



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 09:27 PM EDT

PDB ID : 7CIF  
Title : Crystal structure of L-methionine decarboxylase from Streptomyces sp.590 (internal aldimine form).  
Authors : Okawa, A.; Shiba, T.; Hayashi, M.; Onoue, Y.; Murota, M.; Sato, D.; Inagaki, J.; Tamura, T.; Harada, S.; Inagaki, K.  
Deposited on : 2020-07-07  
Resolution : 1.80 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](mailto: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>.

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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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

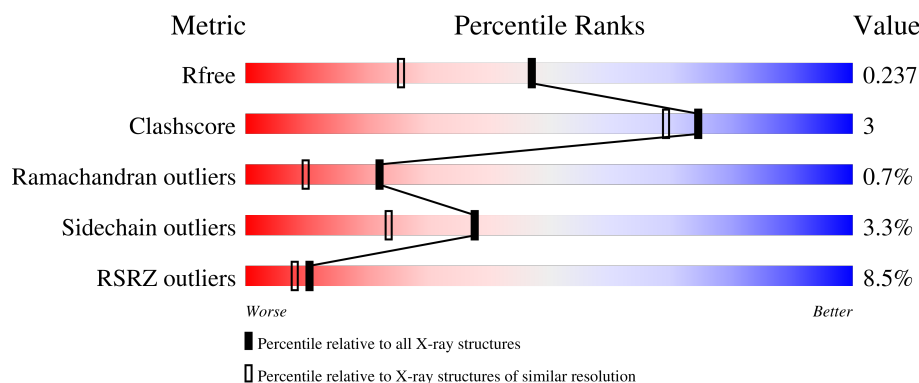
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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  $\geq 3$ , 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	557	<div> <div>9%</div> <div>85%</div> <div>8%</div> <div>6%</div> </div>
1	B	557	<div> <div>7%</div> <div>83%</div> <div>10%</div> <div>7%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8502 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 L-methionine decarboxylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	526	Total	C	N	O	P	S	0	2	0
			4139	2632	722	769	1	15			
1	B	519	Total	C	N	O	P	S	0	0	0
			4082	2598	710	758	1	15			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	132	Total	O	0	0
			132	132		
2	B	149	Total	O	0	0
			149	149		



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.63Å 147.50Å 53.90Å 90.00° 99.87° 90.00°	Depositor
Resolution (Å)	19.89 – 1.80 19.89 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.1 (19.89-1.80) 98.1 (19.89-1.80)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.190 , 0.231 0.199 , 0.237	Depositor DCC
$R_{free}$ test set	4308 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.7	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 43.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8502	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.54% 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, 0.333 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: LLP

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	0.61	0/4234	0.78	4/5773 (0.1%)
1	B	0.64	0/4176	0.78	1/5691 (0.0%)
All	All	0.63	0/8410	0.78	5/11464 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	470	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	A	537	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	425	PRO	N-CA-C	5.13	125.44	112.10
1	A	470	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	150	ARG	NE-CZ-NH1	-5.04	117.78	120.30

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	A	4139	0	3981	24	0
1	B	4082	0	3930	28	0
2	A	132	0	0	0	0
2	B	149	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8502	0	7911	51	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 (51) 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:516:VAL:HG22	1:B:522:THR:HG21	1.56	0.88
1:A:516:VAL:HG22	1:A:522:THR:HG21	1.69	0.72
1:B:482:LEU:HD11	1:B:553:ILE:HG23	1.74	0.68
1:A:284:PHE:O	1:A:528:HIS:HD2	1.82	0.63
1:B:354:PRO:HB2	1:B:360:THR:HG22	1.81	0.63
1:A:537:ARG:NH1	1:A:541:ASP:OD2	2.32	0.62
1:B:284:PHE:O	1:B:528:HIS:HD2	1.83	0.61
1:B:424:ALA:HB1	1:B:425:PRO:CD	2.33	0.59
1:B:354:PRO:CB	1:B:360:THR:HG22	2.34	0.57
1:B:116:HIS:HD2	1:B:369:ASP:OD2	1.87	0.56
1:A:182:ASN:HD21	1:A:217:LYS:NZ	2.04	0.55
1:B:69:MET:HB2	1:B:72:THR:HG23	1.88	0.55
1:B:69:MET:HB2	1:B:72:THR:CG2	2.37	0.54
1:A:516:VAL:HG23	1:A:519:ASP:HB3	1.90	0.53
1:A:313:VAL:HG12	1:A:325:VAL:HG22	1.89	0.53
1:B:208:GLU:HG3	2:B:627:HOH:O	2.10	0.52
1:A:102:VAL:HG22	1:A:105:ARG:NH2	2.27	0.49
1:A:537:ARG:HG2	1:A:537:ARG:HH11	1.78	0.48
1:B:218:TYR:OH	1:B:272:HIS:HE1	1.97	0.48
1:A:265:GLU:OE1	1:A:304:ARG:NH1	2.47	0.48
1:A:178:ARG:HD3	1:A:179:ARG:HA	1.96	0.48
1:B:424:ALA:HB1	1:B:425:PRO:HD2	1.97	0.47
1:B:509:SER:HB3	1:B:528:HIS:CE1	2.50	0.47
1:A:185:HIS:O	1:A:272:HIS:HD2	1.98	0.47
1:B:202:VAL:HG13	1:B:207:VAL:O	2.14	0.47
1:B:62:GLY:HA3	1:B:508:LEU:HA	1.96	0.47
1:B:146:LEU:HG	1:B:207:VAL:HG21	1.96	0.46
1:B:480:VAL:HG23	1:B:482:LEU:HD13	1.97	0.46
1:A:423:GLY:C	1:A:425:PRO:HD2	2.36	0.46
1:B:75:ASP:OD2	1:B:447:ARG:NH2	2.49	0.46
1:B:461:GLN:HE22	1:B:489:GLY:HA2	1.80	0.45
1:A:54:THR:O	1:A:58:LYS:HE3	2.15	0.45
1:A:218:TYR:OH	1:A:272:HIS:HE1	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:SER:HB3	1:A:528:HIS:CE1	2.52	0.45
1:B:444:HIS:HE1	2:B:716:HOH:O	2.01	0.44
1:A:393:HIS:H	1:A:393:HIS:CD2	2.34	0.44
1:A:310[A]:ARG:O	1:A:310[A]:ARG:HG3	2.16	0.44
1:B:110:TYR:CE1	1:B:445:LEU:HD22	2.53	0.44
1:A:190:TYR:HB3	1:A:277:ASN:HB3	2.01	0.43
1:B:337:GLY:O	1:B:338:ALA:C	2.57	0.42
1:B:159:ILE:HG22	1:B:160:GLN:HG2	2.01	0.42
1:B:393:HIS:CD2	1:B:393:HIS:H	2.37	0.42
1:A:344:ALA:N	1:A:345:PRO:CD	2.81	0.42
1:B:185:HIS:O	1:B:272:HIS:HD2	2.03	0.42
1:B:182:ASN:OD1	1:B:217:LYS:NZ	2.53	0.41
1:A:393:HIS:CD2	1:A:401:PRO:HA	2.55	0.41
1:A:258[B]:ASP:OD1	1:A:297:ARG:NH2	2.53	0.41
1:B:146:LEU:HD23	1:B:205:LEU:HD12	2.02	0.41
1:A:89:ASP:HB2	1:A:425:PRO:HA	2.03	0.41
1:A:393:HIS:HE1	1:B:432:SER:OG	2.04	0.40
1:A:516:VAL:HG23	1:A:516:VAL:O	2.21	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	A	523/557 (94%)	497 (95%)	20 (4%)	6 (1%)	14	4
1	B	514/557 (92%)	496 (96%)	17 (3%)	1 (0%)	47	33
All	All	1037/1114 (93%)	993 (96%)	37 (4%)	7 (1%)	22	10

All (7) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	425	PRO
1	B	424	ALA
1	A	319	GLN
1	A	323	PRO
1	A	423	GLY
1	A	180	ASN
1	A	424	ALA

### 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	426/449 (95%)	412 (97%)	14 (3%)	38	23
1	B	421/449 (94%)	406 (96%)	15 (4%)	35	20
All	All	847/898 (94%)	818 (97%)	29 (3%)	38	22

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ARG
1	A	224	LEU
1	A	292	ARG
1	A	309	GLN
1	A	310[A]	ARG
1	A	310[B]	ARG
1	A	322	ARG
1	A	418	GLN
1	A	420	ASP
1	A	421	TYR
1	A	425	PRO
1	A	436	PHE
1	A	494	ARG
1	A	528	HIS
1	B	25	LEU
1	B	57	ARG
1	B	72	THR

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Mol	Chain	Res	Type
1	B	92	GLN
1	B	178	ARG
1	B	179	ARG
1	B	197	SER
1	B	198	PHE
1	B	292	ARG
1	B	319	GLN
1	B	320	THR
1	B	427	THR
1	B	436	PHE
1	B	494	ARG
1	B	528	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	180	ASN
1	A	182	ASN
1	A	184	HIS
1	A	272	HIS
1	A	279	ASN
1	A	393	HIS
1	A	528	HIS
1	B	116	HIS
1	B	272	HIS
1	B	279	ASN
1	B	309	GLN
1	B	319	GLN
1	B	393	HIS
1	B	444	HIS
1	B	461	GLN
1	B	528	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	LLP	A	394	1	23,24,25	2.59	4 (17%)	25,32,34	1.90	7 (28%)
1	LLP	B	394	1	23,24,25	2.69	4 (17%)	25,32,34	1.50	6 (24%)

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
1	LLP	A	394	1	-	4/16/17/19	0/1/1/1
1	LLP	B	394	1	-	4/16/17/19	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	394	LLP	C3-C2	7.95	1.48	1.40
1	A	394	LLP	C3-C2	6.73	1.47	1.40
1	A	394	LLP	C4-C5	6.71	1.50	1.42
1	A	394	LLP	C4'-NZ	5.42	1.45	1.27
1	B	394	LLP	C4-C5	5.39	1.48	1.42
1	B	394	LLP	C4-C3	5.35	1.48	1.40
1	B	394	LLP	C4'-NZ	5.25	1.44	1.27
1	A	394	LLP	C4-C3	4.43	1.47	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	LLP	C4-C3-C2	-4.15	117.62	120.19
1	A	394	LLP	C6-N1-C2	3.88	126.36	119.17
1	A	394	LLP	C4-C4'-NZ	-3.34	108.96	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	394	LLP	C4-C4'-NZ	-3.01	110.48	124.31
1	A	394	LLP	OP3-P-OP1	2.82	121.71	110.68
1	B	394	LLP	C6-N1-C2	2.69	124.16	119.17
1	B	394	LLP	C4-C3-C2	-2.51	118.63	120.19
1	B	394	LLP	OP3-P-OP4	-2.23	100.80	106.73
1	B	394	LLP	OP2-P-OP1	2.22	119.36	110.68
1	B	394	LLP	OP3-P-OP1	2.08	118.82	110.68
1	A	394	LLP	OP4-C5'-C5	-2.03	105.47	109.35
1	A	394	LLP	O3-C3-C2	2.02	121.89	117.49
1	A	394	LLP	OP3-P-OP4	-2.02	101.37	106.73

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	394	LLP	C4-C4'-NZ-CE
1	B	394	LLP	C4-C4'-NZ-CE
1	A	394	LLP	CG-CD-CE-NZ
1	B	394	LLP	CG-CD-CE-NZ
1	A	394	LLP	C3-C4-C4'-NZ
1	B	394	LLP	CD-CE-NZ-C4'
1	A	394	LLP	CD-CE-NZ-C4'
1	B	394	LLP	C3-C4-C4'-NZ

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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

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	525/557 (94%)	0.54	52 (9%) <b>7</b> <b>5</b>	20, 31, 69, 146	0
1	B	518/557 (92%)	0.35	37 (7%) <b>16</b> <b>12</b>	18, 30, 67, 122	0
All	All	1043/1114 (93%)	0.45	89 (8%) <b>10</b> <b>8</b>	18, 30, 69, 146	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	163	THR	14.0
1	A	422	ILE	12.4
1	A	162	PRO	12.2
1	A	161	PRO	12.1
1	B	423	GLY	11.4
1	A	317	CYS	11.2
1	B	421	TYR	11.2
1	A	164	ALA	10.6
1	A	320	THR	10.3
1	A	421	TYR	9.9
1	B	417	SER	9.8
1	B	422	ILE	9.7
1	A	322	ARG	9.5
1	B	424	ALA	8.8
1	A	417	SER	8.3
1	A	556	ALA	8.2
1	B	318	PRO	6.9
1	B	161	PRO	6.8
1	B	419	PRO	6.6
1	A	424	ALA	6.6
1	B	162	PRO	6.6
1	A	419	PRO	6.5
1	B	420	ASP	6.2
1	A	319	GLN	6.1

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Mol	Chain	Res	Type	RSRZ
1	B	418	GLN	6.0
1	A	178	ARG	5.9
1	B	325	VAL	5.9
1	A	423	GLY	5.9
1	A	430	ALA	5.8
1	B	179	ARG	5.8
1	A	416	PRO	5.6
1	B	322	ARG	5.3
1	B	319	GLN	5.0
1	A	418	GLN	4.9
1	A	321	GLY	4.9
1	B	557	PRO	4.8
1	A	420	ASP	4.8
1	A	179	ARG	4.7
1	A	315	GLY	4.7
1	B	324	LEU	4.5
1	B	416	PRO	4.2
1	B	317	CYS	4.2
1	B	25	LEU	4.2
1	A	518	GLY	4.2
1	A	324	LEU	4.2
1	A	323	PRO	4.1
1	B	320	THR	4.0
1	A	318	PRO	4.0
1	B	26	ASP	4.0
1	A	22	GLY	3.9
1	A	316	SER	3.8
1	A	425	PRO	3.8
1	B	24	GLU	3.7
1	B	379	HIS	3.7
1	B	316	SER	3.6
1	B	323	PRO	3.5
1	A	379	HIS	3.5
1	B	518	GLY	3.4
1	A	520	GLU	3.4
1	B	315	GLY	3.2
1	A	429	PHE	3.2
1	B	425	PRO	3.2
1	B	415	PRO	3.1
1	A	93	SER	3.0
1	B	160	GLN	3.0
1	A	314	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	355	GLU	3.0
1	A	18	ALA	2.9
1	A	555	GLY	2.8
1	A	377	ALA	2.8
1	B	216	GLU	2.8
1	A	160	GLN	2.7
1	B	312	VAL	2.6
1	B	313	VAL	2.5
1	A	414	SER	2.5
1	A	68	ASP	2.5
1	A	380	GLY	2.4
1	A	313	VAL	2.3
1	A	232	ARG	2.3
1	A	519	ASP	2.3
1	B	93	SER	2.2
1	A	352	GLU	2.2
1	B	355	GLU	2.1
1	A	378	GLY	2.1
1	A	376	THR	2.1
1	B	426	ASP	2.1
1	A	215	LEU	2.1
1	A	21	PRO	2.0
1	A	24	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
1	LLP	A	394	24/25	0.96	0.09	21,24,28,28	0
1	LLP	B	394	24/25	0.97	0.08	21,24,26,28	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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.