



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:11 AM GMT

PDB ID : 3DL5
Title : Crystal Structure of the A287F Active Site Mutant of TS-DHFR from *Cryptosporidium hominis*
Authors : Vargo, M.A.; Martucci, W.E.; Anderson, K.S.
Deposited on : 2008-06-26
Resolution : 2.74 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

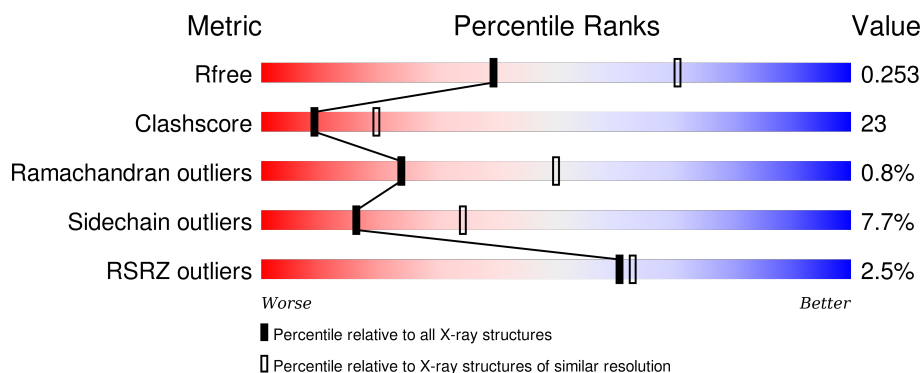
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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	3050 (2.78-2.70)
Clashscore	102246	3424 (2.78-2.70)
Ramachandran outliers	100387	3367 (2.78-2.70)
Sidechain outliers	100360	3368 (2.78-2.70)
RSRZ outliers	91569	3055 (2.78-2.70)

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 $\leq 5\%$. 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	521	<div> <div>2%</div> <div>63% 29% 5% .</div> </div>
1	B	521	<div> <div>2%</div> <div>66% 26% . .</div> </div>
1	C	521	<div> <div>2%</div> <div>60% 31% 6% .</div> </div>
1	D	521	<div> <div>2%</div> <div>54% 37% 6% .</div> </div>
1	E	521	<div> <div>7%</div> <div>55% 38% . .</div> </div>

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	CB3	A	604	-	-	-	X
3	CB3	D	616	X	-	X	X
3	CB3	E	620	X	-	X	-
4	DHF	A	605	X	-	-	-
4	DHF	B	609	X	-	X	-
4	DHF	C	613	-	-	X	X
4	DHF	D	617	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21793 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.

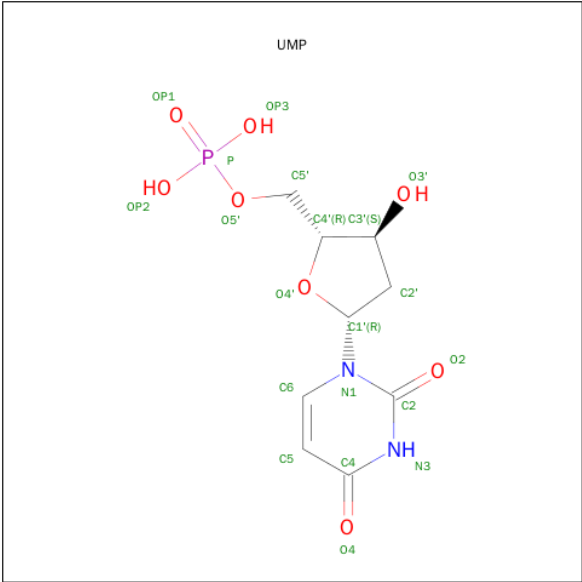
- Molecule 1 is a protein called Dihydrofolate reductase, DHFR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	507	Total	C	N	O	S	0	0	0
			4130	2642	693	773	22			
1	B	508	Total	C	N	O	S	0	0	0
			4143	2650	695	776	22			
1	C	508	Total	C	N	O	S	0	0	0
			4135	2645	694	774	22			
1	D	507	Total	C	N	O	S	0	0	0
			4130	2642	693	773	22			
1	E	508	Total	C	N	O	S	0	0	0
			4135	2645	694	774	22			

There are 5 discrepancies between the modelled and reference sequences:

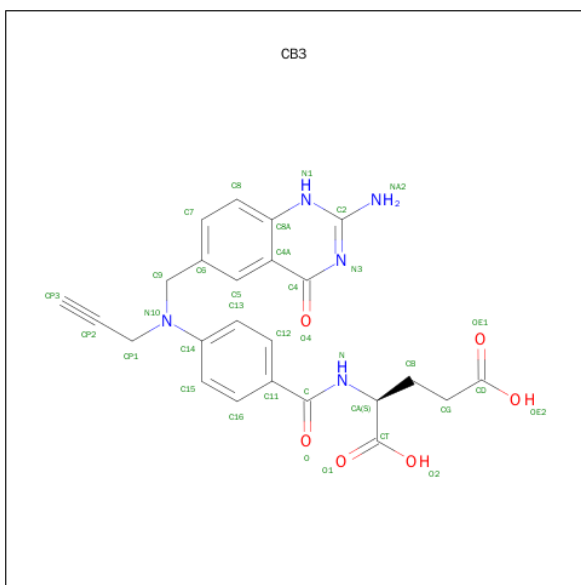
Chain	Residue	Modelled	Actual	Comment	Reference
A	287	PHE	ALA	ENGINEERED	UNP Q5CGA3
B	287	PHE	ALA	ENGINEERED	UNP Q5CGA3
C	287	PHE	ALA	ENGINEERED	UNP Q5CGA3
D	287	PHE	ALA	ENGINEERED	UNP Q5CGA3
E	287	PHE	ALA	ENGINEERED	UNP Q5CGA3

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: C₉H₁₃N₂O₈P).



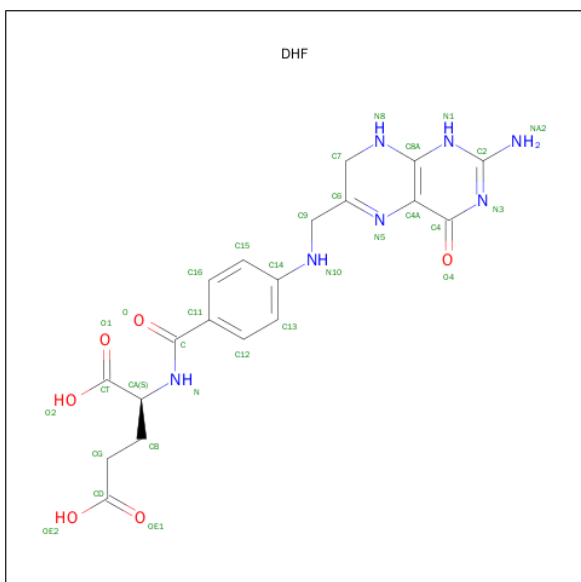
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	D	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	E	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 3 is 10-PROPARGYL-5,8-DIDEAZAFOLIC ACID (three-letter code: CB3) (formula: C₂₄H₂₃N₅O₆).



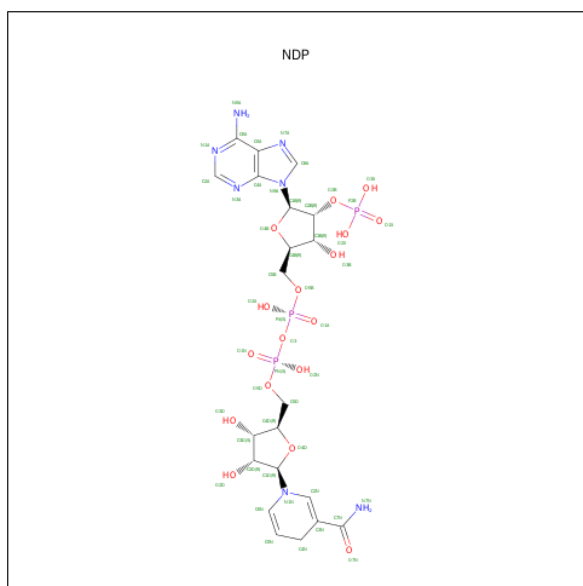
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			35	24	5	6		
3	B	1	Total	C	N	O	0	0
			35	24	5	6		
3	C	1	Total	C	N	O	0	0
			35	24	5	6		
3	D	1	Total	C	N	O	0	0
			35	24	5	6		
3	E	1	Total	C	N	O	0	0
			35	24	5	6		

- Molecule 4 is DIHYDROFOLIC ACID (three-letter code: DHF) (formula: C₁₉H₂₁N₇O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			32	19	7	6		
4	B	1	Total	C	N	O	0	0
			32	19	7	6		
4	C	1	Total	C	N	O	0	0
			32	19	7	6		
4	D	1	Total	C	N	O	0	0
			32	19	7	6		
4	E	1	Total	C	N	O	0	0
			32	19	7	6		

- Molecule 5 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).




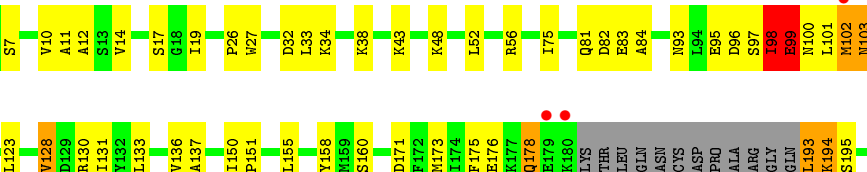
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		


- Molecule 6 is water.

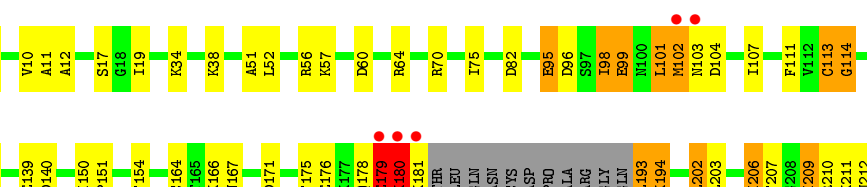
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	114	Total 114	O 114	0	0
6	B	150	Total 150	O 150	0	0
6	C	95	Total 95	O 95	0	0
6	D	62	Total 62	O 62	0	0
6	E	24	Total 24	O 24	0	0

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 ($\text{RSRZ} > 2$). 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.

- Chain A: 

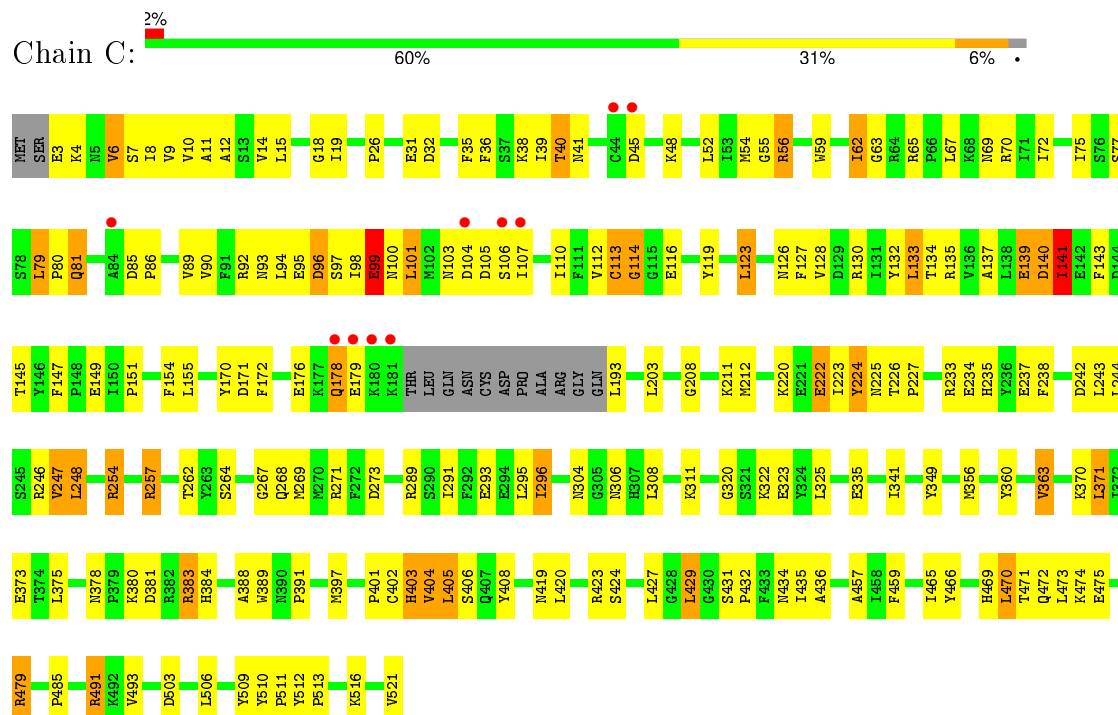


- Chain B: 

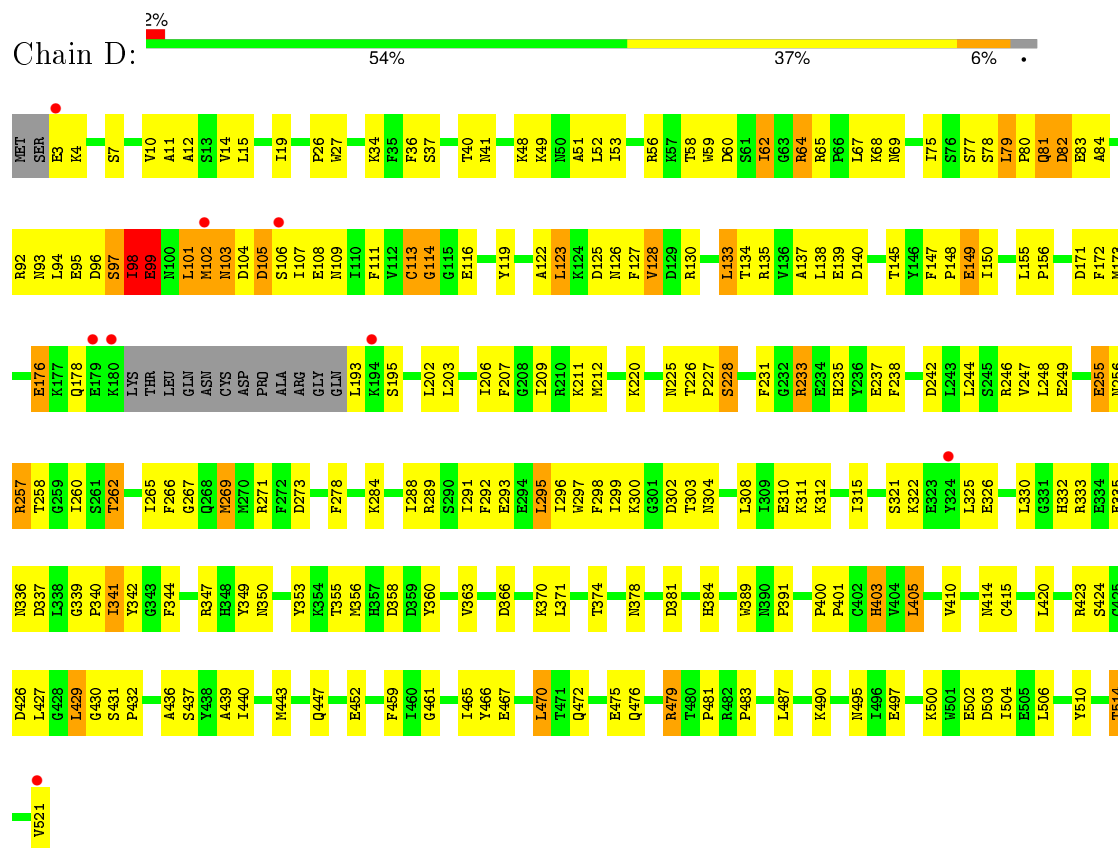


Position	Residue	Category
R130	R130	Green
I131	I131	Green
Y132	Y132	Green
L133	L133	Green
T134	T134	Green
R135	R135	Green
E139	E139	Green
D140	D140	Green
I150	I150	Green
P151	P151	Green
F154	F154	Green
G164	G164	Green
T165	T165	Green
K166	K166	Green
N167	N167	Green
D171	D171	Green
F175	F175	Green
E176	E176	Green
K177	K177	Green
Q178	Q178	Green
E179	E179	Green
K180	K180	Green
K181	K181	Green
T182	T182	Green
L183	L183	Green
G184	G184	Green
A185	A185	Green
C186	C186	Green
S187	S187	Green
P188	P188	Green
A189	A189	Green
G190	G190	Green
L191	L191	Green
L192	L192	Green
L193	L193	Green
K194	K194	Green
L202	L202	Green
L203	L203	Green
L206	L206	Green
F207	F207	Green
G208	G208	Green
L209	L209	Green
R210	R210	Green
K211	K211	Green
N212	N212	Green
R215	R215	Green
R216	R216	Yellow
E221	E221	Yellow
E222	E222	Yellow
Y223	Y223	Yellow
K224	K224	Yellow
K225	K225	Yellow
T226	T226	Yellow
P227	P227	Yellow
R228	R228	Yellow
K229	K229	Yellow
R230	R230	Yellow
E231	E231	Yellow
K232	K232	Yellow
E233	E233	Yellow
E234	E234	Yellow
K235	K235	Yellow
E236	E236	Yellow
E237	E237	Yellow
L243	L243	Yellow
L244	L244	Yellow
V247	V247	Yellow
A252	A252	Yellow
R257	R257	Yellow
Y263	Y263	Yellow
G267	G267	Yellow
Q268	Q268	Yellow
E269	E269	Yellow
R270	R270	Yellow
R271	R271	Yellow
F272	F272	Yellow
D273	D273	Yellow
E276	E276	Yellow
S277	S277	Yellow
K285	K285	Yellow
L288	L288	Yellow
R289	R289	Yellow
F292	F292	Yellow
E293	E293	Yellow
E294	E294	Yellow
L295	L295	Yellow
L296	L296	Yellow
K297	K297	Yellow
L308	L308	Yellow
L315	L315	Yellow
E326	E326	Yellow
E335	E335	Yellow
K336	K336	Yellow
K337	K337	Yellow
L338	L338	Yellow
T341	T341	Yellow
Y342	Y342	Yellow
Y349	Y349	Yellow
V350	V350	Yellow
M351	M351	Yellow
E352	E352	Yellow
A353	A353	Yellow
E354	E354	Yellow
E355	E355	Yellow
E356	E356	Yellow
E357	E357	Yellow
E358	E358	Yellow
E359	E359	Yellow
E360	E360	Yellow
E361	E361	Yellow
E362	E362	Yellow
E363	E363	Yellow
E364	E364	Yellow
E365	E365	Yellow
E366	E366	Yellow
E367	E367	Yellow
E368	E368	Yellow
E369	E369	Yellow
E370	E370	Yellow
E371	E371	Yellow
E372	E372	Yellow
E373	E373	Yellow
E374	E374	Yellow
E375	E375	Yellow
E376	E376	Yellow
E377	E377	Yellow
E378	E378	Yellow
E379	E379	Yellow
E380	E380	Yellow
E381	E381	Yellow
E382	E382	Yellow
E383	E383	Yellow
E384	E384	Yellow
E385	E385	Yellow
E386	E386	Yellow
E387	E387	Yellow
E388	E388	Yellow
E389	E389	Yellow
E390	E390	Yellow
E391	E391	Yellow
E392	E392	Yellow

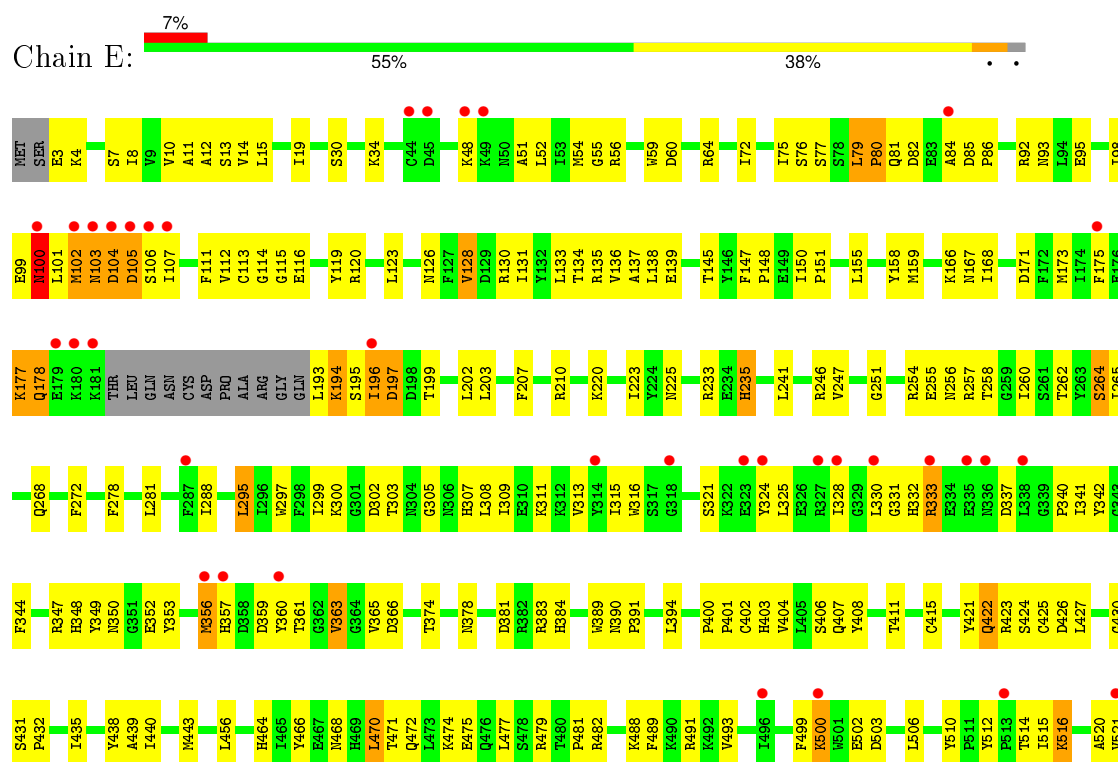
- Molecule 1: Dihydrofolate reductase, DHFR



- Molecule 1: Dihydrofolate reductase, DHFR



- Molecule 1: Dihydrofolate reductase, DHFR



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	214.81Å 116.54Å 219.21Å 90.00° 95.21° 90.00°	Depositor
Resolution (Å)	45.40 – 2.74 45.48 – 2.72	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.40-2.74) 99.4 (45.48-2.72)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.73Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.214 , 0.245 0.225 , 0.253	Depositor DCC
R_{free} test set	7078 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	49.1	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 144186 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21793	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 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: CB3, DHF, UMP, NDP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.38	0/4226	0.65	0/5711
1	B	0.41	0/4239	0.67	0/5727
1	C	0.36	0/4231	0.62	0/5718
1	D	0.36	0/4226	0.61	0/5711
1	E	0.34	0/4231	0.62	1/5718 (0.0%)
All	All	0.37	0/21153	0.63	1/28585 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	4
1	C	0	5
1	D	0	6
1	E	0	2
All	All	0	23

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	357	HIS	CB-CA-C	-5.04	100.33	110.40

There are no chirality outliers.

5 of 23 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	CYS	Peptide
1	A	114	GLY	Peptide
1	A	206	ILE	Peptide
1	A	98	ILE	Peptide
1	A	99	GLU	Peptide

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	4130	0	4057	164	0
1	B	4143	0	4074	160	0
1	C	4135	0	4059	193	1
1	D	4130	0	4057	231	0
1	E	4135	0	4059	224	2
2	A	20	0	11	4	0
2	B	20	0	11	3	0
2	C	20	0	11	3	0
2	D	20	0	11	4	0
2	E	20	0	11	6	0
3	A	35	0	21	4	0
3	B	35	0	21	3	0
3	C	35	0	21	2	0
3	D	35	0	21	9	0
3	E	35	0	21	13	0
4	A	32	0	19	6	0
4	B	32	0	19	10	0
4	C	32	0	19	9	0
4	D	32	0	19	9	0
4	E	32	0	19	5	0
5	A	48	0	26	7	0
5	B	48	0	26	8	0
5	C	48	0	26	11	0
5	D	48	0	26	5	0
5	E	48	0	26	12	0
6	A	114	0	0	18	0
6	B	150	0	0	7	0
6	C	95	0	0	9	0
6	D	62	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	24	0	0	5	0
All	All	21793	0	20691	976	2

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 23.

The worst 5 of 976 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:104:ASP:O	1:D:106:SER:N	1.63	1.26
1:B:179:GLU:C	1:B:180:LYS:HG3	1.52	1.23
1:E:79:LEU:HD23	1:E:80:PRO:CD	1.68	1.21
1:E:79:LEU:CD2	1:E:80:PRO:HD2	1.71	1.18
1:E:178:GLN:HA	1:E:178:GLN:OE1	1.43	1.16

All (2) 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:C:65:ARG:NH2	1:E:251:GLY:O[2_466]	2.11	0.09
1:E:407:GLN:OE1	1:E:421:TYR:OH[2_457]	2.19	0.01

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	503/521 (96%)	476 (95%)	23 (5%)	4 (1%)	24 50
1	B	504/521 (97%)	477 (95%)	23 (5%)	4 (1%)	24 50
1	C	504/521 (97%)	473 (94%)	28 (6%)	3 (1%)	30 57
1	D	503/521 (96%)	469 (93%)	30 (6%)	4 (1%)	24 50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	504/521 (97%)	460 (91%)	38 (8%)	6 (1%)	16	37
All	All	2518/2605 (97%)	2355 (94%)	142 (6%)	21 (1%)	24	50

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	180	LYS
1	C	99	GLU
1	D	105	ASP
1	E	103	ASN
1	A	99	GLU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	457/471 (97%)	427 (93%)	30 (7%)	21	43
1	B	459/471 (98%)	425 (93%)	34 (7%)	17	36
1	C	457/471 (97%)	413 (90%)	44 (10%)	10	23
1	D	457/471 (97%)	415 (91%)	42 (9%)	11	24
1	E	457/471 (97%)	432 (94%)	25 (6%)	27	53
All	All	2287/2355 (97%)	2112 (92%)	175 (8%)	16	34

5 of 175 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	141	ILE
1	C	383	ARG
1	E	235	HIS
1	C	178	GLN
1	C	254	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	100	ASN
1	C	419	ASN
1	D	384	HIS
1	A	384	HIS
1	D	109	ASN

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](#)

20 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	UMP	A	603	-	16,21,21	3.10	3 (18%)	23,31,31	1.96	5 (21%)
3	CB3	A	604	-	31,37,37	1.40	2 (6%)	35,51,51	1.32	4 (11%)
4	DHF	A	605	-	25,34,34	1.14	1 (4%)	24,47,47	1.89	6 (25%)
5	NDP	A	606	-	42,52,52	1.22	3 (7%)	55,80,80	1.71	6 (10%)
2	UMP	B	607	-	16,21,21	3.13	3 (18%)	23,31,31	1.96	4 (17%)
3	CB3	B	608	-	31,37,37	1.42	2 (6%)	35,51,51	1.41	5 (14%)
4	DHF	B	609	-	25,34,34	1.13	1 (4%)	24,47,47	1.86	5 (20%)
5	NDP	B	610	-	42,52,52	1.22	3 (7%)	55,80,80	1.80	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	UMP	C	611	-	16,21,21	3.11	3 (18%)	23,31,31	1.94	5 (21%)
3	CB3	C	612	-	31,37,37	1.44	3 (9%)	35,51,51	1.39	4 (11%)
4	DHF	C	613	-	25,34,34	1.15	1 (4%)	24,47,47	2.01	6 (25%)
5	NDP	C	614	-	42,52,52	1.16	2 (4%)	55,80,80	1.65	4 (7%)
2	UMP	D	615	-	16,21,21	3.12	3 (18%)	23,31,31	1.95	4 (17%)
3	CB3	D	616	-	31,37,37	1.38	3 (9%)	35,51,51	1.37	4 (11%)
4	DHF	D	617	-	25,34,34	1.21	1 (4%)	24,47,47	1.81	5 (20%)
5	NDP	D	618	-	42,52,52	1.19	2 (4%)	55,80,80	1.66	5 (9%)
2	UMP	E	619	-	16,21,21	3.14	3 (18%)	23,31,31	1.95	5 (21%)
3	CB3	E	620	-	31,37,37	1.40	2 (6%)	35,51,51	1.42	5 (14%)
4	DHF	E	621	-	25,34,34	1.19	1 (4%)	24,47,47	1.86	5 (20%)
5	NDP	E	622	-	42,52,52	1.17	2 (4%)	55,80,80	1.77	4 (7%)

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	UMP	A	603	-	-	0/6/22/22	0/2/2/2
3	CB3	A	604	-	-	0/21/28/28	0/3/3/3
4	DHF	A	605	-	1/1/5/8	1/14/31/31	0/3/3/3
5	NDP	A	606	-	-	0/30/77/77	0/5/5/5
2	UMP	B	607	-	-	0/6/22/22	0/2/2/2
3	CB3	B	608	-	-	0/21/28/28	0/3/3/3
4	DHF	B	609	-	1/1/5/8	1/14/31/31	0/3/3/3
5	NDP	B	610	-	-	0/30/77/77	0/5/5/5
2	UMP	C	611	-	-	0/6/22/22	0/2/2/2
3	CB3	C	612	-	-	0/21/28/28	0/3/3/3
4	DHF	C	613	-	-	0/14/31/31	0/3/3/3
5	NDP	C	614	-	-	0/30/77/77	0/5/5/5
2	UMP	D	615	-	-	0/6/22/22	0/2/2/2
3	CB3	D	616	-	1/1/5/6	0/21/28/28	0/3/3/3
4	DHF	D	617	-	-	0/14/31/31	0/3/3/3
5	NDP	D	618	-	-	0/30/77/77	0/5/5/5
2	UMP	E	619	-	-	0/6/22/22	0/2/2/2
3	CB3	E	620	-	1/1/5/6	1/21/28/28	0/3/3/3
4	DHF	E	621	-	-	0/14/31/31	0/3/3/3
5	NDP	E	622	-	-	0/30/77/77	0/5/5/5

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	622	NDP	C4N-C5N	-5.06	1.38	1.49
5	D	618	NDP	C4N-C5N	-5.03	1.38	1.49
5	C	614	NDP	C4N-C5N	-4.96	1.38	1.49
5	B	610	NDP	C4N-C5N	-4.57	1.39	1.49
5	A	606	NDP	C4N-C5N	-4.43	1.39	1.49

The worst 5 of 98 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	622	NDP	N3A-C2A-N1A	-9.84	121.36	128.89
5	A	606	NDP	N3A-C2A-N1A	-9.83	121.37	128.89
5	D	618	NDP	N3A-C2A-N1A	-9.54	121.59	128.89
5	C	614	NDP	N3A-C2A-N1A	-9.51	121.61	128.89
5	B	610	NDP	N3A-C2A-N1A	-9.24	121.82	128.89

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	609	DHF	CA
3	D	616	CB3	CA
4	A	605	DHF	CA
3	E	620	CB3	CA

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	609	DHF	CB-CA-N-C
4	A	605	DHF	CB-CA-N-C
3	E	620	CB3	CB-CA-N-C

There are no ring outliers.

20 monomers are involved in 115 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	603	UMP	4	0
3	A	604	CB3	4	0
4	A	605	DHF	6	0
5	A	606	NDP	7	0
2	B	607	UMP	3	0
3	B	608	CB3	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	609	DHF	10	0
5	B	610	NDP	8	0
2	C	611	UMP	3	0
3	C	612	CB3	2	0
4	C	613	DHF	9	0
5	C	614	NDP	11	0
2	D	615	UMP	4	0
3	D	616	CB3	9	0
4	D	617	DHF	9	0
5	D	618	NDP	5	0
2	E	619	UMP	6	0
3	E	620	CB3	13	0
4	E	621	DHF	5	0
5	E	622	NDP	12	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	507/521 (97%)	-0.13	5 (0%) 84 86	23, 39, 74, 118	0
1	B	508/521 (97%)	-0.27	5 (0%) 84 86	20, 34, 62, 135	0
1	C	508/521 (97%)	-0.06	10 (1%) 68 71	26, 47, 90, 131	0
1	D	507/521 (97%)	0.05	8 (1%) 74 77	29, 50, 84, 158	0
1	E	508/521 (97%)	0.53	36 (7%) 19 18	45, 72, 112, 149	0
All	All	2538/2605 (97%)	0.02	64 (2%) 61 63	20, 48, 96, 158	0

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	521	VAL	5.1
1	E	324	TYR	4.0
1	E	179	GLU	3.8
1	E	106	SER	3.7
1	C	181	LYS	3.5

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	CB3	D	616	35/35	0.78	0.33	4.16	69,75,87,89	0
4	DHF	C	613	32/32	0.91	0.22	3.19	29,35,44,48	0
3	CB3	A	604	35/35	0.84	0.24	3.14	60,67,76,77	0
3	CB3	E	620	35/35	0.73	0.31	1.94	93,98,107,108	0
3	CB3	C	612	35/35	0.90	0.21	1.77	49,60,71,73	0
3	CB3	B	608	35/35	0.92	0.21	1.73	45,50,68,69	0
4	DHF	E	621	32/32	0.93	0.22	1.63	30,33,42,47	0
4	DHF	B	609	32/32	0.91	0.18	1.35	23,26,39,44	0
2	UMP	B	607	20/20	0.93	0.19	0.62	27,44,48,51	0
2	UMP	C	611	20/20	0.93	0.18	0.46	39,50,55,58	0
4	DHF	D	617	32/32	0.92	0.16	0.32	23,31,41,47	0
5	NDP	D	618	48/48	0.93	0.18	0.26	50,61,74,76	0
2	UMP	A	603	20/20	0.92	0.22	0.23	46,57,61,63	0
5	NDP	C	614	48/48	0.91	0.18	0.18	65,77,95,95	0
4	DHF	A	605	32/32	0.92	0.16	-0.02	23,28,38,48	0
5	NDP	B	610	48/48	0.97	0.15	-0.02	31,37,42,43	0
2	UMP	D	615	20/20	0.92	0.20	-0.02	53,66,73,73	0
2	UMP	E	619	20/20	0.88	0.19	-0.21	80,88,89,89	0
5	NDP	E	622	48/48	0.92	0.18	-0.31	66,77,90,92	0
5	NDP	A	606	48/48	0.96	0.14	-0.79	31,40,43,44	0

6.5 Other polymers

There are no such residues in this entry.