Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:21 AM GMT

PDB ID	:	3EDW
Title	:	Replacement of Val3 in Human Thymidylate Synthase Affects Its Kinetic Properties and Intracellular Stability
Authors	:	Huang, X.; Gibson, L.M.; Bell, B.J.; Lovelace, L.L.; Pena, M.M.; Berger, F.G.; Berger, S.H.
Deposited on	:	2008-09-03
Resolution	:	1.75 Å(reported)

The following versions of software and data (see references (i)) 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 1.75 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	Percentile Ranks	Value
Clashscore		7
Ramachandran outliers		0.4%
Sidechain outliers		7.5%
RSRZ outliers		38.1%

Worse　　　　　　　　　　　　　　　　　*Better*

■ Percentile relative to all X-ray structures

◨ Percentile relative to X-ray structures of similar resolution
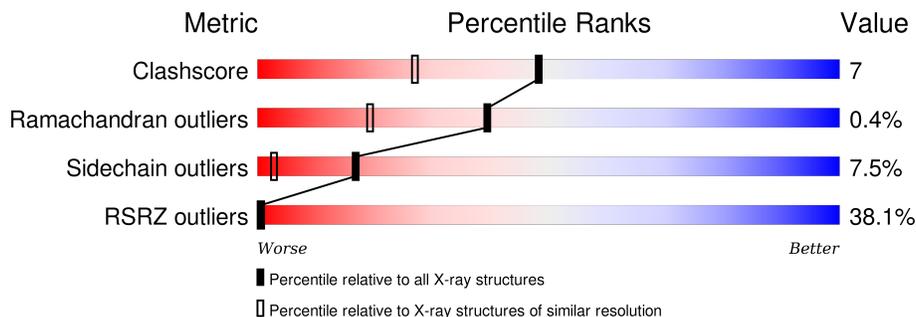
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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	X	313	32% · 65% · 13% · · 17%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2255 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	260	Total	C	N	O	S	0	0	0
			2116	1356	370	379	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	3	PHE	VAL	ENGINEERED	UNP P04818

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
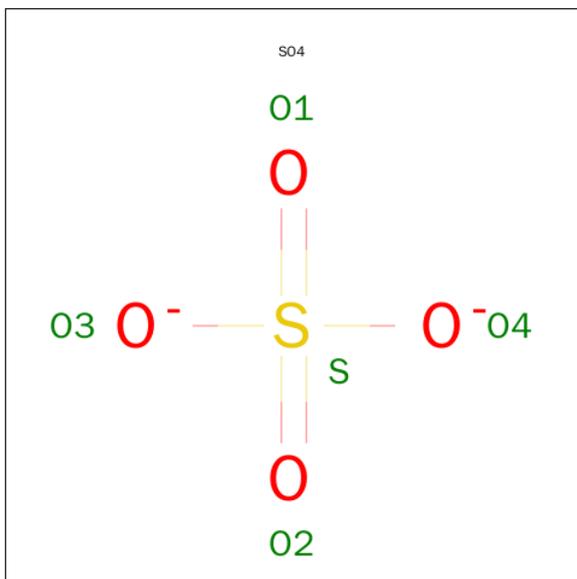
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	X	1	Total	O	S	0	0
			5	4	1		
2	X	1	Total	O	S	0	0
			5	4	1		
2	X	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	X	124	Total 124	O 124	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
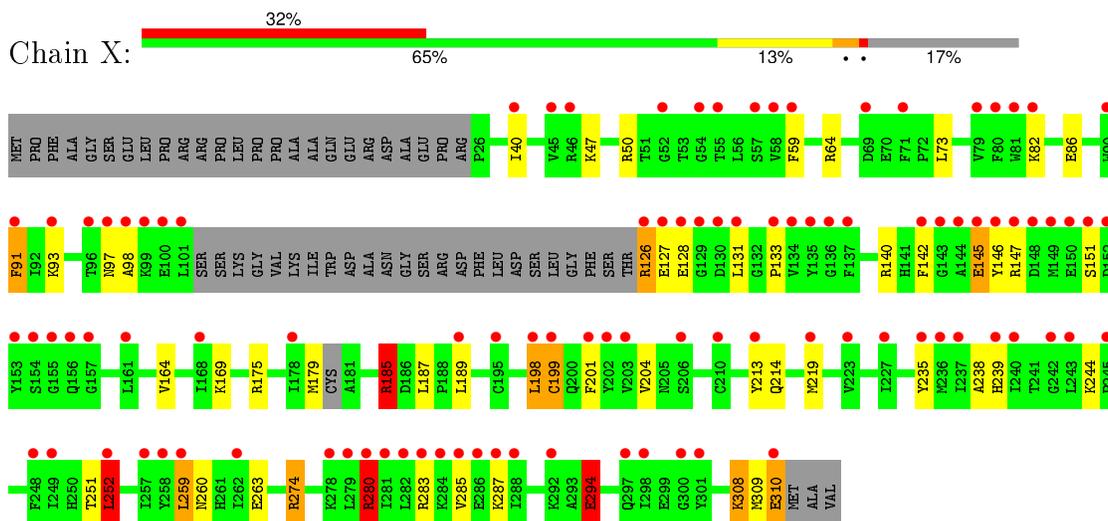
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	96.02Å 96.02Å 80.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.75 48.01 – 1.85	Depositor EDS
% Data completeness (in resolution range)	85.9 (50.00-1.75) 86.0 (48.01-1.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.42 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.229 , 0.268 0.287 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å²)	33.4	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.35 , 49.1	EDS
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
L-test for twinning[2]	$<|L|> = 0.50, <L^2> = 0.33$	Xtriage
Outliers	1 of 33721 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	2255	wwPDB-VP
Average B, all atoms (Å²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	X	1.34	13/2170 (0.6%)	1.17	12/2933 (0.4%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	235	TYR	CG-CD2	7.15	1.48	1.39
1	X	213	TYR	CD1-CE1	7.11	1.50	1.39
1	X	294	GLU	CG-CD	6.88	1.62	1.51
1	X	91	PHE	CE1-CZ	6.75	1.50	1.37
1	X	199	CYS	CB-SG	6.36	1.93	1.82
1	X	64	ARG	CG-CD	6.12	1.67	1.51
1	X	251	THR	CB-CG2	6.06	1.72	1.52
1	X	145	GLU	CG-CD	5.77	1.60	1.51
1	X	164	VAL	CB-CG2	5.73	1.64	1.52
1	X	59	PHE	CE1-CZ	5.55	1.48	1.37
1	X	238	ALA	CA-CB	-5.53	1.40	1.52
1	X	252	LEU	N-CA	-5.27	1.35	1.46
1	X	91	PHE	CG-CD2	5.23	1.46	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	274	ARG	NE-CZ-NH2	10.00	125.30	120.30
1	X	274	ARG	NE-CZ-NH1	-9.45	115.57	120.30
1	X	198	LEU	CB-CG-CD2	-6.83	99.39	111.00
1	X	140	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	X	280	ARG	NE-CZ-NH2	6.00	123.30	120.30
1	X	260	ASN	CB-CA-C	-5.81	98.78	110.40
1	X	73	LEU	CB-CG-CD1	5.58	120.49	111.00
1	X	175	ARG	NE-CZ-NH1	5.50	123.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	283	ARG	NE-CZ-NH2	5.45	123.03	120.30
1	X	47	LYS	CD-CE-NZ	-5.38	99.33	111.70
1	X	175	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	X	185	ARG	NE-CZ-NH1	5.27	122.94	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	X	2116	0	2094	30	0
2	X	15	0	0	0	0
3	X	124	0	0	4	0
All	All	2255	0	2094	30	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 7.

All (30) 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:X:280:ARG:HH21	1:X:280:ARG:HB2	1.02	1.12
1:X:294:GLU:N	1:X:294:GLU:OE1	1.91	1.02
1:X:239:HIS:HE1	1:X:285:VAL:H	1.11	0.95
1:X:126:ARG:HD3	1:X:128:GLU:CG	1.99	0.91
1:X:126:ARG:HD3	1:X:128:GLU:HG3	1.48	0.91
1:X:280:ARG:NH2	1:X:280:ARG:HB2	1.88	0.89
1:X:280:ARG:HH21	1:X:280:ARG:CB	1.92	0.77
1:X:294:GLU:H	1:X:294:GLU:CD	1.89	0.76
1:X:179:MET:C	3:X:415:HOH:O	2.23	0.75
1:X:93:LYS:HE3	3:X:405:HOH:O	1.94	0.67
1:X:239:HIS:CE1	1:X:285:VAL:H	2.04	0.61
1:X:263:GLU:HG3	3:X:418:HOH:O	2.02	0.58
1:X:126:ARG:HD3	1:X:128:GLU:HG2	1.82	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:98:ALA:HB2	1:X:131:LEU:HD21	1.87	0.56
1:X:169:LYS:HD2	3:X:439:HOH:O	2.06	0.55
1:X:126:ARG:CD	1:X:128:GLU:HG3	2.33	0.51
1:X:50:ARG:HD2	1:X:185:ARG:CZ	2.41	0.50
1:X:50:ARG:HD2	1:X:185:ARG:NH2	2.27	0.48
1:X:133:PRO:HB3	1:X:146:TYR:HB2	1.98	0.46
1:X:40:ILE:CD1	1:X:219:MET:HG3	2.47	0.45
1:X:308:LYS:HB3	1:X:308:LYS:HE2	1.70	0.44
1:X:214:GLN:HB2	1:X:252:LEU:HD12	2.00	0.43
1:X:259:LEU:HA	1:X:259:LEU:HD12	1.76	0.43
1:X:244:LYS:HA	1:X:244:LYS:HD3	1.87	0.42
1:X:147:ARG:NH2	1:X:151:SER:HB3	2.35	0.42
1:X:199:CYS:SG	1:X:201:PHE:CZ	3.13	0.41
1:X:187:LEU:HA	1:X:187:LEU:HD23	1.79	0.41
1:X:309:MET:O	1:X:310:GLU:C	2.60	0.41
1:X:142:PHE:C	1:X:142:PHE:CD2	2.95	0.40
1:X:198:LEU:HD12	1:X:198:LEU:C	2.42	0.40

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	X	254/313 (81%)	241 (95%)	12 (5%)	1 (0%)	39 19

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	127	GLU

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	X	228/271 (84%)	211 (92%)	17 (8%)	17 3

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	82	LYS
1	X	86	GLU
1	X	91	PHE
1	X	97	ASN
1	X	126	ARG
1	X	145	GLU
1	X	185	ARG
1	X	189	LEU
1	X	204	VAL
1	X	252	LEU
1	X	259	LEU
1	X	274	ARG
1	X	280	ARG
1	X	287	LYS
1	X	294	GLU
1	X	308	LYS
1	X	310	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	97	ASN
1	X	171	ASN
1	X	239	HIS

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)

3 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	SO4	X	315	-	4,4,4	0.39	0	6,6,6	0.71	0
2	SO4	X	317	-	4,4,4	0.76	0	6,6,6	0.89	0
2	SO4	X	318	-	4,4,4	0.94	0	6,6,6	0.64	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	X	315	-	-	0/0/0/0	0/0/0/0
2	SO4	X	317	-	-	0/0/0/0	0/0/0/0
2	SO4	X	318	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	X	260/313 (83%)	1.93	99 (38%)	0	0	29, 47, 85, 96	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	127	GLU	8.0
1	X	131	LEU	7.1
1	X	128	GLU	6.8
1	X	129	GLY	6.6
1	X	147	ARG	6.6
1	X	148	ASP	6.4
1	X	142	PHE	6.2
1	X	282	LEU	6.2
1	X	98	ALA	5.9
1	X	145	GLU	5.9
1	X	101	LEU	5.7
1	X	281	ILE	5.3
1	X	199	CYS	5.3
1	X	153	TYR	5.0
1	X	126	ARG	4.8
1	X	151	SER	4.8
1	X	144	ALA	4.6
1	X	240	ILE	4.5
1	X	133	PRO	4.5
1	X	152	ASP	4.3
1	X	150	GLU	3.9
1	X	99	LYS	3.8
1	X	146	TYR	3.8
1	X	198	LEU	3.8
1	X	155	GLY	3.7
1	X	100	GLU	3.7
1	X	134	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	X	284	LYS	3.6
1	X	154	SER	3.6
1	X	287	LYS	3.6
1	X	235	TYR	3.5
1	X	288	ILE	3.4
1	X	45	VAL	3.3
1	X	136	GLY	3.3
1	X	149	MET	3.3
1	X	298	ILE	3.2
1	X	286	GLU	3.1
1	X	135	TYR	3.1
1	X	283	ARG	3.1
1	X	157	GLY	3.1
1	X	280	ARG	3.1
1	X	189	LEU	3.0
1	X	242	GLY	3.0
1	X	143	GLY	3.0
1	X	195	CYS	3.0
1	X	79	VAL	3.0
1	X	69	ASP	2.9
1	X	156	GLN	2.9
1	X	239	HIS	2.9
1	X	90	TRP	2.8
1	X	46	ARG	2.8
1	X	97	ASN	2.8
1	X	249	ILE	2.7
1	X	81	TRP	2.7
1	X	82	LYS	2.7
1	X	278	LYS	2.7
1	X	202	TYR	2.7
1	X	236	MET	2.7
1	X	297	GLN	2.7
1	X	178	ILE	2.6
1	X	91	PHE	2.6
1	X	213	TYR	2.6
1	X	223	VAL	2.6
1	X	201	PHE	2.6
1	X	227	ILE	2.5
1	X	210	CYS	2.5
1	X	137	PHE	2.5
1	X	259	LEU	2.5
1	X	130	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	X	203	VAL	2.5
1	X	285	VAL	2.5
1	X	58	VAL	2.4
1	X	54	GLY	2.4
1	X	292	LYS	2.4
1	X	245	PRO	2.4
1	X	59	PHE	2.3
1	X	206	SER	2.3
1	X	96	THR	2.3
1	X	257	ILE	2.3
1	X	219	MET	2.3
1	X	57	SER	2.3
1	X	55	THR	2.2
1	X	80	PHE	2.2
1	X	161	LEU	2.2
1	X	40	ILE	2.2
1	X	52	GLY	2.2
1	X	237	ILE	2.2
1	X	258	TYR	2.2
1	X	301	TYR	2.2
1	X	248	PHE	2.1
1	X	310	GLU	2.1
1	X	71	PHE	2.1
1	X	243	LEU	2.1
1	X	279	LEU	2.1
1	X	93	LYS	2.1
1	X	300	GLY	2.1
1	X	252	LEU	2.0
1	X	168	ILE	2.0
1	X	262	ILE	2.0

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.

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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
2	SO4	X	318	5/5	0.94	0.18	0.36	54,56,57,58	0
2	SO4	X	315	5/5	0.90	0.10	-1.45	79,81,83,83	0
2	SO4	X	317	5/5	0.92	0.12	-1.77	52,61,61,65	0

6.5 Other polymers (i)

There are no such residues in this entry.