



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:08 PM UTC

PDB ID : 1XK7 / pdb_00001xk7
Title : Crystal Structure- C2 form- of Escherichia coli Crotonobetainyl-CoA: carnitine CoA transferase (CaiB)
Authors : Rangarajan, E.S.; Li, Y.; Iannuzzi, P.; Cygler, M.; Matte, A.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)
Deposited on : 2004-09-27
Resolution : 1.60 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

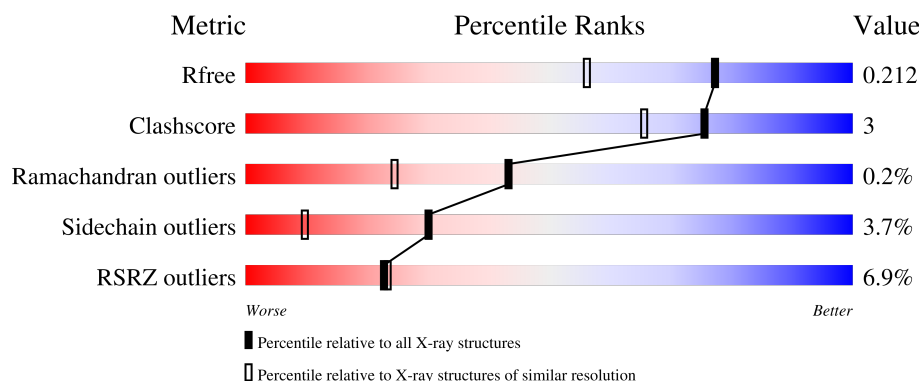
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	A	408	7% 93% 6%
1	B	408	5% 92% 6%
1	C	408	8% 93% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10735 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 Crotonobetainyl-CoA:carnitine CoA-transferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	Se	0	0	0
			3187	2038	531	594	7	17			
1	B	407	Total	C	N	O	S	Se	0	0	0
			3187	2038	531	594	7	17			
1	C	407	Total	C	N	O	S	Se	0	0	0
			3187	2038	531	594	7	17			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	cloning artifact	UNP P31572
A	-1	SER	-	cloning artifact	UNP P31572
A	0	HIS	-	cloning artifact	UNP P31572
B	-2	GLY	-	cloning artifact	UNP P31572
B	-1	SER	-	cloning artifact	UNP P31572
B	0	HIS	-	cloning artifact	UNP P31572
C	-2	GLY	-	cloning artifact	UNP P31572
C	-1	SER	-	cloning artifact	UNP P31572
C	0	HIS	-	cloning artifact	UNP P31572

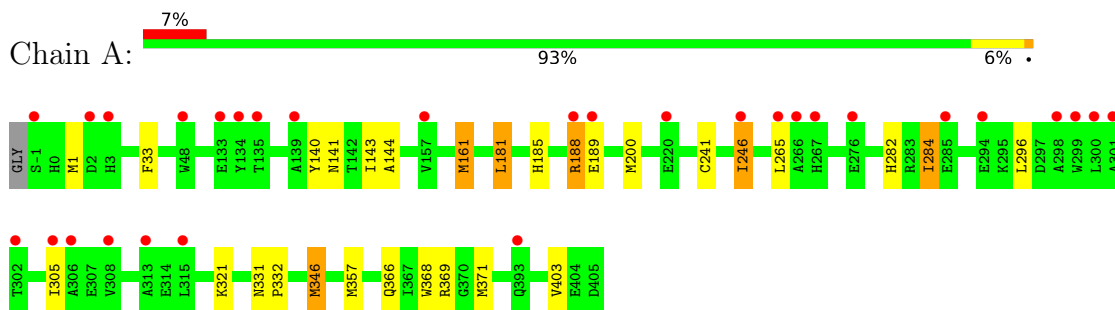
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	381	Total	O	0	0
			381	381		
2	B	383	Total	O	0	0
			383	383		
2	C	410	Total	O	0	0
			410	410		

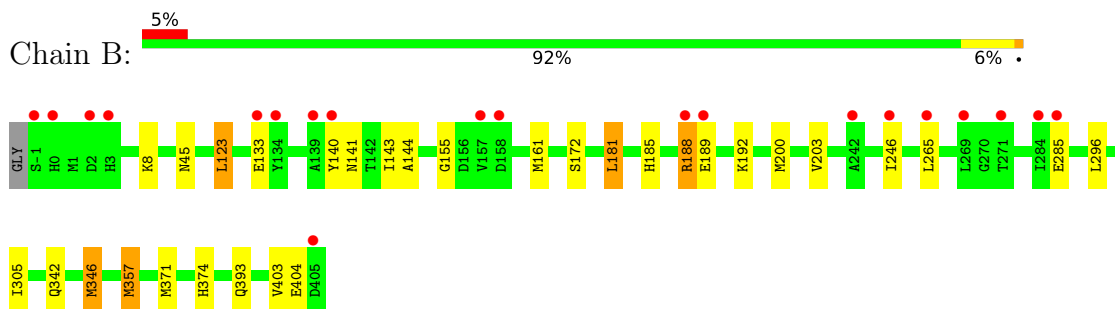
3 Residue-property plots

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.

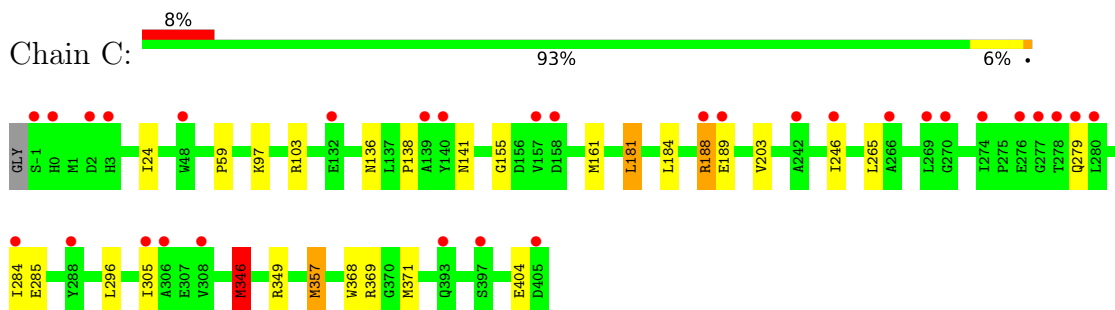
- Molecule 1: Crotonobetainyl-CoA:carnitine CoA-transferase



- Molecule 1: Crotonobetainyl-CoA:carnitine CoA-transferase



- Molecule 1: Crotonobetainyl-CoA:carnitine CoA-transferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	184.28Å 106.17Å 69.68Å 90.00° 107.45° 90.00°	Depositor
Resolution (Å)	45.44 – 1.60 45.44 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.44-1.60) 99.9 (45.44-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.86 (at 1.60Å)	Xtriage
Refinement program	CNS 1.1, REFMAC 5.1.24	Depositor
R, R_{free}	0.187 , 0.213 0.187 , 0.212	Depositor DCC
R_{free} test set	8476 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	14.9	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10735	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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 [i](#)

5.1 Standard geometry [i](#)

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	0/3251	0.77	0/4380
1	B	0.42	0/3251	0.76	0/4380
1	C	0.42	1/3251 (0.0%)	0.77	1/4380 (0.0%)
All	All	0.42	1/9753 (0.0%)	0.77	1/13140 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	346	MSE	SE-CE	5.87	2.13	1.95

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	24	ILE	N-CA-C	5.35	116.50	111.48

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	A	3187	0	3122	19	0
1	B	3187	0	3122	25	0
1	C	3187	0	3122	25	0
2	A	381	0	0	1	0
2	B	383	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	410	0	0	3	0
All	All	10735	0	9366	57	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 3.

All (57) 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:B:185:HIS:HA	1:B:188:ARG:HH22	1.02	1.18
1:A:185:HIS:HA	1:A:188:ARG:HH22	1.08	1.15
1:B:161:MSE:HE1	1:C:155:GLY:HA2	1.32	1.11
1:B:155:GLY:HA2	1:C:161:MSE:HE1	1.35	1.04
1:B:185:HIS:HA	1:B:188:ARG:NH2	1.77	0.99
1:A:185:HIS:HA	1:A:188:ARG:NH2	1.89	0.86
1:A:188:ARG:HH21	1:A:188:ARG:HB2	1.42	0.85
1:B:155:GLY:CA	1:C:161:MSE:HE1	2.06	0.84
1:B:161:MSE:HE1	1:C:155:GLY:CA	2.10	0.81
1:C:184:LEU:HG	1:C:188:ARG:HH12	1.45	0.80
1:A:366:GLN:HE22	1:B:342:GLN:HE22	1.34	0.74
1:C:346:MSE:HG3	1:C:371:MSE:O	1.91	0.71
1:A:346:MSE:HG3	1:A:371:MSE:O	1.93	0.67
1:A:284:ILE:H	1:A:284:ILE:HD12	1.61	0.66
1:B:346:MSE:HG3	1:B:371:MSE:O	1.98	0.62
1:B:161:MSE:HE2	2:C:546:HOH:O	1.99	0.61
1:C:284:ILE:HD12	1:C:284:ILE:H	1.67	0.59
1:A:188:ARG:HH21	1:A:188:ARG:CB	2.15	0.58
1:A:284:ILE:HD12	1:A:284:ILE:N	2.20	0.56
1:C:184:LEU:HG	1:C:188:ARG:NH1	2.19	0.55
1:B:357:MSE:HE1	1:C:203:VAL:HG22	1.88	0.54
1:A:305:ILE:HD13	1:A:321:LYS:HE2	1.90	0.54
1:B:393:GLN:NE2	2:B:741:HOH:O	2.36	0.54
1:B:203:VAL:HG22	1:C:357:MSE:HE1	1.88	0.54
1:C:284:ILE:HD12	1:C:284:ILE:N	2.23	0.52
1:B:357:MSE:CE	1:C:203:VAL:HG22	2.41	0.50
1:A:282:HIS:CE1	1:A:284:ILE:HD13	2.47	0.49
1:B:123:LEU:HD21	1:B:172:SER:HB3	1.95	0.49
1:B:188:ARG:NH2	1:C:188:ARG:HE	2.11	0.49
1:C:97:LYS:HG2	1:C:138:PRO:HA	1.94	0.48
1:B:140:TYR:HB2	1:B:143:ILE:HD12	1.95	0.48
1:A:366:GLN:HE22	1:B:342:GLN:NE2	2.07	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:MSE:HE2	2:C:546:HOH:O	2.14	0.47
1:B:45:ASN:O	1:B:374:HIS:HE1	1.98	0.47
1:B:203:VAL:HG22	1:C:357:MSE:CE	2.46	0.46
1:A:33:PHE:HE2	1:A:181:LEU:HD13	1.84	0.43
1:B:404:GLU:CD	1:B:404:GLU:H	2.26	0.43
1:B:144:ALA:HB2	1:B:200:MSE:HE2	2.01	0.43
1:B:144:ALA:CB	1:B:200:MSE:HE2	2.49	0.43
1:C:184:LEU:HG	1:C:188:ARG:HH22	1.83	0.43
1:B:181:LEU:HB3	1:C:181:LEU:HB3	2.01	0.42
1:C:59:PRO:HB2	1:C:371:MSE:SE	2.68	0.42
1:C:161:MSE:HE2	1:C:161:MSE:HB2	1.73	0.42
1:A:140:TYR:HB2	1:A:143:ILE:HD12	2.00	0.42
1:C:369:ARG:HB3	2:C:461:HOH:O	2.18	0.42
1:C:103:ARG:NH2	1:C:136:ASN:OD1	2.52	0.42
1:A:161:MSE:HE2	1:A:161:MSE:HB2	1.66	0.42
1:C:357:MSE:HE2	1:C:357:MSE:HB2	1.86	0.42
1:A:331:ASN:HA	1:A:332:PRO:HD3	1.95	0.41
1:A:144:ALA:HB2	1:A:200:MSE:HE2	2.02	0.41
1:C:368:TRP:CE3	1:C:369:ARG:HB2	2.55	0.41
1:A:368:TRP:CE3	1:A:369:ARG:HB2	2.54	0.41
1:A:369:ARG:HB3	2:A:567:HOH:O	2.19	0.41
1:B:246:ILE:HG23	1:B:305:ILE:HD12	2.02	0.41
1:B:246:ILE:HG23	1:B:305:ILE:CD1	2.51	0.41
1:C:246:ILE:HG23	1:C:305:ILE:CD1	2.50	0.41
1:A:241:CYS:SG	1:A:246:ILE:HG12	2.62	0.40

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	405/408 (99%)	395 (98%)	9 (2%)	1 (0%)	43 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	405/408 (99%)	395 (98%)	9 (2%)	1 (0%)	43	24
1	C	405/408 (99%)	397 (98%)	8 (2%)	0	100	100
All	All	1215/1224 (99%)	1187 (98%)	26 (2%)	2 (0%)	43	24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	403	VAL
1	B	403	VAL

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	334/317 (105%)	322 (96%)	12 (4%)	31	10
1	B	334/317 (105%)	321 (96%)	13 (4%)	28	9
1	C	334/317 (105%)	322 (96%)	12 (4%)	31	10
All	All	1002/951 (105%)	965 (96%)	37 (4%)	30	10

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	141	ASN
1	A	161	MSE
1	A	181	LEU
1	A	188	ARG
1	A	189	GLU
1	A	246	ILE
1	A	265	LEU
1	A	284	ILE
1	A	296	LEU
1	A	346	MSE
1	A	357	MSE

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Mol	Chain	Res	Type
1	B	8	LYS
1	B	123	LEU
1	B	133	GLU
1	B	141	ASN
1	B	181	LEU
1	B	188	ARG
1	B	189	GLU
1	B	192	LYS
1	B	265	LEU
1	B	285	GLU
1	B	296	LEU
1	B	346	MSE
1	B	357	MSE
1	C	141	ASN
1	C	181	LEU
1	C	188	ARG
1	C	189	GLU
1	C	265	LEU
1	C	279	GLN
1	C	285	GLU
1	C	296	LEU
1	C	346	MSE
1	C	349	ARG
1	C	357	MSE
1	C	404	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	60	GLN
1	A	267	HIS
1	A	374	HIS
1	A	384	ASN
1	B	31	GLN
1	B	153	GLN
1	B	267	HIS
1	B	342	GLN
1	B	374	HIS
1	B	384	ASN
1	C	31	GLN
1	C	57	ASN

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Mol	Chain	Res	Type
1	C	342	GLN
1	C	363	ASN
1	C	374	HIS
1	C	384	ASN
1	C	390	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	A	390/408 (95%)	0.36	30 (7%) 19 20	10, 18, 33, 39	0
1	B	390/408 (95%)	0.18	20 (5%) 33 34	10, 15, 30, 37	0
1	C	390/408 (95%)	0.31	31 (7%) 18 19	9, 16, 29, 35	0
All	All	1170/1224 (95%)	0.28	81 (6%) 23 23	9, 16, 32, 39	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	48	TRP	6.5
1	C	188	ARG	5.0
1	C	189	GLU	4.9
1	A	188	ARG	4.8
1	B	188	ARG	4.7
1	B	140	TYR	4.6
1	A	189	GLU	4.5
1	B	189	GLU	4.0
1	B	3	HIS	3.7
1	C	3	HIS	3.7
1	C	158	ASP	3.6
1	C	246	ILE	3.4
1	A	308	VAL	3.4
1	C	48	TRP	3.4
1	B	405	ASP	3.2
1	C	139	ALA	3.1
1	C	140	TYR	3.1
1	A	3	HIS	3.0
1	C	288	TYR	3.0
1	B	139	ALA	2.9
1	C	284	ILE	2.9
1	C	270	GLY	2.9
1	C	242	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	0	HIS	2.8
1	C	397	SER	2.8
1	B	0	HIS	2.8
1	A	139	ALA	2.8
1	A	246	ILE	2.7
1	A	305	ILE	2.7
1	B	2	ASP	2.6
1	C	280	LEU	2.6
1	C	274	ILE	2.6
1	C	278	THR	2.6
1	C	405	ASP	2.6
1	A	265	LEU	2.6
1	A	306	ALA	2.6
1	C	277	GLY	2.5
1	C	279	GLN	2.5
1	B	285	GLU	2.5
1	A	299	TRP	2.5
1	C	-1	SER	2.5
1	A	285	GLU	2.5
1	A	266	ALA	2.5
1	C	266	ALA	2.5
1	C	2	ASP	2.5
1	A	298	ALA	2.5
1	A	135	THR	2.5
1	A	2	ASP	2.4
1	B	158	ASP	2.4
1	A	313	ALA	2.4
1	B	-1	SER	2.4
1	C	157	VAL	2.4
1	A	133	GLU	2.4
1	C	276	GLU	2.4
1	C	393	GLN	2.4
1	A	315	LEU	2.4
1	A	301	ALA	2.4
1	A	276	GLU	2.4
1	B	265	LEU	2.3
1	C	305	ILE	2.3
1	A	393	GLN	2.3
1	B	242	ALA	2.3
1	B	134	TYR	2.3
1	A	157	VAL	2.3
1	A	302	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	294	GLU	2.3
1	B	271	THR	2.2
1	B	284	ILE	2.2
1	B	133	GLU	2.2
1	C	306	ALA	2.2
1	B	269	LEU	2.2
1	C	269	LEU	2.2
1	A	134	TYR	2.2
1	C	132	GLU	2.1
1	A	267	HIS	2.1
1	A	220	GLU	2.1
1	A	300	LEU	2.1
1	B	246	ILE	2.1
1	A	-1	SER	2.1
1	B	157	VAL	2.0
1	C	308	VAL	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.