



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 01:01 PM GMT

PDB ID : 3DL6  
Title : Crystal Structure of the A287F/S290G Active Site Mutant of TS-DHFR from *Cryptosporidium hominis*  
Authors : Martucci, W.E.; Vargo, M.A.; Anderson, K.S.  
Deposited on : 2008-06-26  
Resolution : 3.25 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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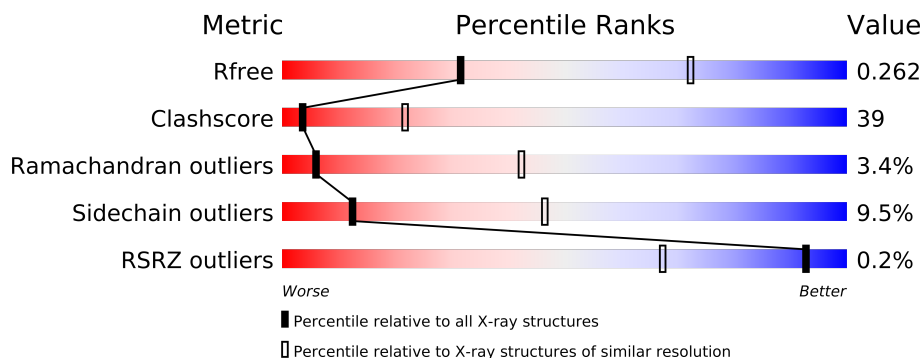
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 3.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1085 (3.32-3.20)
Clashscore	79885	1374 (3.32-3.20)
Ramachandran outliers	78287	1348 (3.32-3.20)
Sidechain outliers	78261	1346 (3.32-3.20)
RSRZ outliers	66119	1086 (3.32-3.20)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	521	
1	B	521	
1	C	521	
1	D	521	
1	E	521	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	UMP	B	607	-	X
3	CB3	A	604	-	X
3	CB3	B	608	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	CB3	C	612	-	X
3	CB3	D	616	-	X
3	CB3	E	620	-	X
4	DHF	A	605	-	X
4	DHF	B	609	-	X
4	DHF	C	613	-	X
4	DHF	D	617	-	X
5	NDP	A	606	-	X
5	NDP	B	610	-	X
5	NDP	C	614	-	X
5	NDP	D	618	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21446 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

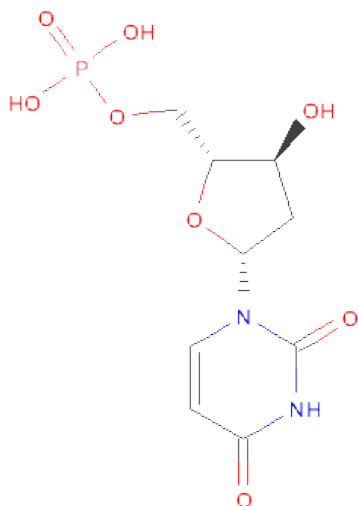
- Molecule 1 is a protein called Dihydrofolate reductase, DHFR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	505	Total	C	N	O	S	0	0	0
			4111	2629	690	770	22			
1	B	508	Total	C	N	O	S	0	0	0
			4126	2638	693	773	22			
1	C	508	Total	C	N	O	S	0	0	0
			4133	2644	694	773	22			
1	D	508	Total	C	N	O	S	0	0	0
			4137	2646	694	775	22			
1	E	507	Total	C	N	O	S	0	0	0
			4121	2635	692	772	22			

There are 10 discrepancies between the modelled and reference sequences:

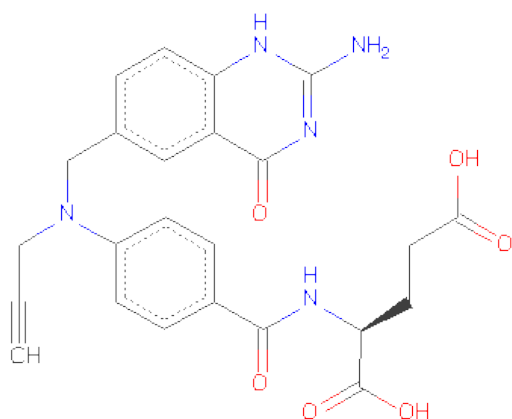
Chain	Residue	Modelled	Actual	Comment	Reference
A	287	PHE	ALA	ENGINEERED	UNP Q5CGA3
A	290	GLY	SER	ENGINEERED	UNP Q5CGA3
B	287	PHE	ALA	ENGINEERED	UNP Q5CGA3
B	290	GLY	SER	ENGINEERED	UNP Q5CGA3
C	287	PHE	ALA	ENGINEERED	UNP Q5CGA3
C	290	GLY	SER	ENGINEERED	UNP Q5CGA3
D	287	PHE	ALA	ENGINEERED	UNP Q5CGA3
D	290	GLY	SER	ENGINEERED	UNP Q5CGA3
E	287	PHE	ALA	ENGINEERED	UNP Q5CGA3
E	290	GLY	SER	ENGINEERED	UNP Q5CGA3

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



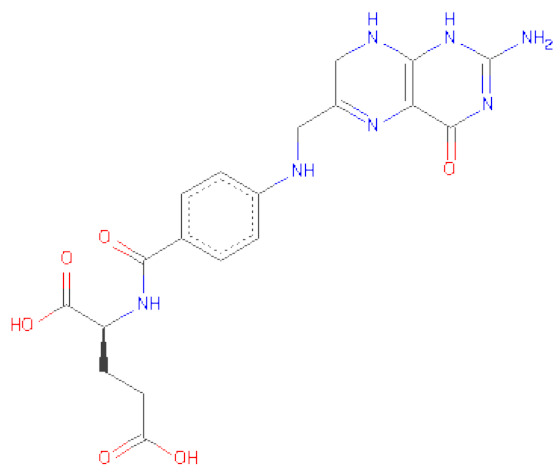
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	D	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	E	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 3 is 10-PROPARGYL-5,8-DIDEAZAFOLICACID (three-letter code: CB3) (formula: C<sub>24</sub>H<sub>23</sub>N<sub>5</sub>O<sub>6</sub>).



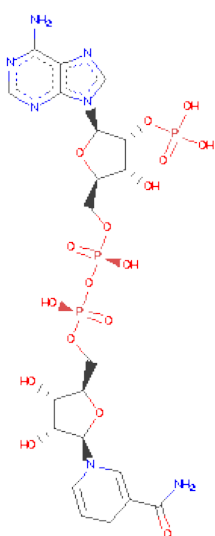
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			35	24	5	6		
3	B	1	Total	C	N	O	0	0
			35	24	5	6		
3	C	1	Total	C	N	O	0	0
			35	24	5	6		
3	D	1	Total	C	N	O	0	0
			35	24	5	6		
3	E	1	Total	C	N	O	0	0
			35	24	5	6		

- Molecule 4 is DIHYDROFOLIC ACID (three-letter code: DHF) (formula:  $C_{19}H_{21}N_7O_6$ ).



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-DINUCLEOTIDEPHOSPHATE (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	35	Total 35	O 35	0	0
6	B	48	Total 48	O 48	0	0
6	C	22	Total 22	O 22	0	0
6	D	23	Total 23	O 23	0	0
6	E	15	Total 15	O 15	0	0

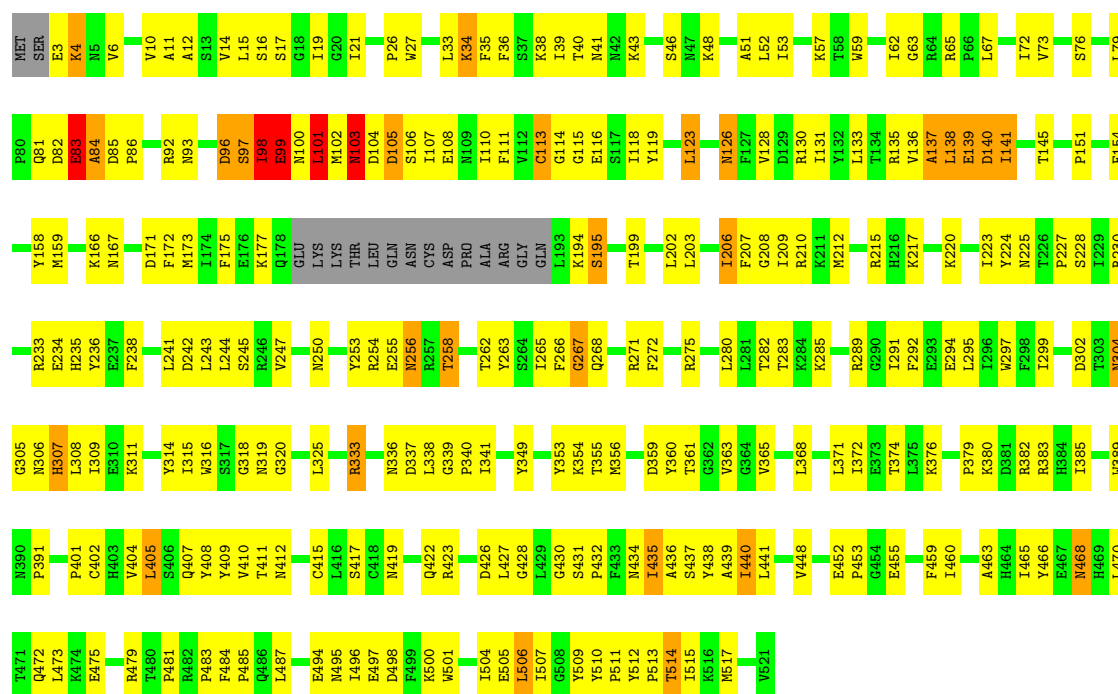


### 3 Residue-property plots

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

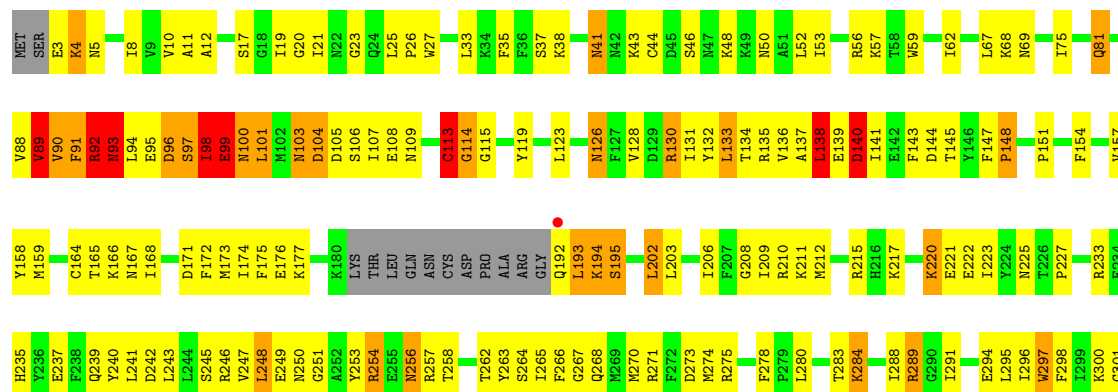
#### • Molecule 1: Dihydrofolate reductase, DHFR

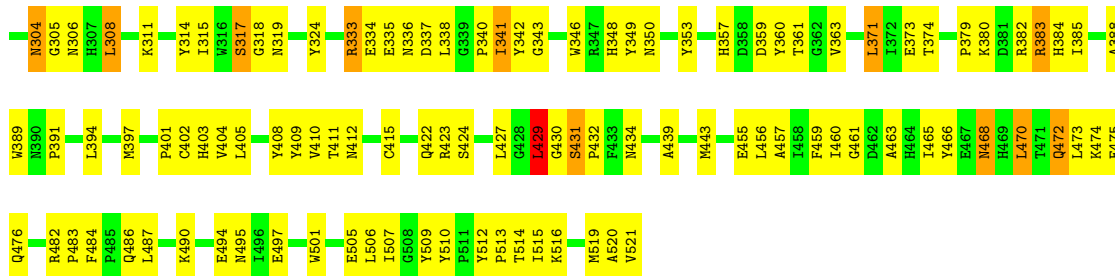
Chain A: 



#### • Molecule 1: Dihydrofolate reductase, DHFR

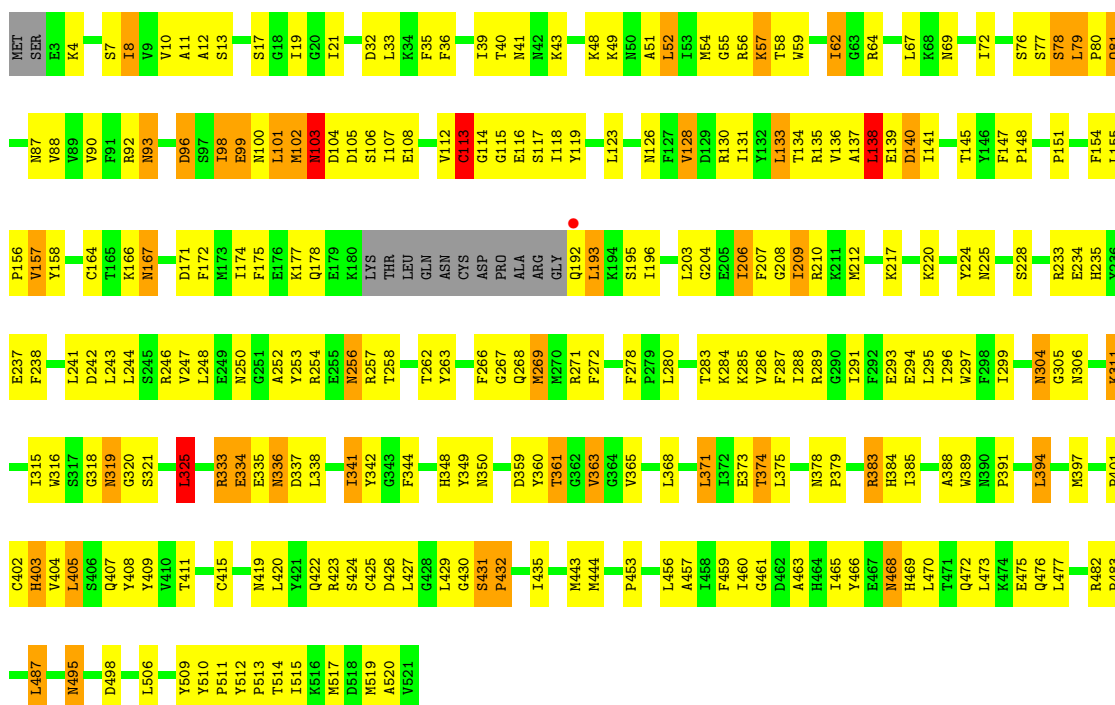
Chain B: 





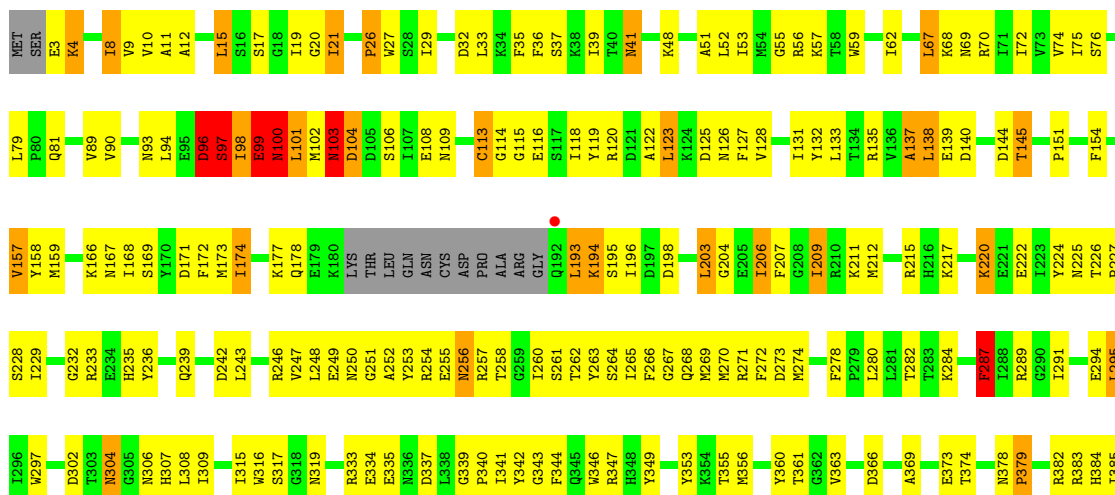
• Molecule 1: Dihydrofolate reductase, DHFR

Chain C:



• Molecule 1: Dihydrofolate reductase, DHFR

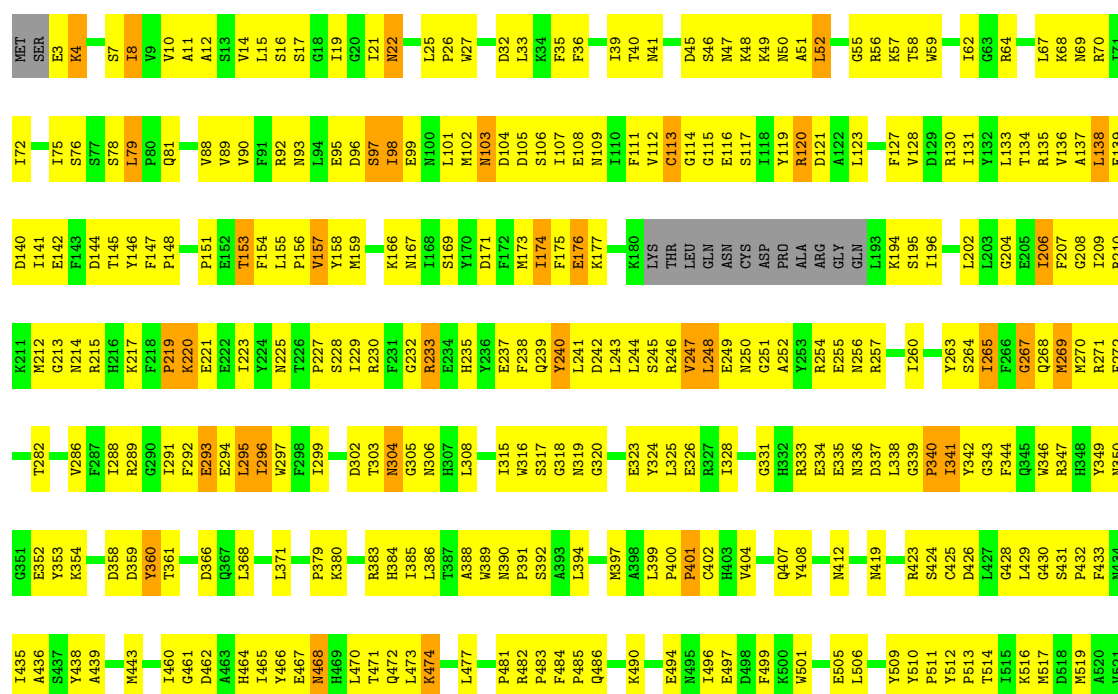
Chain D:





• Molecule 1: Dihydrofolate reductase, DHFR

Chain E:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	214.91Å 116.92Å 220.95Å 90.00° 95.94° 90.00°	Depositor
Resolution (Å)	3.45 – 3.25 46.21 – 3.26	Depositor EDS
% Data completeness (in resolution range)	98.2 (3.45-3.25) 98.2 (46.21-3.26)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.15 (at 3.25Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.225 , 0.276 0.216 , 0.262	Depositor DCC
$R_{free}$ test set	4159 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.4	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 27.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 83352 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	21446	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.40	0/4207	0.68	0/5686
1	B	0.39	0/4222	0.65	0/5707
1	C	0.39	0/4229	0.66	0/5715
1	D	0.38	1/4233 (0.0%)	0.65	0/5720
1	E	0.35	0/4217	0.65	0/5700
All	All	0.38	1/21108 (0.0%)	0.66	0/28528

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	7
1	B	0	9
1	C	0	3
1	D	0	5
1	E	0	2
All	All	0	26

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	379	PRO	N-CD	5.38	1.55	1.47

There are no bond angle outliers.

There are no chirality outliers.

5 of 26 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	LEU	Peptide
1	A	113	CYS	Peptide
1	A	81	GLN	Peptide
1	A	83	GLU	Peptide
1	A	98	ILE	Peptide

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4111	0	4031	311	0
1	B	4126	0	4036	325	0
1	C	4133	0	4057	332	0
1	D	4137	0	4061	343	0
1	E	4121	0	4035	332	0
2	A	20	0	11	8	0
2	B	20	0	11	10	0
2	C	20	0	10	5	0
2	D	20	0	11	3	0
2	E	20	0	11	10	0
3	A	35	0	21	5	0
3	B	35	0	21	14	0
3	C	35	0	21	15	0
3	D	35	0	21	14	0
3	E	35	0	21	13	0
4	A	32	0	19	9	0
4	B	32	0	19	18	0
4	C	32	0	19	24	0
4	D	32	0	19	33	0
4	E	32	0	19	20	0
5	A	48	0	26	18	0
5	B	48	0	26	13	0
5	C	48	0	26	23	0
5	D	48	0	26	14	0
5	E	48	0	26	19	0
6	A	35	0	0	2	0
6	B	48	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	22	0	0	1	0
6	D	23	0	0	5	0
6	E	15	0	0	1	0
All	All	21446	0	20604	1630	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 39.

The worst 5 of 1630 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:349:TYR:CE2	1:B:391:PRO:HD2	1.31	1.63
1:C:349:TYR:CE2	1:D:391:PRO:HD2	1.57	1.39
1:B:81:GLN:OE1	1:B:92:ARG:NH1	1.59	1.34
1:B:67:LEU:HD22	4:B:609:DHF:O2	1.24	1.31
1:D:67:LEU:CD2	4:D:617:DHF:O2	1.81	1.26

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	501/521 (96%)	431 (86%)	51 (10%)	19 (4%)	5	38
1	B	504/521 (97%)	435 (86%)	53 (10%)	16 (3%)	6	44
1	C	504/521 (97%)	445 (88%)	46 (9%)	13 (3%)	8	51
1	D	504/521 (97%)	427 (85%)	56 (11%)	21 (4%)	4	34
1	E	503/521 (96%)	419 (83%)	67 (13%)	17 (3%)	6	42
All	All	2516/2605 (97%)	2157 (86%)	273 (11%)	86 (3%)	6	42

5 of 86 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	LYS

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Mol	Chain	Res	Type
1	A	84	ALA
1	A	103	ASN
1	A	105	ASP
1	A	206	ILE

### 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	454/470 (97%)	422 (93%)	32 (7%)	21	66
1	B	454/470 (97%)	402 (88%)	52 (12%)	8	36
1	C	456/470 (97%)	407 (89%)	49 (11%)	10	40
1	D	457/470 (97%)	413 (90%)	44 (10%)	12	46
1	E	454/470 (97%)	416 (92%)	38 (8%)	16	55
All	All	2275/2350 (97%)	2060 (90%)	215 (10%)	12	46

5 of 215 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	123	LEU
1	C	371	LEU
1	E	265	ILE
1	C	138	LEU
1	C	228	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 104 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	93	ASN
1	C	357	HIS
1	E	304	ASN
1	C	100	ASN
1	C	216	HIS



### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	-	21,21,21	3.25	3 (14%)	26,31,31	2.11	4 (15%)
3	CB3	A	604	-	37,37,37	1.58	5 (13%)	49,51,51	1.67	8 (16%)
4	DHF	A	605	-	34,34,34	1.27	2 (5%)	45,47,47	1.66	6 (13%)
5	NDP	A	606	-	52,52,52	1.34	5 (9%)	80,80,80	1.62	8 (10%)
2	UMP	B	607	-	21,21,21	3.25	4 (19%)	26,31,31	1.97	3 (11%)
3	CB3	B	608	-	37,37,37	1.27	3 (8%)	49,51,51	1.44	8 (16%)
4	DHF	B	609	-	34,34,34	1.28	2 (5%)	45,47,47	1.66	6 (13%)
5	NDP	B	610	-	52,52,52	1.34	5 (9%)	80,80,80	1.62	8 (10%)
2	UMP	C	611	-	21,21,21	3.27	4 (19%)	26,31,31	3.29	7 (26%)
3	CB3	C	612	-	37,37,37	1.28	3 (8%)	49,51,51	1.44	8 (16%)
4	DHF	C	613	-	34,34,34	1.28	2 (5%)	45,47,47	1.67	6 (13%)
5	NDP	C	614	-	52,52,52	1.34	5 (9%)	80,80,80	1.62	8 (10%)
2	UMP	D	615	-	21,21,21	3.27	4 (19%)	26,31,31	1.92	4 (15%)
3	CB3	D	616	-	37,37,37	1.29	3 (8%)	49,51,51	1.45	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	DHF	D	617	-	34,34,34	1.28	2 (5%)	45,47,47	1.66	6 (13%)
5	NDP	D	618	-	52,52,52	1.34	5 (9%)	80,80,80	1.62	8 (10%)
2	UMP	E	619	-	21,21,21	3.28	3 (14%)	26,31,31	2.41	6 (23%)
3	CB3	E	620	-	37,37,37	1.29	3 (8%)	49,51,51	1.44	8 (16%)
4	DHF	E	621	-	34,34,34	1.28	2 (5%)	45,47,47	1.66	6 (13%)
5	NDP	E	622	-	52,52,52	1.34	5 (9%)	80,80,80	1.62	8 (10%)

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	-	-	0/7/22/22	0/2/2/2
3	CB3	A	604	-	-	0/27/28/28	0/1/3/3
4	DHF	A	605	-	-	0/20/31/31	0/1/3/3
5	NDP	A	606	-	-	0/35/77/77	0/3/5/5
2	UMP	B	607	-	-	0/7/22/22	0/2/2/2
3	CB3	B	608	-	-	0/27/28/28	0/1/3/3
4	DHF	B	609	-	1/1/5/8	0/20/31/31	0/1/3/3
5	NDP	B	610	-	-	0/35/77/77	0/3/5/5
2	UMP	C	611	-	-	0/7/22/22	0/2/2/2
3	CB3	C	612	-	-	0/27/28/28	0/1/3/3
4	DHF	C	613	-	-	0/20/31/31	0/1/3/3
5	NDP	C	614	-	-	0/35/77/77	0/3/5/5
2	UMP	D	615	-	-	0/7/22/22	0/2/2/2
3	CB3	D	616	-	-	0/27/28/28	0/1/3/3
4	DHF	D	617	-	-	0/20/31/31	0/1/3/3
5	NDP	D	618	-	-	0/35/77/77	0/3/5/5
2	UMP	E	619	-	-	0/7/22/22	0/2/2/2
3	CB3	E	620	-	-	0/27/28/28	0/1/3/3
4	DHF	E	621	-	-	0/20/31/31	0/1/3/3
5	NDP	E	622	-	-	0/35/77/77	0/3/5/5

The worst 5 of 70 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	619	UMP	C6-C5	10.93	1.53	1.36
2	D	615	UMP	C6-C5	10.80	1.53	1.36
2	C	611	UMP	C6-C5	10.79	1.53	1.36
2	A	603	UMP	C6-C5	10.77	1.53	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	607	UMP	C6-C5	10.72	1.53	1.36

The worst 5 of 134 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	611	UMP	P-O5'-C5'	9.14	144.61	118.19
5	B	610	NDP	N3A-C2A-N1A	-8.84	121.32	128.71
5	E	622	NDP	N3A-C2A-N1A	-8.81	121.34	128.71
5	C	614	NDP	N3A-C2A-N1A	-8.81	121.35	128.71
5	A	606	NDP	N3A-C2A-N1A	-8.80	121.35	128.71

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	609	DHF	CA

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	505/521 (96%)	-0.40	0 100 100	22, 52, 94, 157	0
1	B	508/521 (97%)	-0.41	1 (0%) 93 67	20, 47, 94, 157	0
1	C	508/521 (97%)	-0.34	1 (0%) 93 67	27, 57, 110, 189	0
1	D	508/521 (97%)	-0.33	1 (0%) 93 67	25, 61, 110, 172	0
1	E	507/521 (97%)	-0.23	0 100 100	36, 75, 125, 181	0
All	All	2536/2605 (97%)	-0.34	3 (0%) 93 75	20, 58, 111, 189	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	192	GLN	2.9
1	B	192	GLN	2.5
1	C	192	GLN	2.2

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	DHF	D	617	32/32	0.41	6.73	40,63,63,63	0
3	CB3	B	608	35/35	0.31	5.29	44,50,63,63	0
4	DHF	B	609	32/32	0.34	4.44	33,63,63,63	0
3	CB3	E	620	35/35	0.40	3.12	55,66,89,98	0
5	NDP	C	614	48/48	0.33	2.95	52,63,92,99	0
4	DHF	A	605	32/32	0.24	2.87	33,63,63,64	0
4	DHF	C	613	32/32	0.27	2.79	42,63,63,72	0
5	NDP	A	606	48/48	0.25	2.78	28,63,63,63	0
3	CB3	A	604	35/35	0.32	2.51	60,63,76,80	0
3	CB3	D	616	35/35	0.26	2.39	53,63,65,76	0
2	UMP	B	607	20/20	0.22	2.34	25,63,63,63	0
5	NDP	D	618	48/48	0.28	2.32	49,63,73,88	0
5	NDP	B	610	48/48	0.25	2.30	28,63,63,65	0
3	CB3	C	612	35/35	0.25	2.29	45,58,63,63	0
2	UMP	E	619	20/20	0.22	1.17	63,63,81,84	0
5	NDP	E	622	48/48	0.24	1.15	56,63,90,94	0
4	DHF	E	621	32/32	0.22	0.92	41,63,63,81	0
2	UMP	C	611	20/20	0.18	0.58	45,63,63,66	0
2	UMP	A	603	20/20	0.20	0.36	40,63,66,72	0
2	UMP	D	615	20/20	0.15	-0.54	57,63,65,84	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.