



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:51 PM UTC

PDB ID : 3EDW / pdb_00003edw
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)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

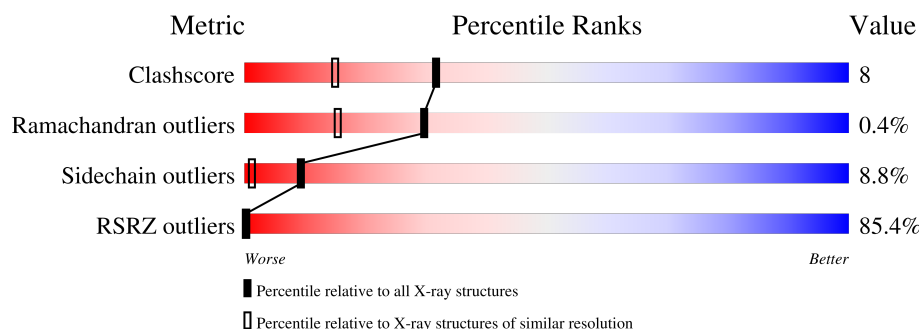
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	X	313	71% 62% 17% • 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
			Total	C	N	O	S			
1	X	260	2116	1356	370	379	11	0	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	X	1	5	4	1	0	0
2	X	1	5	4	1	0	0
2	X	1	5	4	1	0	0

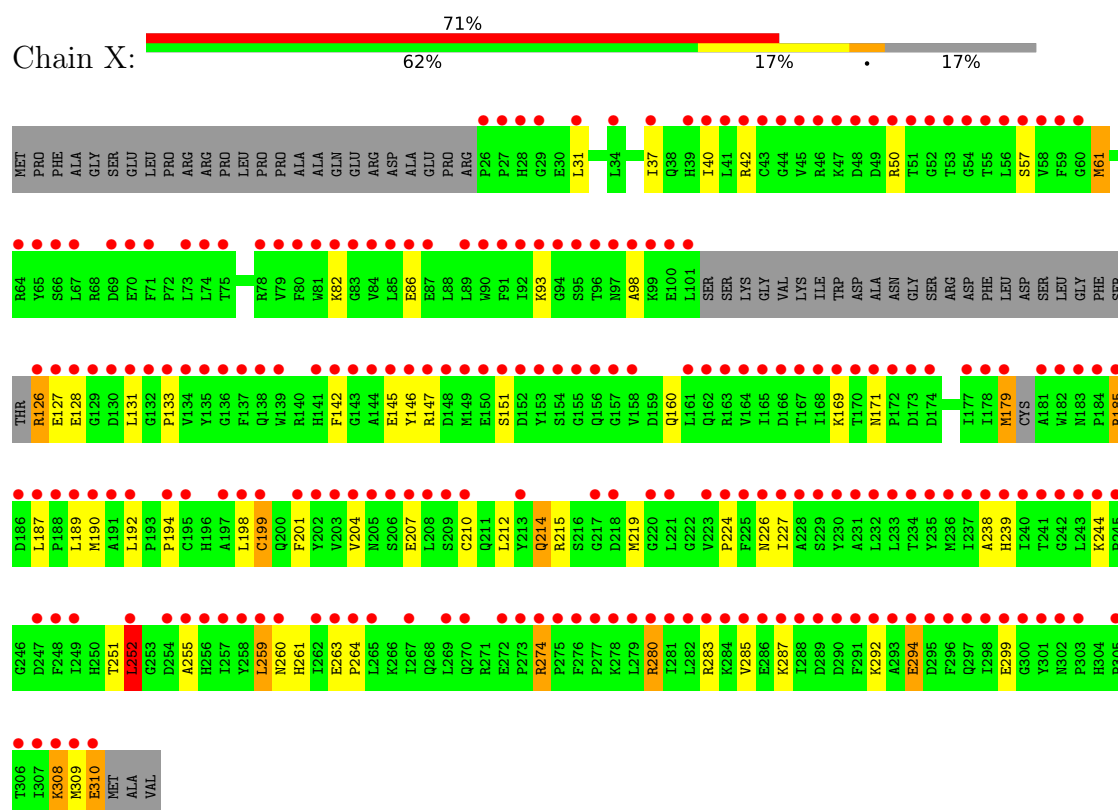
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	X	124	Total 124	O 124	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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

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 50.00 – 1.85	Depositor EDS
% Data completeness (in resolution range)	85.9 (50.00-1.75) 85.9 (50.00-1.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.60 (at 1.86Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.229 , 0.268 0.305 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.513	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	2255	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: 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	1.62	25/2170 (1.2%)	1.38	8/2933 (0.3%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	252	LEU	N-CA	-8.01	1.35	1.45
1	X	238	ALA	CA-CB	-7.99	1.40	1.53
1	X	212	LEU	C-O	-7.19	1.15	1.24
1	X	251	THR	N-CA	7.05	1.54	1.45
1	X	171	ASN	N-CA	-6.68	1.40	1.46
1	X	215	ARG	C-O	6.49	1.32	1.24
1	X	37	ILE	N-CA	6.33	1.53	1.46
1	X	31	LEU	C-O	6.08	1.31	1.24
1	X	251	THR	CB-CG2	6.00	1.72	1.52
1	X	214	GLN	C-O	-5.94	1.16	1.24
1	X	192	LEU	C-O	5.93	1.26	1.23
1	X	255	ALA	CA-CB	-5.89	1.45	1.53
1	X	251	THR	C-N	5.69	1.41	1.33
1	X	199	CYS	CA-C	5.61	1.59	1.52
1	X	207	GLU	C-O	5.45	1.30	1.24
1	X	192	LEU	N-CA	5.39	1.50	1.46
1	X	199	CYS	CA-CB	5.38	1.61	1.53
1	X	179	MET	CB-CG	-5.32	1.36	1.52
1	X	210	CYS	C-O	-5.26	1.18	1.24
1	X	224	PRO	C-O	5.25	1.31	1.24
1	X	160	GLN	CA-C	-5.22	1.46	1.52
1	X	57	SER	N-CA	5.19	1.52	1.46
1	X	192	LEU	CA-CB	5.17	1.57	1.52
1	X	61	MET	CA-C	5.16	1.58	1.52
1	X	179	MET	SD-CE	-5.08	1.66	1.79

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	260	ASN	N-CA-C	6.93	120.83	112.38
1	X	274	ARG	NE-CZ-NH2	6.78	125.30	119.20
1	X	226	ASN	N-CA-C	6.65	118.53	111.28
1	X	274	ARG	NE-CZ-NH1	-5.93	115.57	121.50
1	X	212	LEU	CA-C-O	-5.63	114.44	120.46
1	X	227	ILE	N-CA-C	-5.62	105.02	110.42
1	X	260	ASN	CB-CA-C	-5.47	98.78	110.32
1	X	252	LEU	O-C-N	5.26	129.37	123.27

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	X	2116	0	2094	33	0
2	X	15	0	0	0	0
3	X	124	0	0	4	0
All	All	2255	0	2094	33	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 8.

All (33) 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:HB2	1:X:280:ARG:NH2	1.88	0.89
1:X:294:GLU:H	1:X:294:GLU:CD	1.89	0.80
1:X:179:MET:C	3:X:415:HOH:O	2.23	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:280:ARG:HH21	1:X:280:ARG:CB	1.92	0.77
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
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:190:MET:HE3	1:X:194:PRO:HD2	1.93	0.49
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:309:MET:O	1:X:310:GLU:C	2.60	0.45
1:X:142:PHE:C	1:X:142:PHE:CD2	2.95	0.45
1:X:198:LEU:C	1:X:198:LEU:HD12	2.42	0.45
1:X:40:ILE:CD1	1:X:219:MET:HG3	2.47	0.45
1:X:308:LYS:HE2	1:X:308:LYS:HB3	1.70	0.44
1:X:261:HIS:C	1:X:264:PRO:HD2	2.43	0.44
1:X:214:GLN:HB2	1:X:252:LEU:HD12	2.00	0.43
1:X:259:LEU:HD12	1:X:259:LEU:HA	1.76	0.43
1:X:244:LYS:HD3	1:X:244:LYS:HA	1.87	0.42
1:X:147:ARG:NH2	1:X:151:SER:HB3	2.35	0.42
1:X:187:LEU:HA	1:X:187:LEU:HD23	1.79	0.41
1:X:199:CYS:SG	1:X:201:PHE:CZ	3.13	0.41
1:X:179:MET:HB2	1:X:179:MET:HE2	1.76	0.41

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	X	254/313 (81%)	241 (95%)	12 (5%)	1 (0%)	30 15

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%)	208 (91%)	20 (9%)	9 1

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	42	ARG
1	X	61	MET
1	X	82	LYS
1	X	86	GLU
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	283	ARG
1	X	287	LYS
1	X	292	LYS
1	X	294	GLU
1	X	299	GLU
1	X	308	LYS
1	X	310	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	97	ASN
1	X	171	ASN
1	X	239	HIS
1	X	270	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 oligosaccharides 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	0.43	0	6,6,6	0.72	0
2	SO4	X	318	-	4,4,4	0.35	0	6,6,6	0.93	0
2	SO4	X	317	-	4,4,4	0.61	0	6,6,6	1.08	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

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, 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%)	3.48	222 (85%) 0 0	29, 47, 85, 96	0

All (222) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	189	LEU	7.9
1	X	284	LYS	7.5
1	X	52	GLY	7.4
1	X	298	ILE	7.1
1	X	26	PRO	6.8
1	X	281	ILE	6.8
1	X	288	ILE	6.8
1	X	131	LEU	6.7
1	X	142	PHE	6.7
1	X	136	GLY	6.6
1	X	134	VAL	6.6
1	X	240	ILE	6.5
1	X	153	TYR	6.5
1	X	293	ALA	6.4
1	X	101	LEU	6.3
1	X	147	ARG	6.3
1	X	235	TYR	6.2
1	X	191	ALA	6.2
1	X	242	GLY	6.1
1	X	243	LEU	6.1
1	X	259	LEU	6.1
1	X	282	LEU	6.0
1	X	54	GLY	6.0
1	X	199	CYS	6.0
1	X	98	ALA	6.0
1	X	146	TYR	5.9
1	X	81	TRP	5.9

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Mol	Chain	Res	Type	RSRZ
1	X	91	PHE	5.7
1	X	278	LYS	5.6
1	X	239	HIS	5.6
1	X	45	VAL	5.5
1	X	133	PRO	5.5
1	X	280	ARG	5.4
1	X	279	LEU	5.4
1	X	287	LYS	5.3
1	X	285	VAL	5.3
1	X	148	ASP	5.2
1	X	127	GLU	5.1
1	X	44	GLY	5.1
1	X	53	THR	5.1
1	X	129	GLY	5.1
1	X	204	VAL	5.1
1	X	50	ARG	5.1
1	X	237	ILE	5.0
1	X	203	VAL	5.0
1	X	192	LEU	4.9
1	X	236	MET	4.9
1	X	301	TYR	4.9
1	X	79	VAL	4.9
1	X	232	LEU	4.8
1	X	161	LEU	4.8
1	X	157	GLY	4.7
1	X	69	ASP	4.7
1	X	165	ILE	4.6
1	X	43	CYS	4.6
1	X	41	LEU	4.6
1	X	185	ARG	4.6
1	X	82	LYS	4.6
1	X	135	TYR	4.5
1	X	172	PRO	4.5
1	X	75	THR	4.5
1	X	128	GLU	4.5
1	X	89	LEU	4.5
1	X	51	THR	4.4
1	X	152	ASP	4.4
1	X	71	PHE	4.4
1	X	85	LEU	4.4
1	X	208	LEU	4.4
1	X	55	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	X	144	ALA	4.3
1	X	295	ASP	4.3
1	X	90	TRP	4.2
1	X	283	ARG	4.2
1	X	244	LYS	4.2
1	X	290	ASP	4.2
1	X	92	ILE	4.2
1	X	48	ASP	4.1
1	X	96	THR	4.1
1	X	57	SER	4.1
1	X	245	PRO	4.1
1	X	258	TYR	4.1
1	X	40	ILE	4.1
1	X	198	LEU	4.0
1	X	27	PRO	4.0
1	X	70	GLU	4.0
1	X	238	ALA	4.0
1	X	277	PRO	3.9
1	X	297	GLN	3.9
1	X	187	LEU	3.9
1	X	151	SER	3.9
1	X	168	ILE	3.9
1	X	292	LYS	3.9
1	X	66	SER	3.9
1	X	267	ILE	3.9
1	X	202	TYR	3.9
1	X	46	ARG	3.8
1	X	300	GLY	3.8
1	X	257	ILE	3.8
1	X	275	PRO	3.8
1	X	262	ILE	3.7
1	X	174	ASP	3.7
1	X	260	ASN	3.7
1	X	241	THR	3.7
1	X	194	PRO	3.6
1	X	233	LEU	3.6
1	X	65	TYR	3.6
1	X	206	SER	3.6
1	X	220	GLY	3.6
1	X	94	GLY	3.5
1	X	231	ALA	3.5
1	X	307	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	X	47	LYS	3.5
1	X	154	SER	3.5
1	X	145	GLU	3.5
1	X	170	THR	3.5
1	X	58	VAL	3.5
1	X	190	MET	3.5
1	X	289	ASP	3.4
1	X	138	GLN	3.4
1	X	137	PHE	3.4
1	X	149	MET	3.4
1	X	296	PHE	3.4
1	X	156	GLN	3.4
1	X	188	PRO	3.4
1	X	207	GLU	3.4
1	X	302	ASN	3.4
1	X	178	ILE	3.4
1	X	31	LEU	3.4
1	X	276	PHE	3.4
1	X	67	LEU	3.3
1	X	294	GLU	3.3
1	X	139	TRP	3.3
1	X	34	LEU	3.3
1	X	310	GLU	3.3
1	X	209	SER	3.3
1	X	227	ILE	3.3
1	X	255	ALA	3.2
1	X	248	PHE	3.2
1	X	299	GLU	3.2
1	X	143	GLY	3.2
1	X	150	GLU	3.2
1	X	303	PRO	3.1
1	X	83	GLY	3.1
1	X	80	PHE	3.1
1	X	167	THR	3.1
1	X	234	THR	3.1
1	X	249	ILE	3.1
1	X	181	ALA	3.1
1	X	272	GLU	3.1
1	X	164	VAL	3.0
1	X	305	PRO	3.0
1	X	265	LEU	3.0
1	X	126	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	X	132	GLY	3.0
1	X	308	LYS	3.0
1	X	28	HIS	3.0
1	X	162	GLN	2.9
1	X	93	LYS	2.9
1	X	99	LYS	2.9
1	X	273	PRO	2.9
1	X	173	ASP	2.9
1	X	228	ALA	2.9
1	X	182	TRP	2.9
1	X	270	GLN	2.9
1	X	86	GLU	2.9
1	X	205	ASN	2.9
1	X	247	ASP	2.8
1	X	39	HIS	2.8
1	X	42	ARG	2.8
1	X	201	PHE	2.8
1	X	100	GLU	2.8
1	X	291	PHE	2.8
1	X	225	PHE	2.7
1	X	263	GLU	2.7
1	X	84	VAL	2.7
1	X	256	HIS	2.7
1	X	306	THR	2.7
1	X	87	GLU	2.7
1	X	269	LEU	2.7
1	X	74	LEU	2.6
1	X	158	VAL	2.6
1	X	229	SER	2.6
1	X	97	ASN	2.6
1	X	59	PHE	2.5
1	X	169	LYS	2.5
1	X	78	ARG	2.5
1	X	179	MET	2.5
1	X	184	PRO	2.5
1	X	286	GLU	2.5
1	X	155	GLY	2.4
1	X	186	ASP	2.4
1	X	73	LEU	2.4
1	X	224	PRO	2.4
1	X	37	ILE	2.4
1	X	130	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	X	218	ASP	2.4
1	X	309	MET	2.4
1	X	171	ASN	2.3
1	X	56	LEU	2.3
1	X	223	VAL	2.3
1	X	226	ASN	2.3
1	X	217	GLY	2.3
1	X	252	LEU	2.3
1	X	210	CYS	2.2
1	X	95	SER	2.2
1	X	177	ILE	2.2
1	X	183	ASN	2.2
1	X	213	TYR	2.2
1	X	230	TYR	2.2
1	X	254	ASP	2.2
1	X	195	CYS	2.2
1	X	141	HIS	2.2
1	X	264	PRO	2.2
1	X	49	ASP	2.1
1	X	197	ALA	2.1
1	X	163	ARG	2.1
1	X	29	GLY	2.0
1	X	64	ARG	2.0
1	X	274	ARG	2.0
1	X	221	LEU	2.0
1	X	60	GLY	2.0
1	X	166	ASP	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 oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	X	315	5/5	0.86	0.14	79,81,83,83	0
2	SO4	X	318	5/5	0.86	0.20	54,56,57,58	0
2	SO4	X	317	5/5	0.89	0.14	52,61,61,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.