wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 04:48 PM GMT

PDB ID	:	4FZB
Title	:	Structure of thymidylate synthase ThyX complexed to a new inhibitor
Authors	:	Basta, T.; Boum, Y.; Briffotaux, J.; Becker, H.F.; Lamarre-Jouenne, I.; Lambry, J.C.; Skouloubris, S.; Liebl, U.; van Tilbeurgh, H.; Graille, M.; Myllylkallio, H.
Deposited on	:	2012-07-06
Resolution	:	2.59 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

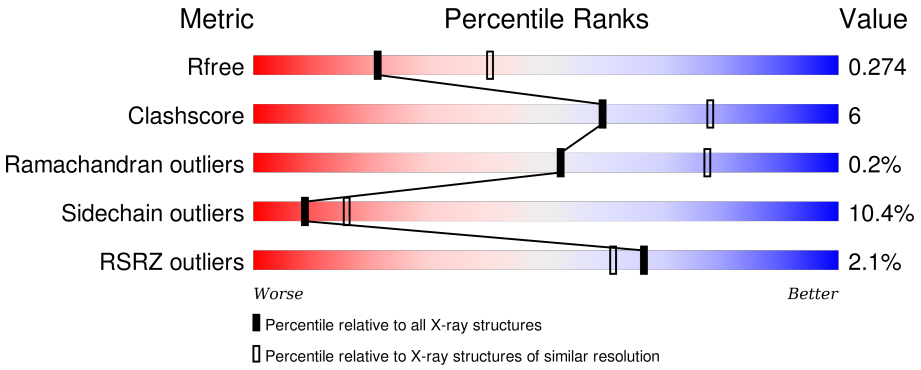
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.59 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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. 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	227	70% 12% • 16%
1	B	227	2% 62% 19% • 17%
1	C	227	76% 13% • 9%
1	D	227	68% 21% • 11%
1	E	227	73% 15% • 9%

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Mol	Chain	Length	Quality of chain
1	F	227	2% 70% 19% 9%
1	G	227	67% 14% 17%
1	H	227	% 65% 13% 21%
1	I	227	% 64% 20% 15%
1	J	227	2% 64% 13% 21%
1	K	227	% 73% 15% 11%
1	L	227	4% 67% 20% 11%
1	M	227	61% 23% 13%
1	N	227	4% 59% 19% 22%
1	O	227	2% 64% 22% 12%
1	P	227	5% 69% 16% 13%

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	0VJ	B	303	-	X	-	-
3	0VJ	G	301	-	-	-	X
4	DMS	A	304	-	-	-	X
4	DMS	C	302	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26503 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 Probable thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	191	Total	C	N	O	S	0	0	0
			1544	984	267	287	6			
1	B	188	Total	C	N	O	S	0	0	0
			1519	971	264	278	6			
1	C	207	Total	C	N	O	S	0	0	0
			1667	1060	291	308	8			
1	D	203	Total	C	N	O	S	0	0	0
			1642	1047	285	303	7			
1	E	206	Total	C	N	O	S	0	1	0
			1668	1060	293	307	8			
1	F	206	Total	C	N	O	S	0	0	0
			1666	1062	289	307	8			
1	G	188	Total	C	N	O	S	0	0	0
			1519	971	264	278	6			
1	H	179	Total	C	N	O	S	0	0	0
			1446	928	250	262	6			
1	I	193	Total	C	N	O	S	0	0	0
			1558	995	270	286	7			
1	J	179	Total	C	N	O	S	0	0	0
			1449	931	251	261	6			
1	K	201	Total	C	N	O	S	0	0	0
			1624	1034	283	300	7			
1	L	201	Total	C	N	O	S	0	0	0
			1624	1034	283	300	7			
1	M	197	Total	C	N	O	S	0	0	0
			1592	1019	275	291	7			
1	N	177	Total	C	N	O	S	0	0	0
			1432	921	247	258	6			
1	O	200	Total	C	N	O	S	0	0	0
			1617	1029	282	299	7			
1	P	197	Total	C	N	O	S	0	0	0
			1592	1015	276	294	7			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MET	-	EXPRESSION TAG	UNP O41156
A	-3	ALA	-	EXPRESSION TAG	UNP O41156
A	-2	SER	-	EXPRESSION TAG	UNP O41156
A	-1	MET	-	EXPRESSION TAG	UNP O41156
A	0	THR	-	EXPRESSION TAG	UNP O41156
A	1	GLY	-	EXPRESSION TAG	UNP O41156
A	217	HIS	-	EXPRESSION TAG	UNP O41156
A	218	HIS	-	EXPRESSION TAG	UNP O41156
A	219	HIS	-	EXPRESSION TAG	UNP O41156
A	220	HIS	-	EXPRESSION TAG	UNP O41156
A	221	HIS	-	EXPRESSION TAG	UNP O41156
A	222	HIS	-	EXPRESSION TAG	UNP O41156
B	-4	MET	-	EXPRESSION TAG	UNP O41156
B	-3	ALA	-	EXPRESSION TAG	UNP O41156
B	-2	SER	-	EXPRESSION TAG	UNP O41156
B	-1	MET	-	EXPRESSION TAG	UNP O41156
B	0	THR	-	EXPRESSION TAG	UNP O41156
B	1	GLY	-	EXPRESSION TAG	UNP O41156
B	217	HIS	-	EXPRESSION TAG	UNP O41156
B	218	HIS	-	EXPRESSION TAG	UNP O41156
B	219	HIS	-	EXPRESSION TAG	UNP O41156
B	220	HIS	-	EXPRESSION TAG	UNP O41156
B	221	HIS	-	EXPRESSION TAG	UNP O41156
B	222	HIS	-	EXPRESSION TAG	UNP O41156
C	-4	MET	-	EXPRESSION TAG	UNP O41156
C	-3	ALA	-	EXPRESSION TAG	UNP O41156
C	-2	SER	-	EXPRESSION TAG	UNP O41156
C	-1	MET	-	EXPRESSION TAG	UNP O41156
C	0	THR	-	EXPRESSION TAG	UNP O41156
C	1	GLY	-	EXPRESSION TAG	UNP O41156
C	217	HIS	-	EXPRESSION TAG	UNP O41156
C	218	HIS	-	EXPRESSION TAG	UNP O41156
C	219	HIS	-	EXPRESSION TAG	UNP O41156
C	220	HIS	-	EXPRESSION TAG	UNP O41156
C	221	HIS	-	EXPRESSION TAG	UNP O41156
C	222	HIS	-	EXPRESSION TAG	UNP O41156
D	-4	MET	-	EXPRESSION TAG	UNP O41156
D	-3	ALA	-	EXPRESSION TAG	UNP O41156
D	-2	SER	-	EXPRESSION TAG	UNP O41156
D	-1	MET	-	EXPRESSION TAG	UNP O41156
D	0	THR	-	EXPRESSION TAG	UNP O41156
D	1	GLY	-	EXPRESSION TAG	UNP O41156

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Chain	Residue	Modelled	Actual	Comment	Reference
D	217	HIS	-	EXPRESSION TAG	UNP O41156
D	218	HIS	-	EXPRESSION TAG	UNP O41156
D	219	HIS	-	EXPRESSION TAG	UNP O41156
D	220	HIS	-	EXPRESSION TAG	UNP O41156
D	221	HIS	-	EXPRESSION TAG	UNP O41156
D	222	HIS	-	EXPRESSION TAG	UNP O41156
E	-4	MET	-	EXPRESSION TAG	UNP O41156
E	-3	ALA	-	EXPRESSION TAG	UNP O41156
E	-2	SER	-	EXPRESSION TAG	UNP O41156
E	-1	MET	-	EXPRESSION TAG	UNP O41156
E	0	THR	-	EXPRESSION TAG	UNP O41156
E	1	GLY	-	EXPRESSION TAG	UNP O41156
E	217	HIS	-	EXPRESSION TAG	UNP O41156
E	218	HIS	-	EXPRESSION TAG	UNP O41156
E	219	HIS	-	EXPRESSION TAG	UNP O41156
E	220	HIS	-	EXPRESSION TAG	UNP O41156
E	221	HIS	-	EXPRESSION TAG	UNP O41156
E	222	HIS	-	EXPRESSION TAG	UNP O41156
F	-4	MET	-	EXPRESSION TAG	UNP O41156
F	-3	ALA	-	EXPRESSION TAG	UNP O41156
F	-2	SER	-	EXPRESSION TAG	UNP O41156
F	-1	MET	-	EXPRESSION TAG	UNP O41156
F	0	THR	-	EXPRESSION TAG	UNP O41156
F	1	GLY	-	EXPRESSION TAG	UNP O41156
F	217	HIS	-	EXPRESSION TAG	UNP O41156
F	218	HIS	-	EXPRESSION TAG	UNP O41156
F	219	HIS	-	EXPRESSION TAG	UNP O41156
F	220	HIS	-	EXPRESSION TAG	UNP O41156
F	221	HIS	-	EXPRESSION TAG	UNP O41156
F	222	HIS	-	EXPRESSION TAG	UNP O41156
G	-4	MET	-	EXPRESSION TAG	UNP O41156
G	-3	ALA	-	EXPRESSION TAG	UNP O41156
G	-2	SER	-	EXPRESSION TAG	UNP O41156
G	-1	MET	-	EXPRESSION TAG	UNP O41156
G	0	THR	-	EXPRESSION TAG	UNP O41156
G	1	GLY	-	EXPRESSION TAG	UNP O41156
G	217	HIS	-	EXPRESSION TAG	UNP O41156
G	218	HIS	-	EXPRESSION TAG	UNP O41156
G	219	HIS	-	EXPRESSION TAG	UNP O41156
G	220	HIS	-	EXPRESSION TAG	UNP O41156
G	221	HIS	-	EXPRESSION TAG	UNP O41156
G	222	HIS	-	EXPRESSION TAG	UNP O41156

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-4	MET	-	EXPRESSION TAG	UNP O41156
H	-3	ALA	-	EXPRESSION TAG	UNP O41156
H	-2	SER	-	EXPRESSION TAG	UNP O41156
H	-1	MET	-	EXPRESSION TAG	UNP O41156
H	0	THR	-	EXPRESSION TAG	UNP O41156
H	1	GLY	-	EXPRESSION TAG	UNP O41156
H	217	HIS	-	EXPRESSION TAG	UNP O41156
H	218	HIS	-	EXPRESSION TAG	UNP O41156
H	219	HIS	-	EXPRESSION TAG	UNP O41156
H	220	HIS	-	EXPRESSION TAG	UNP O41156
H	221	HIS	-	EXPRESSION TAG	UNP O41156
H	222	HIS	-	EXPRESSION TAG	UNP O41156
I	-4	MET	-	EXPRESSION TAG	UNP O41156
I	-3	ALA	-	EXPRESSION TAG	UNP O41156
I	-2	SER	-	EXPRESSION TAG	UNP O41156
I	-1	MET	-	EXPRESSION TAG	UNP O41156
I	0	THR	-	EXPRESSION TAG	UNP O41156
I	1	GLY	-	EXPRESSION TAG	UNP O41156
I	217	HIS	-	EXPRESSION TAG	UNP O41156
I	218	HIS	-	EXPRESSION TAG	UNP O41156
I	219	HIS	-	EXPRESSION TAG	UNP O41156
I	220	HIS	-	EXPRESSION TAG	UNP O41156
I	221	HIS	-	EXPRESSION TAG	UNP O41156
I	222	HIS	-	EXPRESSION TAG	UNP O41156
J	-4	MET	-	EXPRESSION TAG	UNP O41156
J	-3	ALA	-	EXPRESSION TAG	UNP O41156
J	-2	SER	-	EXPRESSION TAG	UNP O41156
J	-1	MET	-	EXPRESSION TAG	UNP O41156
J	0	THR	-	EXPRESSION TAG	UNP O41156
J	1	GLY	-	EXPRESSION TAG	UNP O41156
J	217	HIS	-	EXPRESSION TAG	UNP O41156
J	218	HIS	-	EXPRESSION TAG	UNP O41156
J	219	HIS	-	EXPRESSION TAG	UNP O41156
J	220	HIS	-	EXPRESSION TAG	UNP O41156
J	221	HIS	-	EXPRESSION TAG	UNP O41156
J	222	HIS	-	EXPRESSION TAG	UNP O41156
K	-4	MET	-	EXPRESSION TAG	UNP O41156
K	-3	ALA	-	EXPRESSION TAG	UNP O41156
K	-2	SER	-	EXPRESSION TAG	UNP O41156
K	-1	MET	-	EXPRESSION TAG	UNP O41156
K	0	THR	-	EXPRESSION TAG	UNP O41156
K	1	GLY	-	EXPRESSION TAG	UNP O41156

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Chain	Residue	Modelled	Actual	Comment	Reference
K	217	HIS	-	EXPRESSION TAG	UNP O41156
K	218	HIS	-	EXPRESSION TAG	UNP O41156
K	219	HIS	-	EXPRESSION TAG	UNP O41156
K	220	HIS	-	EXPRESSION TAG	UNP O41156
K	221	HIS	-	EXPRESSION TAG	UNP O41156
K	222	HIS	-	EXPRESSION TAG	UNP O41156
L	-4	MET	-	EXPRESSION TAG	UNP O41156
L	-3	ALA	-	EXPRESSION TAG	UNP O41156
L	-2	SER	-	EXPRESSION TAG	UNP O41156
L	-1	MET	-	EXPRESSION TAG	UNP O41156
L	0	THR	-	EXPRESSION TAG	UNP O41156
L	1	GLY	-	EXPRESSION TAG	UNP O41156
L	217	HIS	-	EXPRESSION TAG	UNP O41156
L	218	HIS	-	EXPRESSION TAG	UNP O41156
L	219	HIS	-	EXPRESSION TAG	UNP O41156
L	220	HIS	-	EXPRESSION TAG	UNP O41156
L	221	HIS	-	EXPRESSION TAG	UNP O41156
L	222	HIS	-	EXPRESSION TAG	UNP O41156
M	-4	MET	-	EXPRESSION TAG	UNP O41156
M	-3	ALA	-	EXPRESSION TAG	UNP O41156
M	-2	SER	-	EXPRESSION TAG	UNP O41156
M	-1	MET	-	EXPRESSION TAG	UNP O41156
M	0	THR	-	EXPRESSION TAG	UNP O41156
M	1	GLY	-	EXPRESSION TAG	UNP O41156
M	217	HIS	-	EXPRESSION TAG	UNP O41156
M	218	HIS	-	EXPRESSION TAG	UNP O41156
M	219	HIS	-	EXPRESSION TAG	UNP O41156
M	220	HIS	-	EXPRESSION TAG	UNP O41156
M	221	HIS	-	EXPRESSION TAG	UNP O41156
M	222	HIS	-	EXPRESSION TAG	UNP O41156
N	-4	MET	-	EXPRESSION TAG	UNP O41156
N	-3	ALA	-	EXPRESSION TAG	UNP O41156
N	-2	SER	-	EXPRESSION TAG	UNP O41156
N	-1	MET	-	EXPRESSION TAG	UNP O41156
N	0	THR	-	EXPRESSION TAG	UNP O41156
N	1	GLY	-	EXPRESSION TAG	UNP O41156
N	217	HIS	-	EXPRESSION TAG	UNP O41156
N	218	HIS	-	EXPRESSION TAG	UNP O41156
N	219	HIS	-	EXPRESSION TAG	UNP O41156
N	220	HIS	-	EXPRESSION TAG	UNP O41156
N	221	HIS	-	EXPRESSION TAG	UNP O41156
N	222	HIS	-	EXPRESSION TAG	UNP O41156

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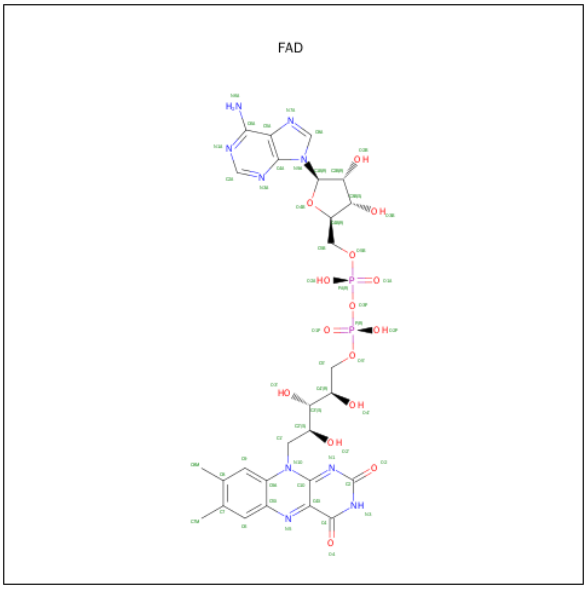
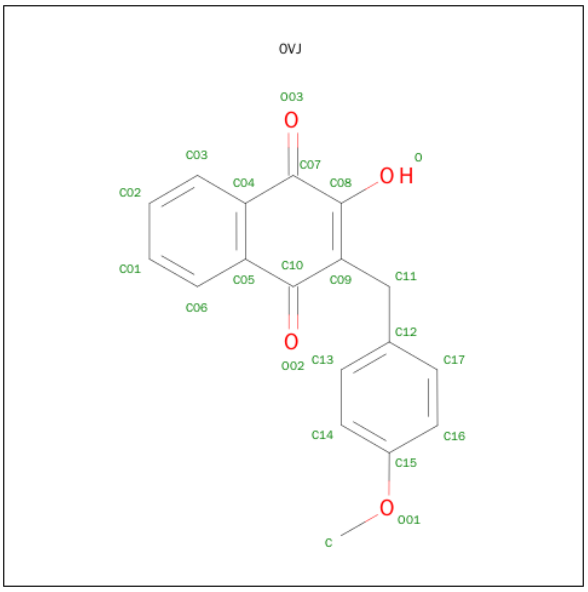
Chain	Residue	Modelled	Actual	Comment	Reference
O	-4	MET	-	EXPRESSION TAG	UNP O41156
O	-3	ALA	-	EXPRESSION TAG	UNP O41156
O	-2	SER	-	EXPRESSION TAG	UNP O41156
O	-1	MET	-	EXPRESSION TAG	UNP O41156
O	0	THR	-	EXPRESSION TAG	UNP O41156
O	1	GLY	-	EXPRESSION TAG	UNP O41156
O	217	HIS	-	EXPRESSION TAG	UNP O41156
O	218	HIS	-	EXPRESSION TAG	UNP O41156
O	219	HIS	-	EXPRESSION TAG	UNP O41156
O	220	HIS	-	EXPRESSION TAG	UNP O41156
O	221	HIS	-	EXPRESSION TAG	UNP O41156
O	222	HIS	-	EXPRESSION TAG	UNP O41156
P	-4	MET	-	EXPRESSION TAG	UNP O41156
P	-3	ALA	-	EXPRESSION TAG	UNP O41156
P	-2	SER	-	EXPRESSION TAG	UNP O41156
P	-1	MET	-	EXPRESSION TAG	UNP O41156
P	0	THR	-	EXPRESSION TAG	UNP O41156
P	1	GLY	-	EXPRESSION TAG	UNP O41156
P	217	HIS	-	EXPRESSION TAG	UNP O41156
P	218	HIS	-	EXPRESSION TAG	UNP O41156
P	219	HIS	-	EXPRESSION TAG	UNP O41156
P	220	HIS	-	EXPRESSION TAG	UNP O41156
P	221	HIS	-	EXPRESSION TAG	UNP O41156
P	222	HIS	-	EXPRESSION TAG	UNP O41156

- 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	A	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		
2	B	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	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	H	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	I	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	I	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	J	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	K	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	M	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	N	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	O	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	P	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is 2-HYDROXY-3-(4-METHOXYBENZYL)NAPHTHALENE-1,4-DIONE (three-letter code: 0VJ) (formula: $C_{18}H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 22 18 4	0	0
3	A	1	Total C O 22 18 4	0	0
3	B	1	Total C O 22 18 4	0	0
3	D	1	Total C O 22 18 4	0	0
3	E	1	Total C O 22 18 4	0	0
3	F	1	Total C O 22 18 4	0	0
3	G	1	Total C O 22 18 4	0	0
3	H	1	Total C O 22 18 4	0	0
3	I	1	Total C O 22 18 4	0	0
3	J	1	Total C O 22 18 4	0	0
3	K	1	Total C O 22 18 4	0	0
3	L	1	Total C O 22 18 4	0	0
3	M	1	Total C O 22 18 4	0	0
3	N	1	Total C O 22 18 4	0	0

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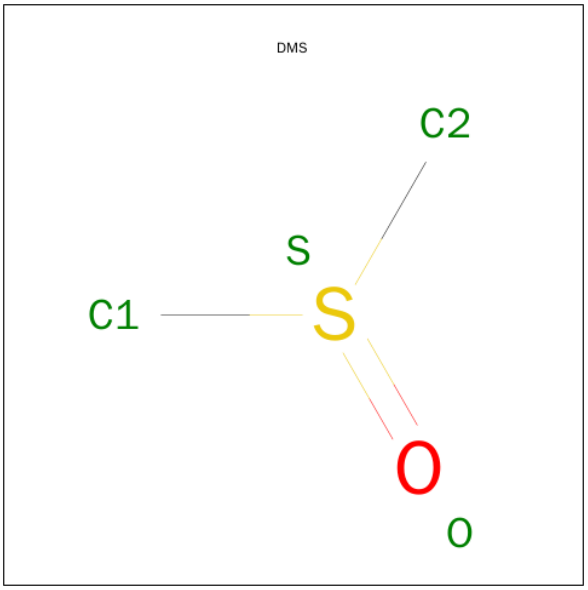
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	O	1	Total C O 22 18 4	0	0
3	P	1	Total C O 22 18 4	0	0

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O S 4 2 1 1	0	0
4	B	1	Total C O S 4 2 1 1	0	0
4	C	1	Total C O S 4 2 1 1	0	0
4	D	1	Total C O S 4 2 1 1	0	0
4	E	1	Total C O S 4 2 1 1	0	0
4	F	1	Total C O S 4 2 1 1	0	0
4	G	1	Total C O S 4 2 1 1	0	0
4	H	1	Total C O S 4 2 1 1	0	0
4	I	1	Total C O S 4 2 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	K	1	Total C O S 4 2 1 1	0	0
4	M	1	Total C O S 4 2 1 1	0	0
4	O	1	Total C O S 4 2 1 1	0	0
4	P	1	Total C O S 4 2 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	11	Total O 11 11	0	0
5	B	7	Total O 7 7	0	0
5	C	2	Total O 2 2	0	0
5	D	7	Total O 7 7	0	0
5	E	8	Total O 8 8	0	0
5	F	13	Total O 13 13	0	0
5	G	13	Total O 13 13	0	0
5	H	5	Total O 5 5	0	0
5	I	3	Total O 3 3	0	0
5	J	5	Total O 5 5	0	0
5	K	2	Total O 2 2	0	0
5	L	6	Total O 6 6	0	0
5	M	3	Total O 3 3	0	0
5	N	5	Total O 5 5	0	0
5	O	1	Total O 1 1	0	0

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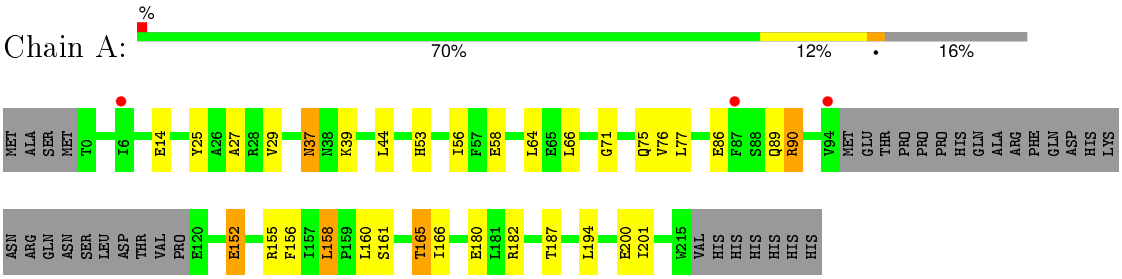
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	P	1	Total O 1 1	0	0

3 Residue-property plots (i)

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

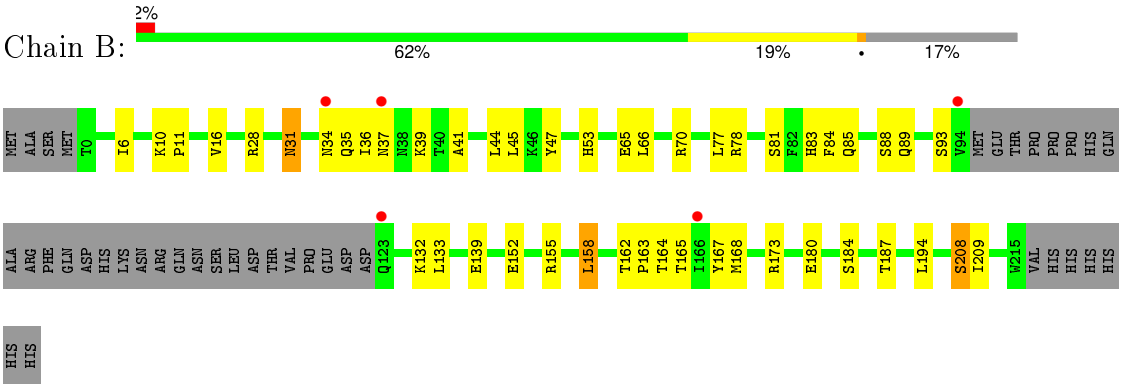
- Molecule 1: Probable thymidylate synthase

Chain A:



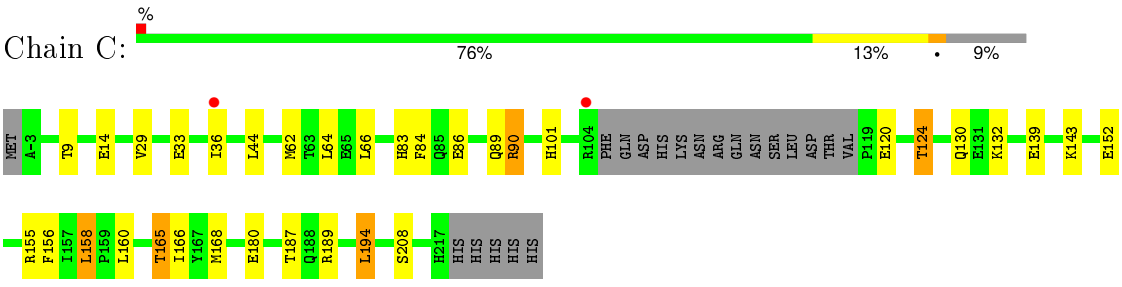
- Molecule 1: Probable thymidylate synthase

Chain B:



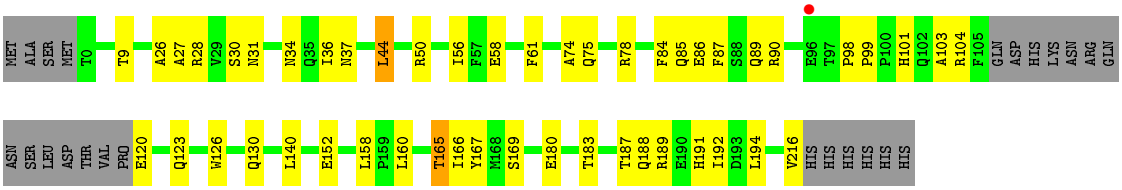
- Molecule 1: Probable thymidylate synthase

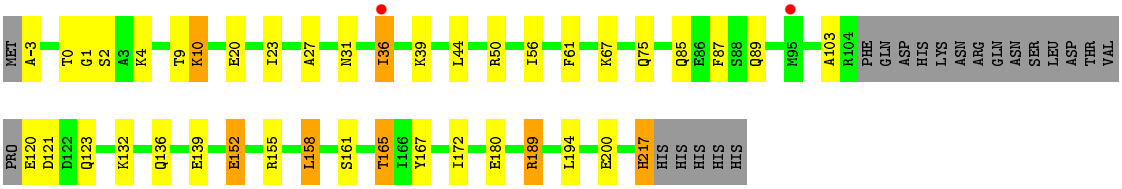
Chain C:



- Molecule 1: Probable thymidylate synthase

Chain D:



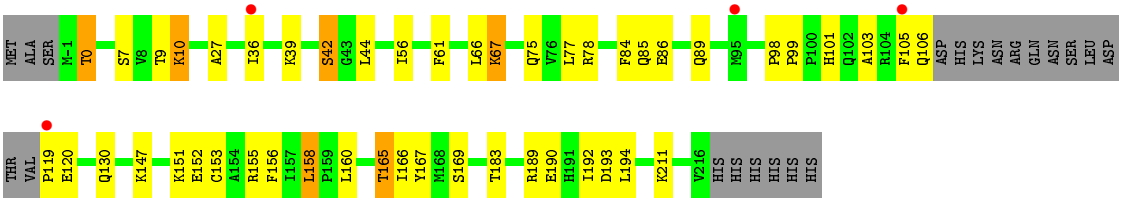


• Molecule 1: Probable thymidylate synthase

Chain E:

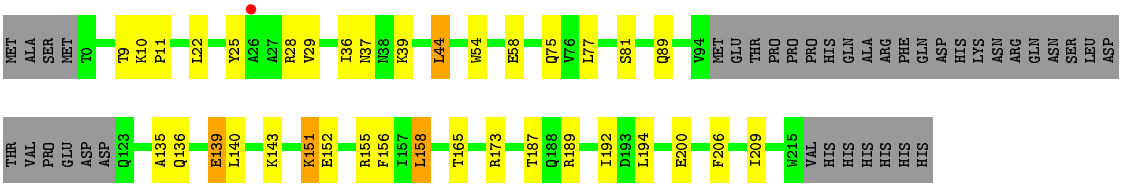
• Molecule 1: Probable thymidylate synthase

Chain F:



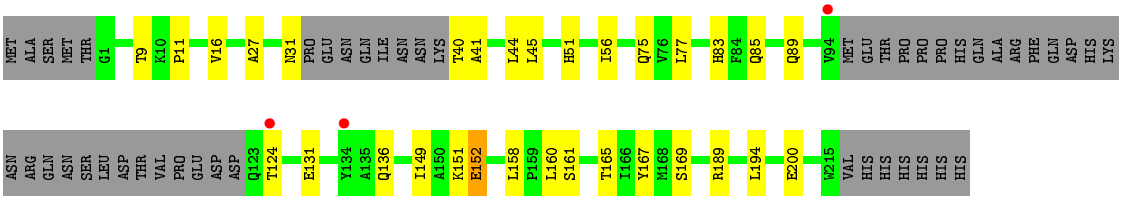
• Molecule 1: Probable thymidylate synthase

Chain G:



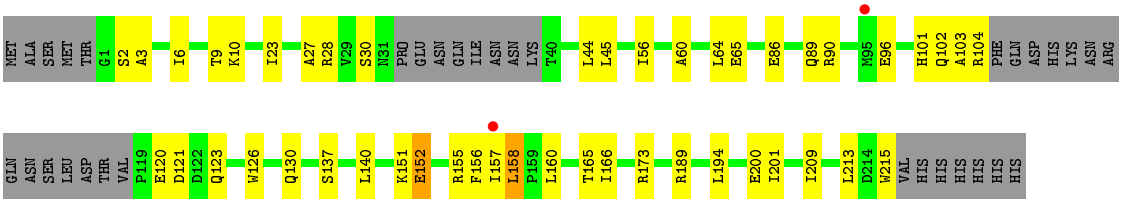
• Molecule 1: Probable thymidylate synthase

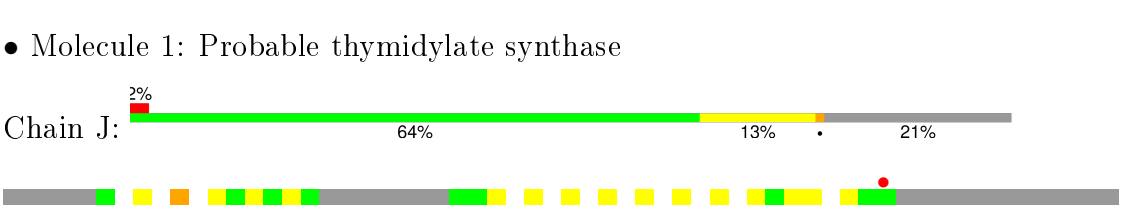
Chain H:



• Molecule 1: Probable thymidylate synthase

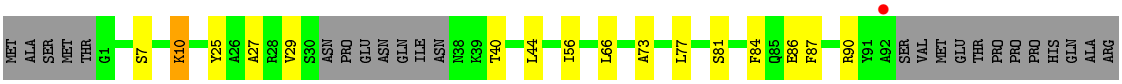
Chain I:

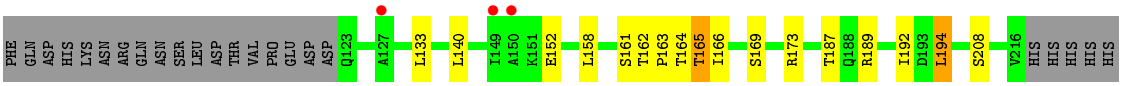




• Molecule 1: Probable thymidylate synthase

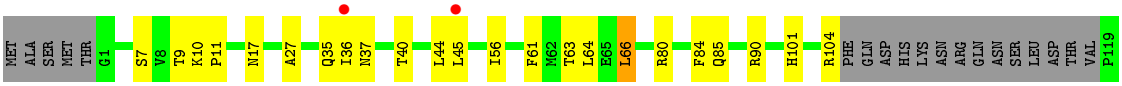
Chain J:

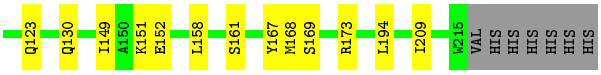




• Molecule 1: Probable thymidylate synthase

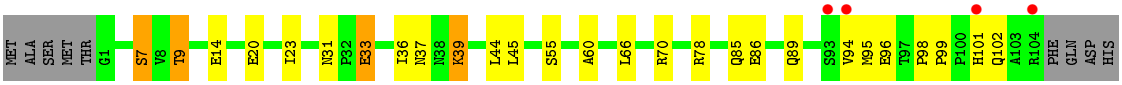
Chain K:

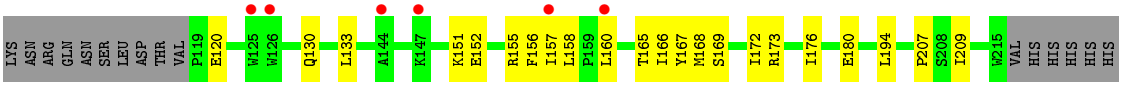




• Molecule 1: Probable thymidylate synthase

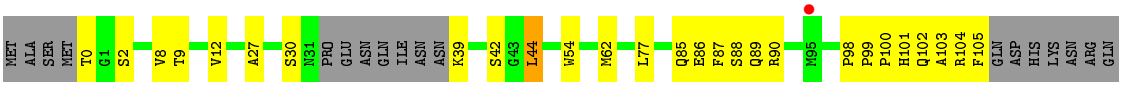
Chain L:

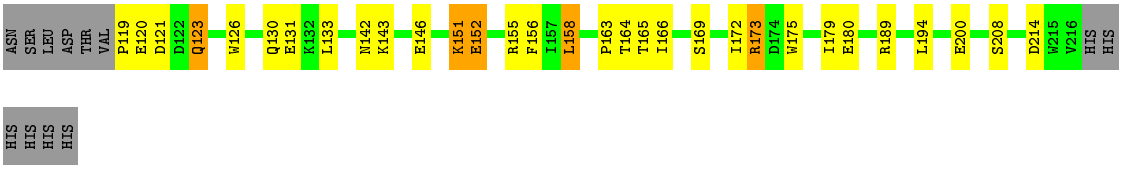




• Molecule 1: Probable thymidylate synthase

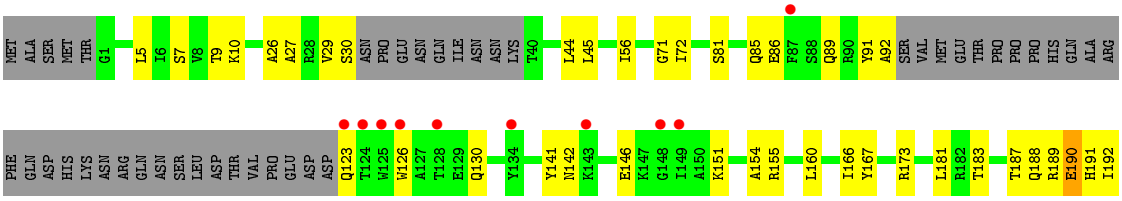
Chain M:





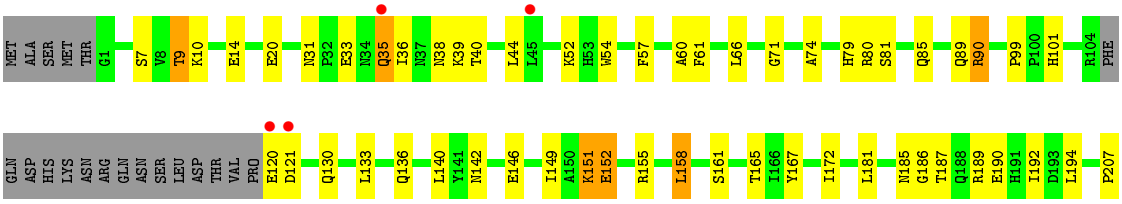
• Molecule 1: Probable thymidylate synthase

Chain N:



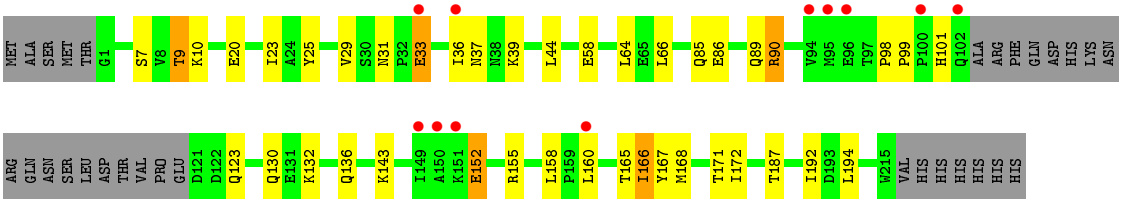
• Molecule 1: Probable thymidylate synthase

Chain O:



• Molecule 1: Probable thymidylate synthase

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	69.97Å 120.58Å 128.25Å 111.65° 91.13° 90.18°	Depositor
Resolution (Å)	34.21 – 2.59 34.21 – 2.59	Depositor EDS
% Data completeness (in resolution range)	(Not available) (34.21-2.59) 81.1 (34.21-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.211 , 0.261 0.222 , 0.274	Depositor DCC
R_{free} test set	5633 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	45.5	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 30.6	EDS
Estimated twinning fraction	0.146 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 111996 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	26503	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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: DMS, 0VJ, 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	0.51	0/1578	0.72	0/2134
1	B	0.51	0/1553	0.72	0/2100
1	C	0.50	0/1707	0.72	0/2311
1	D	0.50	0/1681	0.74	0/2276
1	E	0.51	0/1710	0.73	0/2314
1	F	0.53	0/1706	0.73	0/2309
1	G	0.51	0/1553	0.72	0/2100
1	H	0.51	0/1478	0.72	0/1996
1	I	0.47	0/1595	0.71	0/2157
1	J	0.47	0/1481	0.71	0/1999
1	K	0.52	0/1663	0.70	0/2251
1	L	0.48	0/1663	0.70	0/2251
1	M	0.51	0/1630	0.73	0/2204
1	N	0.48	0/1464	0.71	0/1977
1	O	0.53	0/1655	0.72	0/2240
1	P	0.49	0/1630	0.72	0/2207
All	All	0.50	0/25747	0.72	0/34826

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	1544	0	1533	13	0
1	B	1519	0	1519	22	0
1	C	1667	0	1652	19	0
1	D	1642	0	1627	25	0
1	E	1668	0	1657	20	0
1	F	1666	0	1652	28	0
1	G	1519	0	1519	21	0
1	H	1446	0	1448	12	0
1	I	1558	0	1546	22	0
1	J	1449	0	1456	15	0
1	K	1624	0	1610	13	0
1	L	1624	0	1610	23	0
1	M	1592	0	1584	30	1
1	N	1432	0	1437	23	0
1	O	1617	0	1602	26	1
1	P	1592	0	1578	16	0
2	A	106	0	62	0	0
2	B	53	0	31	1	0
2	C	53	0	31	1	0
2	E	53	0	31	1	0
2	F	106	0	62	3	0
2	H	53	0	31	1	0
2	I	106	0	62	2	0
2	J	53	0	31	3	0
2	K	53	0	31	0	0
2	M	53	0	31	1	0
2	N	53	0	31	2	0
2	O	53	0	31	1	0
2	P	53	0	31	2	0
3	A	44	0	28	0	0
3	B	22	0	14	2	0
3	D	22	0	14	1	0
3	E	22	0	14	0	0
3	F	22	0	14	0	0
3	G	22	0	14	0	0
3	H	22	0	14	0	0
3	I	22	0	14	2	0
3	J	22	0	14	1	0
3	K	22	0	14	0	0
3	L	22	0	14	0	0
3	M	22	0	14	4	0
3	N	22	0	14	4	0
3	O	22	0	14	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	22	0	14	1	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
4	C	4	0	6	0	0
4	D	4	0	6	1	0
4	E	4	0	6	2	0
4	F	4	0	6	0	0
4	G	4	0	6	0	0
4	H	4	0	6	0	0
4	I	4	0	6	0	0
4	K	4	0	6	1	0
4	M	4	0	6	3	0
4	O	4	0	6	0	0
4	P	4	0	6	0	0
5	A	11	0	0	0	0
5	B	7	0	0	0	0
5	C	2	0	0	0	0
5	D	7	0	0	0	0
5	E	8	0	0	0	0
5	F	13	0	0	0	0
5	G	13	0	0	0	0
5	H	5	0	0	0	0
5	I	3	0	0	0	0
5	J	5	0	0	0	0
5	K	2	0	0	0	0
5	L	6	0	0	0	0
5	M	3	0	0	0	0
5	N	5	0	0	0	0
5	O	1	0	0	0	0
5	P	1	0	0	0	0
All	All	26503	0	25828	296	1

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 6.

The worst 5 of 296 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:F:0:THR:HG21	1:F:190:GLU:HA	1.36	1.03
1:C:101:HIS:H	1:C:130:GLN:HE22	1.04	0.98
1:C:155:ARG:HA	1:C:158:LEU:HD22	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:HIS:H	1:C:130:GLN:NE2	1.83	0.76
1:J:87:PHE:HE1	1:J:165:THR:HG23	1.48	0.76

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:0:THR:CG2	1:O:35:GLN:OE1[1_655]	2.11	0.09

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	187/227 (82%)	178 (95%)	7 (4%)	2 (1%)	17 36
1	B	184/227 (81%)	177 (96%)	7 (4%)	0	100 100
1	C	203/227 (89%)	194 (96%)	9 (4%)	0	100 100
1	D	199/227 (88%)	195 (98%)	4 (2%)	0	100 100
1	E	203/227 (89%)	193 (95%)	10 (5%)	0	100 100
1	F	202/227 (89%)	197 (98%)	5 (2%)	0	100 100
1	G	184/227 (81%)	179 (97%)	5 (3%)	0	100 100
1	H	173/227 (76%)	166 (96%)	7 (4%)	0	100 100
1	I	187/227 (82%)	181 (97%)	5 (3%)	1 (0%)	34 60
1	J	173/227 (76%)	170 (98%)	3 (2%)	0	100 100
1	K	197/227 (87%)	191 (97%)	5 (2%)	1 (0%)	34 60
1	L	197/227 (87%)	190 (96%)	7 (4%)	0	100 100
1	M	191/227 (84%)	186 (97%)	5 (3%)	0	100 100
1	N	171/227 (75%)	166 (97%)	4 (2%)	1 (1%)	30 56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	O	196/227 (86%)	190 (97%)	4 (2%)	2 (1%)	19 39
1	P	193/227 (85%)	186 (96%)	7 (4%)	0	100 100
All	All	3040/3632 (84%)	2939 (97%)	94 (3%)	7 (0%)	52 77

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	PHE
1	N	214	ASP
1	O	80	ARG
1	K	80	ARG
1	O	38	ASN

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	165/199 (83%)	151 (92%)	14 (8%)	13 25
1	B	162/199 (81%)	142 (88%)	20 (12%)	6 11
1	C	179/199 (90%)	161 (90%)	18 (10%)	9 17
1	D	176/199 (88%)	162 (92%)	14 (8%)	15 29
1	E	179/199 (90%)	160 (89%)	19 (11%)	8 15
1	F	179/199 (90%)	160 (89%)	19 (11%)	8 15
1	G	162/199 (81%)	150 (93%)	12 (7%)	17 34
1	H	153/199 (77%)	136 (89%)	17 (11%)	8 13
1	I	166/199 (83%)	149 (90%)	17 (10%)	9 17
1	J	153/199 (77%)	138 (90%)	15 (10%)	10 19
1	K	174/199 (87%)	157 (90%)	17 (10%)	10 19
1	L	174/199 (87%)	154 (88%)	20 (12%)	7 12
1	M	170/199 (85%)	146 (86%)	24 (14%)	4 7
1	N	151/199 (76%)	140 (93%)	11 (7%)	17 35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	O	173/199 (87%)	151 (87%)	22 (13%)	5 10
1	P	171/199 (86%)	150 (88%)	21 (12%)	6 11
All	All	2687/3184 (84%)	2407 (90%)	280 (10%)	9 16

5 of 280 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	158	LEU
1	J	152	GLU
1	O	194	LEU
1	H	189	ARG
1	I	152	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	31	ASN
1	I	85	GLN
1	P	34	ASN
1	G	35	GLN
1	G	136	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

45 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FAD	A	301	-	48,58,58	2.25	14 (29%)	54,89,89	2.89	13 (24%)
2	FAD	A	302	-	48,58,58	2.25	14 (29%)	54,89,89	2.89	13 (24%)
3	0VJ	A	303	-	24,24,24	4.21	16 (66%)	30,34,34	3.46	14 (46%)
4	DMS	A	304	-	3,3,3	1.01	0	3,3,3	1.02	0
3	0VJ	A	305	-	24,24,24	4.45	16 (66%)	30,34,34	3.31	14 (46%)
2	FAD	B	301	-	48,58,58	2.40	11 (22%)	54,89,89	2.90	17 (31%)
4	DMS	B	302	-	3,3,3	0.94	0	3,3,3	1.22	0
3	0VJ	B	303	-	24,24,24	5.01	16 (66%)	30,34,34	3.91	19 (63%)
2	FAD	C	301	-	48,58,58	2.26	11 (22%)	54,89,89	2.73	12 (22%)
4	DMS	C	302	-	3,3,3	0.77	0	3,3,3	0.89	0
3	0VJ	D	301	-	24,24,24	4.46	15 (62%)	30,34,34	3.31	11 (36%)
4	DMS	D	302	-	3,3,3	0.93	0	3,3,3	1.02	0
2	FAD	E	301	-	48,58,58	2.25	14 (29%)	54,89,89	2.88	13 (24%)
3	0VJ	E	302	-	24,24,24	4.70	18 (75%)	30,34,34	2.92	11 (36%)
4	DMS	E	303	-	3,3,3	0.65	0	3,3,3	1.23	0
2	FAD	F	301	-	48,58,58	2.33	15 (31%)	54,89,89	2.69	17 (31%)
2	FAD	F	302	-	48,58,58	2.25	14 (29%)	54,89,89	2.88	13 (24%)
4	DMS	F	303	-	3,3,3	0.76	0	3,3,3	0.86	0
3	0VJ	F	304	-	24,24,24	4.40	16 (66%)	30,34,34	3.38	14 (46%)
3	0VJ	G	301	-	24,24,24	4.60	16 (66%)	30,34,34	3.22	10 (33%)
4	DMS	G	302	-	3,3,3	1.05	0	3,3,3	0.77	0
3	0VJ	H	301	-	24,24,24	4.48	18 (75%)	30,34,34	2.95	12 (40%)
2	FAD	H	302	-	48,58,58	1.86	12 (25%)	54,89,89	2.93	14 (25%)
4	DMS	H	303	-	3,3,3	1.05	0	3,3,3	0.84	0
2	FAD	I	301	-	48,58,58	2.25	14 (29%)	54,89,89	2.90	14 (25%)
2	FAD	I	302	-	48,58,58	2.25	14 (29%)	54,89,89	2.89	13 (24%)
4	DMS	I	303	-	3,3,3	0.83	0	3,3,3	0.71	0
3	0VJ	I	304	-	24,24,24	4.32	15 (62%)	30,34,34	3.44	13 (43%)
2	FAD	J	301	-	48,58,58	2.22	11 (22%)	54,89,89	3.04	16 (29%)
3	0VJ	J	302	-	24,24,24	4.87	18 (75%)	30,34,34	3.54	9 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	0VJ	K	301	-	24,24,24	4.69	18 (75%)	30,34,34	3.54	13 (43%)
2	FAD	K	302	-	48,58,58	2.13	10 (20%)	54,89,89	2.48	10 (18%)
4	DMS	K	303	-	3,3,3	0.78	0	3,3,3	0.85	0
3	0VJ	L	301	-	24,24,24	4.82	18 (75%)	30,34,34	3.06	14 (46%)
2	FAD	M	301	-	48,58,58	2.24	14 (29%)	54,89,89	2.88	13 (24%)
4	DMS	M	302	-	3,3,3	0.70	0	3,3,3	0.42	0
3	0VJ	M	303	-	24,24,24	4.60	18 (75%)	30,34,34	3.31	14 (46%)
2	FAD	N	301	-	48,58,58	2.21	10 (20%)	54,89,89	2.79	19 (35%)
3	0VJ	N	302	-	24,24,24	4.76	18 (75%)	30,34,34	3.38	12 (40%)
3	0VJ	O	301	-	24,24,24	4.68	16 (66%)	30,34,34	3.72	14 (46%)
2	FAD	O	302	-	48,58,58	1.96	14 (29%)	54,89,89	2.85	13 (24%)
4	DMS	O	303	-	3,3,3	0.67	0	3,3,3	0.17	0
2	FAD	P	301	-	48,58,58	2.25	14 (29%)	54,89,89	2.89	13 (24%)
3	0VJ	P	302	-	24,24,24	4.46	17 (70%)	30,34,34	3.16	10 (33%)
4	DMS	P	303	-	3,3,3	0.87	0	3,3,3	0.52	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	FAD	A	301	-	-	0/30/50/50	0/6/6/6
2	FAD	A	302	-	-	0/30/50/50	0/6/6/6
3	0VJ	A	303	-	-	0/6/26/26	0/3/3/3
4	DMS	A	304	-	-	0/0/0/0	0/0/0/0
3	0VJ	A	305	-	-	0/6/26/26	0/3/3/3
2	FAD	B	301	-	-	0/30/50/50	0/6/6/6
4	DMS	B	302	-	-	0/0/0/0	0/0/0/0
3	0VJ	B	303	-	-	0/6/26/26	0/3/3/3
2	FAD	C	301	-	-	0/30/50/50	0/6/6/6
4	DMS	C	302	-	-	0/0/0/0	0/0/0/0
3	0VJ	D	301	-	-	0/6/26/26	0/3/3/3
4	DMS	D	302	-	-	0/0/0/0	0/0/0/0
2	FAD	E	301	-	-	0/30/50/50	0/6/6/6
3	0VJ	E	302	-	-	0/6/26/26	0/3/3/3
4	DMS	E	303	-	-	0/0/0/0	0/0/0/0
2	FAD	F	301	-	-	0/30/50/50	0/6/6/6
2	FAD	F	302	-	-	0/30/50/50	0/6/6/6
4	DMS	F	303	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	0VJ	F	304	-	-	0/6/26/26	0/3/3/3
3	0VJ	G	301	-	-	0/6/26/26	0/3/3/3
4	DMS	G	302	-	-	0/0/0/0	0/0/0/0
3	0VJ	H	301	-	-	0/6/26/26	0/3/3/3
2	FAD	H	302	-	-	0/30/50/50	0/6/6/6
4	DMS	H	303	-	-	0/0/0/0	0/0/0/0
2	FAD	I	301	-	-	0/30/50/50	0/6/6/6
2	FAD	I	302	-	-	0/30/50/50	0/6/6/6
4	DMS	I	303	-	-	0/0/0/0	0/0/0/0
3	0VJ	I	304	-	-	0/6/26/26	0/3/3/3
2	FAD	J	301	-	-	0/30/50/50	0/6/6/6
3	0VJ	J	302	-	-	0/6/26/26	0/3/3/3
3	0VJ	K	301	-	-	0/6/26/26	0/3/3/3
2	FAD	K	302	-	-	0/30/50/50	0/6/6/6
4	DMS	K	303	-	-	0/0/0/0	0/0/0/0
3	0VJ	L	301	-	-	0/6/26/26	0/3/3/3
2	FAD	M	301	-	-	0/30/50/50	0/6/6/6
4	DMS	M	302	-	-	0/0/0/0	0/0/0/0
3	0VJ	M	303	-	-	0/6/26/26	0/3/3/3
2	FAD	N	301	-	-	0/30/50/50	0/6/6/6
3	0VJ	N	302	-	-	0/6/26/26	0/3/3/3
3	0VJ	O	301	-	-	0/6/26/26	0/3/3/3
2	FAD	O	302	-	-	0/30/50/50	0/6/6/6
4	DMS	O	303	-	-	0/0/0/0	0/0/0/0
2	FAD	P	301	-	-	0/30/50/50	0/6/6/6
3	0VJ	P	302	-	-	0/6/26/26	0/3/3/3
4	DMS	P	303	-	-	0/0/0/0	0/0/0/0

The worst 5 of 475 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	303	0VJ	C11-C12	-7.20	1.39	1.51
3	K	301	0VJ	C11-C12	-7.18	1.39	1.51
3	A	305	0VJ	C11-C12	-5.97	1.41	1.51
3	I	304	0VJ	C11-C12	-5.89	1.41	1.51
3	H	301	0VJ	C11-C12	-5.74	1.41	1.51

The worst 5 of 427 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	O	301	0VJ	C11-C12-C13	-12.16	102.61	120.86
3	I	304	0VJ	C11-C12-C13	-12.10	102.69	120.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	302	0VJ	C11-C12-C13	-11.89	103.02	120.86
3	B	303	0VJ	C11-C12-C13	-11.85	103.07	120.86
3	A	303	0VJ	C11-C12-C13	-11.59	103.46	120.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

25 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	FAD	1	0
3	B	303	0VJ	2	0
2	C	301	FAD	1	0
3	D	301	0VJ	1	0
4	D	302	DMS	1	0
2	E	301	FAD	1	0
4	E	303	DMS	2	0
2	F	301	FAD	1	0
2	F	302	FAD	2	0
2	H	302	FAD	1	0
2	I	301	FAD	1	0
2	I	302	FAD	2	0
3	I	304	0VJ	2	0
2	J	301	FAD	3	0
3	J	302	0VJ	1	0
4	K	303	DMS	1	0
2	M	301	FAD	1	0
4	M	302	DMS	3	0
3	M	303	0VJ	4	0
2	N	301	FAD	2	0
3	N	302	0VJ	4	0
3	O	301	0VJ	3	0
2	O	302	FAD	1	0
2	P	301	FAD	2	0
3	P	302	0VJ	1	0

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^{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	191/227 (84%)	0.02	3 (1%)	74	69	27, 46, 77, 94	0
1	B	188/227 (82%)	0.14	5 (2%)	58	51	28, 50, 89, 119	0
1	C	207/227 (91%)	0.13	2 (0%)	84	81	27, 51, 91, 104	0
1	D	203/227 (89%)	0.01	1 (0%)	91	90	28, 45, 71, 90	0
1	E	206/227 (90%)	0.03	2 (0%)	84	81	26, 49, 86, 107	0
1	F	206/227 (90%)	0.05	4 (1%)	70	64	24, 44, 74, 111	0
1	G	188/227 (82%)	0.01	1 (0%)	91	90	27, 46, 71, 99	0
1	H	179/227 (78%)	0.07	3 (1%)	73	68	30, 48, 72, 108	0
1	I	193/227 (85%)	-0.01	2 (1%)	84	81	23, 49, 74, 91	0
1	J	179/227 (78%)	0.29	4 (2%)	65	59	32, 57, 91, 101	0
1	K	201/227 (88%)	0.07	2 (0%)	84	81	32, 51, 90, 110	0
1	L	201/227 (88%)	0.29	10 (4%)	32	26	31, 54, 99, 130	0
1	M	197/227 (86%)	0.04	1 (0%)	91	90	29, 51, 78, 92	0
1	N	177/227 (77%)	0.36	10 (5%)	28	21	29, 58, 102, 138	0
1	O	200/227 (88%)	0.13	4 (2%)	68	63	34, 53, 93, 119	0
1	P	197/227 (86%)	0.31	11 (5%)	28	21	29, 60, 101, 120	0
All	All	3113/3632 (85%)	0.12	65 (2%)	67	61	23, 51, 89, 138	0

The worst 5 of 65 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	104	ARG	5.8
1	F	95	MET	5.3
1	N	125	TRP	4.6
1	N	149	ILE	4.3
1	N	126	TRP	4.2

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
4	DMS	A	304	4/4	0.95	0.37	3.44	63,70,74,74	0
3	0VJ	G	301	22/22	0.96	0.18	2.22	30,39,47,47	0
4	DMS	C	302	4/4	0.98	0.23	2.17	63,64,65,65	0
4	DMS	G	302	4/4	0.92	0.24	1.59	70,70,71,76	0
2	FAD	M	301	53/53	0.95	0.17	1.59	33,34,35,37	0
4	DMS	M	302	4/4	0.97	0.21	1.50	80,87,87,88	0
4	DMS	B	302	4/4	0.97	0.24	1.27	44,46,55,55	0
2	FAD	I	301	53/53	0.96	0.16	1.04	33,34,35,37	0
3	0VJ	I	304	22/22	0.94	0.19	0.89	38,44,48,49	0
4	DMS	E	303	4/4	0.97	0.19	0.84	57,64,68,70	0
3	0VJ	M	303	22/22	0.96	0.18	0.82	33,43,52,53	0
3	0VJ	K	301	22/22	0.96	0.17	0.75	21,26,34,35	0
2	FAD	F	302	53/53	0.96	0.16	0.68	33,34,35,37	0
2	FAD	A	302	53/53	0.97	0.16	0.66	33,34,35,37	0
4	DMS	K	303	4/4	0.98	0.17	0.66	54,54,60,61	0
4	DMS	I	303	4/4	0.97	0.19	0.63	81,84,87,89	0
3	0VJ	A	305	22/22	0.94	0.18	0.56	35,40,44,48	0
3	0VJ	F	304	22/22	0.93	0.19	0.31	52,58,61,62	0
4	DMS	H	303	4/4	0.96	0.19	0.28	60,62,63,69	0
3	0VJ	P	302	22/22	0.95	0.19	0.27	44,47,53,57	0
3	0VJ	N	302	22/22	0.93	0.17	0.18	59,65,70,71	0
3	0VJ	A	303	22/22	0.96	0.17	0.16	34,39,43,47	0
3	0VJ	L	301	22/22	0.95	0.18	0.14	39,42,48,51	0
4	DMS	O	303	4/4	0.98	0.17	0.06	53,56,60,63	0
2	FAD	I	302	53/53	0.95	0.15	0.05	33,34,35,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	DMS	P	303	4/4	0.90	0.16	0.02	78,87,87,91	0
3	0VJ	J	302	22/22	0.95	0.17	-0.03	51,55,59,60	0
2	FAD	E	301	53/53	0.95	0.15	-0.04	33,34,35,37	0
2	FAD	A	301	53/53	0.98	0.14	-0.06	33,34,35,37	0
2	FAD	H	302	53/53	0.97	0.15	-0.09	45,46,47,49	0
2	FAD	O	302	53/53	0.96	0.15	-0.11	40,41,43,44	0
2	FAD	K	302	53/53	0.97	0.14	-0.21	37,38,40,40	0
2	FAD	P	301	53/53	0.96	0.15	-0.22	33,34,35,37	0
3	0VJ	D	301	22/22	0.96	0.15	-0.26	45,50,56,56	0
3	0VJ	O	301	22/22	0.97	0.16	-0.26	18,27,33,36	0
2	FAD	F	301	53/53	0.98	0.14	-0.34	28,29,30,32	0
3	0VJ	E	302	22/22	0.96	0.14	-0.52	32,39,43,44	0
2	FAD	B	301	53/53	0.97	0.14	-0.59	40,41,43,44	0
2	FAD	C	301	53/53	0.98	0.13	-0.60	33,34,36,38	0
3	0VJ	H	301	22/22	0.96	0.14	-0.64	27,33,39,39	0
2	FAD	J	301	53/53	0.96	0.13	-0.71	42,44,46,48	0
2	FAD	N	301	53/53	0.96	0.14	-0.81	44,45,47,48	0
3	0VJ	B	303	22/22	0.97	0.15	-0.82	24,27,36,40	0
4	DMS	F	303	4/4	0.98	0.12	-1.49	60,63,67,74	0
4	DMS	D	302	4/4	0.98	0.11	-1.84	63,63,67,74	0

6.5 Other polymers (i)

There are no such residues in this entry.