



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:12 AM GMT

PDB ID : 3HJ3  
Title : Crystal Structure of the ChTS-DHFR F207A Non-Active Site Mutant  
Authors : Anderson, K.S.; Martucci, W.E.  
Deposited on : 2009-05-20  
Resolution : 2.70 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](mailto: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.

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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 : 1.7 (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

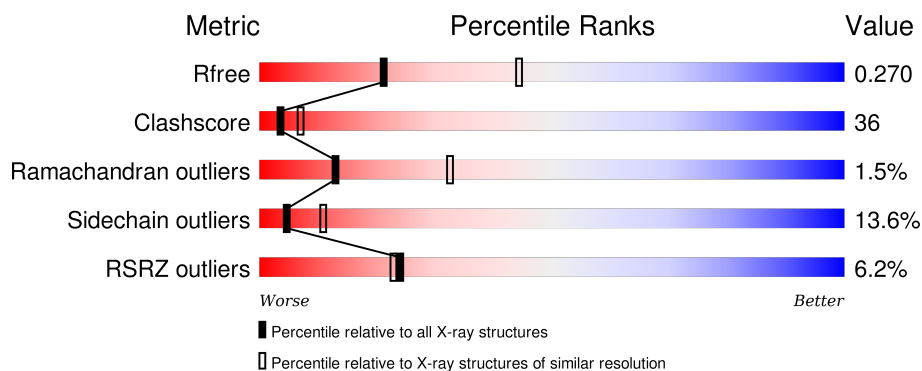
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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  $\geq 3$ , 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	 3% 56% 32% 9% ..
1	B	521	 3% 55% 34% 8% ..
1	C	521	 8% 47% 40% 10% ..
1	D	521	 11% 42% 45% 9% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UMP	A	603	-	-	X	X
2	UMP	B	607	-	-	X	X
2	UMP	C	611	-	-	X	-
3	CB3	A	604	X	-	X	X
3	CB3	B	608	X	-	-	X
3	CB3	C	612	X	-	X	X
4	MTX	D	615	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17282 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.

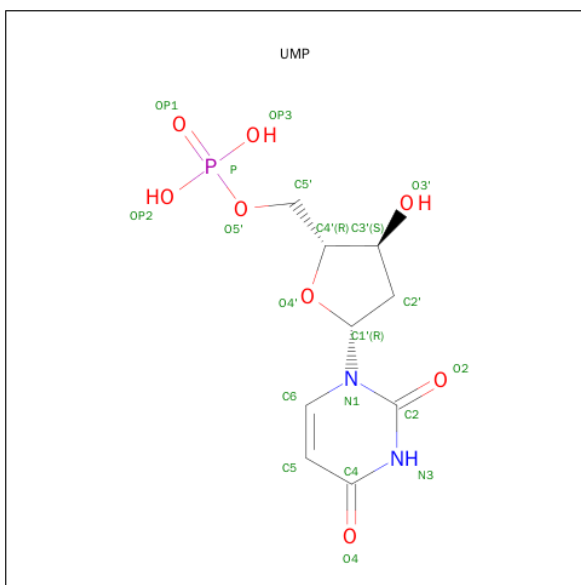
- Molecule 1 is a protein called Chain A, crystal structure of Dhfr.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	508	Total	C	N	O	S	0	0	0
			4131	2638	695	776	22			
1	B	510	Total	C	N	O	S	0	0	0
			4144	2645	698	779	22			
1	C	510	Total	C	N	O	S	0	0	0
			4147	2648	698	779	22			
1	D	505	Total	C	N	O	S	0	0	0
			4104	2622	690	770	22			

There are 4 discrepancies between the modelled and reference sequences:

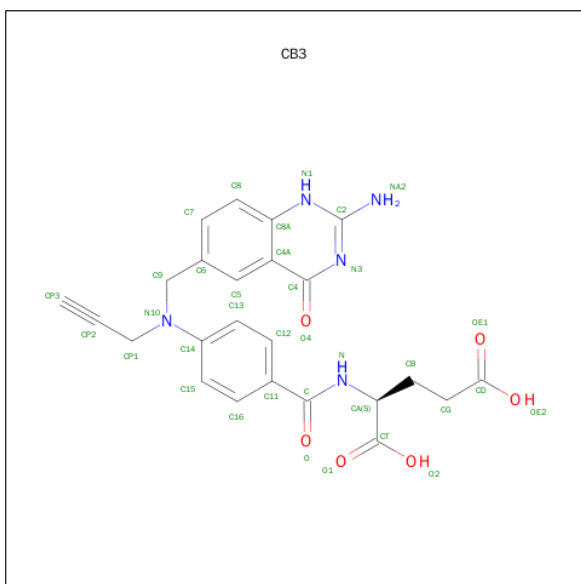
Chain	Residue	Modelled	Actual	Comment	Reference
A	207	ALA	PHE	ENGINEERED	UNP Q5CGA3
B	207	ALA	PHE	ENGINEERED	UNP Q5CGA3
C	207	ALA	PHE	ENGINEERED	UNP Q5CGA3
D	207	ALA	PHE	ENGINEERED	UNP Q5CGA3

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



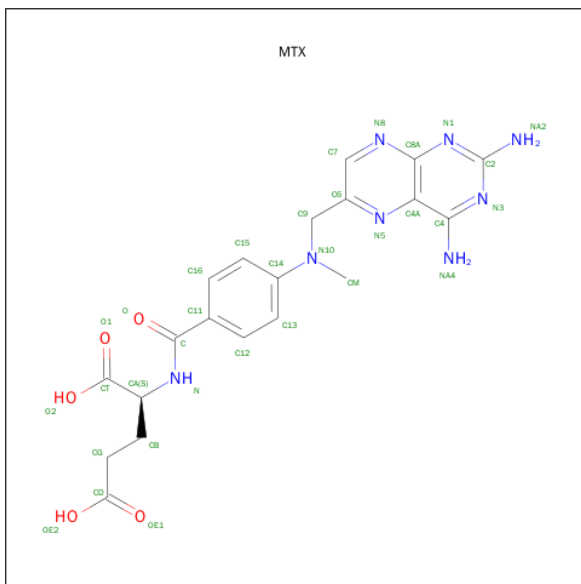
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 3 is 10-PROPARGYL-5,8-DIDEAZAFOLIC ACID (three-letter code: CB3) (formula:  $C_{24}H_{23}N_5O_6$ ).



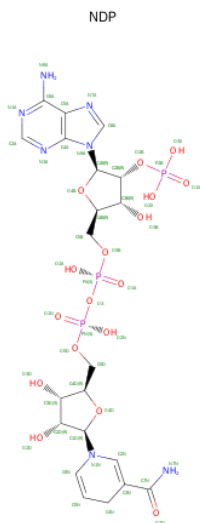
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 35	C 24	N 5	O 6	0	0
3	B	1	Total 35	C 24	N 5	O 6	0	0
3	C	1	Total 35	C 24	N 5	O 6	0	0

- Molecule 4 is METHOTREXATE (three-letter code: MTX) (formula:  $C_{20}H_{22}N_8O_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 33	C 20	N 8	O 5	0	0
4	B	1	Total 33	C 20	N 8	O 5	0	0
4	C	1	Total 33	C 20	N 8	O 5	0	0
4	D	1	Total 33	C 20	N 8	O 5	0	0

- 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 48	C 21	N 7	O 17	P 3	0	0
5	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
5	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
5	D	1	Total 48	C 21	N 7	O 17	P 3	0	0

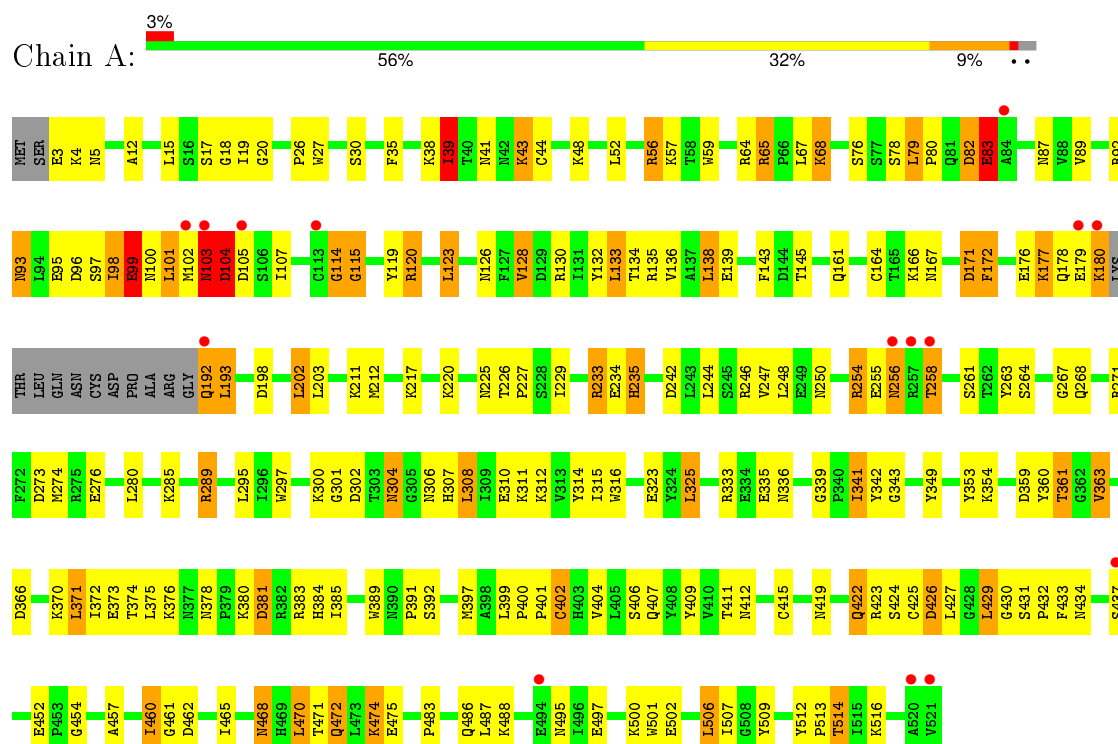
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	98	Total O 98 98	0	0
6	B	86	Total O 86 86	0	0
6	C	47	Total O 47 47	0	0
6	D	36	Total O 36 36	0	0

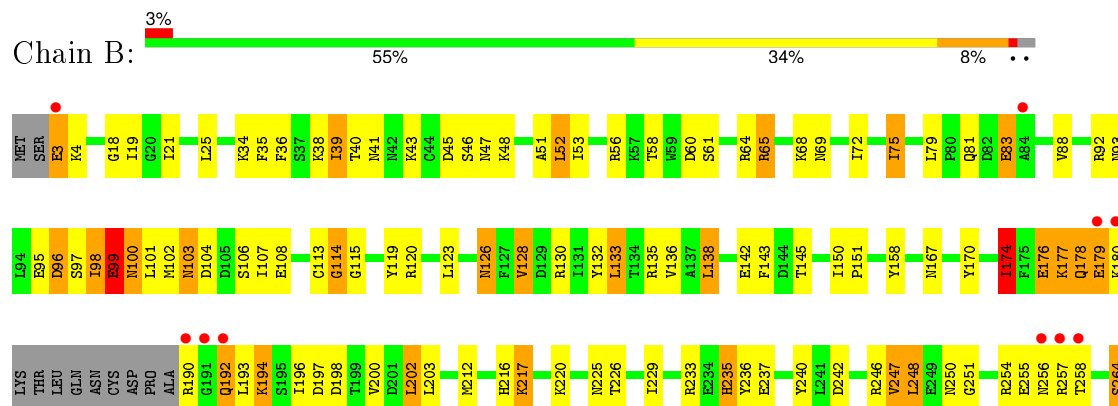
### 3 Residue-property plots

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.

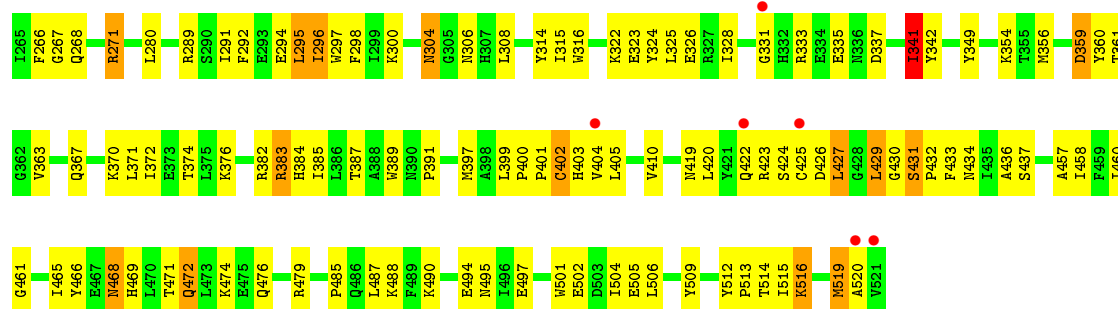
- Molecule 1: Chain A, crystal structure of Dhfr



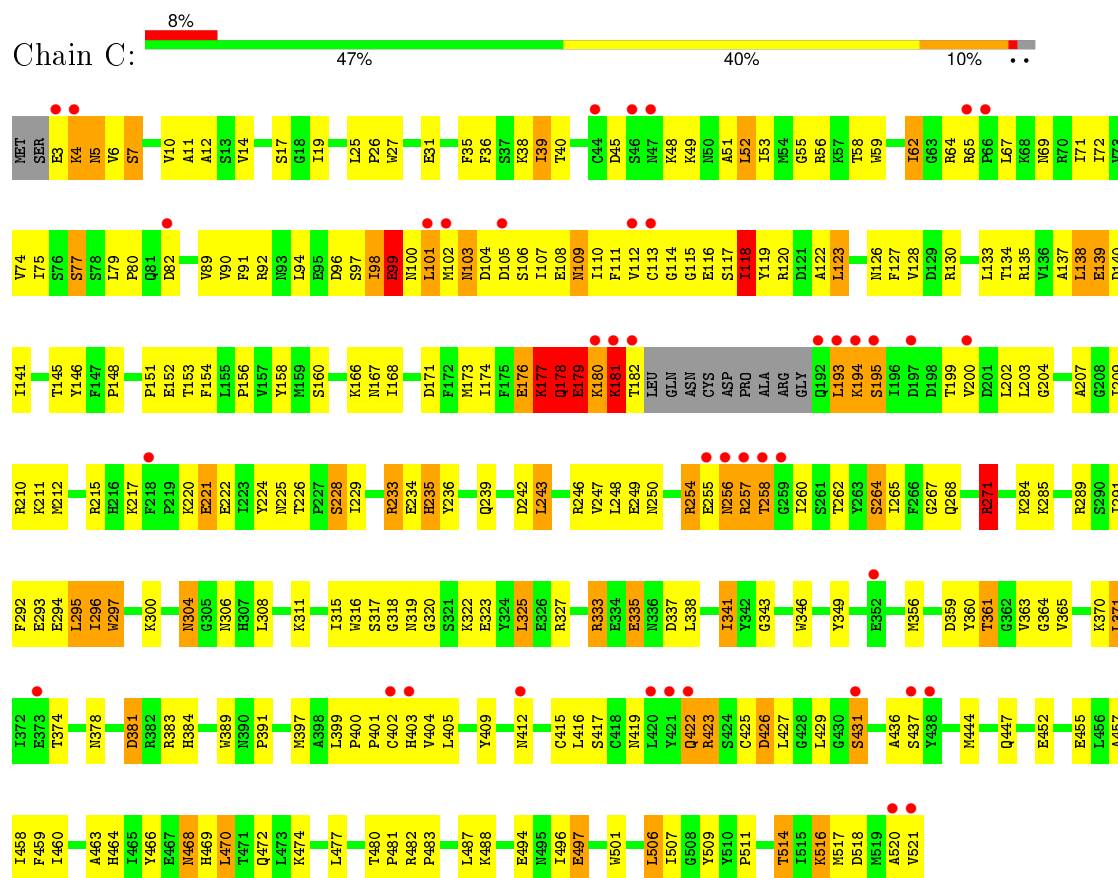
- Molecule 1: Chain A, crystal structure of Dhfr



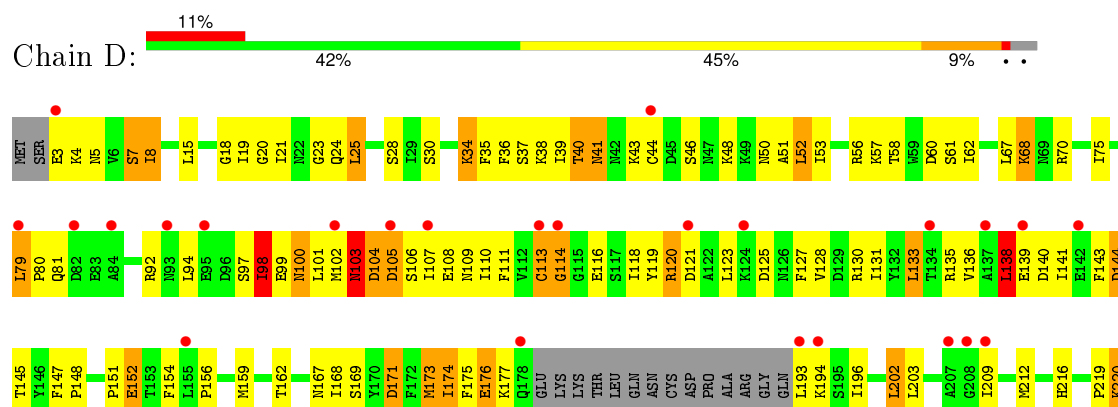




• Molecule 1: Chain A, crystal structure of Dhfr



• Molecule 1: Chain A, crystal structure of Dhfr





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.86Å 121.86Å 342.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.70 34.47 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-2.70) 99.5 (34.47-2.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 2.68Å)	Xtriage
Refinement program	Refmac and CNS	Depositor
R, $R_{free}$	0.228 , 0.274 0.225 , 0.270	Depositor DCC
$R_{free}$ test set	4070 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.6	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 45.4	EDS
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 81139 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	17282	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CB3, MTX, 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	0.84	1/4225 (0.0%)	0.86	4/5709 (0.1%)
1	B	0.87	2/4238 (0.0%)	0.83	4/5726 (0.1%)
1	C	0.82	1/4241 (0.0%)	0.86	5/5730 (0.1%)
1	D	0.74	1/4198 (0.0%)	0.79	2/5674 (0.0%)
All	All	0.82	5/16902 (0.0%)	0.83	15/22839 (0.1%)

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	8
1	C	0	12
1	D	0	6
All	All	0	32

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	402	CYS	CB-SG	-9.21	1.66	1.82
1	B	402	CYS	CB-SG	-9.01	1.67	1.82
1	D	521	VAL	C-OXT	6.37	1.35	1.23
1	C	521	VAL	C-OXT	6.01	1.34	1.23
1	B	240	TYR	CE1-CZ	5.49	1.45	1.38

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	423	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	C	423	ARG	NE-CZ-NH2	-8.69	115.96	120.30
1	B	75	ILE	CG1-CB-CG2	-7.13	95.72	111.40
1	B	402	CYS	CA-CB-SG	-6.15	102.93	114.00
1	A	402	CYS	CA-CB-SG	-5.80	103.55	114.00

There are no chirality outliers.

5 of 32 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	GLY	Peptide
1	A	171	ASP	Peptide
1	A	192	GLN	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	4131	0	4066	271	0
1	B	4144	0	4077	280	3
1	C	4147	0	4086	333	3
1	D	4104	0	4039	351	0
2	A	20	0	11	7	0
2	B	20	0	11	9	0
2	C	20	0	11	9	0
3	A	35	0	21	11	0
3	B	35	0	21	8	0
3	C	35	0	21	10	0
4	A	33	0	19	1	0
4	B	33	0	19	4	0
4	C	33	0	19	6	0
4	D	33	0	20	13	0
5	A	48	0	26	4	0
5	B	48	0	26	6	0
5	C	48	0	26	7	0
5	D	48	0	26	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	98	0	0	32	0
6	B	86	0	0	30	0
6	C	47	0	0	29	0
6	D	36	0	0	47	0
All	All	17282	0	16545	1208	3

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 36.

The worst 5 of 1208 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:C:402:CYS:SG	2:C:611:UMP:C6	2.20	1.33
1:B:65:ARG:HD2	6:B:593:HOH:O	1.41	1.19
1:C:211:LYS:HB3	6:C:561:HOH:O	1.39	1.18
1:C:374:THR:HG22	1:C:384:HIS:CE1	1.81	1.14
1:A:381:ASP:HB2	6:A:591:HOH:O	1.47	1.12

All (3) 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:B:3:GLU:OE1	1:C:166:LYS:NZ[5_555]	1.67	0.53
1:B:3:GLU:OE1	1:C:166:LYS:CE[5_555]	1.99	0.21
1:B:3:GLU:CD	1:C:166:LYS:NZ[5_555]	2.07	0.13

## 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	504/521 (97%)	468 (93%)	28 (6%)	8 (2%)	12 30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	506/521 (97%)	473 (94%)	28 (6%)	5 (1%)	19	45
1	C	506/521 (97%)	462 (91%)	37 (7%)	7 (1%)	14	35
1	D	501/521 (96%)	439 (88%)	51 (10%)	11 (2%)	8	22
All	All	2017/2084 (97%)	1842 (91%)	144 (7%)	31 (2%)	13	32

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	GLU
1	C	118	ILE
1	C	178	GLN
1	C	181	LYS
1	D	103	ASN

### 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	457/469 (97%)	399 (87%)	58 (13%)	5	13
1	B	458/469 (98%)	405 (88%)	53 (12%)	7	16
1	C	459/469 (98%)	385 (84%)	74 (16%)	3	7
1	D	454/469 (97%)	391 (86%)	63 (14%)	4	10
All	All	1828/1876 (97%)	1580 (86%)	248 (14%)	5	11

5 of 248 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	5	ASN
1	C	193	LEU
1	D	371	LEU
1	C	52	LEU
1	C	109	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	434	ASN
1	C	103	ASN
1	D	414	ASN
1	B	468	ASN
1	C	5	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](#)

14 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	3.71	5 (31%)	23,31,31	2.54	5 (21%)
3	CB3	A	604	-	31,37,37	2.26	10 (32%)	35,51,51	1.36	2 (5%)
4	MTX	A	605	-	27,35,35	1.88	8 (29%)	30,49,49	1.65	6 (20%)
5	NDP	A	606	-	42,52,52	1.27	4 (9%)	55,80,80	1.70	5 (9%)
2	UMP	B	607	-	16,21,21	3.65	3 (18%)	23,31,31	2.50	5 (21%)
3	CB3	B	608	-	31,37,37	2.15	10 (32%)	35,51,51	1.38	2 (5%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MTX	B	609	-	27,35,35	2.00	8 (29%)	30,49,49	1.91	6 (20%)
5	NDP	B	610	-	42,52,52	1.15	3 (7%)	55,80,80	1.75	6 (10%)
2	UMP	C	611	-	16,21,21	3.63	3 (18%)	23,31,31	2.52	5 (21%)
3	CB3	C	612	-	31,37,37	2.11	10 (32%)	35,51,51	1.39	3 (8%)
4	MTX	C	613	-	27,35,35	1.77	6 (22%)	30,49,49	2.00	9 (30%)
5	NDP	C	614	-	42,52,52	1.08	3 (7%)	55,80,80	1.85	9 (16%)
4	MTX	D	615	-	27,35,35	1.69	6 (22%)	30,49,49	1.88	6 (20%)
5	NDP	D	616	-	42,52,52	1.14	4 (9%)	55,80,80	1.97	9 (16%)

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	-	1/1/5/6	0/21/28/28	0/3/3/3
4	MTX	A	605	-	-	0/19/25/25	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	-	1/1/5/6	0/21/28/28	0/3/3/3
4	MTX	B	609	-	-	0/19/25/25	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	-	1/1/5/6	0/21/28/28	0/3/3/3
4	MTX	C	613	-	-	0/19/25/25	0/3/3/3
5	NDP	C	614	-	-	0/30/77/77	0/5/5/5
4	MTX	D	615	-	-	0/19/25/25	0/3/3/3
5	NDP	D	616	-	-	0/30/77/77	0/5/5/5

The worst 5 of 83 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	613	MTX	C-N	-5.20	1.22	1.34
4	B	609	MTX	C-N	-5.14	1.22	1.34
5	A	606	NDP	C4N-C5N	-4.95	1.38	1.49
5	C	614	NDP	C4N-C5N	-4.28	1.39	1.49
4	A	605	MTX	C-N	-4.24	1.24	1.34

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	616	NDP	N3A-C2A-N1A	-11.20	120.32	128.89
5	B	610	NDP	N3A-C2A-N1A	-10.30	121.01	128.89
5	C	614	NDP	N3A-C2A-N1A	-9.91	121.30	128.89
5	A	606	NDP	N3A-C2A-N1A	-9.29	121.78	128.89
4	B	609	MTX	C6-C9-N10	-6.10	103.18	113.78

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	604	CB3	CA
3	B	608	CB3	CA
3	C	612	CB3	CA

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 96 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	603	UMP	7	0
3	A	604	CB3	11	0
4	A	605	MTX	1	0
5	A	606	NDP	4	0
2	B	607	UMP	9	0
3	B	608	CB3	8	0
4	B	609	MTX	4	0
5	B	610	NDP	6	0
2	C	611	UMP	9	0
3	C	612	CB3	10	0
4	C	613	MTX	6	0
5	C	614	NDP	7	0
4	D	615	MTX	13	0
5	D	616	NDP	8	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, 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	508/521 (97%)	-0.11	15 (2%) 54 54	19, 38, 67, 100	0
1	B	510/521 (97%)	-0.09	16 (3%) 52 52	22, 39, 75, 129	0
1	C	510/521 (97%)	0.41	41 (8%) 15 13	33, 54, 98, 126	0
1	D	505/521 (96%)	0.71	55 (10%) 7 5	41, 73, 101, 126	0
All	All	2033/2084 (97%)	0.23	127 (6%) 24 23	19, 50, 94, 129	0

The worst 5 of 127 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	192	GLN	9.8
1	B	191	GLY	8.3
1	C	182	THR	7.1
1	D	257	ARG	7.0
1	D	256	ASN	6.9

### 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<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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	UMP	B	607	20/20	0.65	0.54	4.96	52,66,72,72	0
3	CB3	B	608	35/35	0.66	0.44	2.72	63,69,76,76	0
2	UMP	A	603	20/20	0.76	0.45	2.69	55,68,73,73	0
3	CB3	C	612	35/35	0.57	0.54	2.34	65,69,76,76	0
3	CB3	A	604	35/35	0.70	0.38	2.03	66,71,77,78	0
2	UMP	C	611	20/20	0.78	0.36	0.78	55,66,73,73	0
4	MTX	C	613	33/33	0.90	0.19	-0.26	52,63,100,144	0
4	MTX	B	609	33/33	0.95	0.14	-0.28	27,38,51,73	0
5	NDP	C	614	48/48	0.91	0.17	-0.35	50,74,118,195	0
4	MTX	D	615	33/33	0.87	0.21	-0.42	65,70,133,151	0
4	MTX	A	605	33/33	0.94	0.17	-0.46	28,40,56,79	0
5	NDP	D	616	48/48	0.88	0.20	-0.59	54,74,151,159	0
5	NDP	A	606	48/48	0.97	0.14	-0.89	27,38,50,69	0
5	NDP	B	610	48/48	0.98	0.11	-1.26	24,33,46,49	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.