wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 12:27 AM GMT

PDB ID	:	2AF6
Title	:	Crystal structure of Mycobacterium tuberculosis Flavin dependent thymidylate synthase (Mtb ThyX) in the presence of co-factor FAD and substrate analog 5-Bromo-2'-Deoxyuridine-5'-Monophosphate (BrdUMP)
Authors	:	Sampathkumar, P.; Turley, S.; Ulmer, J.E.; Rhie, H.G.; Sibley, C.H.; Hol, W.G.
Deposited on	:	2005-07-25
Resolution	:	2.01 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:

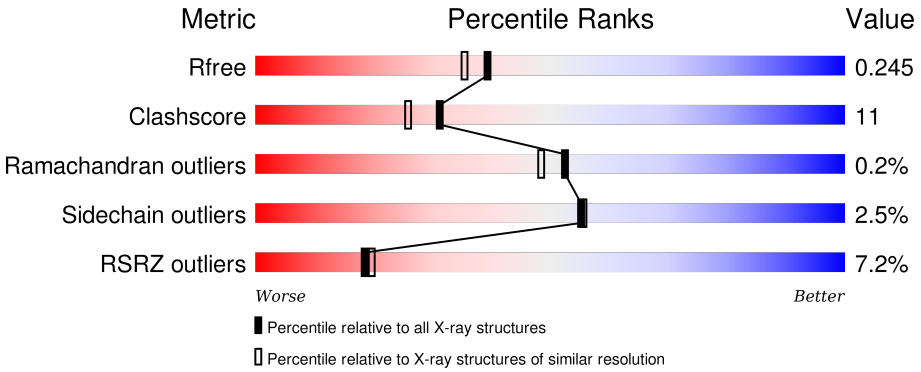
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.01 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	258	8% 77% 17% 5%
1	B	258	5% 78% 16% 5%
1	C	258	6% 80% 13% • 6%
1	D	258	9% 79% 13% • 6%
1	E	258	9% 80% 12% • 6%

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Mol	Chain	Length	Quality of chain
1	F	258	9% 78% 15% • 6%
1	G	258	6% 79% 16% • 5%
1	H	258	2% 81% 11% • 6%

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
2	IOD	A	3001	-	-	X	-
2	IOD	D	3002	-	-	X	-
2	IOD	D	3004	-	-	X	X
2	IOD	E	3006	-	-	X	-
2	IOD	F	3005	-	-	X	-
2	IOD	F	3010	-	-	X	-
4	GOL	A	2001	-	-	X	-
4	GOL	A	2013	-	-	-	X
4	GOL	B	2002	-	-	X	X
4	GOL	B	2008	-	-	X	X
4	GOL	C	2003	-	-	X	X
4	GOL	D	2012	-	-	X	X
4	GOL	E	2004	-	-	X	X
4	GOL	E	2011	-	-	X	X
4	GOL	F	2014	-	-	-	X
4	GOL	G	2005	-	-	X	X
4	GOL	H	2006	-	-	X	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16789 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	245	Total	C	N	O	S	Se	0	1	0
			1890	1187	342	353	3	5			
1	B	245	Total	C	N	O	S	Se	0	1	0
			1904	1196	346	354	3	5			
1	C	242	Total	C	N	O	S	Se	0	1	0
			1877	1179	339	351	3	5			
1	D	242	Total	C	N	O	S	Se	0	1	0
			1882	1182	341	351	3	5			
1	E	243	Total	C	N	O	S	Se	0	1	0
			1882	1182	340	352	3	5			
1	F	242	Total	C	N	O	S	Se	0	1	0
			1886	1185	342	351	3	5			
1	G	246	Total	C	N	O	S	Se	0	1	0
			1909	1200	345	356	3	5			
1	H	243	Total	C	N	O	S	Se	0	1	0
			1884	1184	340	352	3	5			

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P66930
A	65	MSE	ILE	ENGINEERED	UNP P66930
A	122	MSE	MET	MODIFIED RESIDUE	UNP P66930
A	175	MSE	LEU	ENGINEERED	UNP P66930
A	198	MSE	MET	MODIFIED RESIDUE	UNP P66930
A	251	LEU	-	CLONING ARTIFACT	UNP P66930
A	252	GLU	-	CLONING ARTIFACT	UNP P66930
A	253	HIS	-	EXPRESSION TAG	UNP P66930
A	254	HIS	-	EXPRESSION TAG	UNP P66930
A	255	HIS	-	EXPRESSION TAG	UNP P66930
A	256	HIS	-	EXPRESSION TAG	UNP P66930
A	257	HIS	-	EXPRESSION TAG	UNP P66930
A	258	HIS	-	EXPRESSION TAG	UNP P66930

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MSE	MET	MODIFIED RESIDUE	UNP P66930
B	65	MSE	ILE	ENGINEERED	UNP P66930
B	122	MSE	MET	MODIFIED RESIDUE	UNP P66930
B	175	MSE	LEU	ENGINEERED	UNP P66930
B	198	MSE	MET	MODIFIED RESIDUE	UNP P66930
B	251	LEU	-	CLONING ARTIFACT	UNP P66930
B	252	GLU	-	CLONING ARTIFACT	UNP P66930
B	253	HIS	-	EXPRESSION TAG	UNP P66930
B	254	HIS	-	EXPRESSION TAG	UNP P66930
B	255	HIS	-	EXPRESSION TAG	UNP P66930
B	256	HIS	-	EXPRESSION TAG	UNP P66930
B	257	HIS	-	EXPRESSION TAG	UNP P66930
B	258	HIS	-	EXPRESSION TAG	UNP P66930
C	1	MSE	MET	MODIFIED RESIDUE	UNP P66930
C	65	MSE	ILE	ENGINEERED	UNP P66930
C	122	MSE	MET	MODIFIED RESIDUE	UNP P66930
C	175	MSE	LEU	ENGINEERED	UNP P66930
C	198	MSE	MET	MODIFIED RESIDUE	UNP P66930
C	251	LEU	-	CLONING ARTIFACT	UNP P66930
C	252	GLU	-	CLONING ARTIFACT	UNP P66930
C	253	HIS	-	EXPRESSION TAG	UNP P66930
C	254	HIS	-	EXPRESSION TAG	UNP P66930
C	255	HIS	-	EXPRESSION TAG	UNP P66930
C	256	HIS	-	EXPRESSION TAG	UNP P66930
C	257	HIS	-	EXPRESSION TAG	UNP P66930
C	258	HIS	-	EXPRESSION TAG	UNP P66930
D	1	MSE	MET	MODIFIED RESIDUE	UNP P66930
D	65	MSE	ILE	ENGINEERED	UNP P66930
D	122	MSE	MET	MODIFIED RESIDUE	UNP P66930
D	175	MSE	LEU	ENGINEERED	UNP P66930
D	198	MSE	MET	MODIFIED RESIDUE	UNP P66930
D	251	LEU	-	CLONING ARTIFACT	UNP P66930
D	252	GLU	-	CLONING ARTIFACT	UNP P66930
D	253	HIS	-	EXPRESSION TAG	UNP P66930
D	254	HIS	-	EXPRESSION TAG	UNP P66930
D	255	HIS	-	EXPRESSION TAG	UNP P66930
D	256	HIS	-	EXPRESSION TAG	UNP P66930
D	257	HIS	-	EXPRESSION TAG	UNP P66930
D	258	HIS	-	EXPRESSION TAG	UNP P66930
E	1	MSE	MET	MODIFIED RESIDUE	UNP P66930
E	65	MSE	ILE	ENGINEERED	UNP P66930
E	122	MSE	MET	MODIFIED RESIDUE	UNP P66930

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Chain	Residue	Modelled	Actual	Comment	Reference
E	175	MSE	LEU	ENGINEERED	UNP P66930
E	198	MSE	MET	MODIFIED RESIDUE	UNP P66930
E	251	LEU	-	CLONING ARTIFACT	UNP P66930
E	252	GLU	-	CLONING ARTIFACT	UNP P66930
E	253	HIS	-	EXPRESSION TAG	UNP P66930
E	254	HIS	-	EXPRESSION TAG	UNP P66930
E	255	HIS	-	EXPRESSION TAG	UNP P66930
E	256	HIS	-	EXPRESSION TAG	UNP P66930
E	257	HIS	-	EXPRESSION TAG	UNP P66930
E	258	HIS	-	EXPRESSION TAG	UNP P66930
F	1	MSE	MET	MODIFIED RESIDUE	UNP P66930
F	65	MSE	ILE	ENGINEERED	UNP P66930
F	122	MSE	MET	MODIFIED RESIDUE	UNP P66930
F	175	MSE	LEU	ENGINEERED	UNP P66930
F	198	MSE	MET	MODIFIED RESIDUE	UNP P66930
F	251	LEU	-	CLONING ARTIFACT	UNP P66930
F	252	GLU	-	CLONING ARTIFACT	UNP P66930
F	253	HIS	-	EXPRESSION TAG	UNP P66930
F	254	HIS	-	EXPRESSION TAG	UNP P66930
F	255	HIS	-	EXPRESSION TAG	UNP P66930
F	256	HIS	-	EXPRESSION TAG	UNP P66930
F	257	HIS	-	EXPRESSION TAG	UNP P66930
F	258	HIS	-	EXPRESSION TAG	UNP P66930
G	1	MSE	MET	MODIFIED RESIDUE	UNP P66930
G	65	MSE	ILE	ENGINEERED	UNP P66930
G	122	MSE	MET	MODIFIED RESIDUE	UNP P66930
G	175	MSE	LEU	ENGINEERED	UNP P66930
G	198	MSE	MET	MODIFIED RESIDUE	UNP P66930
G	251	LEU	-	CLONING ARTIFACT	UNP P66930
G	252	GLU	-	CLONING ARTIFACT	UNP P66930
G	253	HIS	-	EXPRESSION TAG	UNP P66930
G	254	HIS	-	EXPRESSION TAG	UNP P66930
G	255	HIS	-	EXPRESSION TAG	UNP P66930
G	256	HIS	-	EXPRESSION TAG	UNP P66930
G	257	HIS	-	EXPRESSION TAG	UNP P66930
G	258	HIS	-	EXPRESSION TAG	UNP P66930
H	1	MSE	MET	MODIFIED RESIDUE	UNP P66930
H	65	MSE	ILE	ENGINEERED	UNP P66930
H	122	MSE	MET	MODIFIED RESIDUE	UNP P66930
H	175	MSE	LEU	ENGINEERED	UNP P66930
H	198	MSE	MET	MODIFIED RESIDUE	UNP P66930
H	251	LEU	-	CLONING ARTIFACT	UNP P66930

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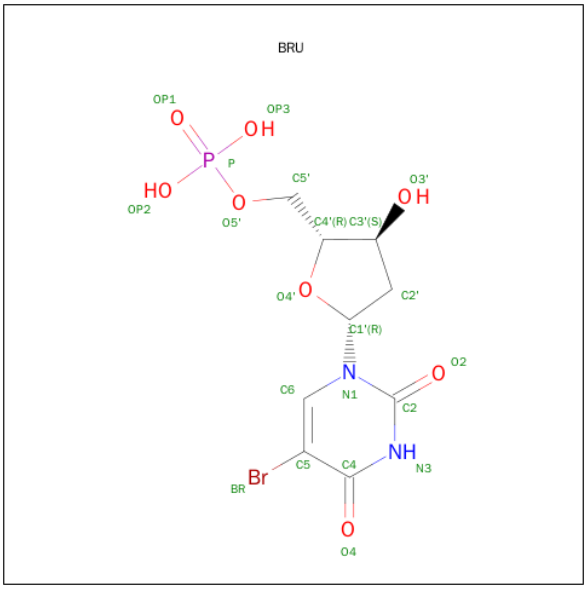
Chain	Residue	Modelled	Actual	Comment	Reference
H	252	GLU	-	CLONING ARTIFACT	UNP P66930
H	253	HIS	-	EXPRESSION TAG	UNP P66930
H	254	HIS	-	EXPRESSION TAG	UNP P66930
H	255	HIS	-	EXPRESSION TAG	UNP P66930
H	256	HIS	-	EXPRESSION TAG	UNP P66930
H	257	HIS	-	EXPRESSION TAG	UNP P66930
H	258	HIS	-	EXPRESSION TAG	UNP P66930

- Molecule 2 is IODIDE ION (three-letter code: IOD) (formula: I).

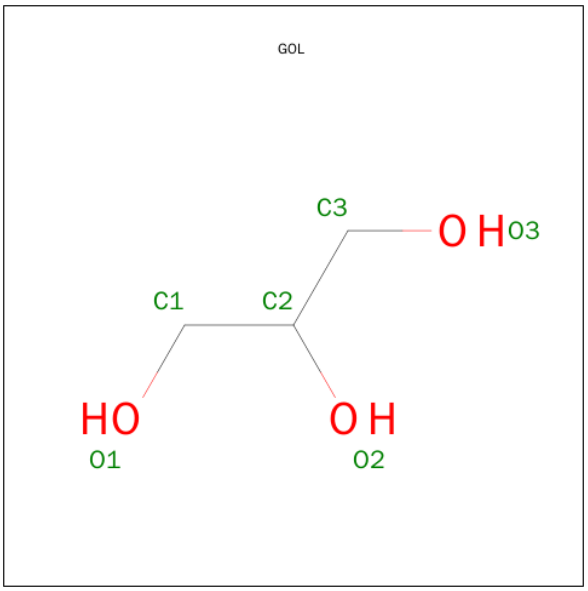
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total I 1 1	0	0
2	D	2	Total I 2 2	0	0
2	E	2	Total I 2 2	0	0
2	C	1	Total I 1 1	0	0
2	A	2	Total I 2 2	0	0
2	F	2	Total I 2 2	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: BRU, FAD) (formula: $C_9H_{12}BrN_2O_8P$, $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	D	2	Total	Br	C	N	O	P	0	0
			74	1	36	11	23	3		
3	C	2	Total	Br	C	N	O	P	0	0
			74	1	36	11	23	3		
3	B	2	Total	Br	C	N	O	P	0	0
			74	1	36	11	23	3		
3	A	2	Total	Br	C	N	O	P	0	0
			74	1	36	11	23	3		
3	H	2	Total	Br	C	N	O	P	0	0
			74	1	36	11	23	3		
3	G	2	Total	Br	C	N	O	P	0	0
			74	1	36	11	23	3		
3	F	2	Total	Br	C	N	O	P	0	0
			74	1	36	11	23	3		
3	E	2	Total	Br	C	N	O	P	0	0
			74	1	36	11	23	3		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O		0	0
			6	3	3			
4	B	1	Total	C	O		0	0
			6	3	3			
4	C	1	Total	C	O		0	0
			6	3	3			
4	E	1	Total	C	O		0	0
			6	3	3			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	F	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	F	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

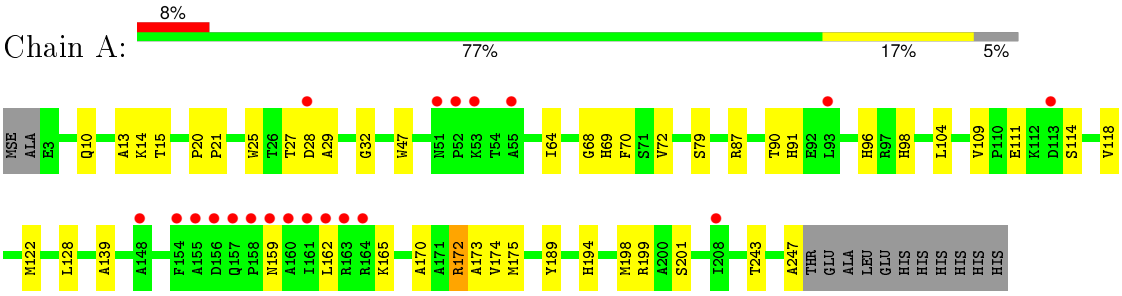
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	135	Total O 135 135	0	0
5	B	129	Total O 129 129	0	0
5	C	116	Total O 116 116	0	0
5	D	120	Total O 120 120	0	0
5	E	130	Total O 130 130	0	0
5	F	106	Total O 106 106	0	0
5	G	114	Total O 114 114	0	0
5	H	139	Total O 139 139	0	0

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.

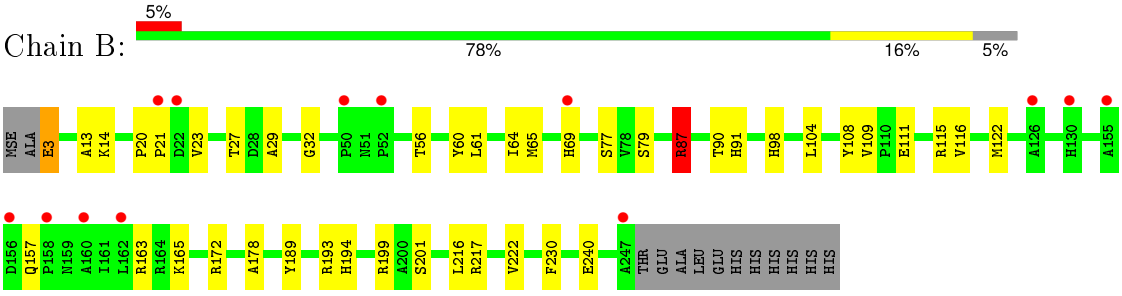
- Molecule 1: Thymidylate synthase thyX

Chain A:



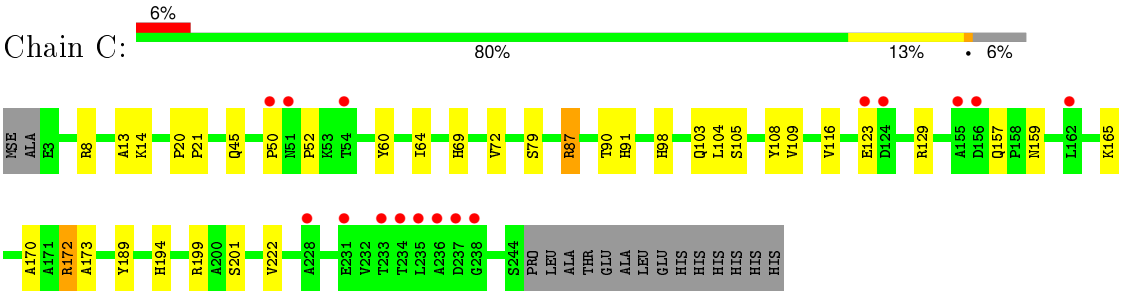
- Molecule 1: Thymidylate synthase thyX

Chain B:



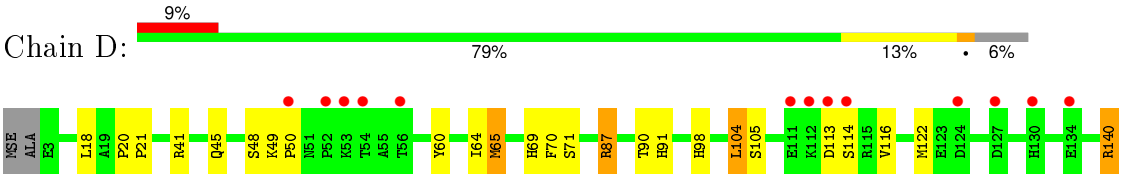
- Molecule 1: Thymidylate synthase thyX

Chain C:



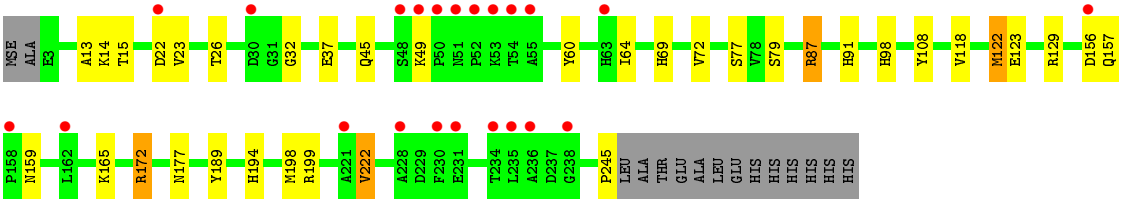
- Molecule 1: Thymidylate synthase thyX

Chain D:



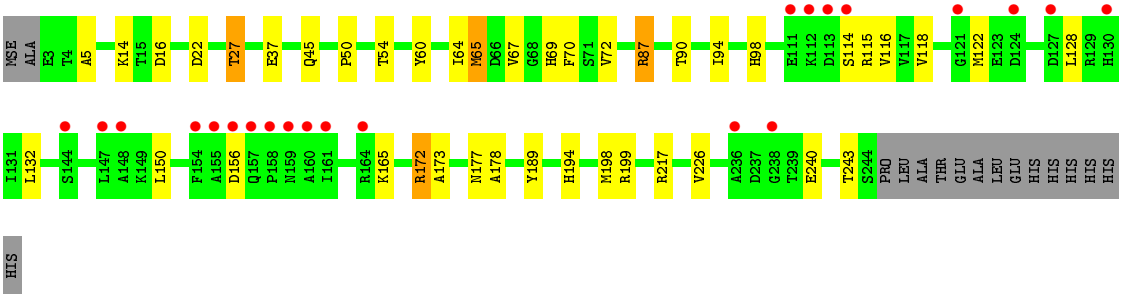
• Molecule 1: Thymidylate synthase thyX

Chain E:



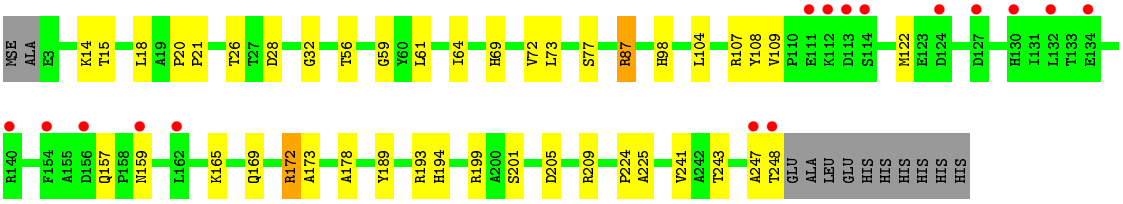
• Molecule 1: Thymidylate synthase thyX

Chain F:



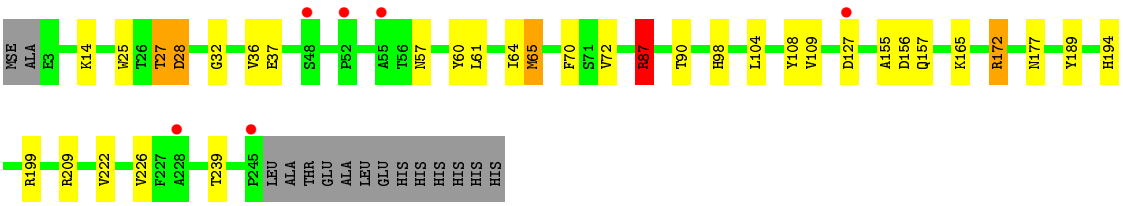
• Molecule 1: Thymidylate synthase thyX

Chain G:



• Molecule 1: Thymidylate synthase thyX

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.09Å 78.30Å 168.72Å 90.00° 96.80° 90.00°	Depositor
Resolution (Å)	44.95 – 2.01 44.95 – 2.01	Depositor EDS
% Data completeness (in resolution range)	95.5 (44.95-2.01) 95.4 (44.95-2.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.23 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.195 , 0.243 0.197 , 0.245	Depositor DCC
R_{free} test set	6506 reflections (5.15%)	DCC
Wilson B-factor (Å^2)	21.5	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 50.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 132836 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16789	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.36% 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: GOL, BRU, IOD, 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	0.48	0/1931	0.62	1/2626 (0.0%)
1	B	0.48	0/1947	0.61	2/2648 (0.1%)
1	C	0.49	0/1918	0.63	2/2607 (0.1%)
1	D	0.47	0/1924	0.63	3/2615 (0.1%)
1	E	0.49	0/1923	0.63	3/2614 (0.1%)
1	F	0.48	0/1928	0.62	2/2619 (0.1%)
1	G	0.46	0/1952	0.60	2/2655 (0.1%)
1	H	0.48	0/1926	0.64	3/2619 (0.1%)
All	All	0.48	0/15449	0.62	18/21003 (0.1%)

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	87	ARG	NE-CZ-NH2	-8.69	115.96	120.30
1	E	87	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	H	87	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	E	172	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	B	172	ARG	NE-CZ-NH2	-6.56	117.02	120.30

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	1890	0	1851	54	0
1	B	1904	0	1863	50	0
1	C	1877	0	1835	37	0
1	D	1882	0	1840	48	0
1	E	1882	0	1836	48	0
1	F	1886	0	1851	38	0
1	G	1909	0	1870	38	0
1	H	1884	0	1842	50	0
2	A	2	0	0	2	0
2	C	1	0	0	0	0
2	D	2	0	0	11	0
2	E	2	0	0	3	0
2	F	2	0	0	4	0
2	G	1	0	0	1	0
3	A	74	0	41	12	0
3	B	74	0	41	8	0
3	C	74	0	41	5	0
3	D	74	0	41	8	0
3	E	74	0	41	6	0
3	F	74	0	41	6	0
3	G	74	0	41	7	0
3	H	74	0	41	7	0
4	A	18	0	24	8	0
4	B	12	0	16	15	0
4	C	6	0	8	9	0
4	D	12	0	16	11	0
4	E	12	0	16	27	0
4	F	12	0	14	1	0
4	G	6	0	8	9	0
4	H	6	0	8	12	0
5	A	135	0	0	3	0
5	B	129	0	0	2	0
5	C	116	0	0	0	0
5	D	120	0	0	10	0
5	E	130	0	0	2	0
5	F	106	0	0	4	0
5	G	114	0	0	3	0
5	H	139	0	0	2	0
All	All	16789	0	15226	336	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 11.

The worst 5 of 336 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:D:222:VAL:CG1	2:D:3004:IOD:I	2.54	1.25
2:D:3004:IOD:I	5:D:3123:HOH:O	2.20	1.24
2:D:3004:IOD:I	5:D:3122:HOH:O	2.23	1.19
4:E:2011:GOL:H31	1:H:177:ASN:ND2	1.66	1.09
1:F:199:ARG:HH12	3:F:7603:BRU:HN3	1.04	1.04

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	244/258 (95%)	239 (98%)	4 (2%)	1 (0%)	39	33
1	B	244/258 (95%)	241 (99%)	3 (1%)	0	100	100
1	C	241/258 (93%)	236 (98%)	5 (2%)	0	100	100
1	D	241/258 (93%)	236 (98%)	5 (2%)	0	100	100
1	E	242/258 (94%)	239 (99%)	3 (1%)	0	100	100
1	F	241/258 (93%)	235 (98%)	6 (2%)	0	100	100
1	G	245/258 (95%)	237 (97%)	7 (3%)	1 (0%)	39	33
1	H	242/258 (94%)	237 (98%)	4 (2%)	1 (0%)	39	33
All	All	1940/2064 (94%)	1900 (98%)	37 (2%)	3 (0%)	52	48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	247	ALA
1	A	28	ASP
1	H	156	ASP

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	194/204 (95%)	191 (98%)	3 (2%)	72	75
1	B	196/204 (96%)	192 (98%)	4 (2%)	63	65
1	C	193/204 (95%)	189 (98%)	4 (2%)	61	63
1	D	194/204 (95%)	187 (96%)	7 (4%)	42	39
1	E	193/204 (95%)	188 (97%)	5 (3%)	54	54
1	F	195/204 (96%)	186 (95%)	9 (5%)	33	28
1	G	197/204 (97%)	191 (97%)	6 (3%)	48	47
1	H	194/204 (95%)	191 (98%)	3 (2%)	72	75
All	All	1556/1632 (95%)	1515 (97%)	41 (3%)	55	54

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	122	MSE
1	E	222	VAL
1	G	243	THR
1	E	156	ASP
1	E	198[A]	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	69	HIS
1	E	57	ASN
1	H	91	HIS
1	D	91	HIS
1	D	157	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)

Of 40 ligands modelled in this entry, 10 are monoatomic - leaving 30 for Mogul analysis.

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	$\#\|Z\| > 2$
4	GOL	A	2001	-	5,5,5	0.66	0	5,5,5	0.52	0
4	GOL	A	2010	-	5,5,5	0.28	0	5,5,5	0.28	0
4	GOL	A	2013	-	5,5,5	0.39	0	5,5,5	0.25	0
3	FAD	A	4600	-	48,58,58	1.35	6 (12%)	54,89,89	2.22	9 (16%)
3	BRU	A	4603	-	18,22,22	1.85	1 (5%)	22,33,33	2.33	3 (13%)
4	GOL	B	2002	-	5,5,5	0.45	0	5,5,5	1.32	1 (20%)
4	GOL	B	2008	-	5,5,5	0.41	0	5,5,5	0.52	0
3	FAD	B	3600	-	48,58,58	1.30	6 (12%)	54,89,89	2.18	9 (16%)
3	BRU	B	3603	-	18,22,22	1.98	1 (5%)	22,33,33	1.88	3 (13%)
4	GOL	C	2003	-	5,5,5	0.50	0	5,5,5	0.38	0
3	FAD	C	2600	-	48,58,58	1.19	4 (8%)	54,89,89	2.17	6 (11%)
3	BRU	C	2603	-	18,22,22	1.96	2 (11%)	22,33,33	2.29	4 (18%)
3	FAD	D	1600	-	48,58,58	1.29	6 (12%)	54,89,89	2.30	10 (18%)
3	BRU	D	1603	-	18,22,22	1.85	1 (5%)	22,33,33	1.96	2 (9%)
4	GOL	D	2009	-	5,5,5	0.40	0	5,5,5	0.28	0
4	GOL	D	2012	-	5,5,5	0.38	0	5,5,5	0.28	0
4	GOL	E	2004	-	5,5,5	0.51	0	5,5,5	0.48	0
4	GOL	E	2011	-	5,5,5	0.73	0	5,5,5	0.82	0
3	FAD	E	8600	-	48,58,58	1.22	6 (12%)	54,89,89	2.14	6 (11%)
3	BRU	E	8603	-	18,22,22	2.09	2 (11%)	22,33,33	2.12	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GOL	F	2007	-	5,5,5	0.41	0	5,5,5	0.40	0
4	GOL	F	2014	-	5,5,5	0.40	0	5,5,5	0.26	0
3	FAD	F	7600	-	48,58,58	1.32	6 (12%)	54,89,89	2.31	7 (12%)
3	BRU	F	7603	-	18,22,22	2.02	1 (5%)	22,33,33	2.14	3 (13%)
4	GOL	G	2005	-	5,5,5	0.55	0	5,5,5	0.47	0
3	FAD	G	6600	-	48,58,58	1.32	6 (12%)	54,89,89	2.25	9 (16%)
3	BRU	G	6603	-	18,22,22	2.08	1 (5%)	22,33,33	1.92	3 (13%)
4	GOL	H	2006	-	5,5,5	0.57	0	5,5,5	0.40	0
3	FAD	H	5600	-	48,58,58	1.21	4 (8%)	54,89,89	2.27	8 (14%)
3	BRU	H	5603	-	18,22,22	1.86	1 (5%)	22,33,33	1.90	3 (13%)

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
4	GOL	A	2001	-	-	0/4/4/4	0/0/0/0
4	GOL	A	2010	-	-	0/4/4/4	0/0/0/0
4	GOL	A	2013	-	-	0/4/4/4	0/0/0/0
3	FAD	A	4600	-	-	0/30/50/50	0/6/6/6
3	BRU	A	4603	-	-	0/6/22/22	0/2/2/2
4	GOL	B	2002	-	-	0/4/4/4	0/0/0/0
4	GOL	B	2008	-	-	0/4/4/4	0/0/0/0
3	FAD	B	3600	-	-	0/30/50/50	0/6/6/6
3	BRU	B	3603	-	-	0/6/22/22	0/2/2/2
4	GOL	C	2003	-	-	0/4/4/4	0/0/0/0
3	FAD	C	2600	-	-	0/30/50/50	0/6/6/6
3	BRU	C	2603	-	-	0/6/22/22	0/2/2/2
3	FAD	D	1600	-	-	0/30/50/50	0/6/6/6
3	BRU	D	1603	-	-	0/6/22/22	0/2/2/2
4	GOL	D	2009	-	-	0/4/4/4	0/0/0/0
4	GOL	D	2012	-	-	0/4/4/4	0/0/0/0
4	GOL	E	2004	-	-	0/4/4/4	0/0/0/0
4	GOL	E	2011	-	-	0/4/4/4	0/0/0/0
3	FAD	E	8600	-	-	0/30/50/50	0/6/6/6
3	BRU	E	8603	-	-	0/6/22/22	0/2/2/2
4	GOL	F	2007	-	-	0/4/4/4	0/0/0/0
4	GOL	F	2014	-	-	0/4/4/4	0/0/0/0
3	FAD	F	7600	-	-	0/30/50/50	0/6/6/6
3	BRU	F	7603	-	-	0/6/22/22	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	G	2005	-	-	0/4/4/4	0/0/0/0
3	FAD	G	6600	-	-	0/30/50/50	0/6/6/6
3	BRU	G	6603	-	-	0/6/22/22	0/2/2/2
4	GOL	H	2006	-	-	0/4/4/4	0/0/0/0
3	FAD	H	5600	-	-	0/30/50/50	0/6/6/6
3	BRU	H	5603	-	-	0/6/22/22	0/2/2/2

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	8603	BRU	P-OP3	-2.08	1.47	1.54
3	C	2603	BRU	P-OP3	-2.05	1.47	1.54
3	D	1600	FAD	C1'-N10	2.17	1.50	1.48
3	A	4600	FAD	C2A-N1A	2.23	1.38	1.33
3	B	3600	FAD	C2A-N1A	2.26	1.38	1.33

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	7600	FAD	N3A-C2A-N1A	-13.06	118.89	128.89
3	H	5600	FAD	N3A-C2A-N1A	-12.99	118.95	128.89
3	A	4600	FAD	N3A-C2A-N1A	-12.57	119.27	128.89
3	E	8600	FAD	N3A-C2A-N1A	-12.41	119.39	128.89
3	C	2600	FAD	N3A-C2A-N1A	-12.37	119.42	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

28 monomers are involved in 151 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2001	GOL	7	0
4	A	2013	GOL	1	0
3	A	4600	FAD	7	0
3	A	4603	BRU	5	0
4	B	2002	GOL	11	0
4	B	2008	GOL	4	0
3	B	3600	FAD	2	0
3	B	3603	BRU	6	0
4	C	2003	GOL	9	0
3	C	2600	FAD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2603	BRU	3	0
3	D	1600	FAD	2	0
3	D	1603	BRU	6	0
4	D	2009	GOL	3	0
4	D	2012	GOL	8	0
4	E	2004	GOL	12	0
4	E	2011	GOL	15	0
3	E	8600	FAD	2	0
3	E	8603	BRU	4	0
4	F	2007	GOL	1	0
3	F	7600	FAD	1	0
3	F	7603	BRU	5	0
4	G	2005	GOL	9	0
3	G	6600	FAD	2	0
3	G	6603	BRU	5	0
4	H	2006	GOL	12	0
3	H	5600	FAD	2	0
3	H	5603	BRU	5	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	241/258 (93%)	0.53	20 (8%) 14 15	10, 25, 41, 50	0
1	B	241/258 (93%)	0.30	13 (5%) 29 31	10, 24, 41, 50	1 (0%)
1	C	238/258 (92%)	0.27	16 (6%) 21 22	10, 25, 42, 51	0
1	D	238/258 (92%)	0.39	23 (9%) 10 10	11, 25, 42, 50	1 (0%)
1	E	239/258 (92%)	0.37	22 (9%) 11 12	10, 24, 42, 50	0
1	F	238/258 (92%)	0.39	22 (9%) 11 12	11, 25, 41, 51	1 (0%)
1	G	242/258 (93%)	0.40	16 (6%) 22 22	11, 25, 42, 51	1 (0%)
1	H	239/258 (92%)	0.14	6 (2%) 61 61	10, 24, 42, 50	0
All	All	1916/2064 (92%)	0.35	138 (7%) 18 20	10, 25, 42, 51	4 (0%)

The worst 5 of 138 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	50	PRO	7.3
1	D	52	PRO	6.7
1	B	52	PRO	6.5
1	A	160	ALA	6.4
1	B	247	ALA	6.4

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 (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	IOD	D	3004	1/1	0.76	0.26	11.95	66,66,66,66	1
4	GOL	D	2012	6/6	0.77	0.63	11.91	25,26,27,27	6
4	GOL	B	2008	6/6	0.86	0.24	6.60	29,35,36,38	0
4	GOL	H	2006	6/6	0.90	0.20	5.76	25,25,28,30	0
4	GOL	F	2014	6/6	0.94	0.18	4.25	24,25,26,27	6
4	GOL	A	2013	6/6	0.86	0.22	3.77	42,42,43,44	0
4	GOL	C	2003	6/6	0.95	0.26	3.70	28,28,29,33	0
4	GOL	B	2002	6/6	0.87	0.19	3.62	18,18,23,25	0
4	GOL	G	2005	6/6	0.89	0.22	3.36	25,27,27,30	0
4	GOL	E	2004	6/6	0.93	0.22	2.65	26,27,27,30	0
4	GOL	E	2011	6/6	0.91	0.21	2.50	19,25,29,30	0
4	GOL	A	2001	6/6	0.93	0.14	0.73	25,26,28,29	0
2	IOD	C	3009	1/1	0.97	0.14	0.62	20,20,20,20	1
2	IOD	A	3001	1/1	0.95	0.13	0.59	41,41,41,41	1
2	IOD	E	3007	1/1	0.99	0.14	0.48	16,16,16,16	1
4	GOL	D	2009	6/6	0.75	0.21	0.40	43,46,47,48	0
3	FAD	G	6600	53/53	0.95	0.14	0.40	13,23,26,28	0
3	FAD	F	7600	53/53	0.95	0.13	0.38	16,22,24,26	0
3	FAD	E	8600	53/53	0.96	0.14	0.15	13,16,23,27	0
2	IOD	G	3003	1/1	0.80	0.14	0.06	64,64,64,64	1
3	FAD	C	2600	53/53	0.96	0.14	-0.01	14,16,22,24	0
3	FAD	D	1600	53/53	0.95	0.13	-0.12	13,21,24,25	0
3	FAD	A	4600	53/53	0.97	0.13	-0.15	12,15,21,24	0
3	FAD	H	5600	53/53	0.96	0.13	-0.18	13,17,21,22	0
4	GOL	A	2010	6/6	0.82	0.16	-0.22	48,50,50,50	0
3	FAD	B	3600	53/53	0.96	0.13	-0.32	12,16,21,24	0
3	BRU	F	7603	21/21	0.97	0.10	-0.87	18,22,26,28	0
3	BRU	A	4603	21/21	0.98	0.09	-1.05	12,15,16,18	0
3	BRU	D	1603	21/21	0.97	0.09	-1.18	15,17,25,27	0
3	BRU	E	8603	21/21	0.98	0.11	-1.21	8,11,14,18	0
3	BRU	G	6603	21/21	0.99	0.08	-1.48	16,21,24,26	0
3	BRU	C	2603	21/21	0.99	0.10	-1.53	8,11,15,20	0
3	BRU	B	3603	21/21	0.99	0.10	-1.54	8,12,13,17	0
3	BRU	H	5603	21/21	0.99	0.09	-2.10	8,12,14,18	0
2	IOD	F	3005	1/1	0.97	0.04	-3.02	38,38,38,38	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	IOD	F	3010	1/1	0.98	0.04	-6.02	45,45,45,45	1
2	IOD	E	3006	1/1	0.95	0.14	-	37,37,37,37	1
4	GOL	F	2007	6/6	0.90	0.21	-	41,41,42,43	0
2	IOD	A	3008	1/1	0.97	0.09	-	34,34,34,34	1
2	IOD	D	3002	1/1	0.92	0.13	-	49,49,49,49	1

6.5 Other polymers (i)

There are no such residues in this entry.