2.18	0.44
1:A:122:ILE:O	1:A:125:ILE:HG22	2.18	0.44
1:A:19:ASN:HB2	5:A:433:HOH:O	2.17	0.43
1:C:25:ARG:HG2	1:C:35:LEU:CD2	2.44	0.43
1:B:45:ILE:HD12	1:B:200:TRP:HE3	1.84	0.43
1:D:1:MET:HE2	1:D:197:LYS:HE2	2.01	0.43
1:C:36:LYS:HD3	1:C:40:ARG:HH11	1.84	0.43
1:C:31:PHE:CE2	1:D:91:TYR:HB3	2.53	0.43
1:A:74:ARG:HG2	4:D:620:PGE:H2	2.01	0.43
1:C:175:ALA:HA	1:C:214:ILE:HD11	2.01	0.43
1:B:39:GLU:HG3	1:B:40:ARG:N	2.33	0.43
1:B:54:GLU:H	4:B:630:PGE:H22	1.84	0.42
1:B:130:TYR:CE2	1:B:134:LEU:HD11	2.54	0.42
1:A:114:PRO:O	1:A:117:ARG:HB2	2.20	0.42
1:B:117:ARG:HH11	1:B:117:ARG:HG3	1.83	0.42
1:C:117:ARG:NH1	1:C:117:ARG:HG3	2.34	0.42
1:C:26:ALA:O	1:C:29:VAL:HG12	2.19	0.42
1:A:50:LYS:HE3	1:A:208:TYR:CZ	2.55	0.42
1:A:5:ILE:HG22	1:A:6:LEU:HG	2.02	0.42
1:C:25:ARG:CG	1:C:35:LEU:HD21	2.47	0.42
1:B:219:GLN:O	1:B:220:VAL:OXT	2.37	0.42
1:D:1:MET:CE	1:D:197:LYS:HE2	2.50	0.41
1:A:210:TYR:CZ	1:A:215:LEU:HB2	2.55	0.41
1:A:163:ASN:ND2	1:A:166:SER:H	2.18	0.41
1:A:114:PRO:HA	1:A:115:PRO:HD3	1.96	0.41
1:A:118:VAL:HG13	1:D:136:LEU:HD22	2.02	0.41
1:A:192:ARG:HH11	1:A:192:ARG:CG	2.32	0.41
1:D:113:ILE:CG2	1:D:117:ARG:HB3	2.51	0.40
1:A:50:LYS:HG2	1:A:208:TYR:CD2	2.56	0.40
1:B:113:ILE:HD12	1:B:117:ARG:HD3	2.03	0.40
1:C:210:TYR:CE2	1:C:215:LEU:HB2	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	217/232 (94%)	212 (98%)	4 (2%)	1 (0%)	38	13
1	B	219/232 (94%)	215 (98%)	4 (2%)	0	100	100
1	C	216/232 (93%)	213 (99%)	3 (1%)	0	100	100
1	D	216/232 (93%)	212 (98%)	4 (2%)	0	100	100
All	All	868/928 (94%)	852 (98%)	15 (2%)	1 (0%)	59	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	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	194/207 (94%)	190 (98%)	4 (2%)	66	37
1	B	197/207 (95%)	194 (98%)	3 (2%)	76	53
1	C	194/207 (94%)	193 (100%)	1 (0%)	94	87
1	D	194/207 (94%)	192 (99%)	2 (1%)	85	70
All	All	779/828 (94%)	769 (99%)	10 (1%)	80	60

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

Mol	Chain	Res	Type
1	A	2	LYS
1	A	44	LEU

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Mol	Chain	Res	Type
1	A	147	ARG
1	A	163	ASN
1	B	147	ARG
1	B	192	ARG
1	B	211	LYS
1	C	147	ARG
1	D	53	HIS
1	D	147	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

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

13 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	UMP	A	603	-	21,21,21	2.38	8 (38%)	26,31,31	2.19	5 (19%)
2	FAD	A	615	-	58,58,58	2.42	24 (41%)	85,89,89	2.61	22 (25%)
4	PGE	A	635	-	9,9,9	0.77	0	8,8,8	0.66	0
3	UMP	B	608	-	21,21,21	2.20	6 (28%)	26,31,31	2.11	6 (23%)
2	FAD	B	610	-	58,58,58	2.46	28 (48%)	85,89,89	2.67	22 (25%)
4	PGE	B	625	-	9,9,9	0.48	0	8,8,8	0.99	0
4	PGE	B	630	-	9,9,9	0.73	0	8,8,8	0.77	0
2	FAD	C	605	-	58,58,58	2.36	26 (44%)	85,89,89	2.61	22 (25%)
3	UMP	C	613	-	21,21,21	2.24	8 (38%)	26,31,31	2.14	5 (19%)
2	FAD	D	600	-	58,58,58	2.46	23 (39%)	85,89,89	2.63	21 (24%)
3	UMP	D	618	-	21,21,21	2.14	7 (33%)	26,31,31	2.15	6 (23%)
4	PGE	D	620	-	9,9,9	0.62	0	8,8,8	0.87	0
4	PGE	D	640	-	9,9,9	0.74	0	8,8,8	0.76	0

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	UMP	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
4	PGE	A	635	-	-	0/7/7/7	0/0/0/0
3	UMP	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
4	PGE	B	625	-	-	0/7/7/7	0/0/0/0
4	PGE	B	630	-	-	0/7/7/7	0/0/0/0
2	FAD	C	605	-	1/1/9/9	0/34/50/50	0/1/6/6
3	UMP	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	UMP	D	618	-	-	0/7/22/22	0/2/2/2
4	PGE	D	620	-	-	0/7/7/7	0/0/0/0
4	PGE	D	640	-	-	0/7/7/7	0/0/0/0

All (130) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	603	UMP	C2-N1	6.30	1.45	1.38
2	B	610	FAD	C4A-N3A	5.61	1.44	1.35
2	C	605	FAD	C4A-N3A	5.55	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	608	UMP	C6-N1	5.43	1.44	1.35
3	C	613	UMP	C2-N1	5.40	1.44	1.38
2	D	600	FAD	C2B-C1B	5.35	1.61	1.53
2	D	600	FAD	C4A-N3A	5.33	1.43	1.35
2	C	605	FAD	C2B-C1B	5.32	1.61	1.53
3	C	613	UMP	C6-N1	5.23	1.44	1.35
3	A	603	UMP	C6-N1	5.22	1.44	1.35
2	B	610	FAD	C2B-C1B	5.06	1.60	1.53
3	D	618	UMP	C6-N1	5.06	1.44	1.35
2	A	615	FAD	C4A-N3A	5.04	1.43	1.35
2	A	615	FAD	C2B-C1B	5.03	1.60	1.53
2	D	600	FAD	C8A-N7A	-4.91	1.24	1.34
2	A	615	FAD	C4X-C10	4.86	1.49	1.40
2	B	610	FAD	C8A-N7A	-4.79	1.25	1.34
2	A	615	FAD	C8A-N7A	-4.75	1.25	1.34
2	D	600	FAD	C4X-C10	4.74	1.49	1.40
3	B	608	UMP	C2-N1	4.70	1.43	1.38
3	D	618	UMP	C2-N1	4.52	1.43	1.38
2	C	605	FAD	C9A-C5X	4.47	1.51	1.42
2	C	605	FAD	C4X-C10	4.40	1.48	1.40
2	B	610	FAD	C4X-C10	4.39	1.48	1.40
2	D	600	FAD	C9A-C5X	4.37	1.51	1.42
2	B	610	FAD	C9A-C5X	4.36	1.51	1.42
2	A	615	FAD	C9A-C5X	4.23	1.51	1.42
2	C	605	FAD	C8A-N7A	-4.12	1.26	1.34
2	C	605	FAD	C6-C5X	4.08	1.46	1.41
2	D	600	FAD	C6-C5X	4.05	1.46	1.41
2	B	610	FAD	C6-C5X	4.05	1.46	1.41
2	A	615	FAD	C4-N3	4.00	1.43	1.37
2	B	610	FAD	C4-N3	3.98	1.43	1.37
3	D	618	UMP	C4-N3	3.73	1.43	1.37
2	A	615	FAD	C6-C5X	3.71	1.46	1.41
2	B	610	FAD	C6-C7	3.70	1.48	1.37
2	A	615	FAD	C2-N3	3.66	1.44	1.37
2	A	615	FAD	C8-C7	3.60	1.51	1.40
2	D	600	FAD	C4-N3	3.58	1.43	1.37
3	B	608	UMP	C4-N3	3.56	1.43	1.37
2	B	610	FAD	C4-C4X	3.56	1.47	1.41
2	C	605	FAD	C8-C7	3.55	1.51	1.40
2	D	600	FAD	C8-C7	3.54	1.51	1.40
2	C	605	FAD	C4-N3	3.53	1.43	1.37
2	D	600	FAD	C4-C4X	3.50	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	613	UMP	C4-N3	3.48	1.43	1.37
2	D	600	FAD	C6-C7	3.48	1.47	1.37
2	C	605	FAD	C1B-N9A	-3.45	1.37	1.48
2	D	600	FAD	C1B-N9A	-3.44	1.37	1.48
2	D	600	FAD	C9-C9A	3.42	1.47	1.40
2	D	600	FAD	C2-N3	3.38	1.43	1.37
3	A	603	UMP	C4-N3	3.37	1.42	1.37
2	B	610	FAD	C2-N3	3.37	1.43	1.37
2	B	610	FAD	C8-C7	3.36	1.50	1.40
2	A	615	FAD	C4-C4X	3.34	1.46	1.41
2	A	615	FAD	C9-C9A	3.33	1.47	1.40
2	B	610	FAD	C1'-C2'	3.32	1.54	1.51
2	B	610	FAD	C1B-N9A	-3.32	1.38	1.48
2	A	615	FAD	C5X-N5	3.27	1.40	1.35
2	D	600	FAD	C5X-N5	3.27	1.40	1.35
2	A	615	FAD	C1B-N9A	-3.23	1.38	1.48
2	B	610	FAD	C2A-N1A	3.23	1.40	1.33
2	A	615	FAD	C6-C7	3.23	1.46	1.37
2	C	605	FAD	C6-C7	3.19	1.46	1.37
2	B	610	FAD	C2A-N3A	3.16	1.38	1.32
2	C	605	FAD	C4-C4X	3.11	1.46	1.41
2	B	610	FAD	C10-N1	3.08	1.41	1.35
2	B	610	FAD	C9-C9A	3.08	1.46	1.40
2	D	600	FAD	C2A-N3A	3.07	1.38	1.32
2	B	610	FAD	C5X-N5	3.07	1.40	1.35
2	C	605	FAD	C2-N3	3.02	1.43	1.37
2	A	615	FAD	C1'-C2'	3.02	1.54	1.51
3	A	603	UMP	O4'-C1'	3.01	1.49	1.42
2	D	600	FAD	C10-N1	2.94	1.40	1.35
2	A	615	FAD	C2A-N3A	2.89	1.37	1.32
2	A	615	FAD	C2A-N1A	2.88	1.39	1.33
2	A	615	FAD	O4B-C1B	2.87	1.45	1.41
2	D	600	FAD	C2A-N1A	2.86	1.39	1.33
3	D	618	UMP	C2'-C3'	2.85	1.60	1.52
2	D	600	FAD	C8A-N9A	2.84	1.40	1.36
3	B	608	UMP	C2'-C3'	2.84	1.60	1.52
2	C	605	FAD	C8A-N9A	2.82	1.40	1.36
3	A	603	UMP	C2'-C3'	2.82	1.60	1.52
2	B	610	FAD	C5A-C4A	2.81	1.46	1.40
2	D	600	FAD	C5A-C4A	2.79	1.46	1.40
2	C	605	FAD	C5A-C4A	2.77	1.46	1.40
2	C	605	FAD	C2A-N3A	2.74	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	FAD	C1'-C2'	2.71	1.54	1.51
2	C	605	FAD	C10-N1	2.68	1.40	1.35
2	A	615	FAD	C8A-N9A	2.59	1.40	1.36
3	C	613	UMP	C2'-C3'	2.60	1.60	1.52
2	C	605	FAD	C9-C9A	2.58	1.45	1.40
2	A	615	FAD	C5A-C4A	2.56	1.46	1.40
2	C	605	FAD	P-O3P	-2.55	1.55	1.59
2	A	615	FAD	C10-N1	2.54	1.40	1.35
2	C	605	FAD	C2A-N1A	2.53	1.38	1.33
2	B	610	FAD	C4X-N5	2.46	1.41	1.36
2	A	615	FAD	C9-C8	2.44	1.44	1.37
3	C	613	UMP	C2-N3	2.43	1.42	1.37
2	C	605	FAD	O4B-C1B	2.42	1.45	1.41
3	C	613	UMP	O4'-C1'	2.41	1.48	1.42
3	B	608	UMP	C2-N3	2.40	1.42	1.37
3	A	603	UMP	P-OP2	-2.38	1.46	1.54
2	D	600	FAD	O4B-C1B	2.38	1.45	1.41
2	B	610	FAD	O4B-C1B	2.35	1.45	1.41
2	B	610	FAD	C8A-N9A	2.34	1.40	1.36
2	D	600	FAD	C4X-N5	2.33	1.41	1.36
2	D	600	FAD	C9-C8	2.33	1.44	1.37
2	C	605	FAD	C5X-N5	2.31	1.38	1.35
3	B	608	UMP	P-OP3	-2.30	1.46	1.54
2	C	605	FAD	C4X-N5	2.27	1.40	1.36
2	C	605	FAD	C9-C8	2.23	1.43	1.37
2	B	610	FAD	P-O3P	-2.23	1.55	1.59
3	A	603	UMP	P-OP3	-2.22	1.46	1.54
2	B	610	FAD	C9-C8	2.21	1.43	1.37
3	D	618	UMP	O4'-C1'	2.18	1.47	1.42
3	A	603	UMP	C2-N3	2.17	1.41	1.37
2	C	605	FAD	C1'-C2'	2.15	1.53	1.51
2	B	610	FAD	PA-O5B	-2.14	1.49	1.59
3	D	618	UMP	C2-N3	2.13	1.41	1.37
3	C	613	UMP	P-OP3	-2.13	1.46	1.54
2	A	615	FAD	C4X-N5	2.09	1.40	1.36
2	B	610	FAD	O5B-C5B	2.08	1.53	1.44
2	B	610	FAD	C10-N10	2.07	1.43	1.38
3	D	618	UMP	P-OP2	-2.03	1.47	1.54
3	C	613	UMP	P-OP2	-2.03	1.47	1.54
2	C	605	FAD	C10-N10	2.02	1.43	1.38
2	A	615	FAD	PA-O5B	-2.02	1.50	1.59
2	C	605	FAD	P-O5'	-2.01	1.50	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	610	FAD	P-O5'	-2.01	1.50	1.59

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	610	FAD	C2B-C1B-N9A	9.10	136.62	113.27
2	A	615	FAD	C2B-C1B-N9A	9.00	136.36	113.27
2	C	605	FAD	C2B-C1B-N9A	8.99	136.34	113.27
2	B	610	FAD	C4B-O4B-C1B	-8.98	99.99	109.75
2	D	600	FAD	C2B-C1B-N9A	8.94	136.22	113.27
2	C	605	FAD	C4B-O4B-C1B	-8.94	100.04	109.75
2	D	600	FAD	O4B-C1B-N9A	8.85	116.67	108.44
2	C	605	FAD	O4B-C1B-N9A	8.83	116.65	108.44
2	D	600	FAD	C4B-O4B-C1B	-8.73	100.27	109.75
2	A	615	FAD	C4B-O4B-C1B	-8.70	100.30	109.75
2	A	615	FAD	O4B-C1B-N9A	8.60	116.44	108.44
2	B	610	FAD	O4B-C1B-N9A	8.40	116.25	108.44
2	B	610	FAD	C3B-C2B-C1B	-8.09	88.25	100.91
2	D	600	FAD	C3B-C2B-C1B	-8.07	88.28	100.91
2	A	615	FAD	C3B-C2B-C1B	-7.78	88.72	100.91
2	C	605	FAD	C3B-C2B-C1B	-7.60	89.02	100.91
3	C	613	UMP	C2'-C1'-N1	-7.39	94.89	114.08
3	A	603	UMP	C2'-C1'-N1	-7.33	95.03	114.08
3	B	608	UMP	C2'-C1'-N1	-7.12	95.60	114.08
3	D	618	UMP	C2'-C1'-N1	-6.95	96.02	114.08
2	D	600	FAD	C2-N1-C10	6.42	121.45	114.98
2	B	610	FAD	N3A-C2A-N1A	-6.40	123.36	128.71
2	A	615	FAD	N3A-C2A-N1A	-6.25	123.48	128.71
2	C	605	FAD	C2-N1-C10	6.19	121.22	114.98
2	B	610	FAD	C2-N1-C10	6.19	121.21	114.98
2	A	615	FAD	C2-N1-C10	6.18	121.20	114.98
2	D	600	FAD	N3A-C2A-N1A	-6.16	123.56	128.71
2	C	605	FAD	N3A-C2A-N1A	-6.11	123.60	128.71
2	B	610	FAD	O2B-C2B-C1B	5.84	128.90	111.23
2	C	605	FAD	O2B-C2B-C1B	5.71	128.50	111.23
2	D	600	FAD	O2B-C2B-C1B	5.68	128.42	111.23
2	A	615	FAD	O2B-C2B-C1B	5.59	128.15	111.23
3	A	603	UMP	O4'-C1'-N1	5.14	117.35	107.68
2	B	610	FAD	C4X-C10-N10	-4.80	118.11	120.51
3	B	608	UMP	O4'-C1'-N1	4.72	116.55	107.68
2	C	605	FAD	C4X-C10-N10	-4.68	118.17	120.51
3	C	613	UMP	O4'-C1'-N1	4.63	116.38	107.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	618	UMP	O4'-C1'-N1	4.60	116.32	107.68
2	D	600	FAD	C4X-C10-N10	-4.60	118.21	120.51
2	A	615	FAD	C4X-C10-N10	-4.52	118.25	120.51
2	A	615	FAD	C1'-N10-C9A	4.16	122.92	118.87
2	B	610	FAD	C1'-N10-C9A	4.02	122.78	118.87
2	B	610	FAD	C4A-C5A-N7A	-3.84	106.24	109.52
2	A	615	FAD	C4A-C5A-N7A	-3.83	106.24	109.52
2	C	605	FAD	C1'-N10-C9A	3.78	122.55	118.87
3	D	618	UMP	C5-C6-N1	3.67	125.36	121.21
2	C	605	FAD	C4A-C5A-N7A	-3.65	106.39	109.52
2	D	600	FAD	C4A-C5A-N7A	-3.63	106.41	109.52
2	D	600	FAD	C1'-N10-C9A	3.47	122.25	118.87
3	C	613	UMP	C5-C6-N1	3.40	125.06	121.21
2	B	610	FAD	C1'-N10-C10	-3.36	114.40	119.17
3	B	608	UMP	C5-C6-N1	3.31	124.95	121.21
2	A	615	FAD	C1'-N10-C10	-3.26	114.54	119.17
3	A	603	UMP	C5-C6-N1	3.25	124.89	121.21
3	D	618	UMP	C4'-O4'-C1'	3.12	117.34	109.44
2	B	610	FAD	C4X-N5-C5X	3.04	120.10	116.69
2	D	600	FAD	C1'-N10-C10	-2.98	114.93	119.17
3	A	603	UMP	C4'-O4'-C1'	2.97	116.96	109.44
3	B	608	UMP	C4'-O4'-C1'	2.96	116.94	109.44
2	D	600	FAD	P-O3P-PA	2.89	140.17	131.68
2	D	600	FAD	N3A-C4A-N9A	2.85	130.58	125.43
2	B	610	FAD	N3A-C4A-N9A	2.84	130.57	125.43
2	D	600	FAD	C4X-N5-C5X	2.84	119.88	116.69
2	B	610	FAD	C8A-N9A-C4A	2.82	109.05	106.90
2	A	615	FAD	C8A-N9A-C4A	2.79	109.03	106.90
2	C	605	FAD	C8A-N9A-C4A	2.75	109.00	106.90
3	C	613	UMP	C4'-O4'-C1'	2.75	116.40	109.44
2	A	615	FAD	O3B-C3B-C4B	2.72	119.09	111.08
2	C	605	FAD	O3B-C3B-C4B	2.71	119.07	111.08
2	B	610	FAD	P-O3P-PA	2.71	139.62	131.68
2	C	605	FAD	C1'-N10-C10	-2.71	115.33	119.17
2	C	605	FAD	P-O3P-PA	2.69	139.58	131.68
2	D	600	FAD	C8A-N7A-C5A	2.63	111.73	103.58
2	D	600	FAD	O3B-C3B-C4B	2.62	118.79	111.08
2	B	610	FAD	C8A-N7A-C5A	2.61	111.67	103.58
2	D	600	FAD	C8A-N9A-C4A	2.59	108.88	106.90
2	C	605	FAD	C4X-N5-C5X	2.59	119.61	116.69
2	B	610	FAD	O3B-C3B-C4B	2.59	118.70	111.08
2	A	615	FAD	C4X-N5-C5X	2.59	119.59	116.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	605	FAD	O4B-C4B-C3B	2.57	110.38	105.17
2	B	610	FAD	C5A-C4A-N9A	-2.51	103.54	107.16
2	A	615	FAD	C8A-N7A-C5A	2.50	111.34	103.58
2	C	605	FAD	N3A-C4A-N9A	2.49	129.92	125.43
2	D	600	FAD	C5A-C4A-N9A	-2.48	103.59	107.16
2	B	610	FAD	C5B-C4B-C3B	-2.48	105.29	115.21
2	A	615	FAD	O4B-C4B-C3B	2.47	110.19	105.17
2	C	605	FAD	C5B-C4B-C3B	-2.47	105.32	115.21
2	C	605	FAD	C2A-N1A-C6A	2.43	123.17	118.77
2	B	610	FAD	O4B-C4B-C3B	2.43	110.10	105.17
2	D	600	FAD	C5B-C4B-C3B	-2.43	105.48	115.21
2	C	605	FAD	C8A-N7A-C5A	2.42	111.10	103.58
2	D	600	FAD	O4B-C4B-C3B	2.42	110.07	105.17
2	A	615	FAD	P-O3P-PA	2.41	138.76	131.68
2	A	615	FAD	C2A-N1A-C6A	2.39	123.08	118.77
3	D	618	UMP	N3-C2-N1	-2.38	113.99	115.97
2	A	615	FAD	C5B-C4B-C3B	-2.37	105.72	115.21
2	A	615	FAD	N3A-C4A-N9A	2.35	129.67	125.43
2	B	610	FAD	C2'-C1'-N10	-2.34	109.34	112.45
3	C	613	UMP	N3-C2-N1	-2.27	114.08	115.97
3	D	618	UMP	O4'-C4'-C3'	-2.26	99.93	105.66
2	A	615	FAD	C5A-C4A-N9A	-2.22	103.96	107.16
2	B	610	FAD	C2A-N1A-C6A	2.20	122.73	118.77
2	D	600	FAD	C2A-N1A-C6A	2.19	122.72	118.77
3	B	608	UMP	N3-C2-N1	-2.17	114.17	115.97
2	C	605	FAD	C5A-C4A-N9A	-2.16	104.04	107.16
3	A	603	UMP	O4'-C4'-C3'	-2.05	100.45	105.66
2	C	605	FAD	P-O5'-C5'	2.05	136.75	122.03
2	A	615	FAD	P-O5'-C5'	2.05	136.73	122.03
3	B	608	UMP	O4'-C4'-C3'	-2.02	100.53	105.66

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	600	FAD	C1B
2	A	615	FAD	C1B
2	C	605	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	219/232 (94%)	0.64	22 (10%) 8 7	15, 29, 57, 64	0
1	B	221/232 (95%)	0.62	27 (12%) 5 4	17, 31, 57, 62	0
1	C	218/232 (93%)	0.57	20 (9%) 9 8	16, 28, 51, 58	0
1	D	218/232 (93%)	0.60	26 (11%) 5 4	16, 31, 56, 60	0
All	All	876/928 (94%)	0.61	95 (10%) 6 5	15, 30, 56, 64	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	220	VAL	8.8
1	A	113	ILE	7.2
1	D	35	LEU	6.6
1	D	40	ARG	5.4
1	B	219	GLN	4.8
1	D	37	ASP	4.8
1	B	35	LEU	4.4
1	D	36	LYS	4.3
1	A	112	THR	4.3
1	B	109	TYR	4.2
1	B	36	LYS	4.2
1	D	138	GLU	3.9
1	B	37	ASP	3.7
1	C	39	GLU	3.7
1	A	107	GLU	3.6
1	C	96	TYR	3.6
1	B	107	GLU	3.5
1	C	91	TYR	3.5
1	D	110	LYS	3.5
1	D	218	VAL	3.5
1	A	117	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	34	GLY	3.4
1	A	110	LYS	3.4
1	B	43	HIS	3.4
1	B	47	TYR	3.3
1	A	33	MET	3.2
1	D	31	PHE	3.2
1	C	113	ILE	3.1
1	D	111	THR	3.1
1	A	-1	HIS	3.1
1	D	47	TYR	3.0
1	B	113	ILE	3.0
1	D	96	TYR	3.0
1	D	107	GLU	3.0
1	C	104	GLU	3.0
1	C	35	LEU	2.9
1	A	39	GLU	2.9
1	B	38	GLU	2.9
1	D	109	TYR	2.9
1	A	114	PRO	2.9
1	B	138	GLU	2.8
1	A	111	THR	2.8
1	C	131	ARG	2.8
1	C	94	LEU	2.8
1	A	37	ASP	2.8
1	D	38	GLU	2.8
1	A	120	GLU	2.8
1	B	120	GLU	2.7
1	B	40	ARG	2.7
1	A	43	HIS	2.7
1	A	208	TYR	2.7
1	C	25	ARG	2.7
1	B	112	THR	2.6
1	D	131	ARG	2.6
1	D	43	HIS	2.6
1	B	200	TRP	2.6
1	B	42	ARG	2.6
1	D	113	ILE	2.6
1	D	39	GLU	2.6
1	A	217	GLU	2.5
1	A	0	HIS	2.5
1	B	117	ARG	2.5
1	A	38	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	107	GLU	2.5
1	D	135	GLU	2.4
1	D	34	GLY	2.4
1	B	0	HIS	2.4
1	D	25	ARG	2.4
1	C	36	LYS	2.3
1	B	104	GLU	2.3
1	B	131	ARG	2.3
1	C	137	ILE	2.3
1	D	203	GLU	2.3
1	B	135	GLU	2.2
1	D	33	MET	2.2
1	D	137	ILE	2.2
1	B	108	GLY	2.2
1	A	109	TYR	2.2
1	B	114	PRO	2.2
1	B	31	PHE	2.2
1	A	47	TYR	2.1
1	A	104	GLU	2.1
1	C	93	LYS	2.1
1	C	173	LEU	2.1
1	B	116	GLU	2.1
1	C	203	GLU	2.1
1	C	217	GLU	2.1
1	D	104	GLU	2.1
1	C	32	ASP	2.1
1	C	31	PHE	2.0
1	C	120	GLU	2.0
1	C	138	GLU	2.0
1	A	40	ARG	2.0
1	D	116	GLU	2.0
1	A	115	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	PGE	B	630	10/10	0.18	3.16	52,53,54,54	0
4	PGE	A	635	10/10	0.23	3.14	48,50,53,54	0
4	PGE	D	640	10/10	0.20	1.41	54,55,56,56	0
4	PGE	B	625	10/10	0.12	0.98	36,37,40,42	0
3	UMP	B	608	20/20	0.12	0.73	17,20,22,22	0
4	PGE	D	620	10/10	0.12	0.27	37,38,40,43	0
2	FAD	C	605	53/53	0.13	0.11	16,19,22,23	0
2	FAD	A	615	53/53	0.12	-0.08	16,20,23,24	0
3	UMP	C	613	20/20	0.09	-0.18	21,22,24,25	0
3	UMP	D	618	20/20	0.10	-0.19	18,21,24,24	0
2	FAD	B	610	53/53	0.10	-0.41	17,22,25,26	0
2	FAD	D	600	53/53	0.10	-0.46	17,22,25,26	0
3	UMP	A	603	20/20	0.09	-0.55	20,21,25,25	0

6.5 Other polymers ⓘ

There are no such residues in this entry.