Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:14 PM GMT

PDB ID	:	1O2B
Title	:	Crystal structure of Thymidylate Synthase Complementing Protein (TM0449) from Thermotoga maritima with FAD and PO4 at 2.45 A 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	:	2.45 Å(reported)

This is a Full wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

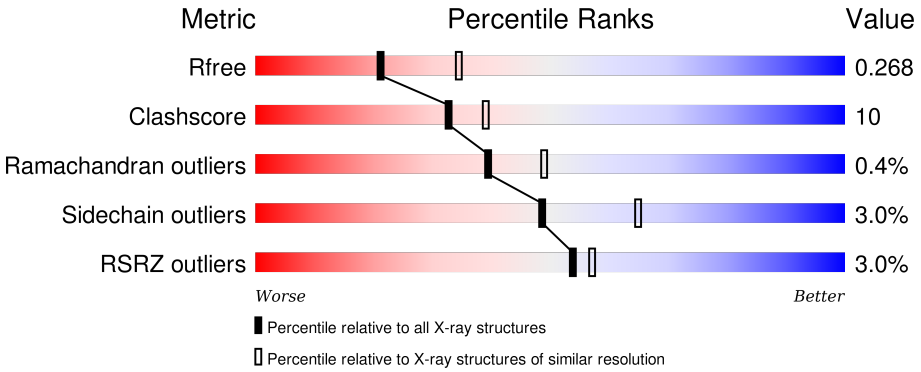
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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}	91344	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	232	4% 67% 24% • 8%
1	B	232	3% 72% 20% • 7%
1	C	232	2% 74% 17% • 8%
1	D	232	3% 72% 20% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FAD	A	615	X	-	-	-
3	FAD	B	610	X	-	-	-
3	FAD	C	605	X	-	-	-
3	FAD	D	600	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7603 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	213	Total	C	N	O	S	0	0	0
			1768	1151	304	307	6			
1	B	215	Total	C	N	O	S	0	0	0
			1803	1174	308	315	6			
1	C	214	Total	C	N	O	S	0	0	0
			1796	1168	307	316	5			
1	D	212	Total	C	N	O	S	0	0	0
			1769	1153	300	311	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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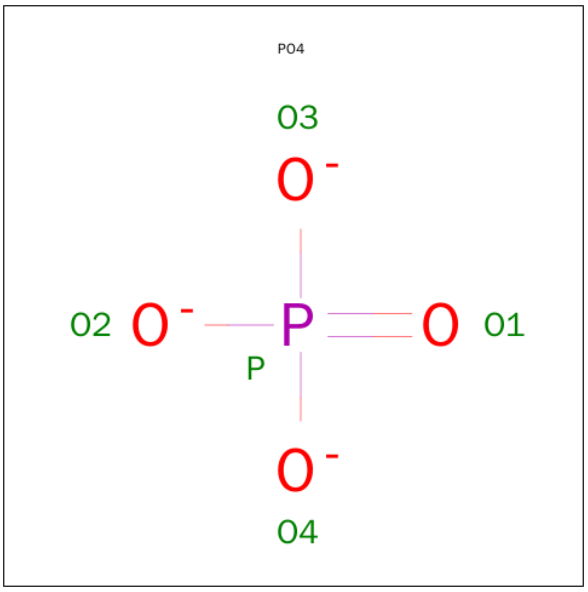
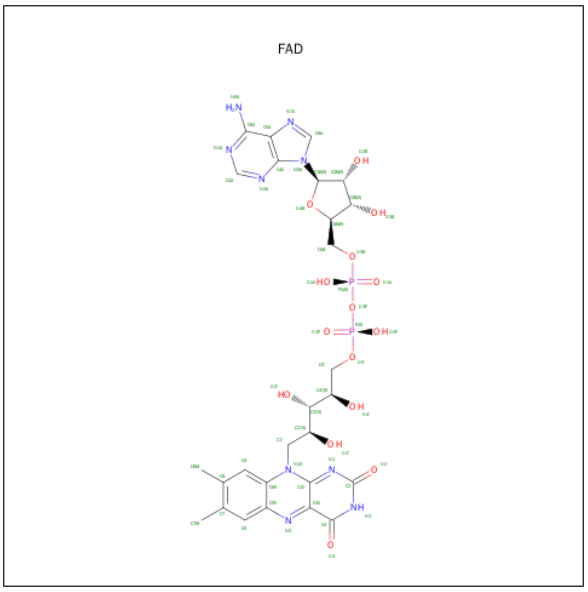
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
B	-1	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
B	0	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
C	-11	MET	-	LEADER SEQUENCE	UNP Q9WYT0
C	-10	GLY	-	LEADER SEQUENCE	UNP Q9WYT0
C	-9	SER	-	LEADER SEQUENCE	UNP Q9WYT0
C	-8	ASP	-	LEADER SEQUENCE	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 PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 4 is water.

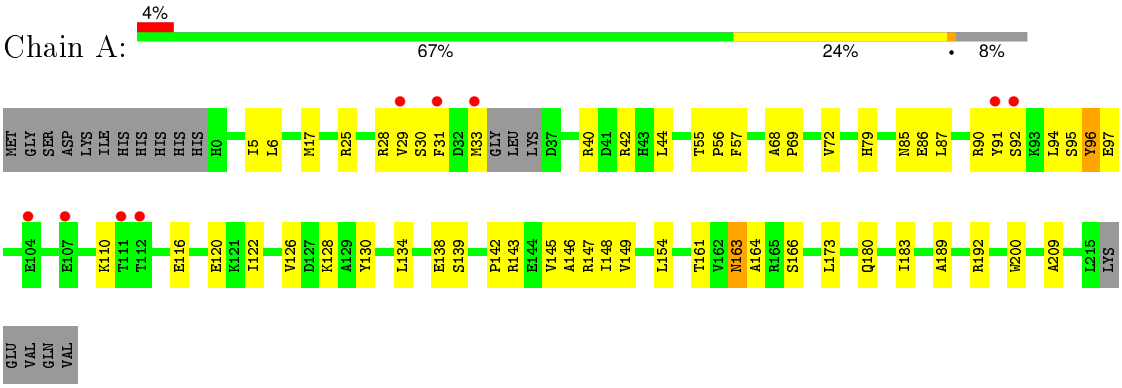
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	56	Total	O	0	0
			56	56		
4	B	64	Total	O	0	0
			64	64		
4	C	63	Total	O	0	0
			63	63		
4	D	57	Total	O	0	0
			57	57		

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.

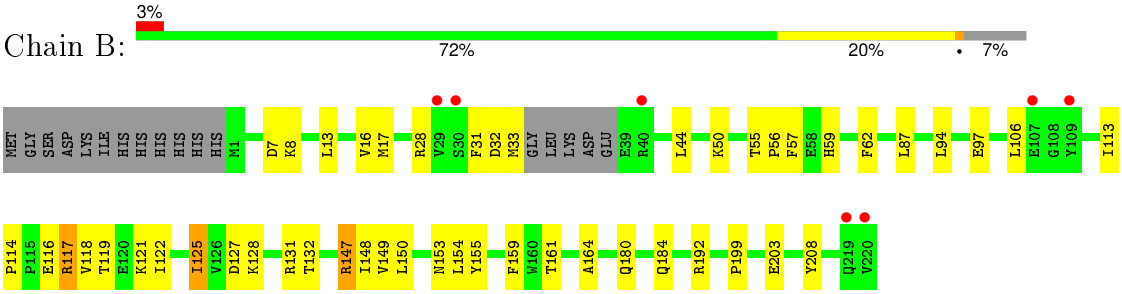
- Molecule 1: Thymidylate synthase thyX

Chain A:



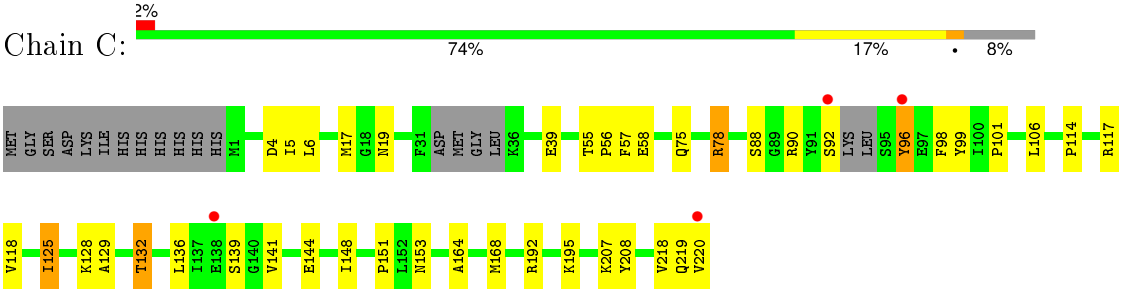
- Molecule 1: Thymidylate synthase thyX

Chain B:



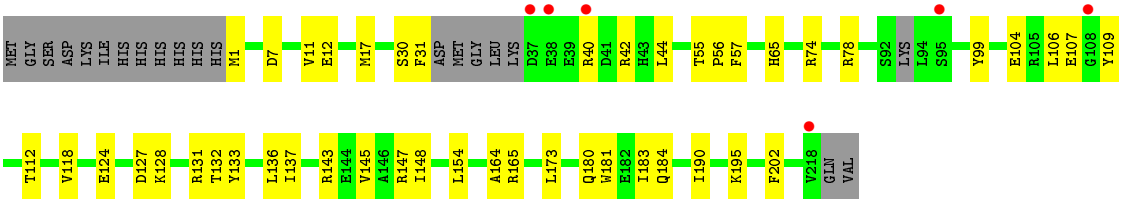
- Molecule 1: Thymidylate synthase thyX

Chain C:



- Molecule 1: Thymidylate synthase thyX

Chain D:


MET GLY SER ASP LYS ILE HIS HIS HIS HIS HIS HIS M1 D7 V11 E12 M17 S30 F31 ASP MET GLY LEU LYS D37 E38 E39 R40 D41 R42 H43 L44 T55 P56 F57 H65 R74 R78 S92 LYS L94 S95 Y99 E104 R105 L106 E107 G108 Y109
T112 V118 E124 D127 K128 R131 T132 Y133 L136 I137 R143 E144 V145 A146 R147 I148 L154 A164 R165 L173 Q180 W181 E182 I183 Q184 I190 K195 F202 V218 GLN VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	54.99Å 118.15Å 145.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.45 47.16 – 2.45	Depositor EDS
% Data completeness (in resolution range)	93.0 (20.00-2.45) 94.7 (47.16-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 2.45Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.203 , 0.265 0.207 , 0.268	Depositor DCC
R_{free} test set	1673 reflections (4.96%)	DCC
Wilson B-factor (Å^2)	40.7	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 53.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 33811 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7603	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 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	0.40	0/1816	0.59	0/2454
1	B	0.40	0/1851	0.61	0/2501
1	C	0.39	0/1843	0.62	0/2489
1	D	0.40	0/1816	0.59	0/2455
All	All	0.40	0/7326	0.60	0/9899

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1768	0	1754	43	0
1	B	1803	0	1801	47	0
1	C	1796	0	1786	45	0
1	D	1769	0	1751	38	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
2	D	5	0	0	0	0
3	A	53	0	30	1	0
3	B	53	0	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	53	0	30	1	0
3	D	53	0	30	3	0
4	A	56	0	0	0	0
4	B	64	0	0	4	0
4	C	63	0	0	2	0
4	D	57	0	0	5	0
All	All	7603	0	7212	152	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (152) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:LYS:HB3	1:B:208:TYR:CD2	2.12	0.85
1:A:17:MET:HB2	1:B:17:MET:HB2	1.64	0.80
1:C:106:LEU:HD11	1:C:118:VAL:HG11	1.64	0.79
1:C:17:MET:HB2	1:D:17:MET:HB2	1.65	0.79
1:A:180:GLN:O	1:A:183:ILE:HG22	1.86	0.75
1:B:149:VAL:HB	1:C:125:ILE:HD12	1.68	0.75
1:D:127:ASP:HB3	1:D:131:ARG:NH2	2.01	0.75
1:D:106:LEU:HD21	1:D:118:VAL:HG11	1.69	0.74
1:A:116:GLU:O	1:A:120:GLU:HG2	1.89	0.72
1:C:78:ARG:HG3	1:C:78:ARG:HH11	1.52	0.72
1:B:94:LEU:HD13	1:B:154:LEU:HD21	1.72	0.70
1:C:151:PRO:HB2	1:C:153:ASN:OD1	1.93	0.69
1:B:128:LYS:HD2	1:C:128:LYS:NZ	2.07	0.69
1:B:127:ASP:HB3	1:B:131:ARG:CZ	2.23	0.68
1:B:128:LYS:HD2	1:C:128:LYS:HZ3	1.60	0.67
1:B:132:THR:HG21	1:C:125:ILE:HD13	1.82	0.62
1:C:195:LYS:HD3	1:C:220:VAL:HG12	1.82	0.62
1:D:180:GLN:O	1:D:183:ILE:HG22	2.00	0.62
1:A:28:ARG:HH11	1:A:28:ARG:HG3	1.64	0.61
1:A:5:ILE:HG22	1:A:6:LEU:HG	1.82	0.61
1:B:114:PRO:HG2	1:B:117:ARG:HB2	1.82	0.60
1:D:57:PHE:O	1:D:164:ALA:HB3	2.02	0.59
1:A:55:THR:OG1	1:A:56:PRO:HD3	2.01	0.59
1:D:30:SER:O	1:D:31:PHE:HB2	2.03	0.59
1:A:30:SER:HA	1:B:87:LEU:HA	1.84	0.58
1:B:31:PHE:C	1:B:33:MET:H	2.06	0.58
1:A:163:ASN:HD22	1:A:163:ASN:C	2.06	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:ARG:HD3	4:D:439:HOH:O	2.04	0.58
1:D:42:ARG:HB2	4:D:507:HOH:O	2.03	0.58
1:A:95:SER:O	1:A:97:GLU:N	2.36	0.57
1:C:19:ASN:HB2	4:C:441:HOH:O	2.03	0.57
1:A:92:SER:O	1:A:143:ARG:HD3	2.05	0.56
1:D:133:TYR:CZ	1:D:137:ILE:HD11	2.41	0.56
1:D:145:VAL:O	1:D:148:ILE:HG12	2.06	0.56
1:C:129:ALA:O	1:C:132:THR:HG23	2.05	0.56
1:B:13:LEU:HD21	1:B:16:VAL:CG2	2.35	0.56
1:B:55:THR:OG1	1:B:56:PRO:HD3	2.06	0.55
1:C:75:GLN:O	1:C:78:ARG:HB2	2.07	0.55
1:B:113:ILE:HG12	1:C:139:SER:OG	2.07	0.54
1:A:29:VAL:HG21	1:B:159:PHE:CE1	2.43	0.54
1:A:116:GLU:N	1:A:116:GLU:OE1	2.40	0.54
1:C:78:ARG:HG3	1:C:78:ARG:NH1	2.22	0.54
1:C:164:ALA:O	1:C:168:MET:HG3	2.08	0.54
1:D:137:ILE:HD13	1:D:143:ARG:NH1	2.23	0.53
1:A:79:HIS:HE1	1:A:173:LEU:HD12	1.73	0.53
1:C:98:PHE:HE2	1:C:151:PRO:HD2	1.74	0.53
1:C:114:PRO:HB2	1:C:117:ARG:HG2	1.91	0.52
1:A:122:ILE:O	1:A:126:VAL:HG23	2.09	0.52
1:D:132:THR:O	1:D:136:LEU:HG	2.10	0.52
1:D:1:MET:N	4:D:538:HOH:O	2.42	0.52
1:D:127:ASP:HB3	1:D:131:ARG:CZ	2.39	0.52
1:A:142:PRO:HG3	1:D:109:TYR:CE2	2.45	0.51
1:D:78:ARG:HH12	3:D:600:FAD:C2	2.23	0.51
1:D:147:ARG:HD2	4:D:440:HOH:O	2.11	0.51
1:B:199:PRO:O	1:B:203:GLU:HG2	2.09	0.51
1:C:192:ARG:NH2	4:C:386:HOH:O	2.34	0.51
1:A:25:ARG:O	1:A:29:VAL:HG23	2.11	0.51
1:B:50:LYS:HD3	1:B:208:TYR:CE2	2.46	0.51
1:D:42:ARG:HD2	4:D:507:HOH:O	2.11	0.51
1:A:42:ARG:HG2	1:A:200:TRP:CD2	2.46	0.51
1:C:114:PRO:HD2	1:C:117:ARG:HG3	1.94	0.50
1:A:69:PRO:HG2	1:A:72:VAL:HG23	1.92	0.50
1:A:86:GLU:HG2	1:A:87:LEU:N	2.27	0.50
1:D:104:GLU:O	1:D:107:GLU:HB2	2.13	0.49
1:A:40:ARG:HH11	1:A:40:ARG:HG3	1.77	0.49
1:B:122:ILE:O	1:B:125:ILE:HG22	2.12	0.49
1:D:124:GLU:HG2	1:D:128:LYS:HE2	1.94	0.49
1:A:173:LEU:HD13	3:A:615:FAD:O4'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:GLU:HG2	1:A:87:LEU:H	1.78	0.49
1:B:57:PHE:O	1:B:164:ALA:HB3	2.13	0.49
1:B:180:GLN:O	1:B:184:GLN:HG3	2.13	0.49
1:D:124:GLU:CG	1:D:128:LYS:HE2	2.42	0.49
1:B:97:GLU:HA	4:B:345:HOH:O	2.12	0.49
1:C:99:TYR:CE1	1:C:101:PRO:HG3	2.48	0.49
1:C:78:ARG:NH2	3:C:605:FAD:O2	2.46	0.49
1:B:148:ILE:HB	1:C:153:ASN:HB3	1.95	0.48
1:B:147:ARG:HD2	1:B:148:ILE:N	2.28	0.48
1:C:195:LYS:CD	1:C:220:VAL:HG12	2.43	0.48
1:D:55:THR:OG1	1:D:56:PRO:HD3	2.14	0.48
1:A:31:PHE:HB2	1:A:33:MET:CE	2.44	0.48
1:A:146:ALA:O	1:A:149:VAL:HG22	2.13	0.48
1:D:11:VAL:HG11	1:D:190:ILE:HD13	1.96	0.47
1:B:94:LEU:HD12	1:B:150:LEU:HD12	1.95	0.47
1:C:4:ASP:O	1:C:5:ILE:HD13	2.13	0.47
1:C:192:ARG:HH12	1:C:220:VAL:HG23	1.79	0.47
1:B:180:GLN:HG3	1:C:144:GLU:OE2	2.15	0.47
1:D:12:GLU:HG3	1:D:65:HIS:HB3	1.96	0.47
1:A:28:ARG:NH1	1:A:28:ARG:HG3	2.29	0.47
1:B:106:LEU:HD11	1:C:141:VAL:HG13	1.96	0.47
3:B:610:FAD:O2B	3:D:600:FAD:H4B	2.15	0.47
1:C:55:THR:O	1:C:58:GLU:HG3	2.15	0.47
1:C:218:VAL:HG12	1:C:219:GLN:N	2.30	0.47
1:D:106:LEU:HD12	1:D:106:LEU:N	2.31	0.46
1:A:139:SER:HB2	1:D:112:THR:HB	1.95	0.46
1:C:55:THR:N	1:C:56:PRO:CD	2.79	0.46
1:C:195:LYS:CE	1:C:220:VAL:HG12	2.45	0.46
1:D:180:GLN:O	1:D:184:GLN:HG3	2.16	0.46
1:A:55:THR:N	1:A:56:PRO:CD	2.78	0.46
1:C:57:PHE:O	1:C:164:ALA:HB3	2.16	0.46
1:D:7:ASP:OD1	1:D:99:TYR:HD2	1.99	0.46
1:B:127:ASP:HB3	1:B:131:ARG:NH2	2.31	0.46
1:D:143:ARG:O	1:D:147:ARG:HG2	2.16	0.45
1:A:145:VAL:O	1:A:148:ILE:HG12	2.16	0.45
1:A:92:SER:C	1:A:143:ARG:HD3	2.37	0.45
1:A:85:ASN:ND2	1:B:59:HIS:NE2	2.63	0.45
1:C:98:PHE:CE2	1:C:151:PRO:HD2	2.51	0.45
1:C:192:ARG:NH1	1:C:220:VAL:HG23	2.30	0.45
1:D:173:LEU:HD13	3:D:600:FAD:O4'	2.16	0.45
1:D:127:ASP:HB3	1:D:131:ARG:HH22	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:ILE:CG1	1:C:132:THR:HG21	2.46	0.44
1:B:13:LEU:HD21	1:B:16:VAL:HG21	1.98	0.44
1:A:40:ARG:HG3	1:A:40:ARG:NH1	2.31	0.44
1:C:5:ILE:HG22	1:C:6:LEU:HG	1.99	0.44
1:B:50:LYS:HE3	4:B:506:HOH:O	2.17	0.44
1:B:117:ARG:NH1	1:B:121:LYS:NZ	2.66	0.44
1:C:132:THR:O	1:C:136:LEU:HG	2.18	0.44
1:D:30:SER:O	1:D:31:PHE:CB	2.63	0.44
1:A:163:ASN:ND2	1:A:166:SER:H	2.16	0.44
1:A:5:ILE:HD11	1:A:189:ALA:HB2	1.99	0.44
1:B:62:PHE:O	1:B:161:THR:HA	2.18	0.44
1:A:90:ARG:HG2	2:A:603:PO4:O3	2.18	0.43
1:B:117:ARG:O	1:B:121:LYS:HG3	2.18	0.43
1:A:69:PRO:HG2	1:A:72:VAL:CG2	2.48	0.43
1:D:106:LEU:HD12	1:D:106:LEU:H	1.82	0.43
1:B:7:ASP:HB3	4:B:338:HOH:O	2.18	0.43
1:C:88:SER:O	1:C:92:SER:HB2	2.19	0.43
1:A:94:LEU:HD13	1:A:154:LEU:HD21	2.00	0.43
1:A:130:TYR:CE2	1:A:134:LEU:HD11	2.54	0.42
1:D:40:ARG:HH11	1:D:40:ARG:HG2	1.85	0.42
1:B:127:ASP:O	1:B:131:ARG:HG3	2.20	0.42
1:D:143:ARG:HG2	1:D:143:ARG:HH11	1.85	0.42
1:A:161:THR:OG1	1:B:59:HIS:ND1	2.44	0.42
1:A:96:TYR:CD1	1:A:130:TYR:CD2	3.08	0.42
1:B:28:ARG:HG3	4:B:536:HOH:O	2.18	0.42
1:B:125:ILE:HG13	1:C:132:THR:HG21	2.00	0.42
1:D:12:GLU:CG	1:D:65:HIS:HB3	2.50	0.42
1:C:207:LYS:HD2	1:C:208:TYR:CE1	2.55	0.42
1:A:57:PHE:O	1:A:164:ALA:HB3	2.19	0.42
1:A:91:TYR:HB3	1:B:31:PHE:CE2	2.55	0.41
1:A:163:ASN:C	1:A:163:ASN:ND2	2.73	0.41
1:C:96:TYR:CG	1:C:96:TYR:O	2.73	0.41
1:B:153:ASN:HB3	1:C:148:ILE:HB	2.02	0.41
1:B:128:LYS:HD2	1:C:128:LYS:HZ2	1.84	0.41
1:B:125:ILE:HD13	1:B:125:ILE:O	2.20	0.41
1:B:149:VAL:HG11	1:C:125:ILE:HD11	2.01	0.41
1:A:68:ALA:HB1	1:A:69:PRO:HD2	2.02	0.40
1:D:195:LYS:HG3	1:D:202:PHE:CD2	2.56	0.40
1:B:118:VAL:O	1:B:122:ILE:HG13	2.21	0.40
1:C:78:ARG:CG	1:C:78:ARG:NH1	2.80	0.40
1:B:8:LYS:HB2	1:B:155:TYR:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:TRP:O	1:D:184:GLN:HB2	2.22	0.40
1:B:31:PHE:C	1:B:33:MET:N	2.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	209/232 (90%)	198 (95%)	9 (4%)	2 (1%)	19 21
1	B	211/232 (91%)	205 (97%)	6 (3%)	0	100 100
1	C	208/232 (90%)	198 (95%)	9 (4%)	1 (0%)	34 41
1	D	206/232 (89%)	197 (96%)	9 (4%)	0	100 100
All	All	834/928 (90%)	798 (96%)	33 (4%)	3 (0%)	39 49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	TYR
1	C	96	TYR
1	A	209	ALA

5.3.2 Protein sidechains (i)

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	186/207 (90%)	179 (96%)	7 (4%)	40 55
1	B	192/207 (93%)	184 (96%)	8 (4%)	36 51
1	C	191/207 (92%)	186 (97%)	5 (3%)	54 70
1	D	187/207 (90%)	184 (98%)	3 (2%)	70 83
All	All	756/828 (91%)	733 (97%)	23 (3%)	48 65

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	110	LYS
1	A	128	LYS
1	A	138	GLU
1	A	147	ARG
1	A	163	ASN
1	A	192	ARG
1	B	32	ASP
1	B	44	LEU
1	B	116	GLU
1	B	117	ARG
1	B	119	THR
1	B	125	ILE
1	B	147	ARG
1	B	192	ARG
1	C	39	GLU
1	C	78	ARG
1	C	90	ARG
1	C	125	ILE
1	C	132	THR
1	D	44	LEU
1	D	154	LEU
1	D	165	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	163	ASN
1	D	184	GLN

5.3.3 RNA

There are no RNA molecules 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

7 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	PO4	A	603	-	4,4,4	1.09	0	6,6,6	0.27	0
3	FAD	A	615	-	48,58,58	3.19	22 (45%)	54,89,89	3.40	17 (31%)
2	PO4	B	608	-	4,4,4	1.08	0	6,6,6	0.27	0
3	FAD	B	610	-	48,58,58	3.15	22 (45%)	54,89,89	3.40	17 (31%)
3	FAD	C	605	-	48,58,58	3.18	23 (47%)	54,89,89	3.38	17 (31%)
3	FAD	D	600	-	48,58,58	3.15	21 (43%)	54,89,89	3.37	16 (29%)
2	PO4	D	618	-	4,4,4	1.05	0	6,6,6	0.27	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
2	PO4	A	603	-	-	0/0/0/0	0/0/0/0
3	FAD	A	615	-	1/1/9/9	0/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	B	608	-	-	0/0/0/0	0/0/0/0
3	FAD	B	610	-	1/1/9/9	0/30/50/50	0/6/6/6
3	FAD	C	605	-	1/1/9/9	0/30/50/50	0/6/6/6
3	FAD	D	600	-	1/1/9/9	0/30/50/50	0/6/6/6
2	PO4	D	618	-	-	0/0/0/0	0/0/0/0

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	615	FAD	C8A-N7A	-4.77	1.25	1.34
3	C	605	FAD	C8A-N7A	-4.71	1.25	1.34
3	B	610	FAD	C8A-N7A	-4.70	1.25	1.34
3	D	600	FAD	C8A-N7A	-4.42	1.26	1.34
3	A	615	FAD	P-O5'	-2.14	1.49	1.59
3	C	605	FAD	C2B-C3B	2.01	1.58	1.53
3	A	615	FAD	C5B-C4B	2.04	1.58	1.51
3	B	610	FAD	O5B-C5B	2.04	1.53	1.44
3	B	610	FAD	C2'-C3'	2.04	1.57	1.53
3	D	600	FAD	O5B-C5B	2.09	1.53	1.44
3	A	615	FAD	C1'-N10	2.10	1.50	1.48
3	C	605	FAD	C4'-C3'	2.20	1.58	1.53
3	D	600	FAD	C5B-C4B	2.29	1.59	1.51
3	B	610	FAD	C5B-C4B	2.31	1.59	1.51
3	C	605	FAD	C2'-C3'	2.39	1.58	1.53
3	C	605	FAD	C1'-N10	2.47	1.51	1.48
3	B	610	FAD	C9-C8	2.69	1.45	1.37
3	A	615	FAD	C9-C8	2.69	1.45	1.37
3	D	600	FAD	C9-C8	2.70	1.45	1.37
3	C	605	FAD	C9-C8	2.82	1.45	1.37
3	B	610	FAD	C5A-C4A	2.89	1.47	1.40
3	D	600	FAD	C5A-C4A	3.03	1.47	1.40
3	C	605	FAD	C5A-C4A	3.16	1.47	1.40
3	B	610	FAD	C2A-N3A	3.35	1.38	1.32
3	C	605	FAD	C2A-N3A	3.52	1.38	1.32
3	B	610	FAD	C2A-N1A	3.54	1.40	1.33
3	A	615	FAD	C5A-C4A	3.54	1.48	1.40
3	D	600	FAD	C2A-N1A	3.57	1.40	1.33
3	A	615	FAD	O4B-C1B	3.64	1.45	1.41
3	C	605	FAD	C2A-N1A	3.65	1.40	1.33
3	B	610	FAD	O4B-C1B	3.67	1.45	1.41
3	A	615	FAD	C2A-N1A	3.69	1.40	1.33
3	C	605	FAD	C6-C7	3.74	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	605	FAD	C6-C5X	3.87	1.47	1.41
3	D	600	FAD	C6-C7	4.02	1.48	1.37
3	D	600	FAD	C9-C9A	4.04	1.49	1.40
3	A	615	FAD	C2A-N3A	4.06	1.39	1.32
3	A	615	FAD	C6-C5X	4.06	1.47	1.41
3	A	615	FAD	C6-C7	4.10	1.49	1.37
3	B	610	FAD	C9-C9A	4.16	1.49	1.40
3	B	610	FAD	C6-C7	4.16	1.49	1.37
3	B	610	FAD	C8-C7	4.16	1.52	1.41
3	C	605	FAD	C9-C9A	4.19	1.49	1.40
3	B	610	FAD	C6-C5X	4.19	1.48	1.41
3	A	615	FAD	C9-C9A	4.20	1.49	1.40
3	A	615	FAD	C8-C7	4.21	1.52	1.41
3	D	600	FAD	C8-C7	4.21	1.52	1.41
3	D	600	FAD	C2A-N3A	4.22	1.39	1.32
3	D	600	FAD	C6-C5X	4.25	1.48	1.41
3	C	605	FAD	C8-C7	4.28	1.52	1.41
3	B	610	FAD	C10-N1	4.28	1.42	1.35
3	A	615	FAD	C10-N1	4.29	1.42	1.35
3	C	605	FAD	C5X-N5	4.32	1.42	1.35
3	D	600	FAD	C10-N1	4.37	1.42	1.35
3	D	600	FAD	C5X-N5	4.45	1.42	1.35
3	C	605	FAD	O4B-C1B	4.48	1.46	1.41
3	C	605	FAD	C10-N1	4.48	1.43	1.35
3	D	600	FAD	C4X-C10	4.58	1.49	1.41
3	B	610	FAD	C5X-N5	4.59	1.42	1.35
3	D	600	FAD	C4-C4X	4.62	1.50	1.41
3	A	615	FAD	C4X-C10	4.63	1.49	1.41
3	D	600	FAD	O4B-C1B	4.63	1.47	1.41
3	C	605	FAD	C4-C4X	4.68	1.50	1.41
3	A	615	FAD	C5X-N5	4.71	1.42	1.35
3	B	610	FAD	C4X-C10	4.96	1.50	1.41
3	A	615	FAD	C9A-C5X	5.00	1.52	1.42
3	D	600	FAD	C9A-C5X	5.01	1.52	1.42
3	C	605	FAD	C4X-C10	5.02	1.50	1.41
3	B	610	FAD	C9A-C5X	5.04	1.52	1.42
3	A	615	FAD	C4-C4X	5.13	1.51	1.41
3	C	605	FAD	C9A-C5X	5.34	1.53	1.42
3	B	610	FAD	C4-C4X	5.46	1.52	1.41
3	C	605	FAD	C4X-N5	5.86	1.42	1.33
3	B	610	FAD	C4-N3	6.09	1.44	1.33
3	D	600	FAD	C4-N3	6.22	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	600	FAD	C4X-N5	6.24	1.43	1.33
3	A	615	FAD	C4-N3	6.28	1.44	1.33
3	C	605	FAD	C4-N3	6.34	1.44	1.33
3	A	615	FAD	C4X-N5	6.47	1.43	1.33
3	B	610	FAD	C4X-N5	6.49	1.43	1.33
3	A	615	FAD	C4A-N3A	6.61	1.45	1.35
3	D	600	FAD	C10-N10	6.62	1.46	1.39
3	B	610	FAD	C10-N10	6.75	1.47	1.39
3	B	610	FAD	C4A-N3A	6.80	1.45	1.35
3	C	605	FAD	C10-N10	6.85	1.47	1.39
3	D	600	FAD	C4A-N3A	6.98	1.46	1.35
3	C	605	FAD	C4A-N3A	7.01	1.46	1.35
3	A	615	FAD	C10-N10	7.36	1.47	1.39

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	610	FAD	C4B-O4B-C1B	-8.82	100.02	109.72
3	C	605	FAD	C4B-O4B-C1B	-8.72	100.14	109.72
3	A	615	FAD	C4B-O4B-C1B	-8.33	100.57	109.72
3	D	600	FAD	C4B-O4B-C1B	-8.19	100.72	109.72
3	B	610	FAD	N3A-C2A-N1A	-7.56	123.11	128.89
3	D	600	FAD	N3A-C2A-N1A	-7.27	123.33	128.89
3	C	605	FAD	N3A-C2A-N1A	-7.13	123.44	128.89
3	A	615	FAD	N3A-C2A-N1A	-6.93	123.59	128.89
3	A	615	FAD	C4-C4X-C10	-5.24	116.58	119.94
3	D	600	FAD	C4-C4X-C10	-5.03	116.72	119.94
3	B	610	FAD	C4-C4X-C10	-4.97	116.76	119.94
3	C	605	FAD	C4X-C4-N3	-4.63	117.26	123.59
3	A	615	FAD	C4X-C4-N3	-4.54	117.38	123.59
3	C	605	FAD	C4-C4X-C10	-4.52	117.05	119.94
3	B	610	FAD	C4X-C4-N3	-4.44	117.51	123.59
3	D	600	FAD	C4X-C4-N3	-4.39	117.58	123.59
3	D	600	FAD	C4X-C10-N10	-4.01	118.15	120.52
3	C	605	FAD	C4X-C10-N10	-3.90	118.22	120.52
3	B	610	FAD	C4X-C10-N10	-3.74	118.32	120.52
3	A	615	FAD	C4A-C5A-N7A	-3.72	106.06	109.48
3	C	605	FAD	C4A-C5A-N7A	-3.62	106.15	109.48
3	A	615	FAD	C4X-C10-N10	-3.57	118.42	120.52
3	D	600	FAD	C4A-C5A-N7A	-3.49	106.27	109.48
3	B	610	FAD	C4A-C5A-N7A	-3.47	106.29	109.48
3	C	605	FAD	C5B-C4B-C3B	-2.60	104.88	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	600	FAD	C5B-C4B-C3B	-2.53	105.17	115.21
3	B	610	FAD	C5B-C4B-C3B	-2.50	105.27	115.21
3	A	615	FAD	C5B-C4B-C3B	-2.38	105.76	115.21
3	B	610	FAD	C2A-N1A-C6A	2.12	122.55	118.77
3	A	615	FAD	C2A-N1A-C6A	2.17	122.65	118.77
3	C	605	FAD	C2A-N1A-C6A	2.22	122.74	118.77
3	A	615	FAD	O4B-C4B-C3B	2.50	110.19	105.15
3	C	605	FAD	O3B-C3B-C4B	2.55	118.70	111.05
3	D	600	FAD	O4B-C4B-C3B	2.55	110.29	105.15
3	B	610	FAD	O4B-C4B-C3B	2.60	110.38	105.15
3	C	605	FAD	O4B-C4B-C3B	2.65	110.49	105.15
3	B	610	FAD	O3B-C3B-C4B	2.72	119.22	111.05
3	A	615	FAD	O3B-C3B-C4B	2.74	119.27	111.05
3	D	600	FAD	O3B-C3B-C4B	2.82	119.50	111.05
3	A	615	FAD	C1'-N10-C9A	2.93	122.16	118.86
3	B	610	FAD	C1'-N10-C9A	3.05	122.29	118.86
3	D	600	FAD	C1'-N10-C9A	3.12	122.36	118.86
3	D	600	FAD	C4X-N5-C5X	3.33	120.59	116.76
3	C	605	FAD	C4X-N5-C5X	3.37	120.63	116.76
3	B	610	FAD	C4X-N5-C5X	3.39	120.66	116.76
3	A	615	FAD	C4X-N5-C5X	3.40	120.67	116.76
3	C	605	FAD	C4-C4X-N5	3.41	122.86	118.72
3	C	605	FAD	C1'-N10-C9A	3.47	122.76	118.86
3	A	615	FAD	P-O3P-PA	3.53	142.63	132.73
3	B	610	FAD	P-O3P-PA	3.55	142.71	132.73
3	D	600	FAD	C4-C4X-N5	3.81	123.35	118.72
3	B	610	FAD	O4B-C1B-N9A	3.94	116.34	108.10
3	A	615	FAD	O4B-C1B-N9A	3.98	116.43	108.10
3	B	610	FAD	C4-C4X-N5	4.10	123.70	118.72
3	C	605	FAD	O4B-C1B-N9A	4.19	116.88	108.10
3	A	615	FAD	C4-C4X-N5	4.22	123.84	118.72
3	D	600	FAD	P-O3P-PA	4.22	144.58	132.73
3	C	605	FAD	P-O3P-PA	4.27	144.73	132.73
3	D	600	FAD	O4B-C1B-N9A	4.40	117.30	108.10
3	B	610	FAD	C4-N3-C2	8.59	122.67	115.25
3	A	615	FAD	C4-N3-C2	8.75	122.81	115.25
3	C	605	FAD	C4-N3-C2	8.82	122.87	115.25
3	D	600	FAD	C4-N3-C2	8.89	122.93	115.25
3	C	605	FAD	C2B-C1B-N9A	14.76	136.85	114.29
3	D	600	FAD	C2B-C1B-N9A	14.83	136.95	114.29
3	B	610	FAD	C2B-C1B-N9A	15.13	137.40	114.29
3	A	615	FAD	C2B-C1B-N9A	15.55	138.05	114.29

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	600	FAD	C1B
3	C	605	FAD	C1B
3	A	615	FAD	C1B
3	B	610	FAD	C1B

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	603	PO4	1	0
3	A	615	FAD	1	0
3	B	610	FAD	1	0
3	C	605	FAD	1	0
3	D	600	FAD	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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^{th} 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	213/232 (91%)	-0.03	9 (4%) 40 43	20, 35, 65, 77	0
1	B	215/232 (92%)	-0.07	7 (3%) 50 53	21, 37, 65, 78	0
1	C	214/232 (92%)	-0.23	4 (1%) 70 72	20, 33, 60, 72	0
1	D	212/232 (91%)	-0.02	6 (2%) 56 60	23, 37, 56, 69	0
All	All	854/928 (92%)	-0.09	26 (3%) 54 57	20, 35, 62, 78	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	33	MET	4.7
1	C	96	TYR	4.4
1	A	92	SER	4.4
1	D	40	ARG	4.1
1	C	138	GLU	3.6
1	B	29	VAL	3.6
1	D	218	VAL	3.2
1	A	107	GLU	2.9
1	C	220	VAL	2.9
1	D	37	ASP	2.8
1	D	108	GLY	2.8
1	D	38	GLU	2.7
1	A	29	VAL	2.6
1	A	112	THR	2.6
1	B	220	VAL	2.5
1	A	91	TYR	2.5
1	D	95	SER	2.3
1	B	109	TYR	2.3
1	A	104	GLU	2.2
1	B	30	SER	2.2
1	B	40	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	92	SER	2.1
1	A	31	PHE	2.1
1	B	107	GLU	2.1
1	A	111	THR	2.1
1	B	219	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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^{th} 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	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	PO4	D	618	5/5	0.88	0.21	1.75	97,98,98,98	0
3	FAD	A	615	53/53	0.92	0.19	0.73	31,41,65,65	0
2	PO4	B	608	5/5	0.96	0.17	0.71	72,72,73,74	0
3	FAD	B	610	53/53	0.93	0.16	0.14	32,44,59,60	0
3	FAD	C	605	53/53	0.95	0.17	0.05	27,39,51,52	0
3	FAD	D	600	53/53	0.95	0.17	-0.33	29,45,55,56	0
2	PO4	A	603	5/5	0.94	0.15	-0.96	73,74,74,75	0

6.5 Other polymers (i)

There are no such residues in this entry.