Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2023 – 07:07 PM JST

PDB ID	:	6M2O
Title	:	Double mutant(H333A/I334A) crystal structure of benzoate coenzyme A ligase
Authors	:	Li, T.L.; Adhikari, K.
Deposited on	:	2020-02-28
Resolution	:	1.57 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:

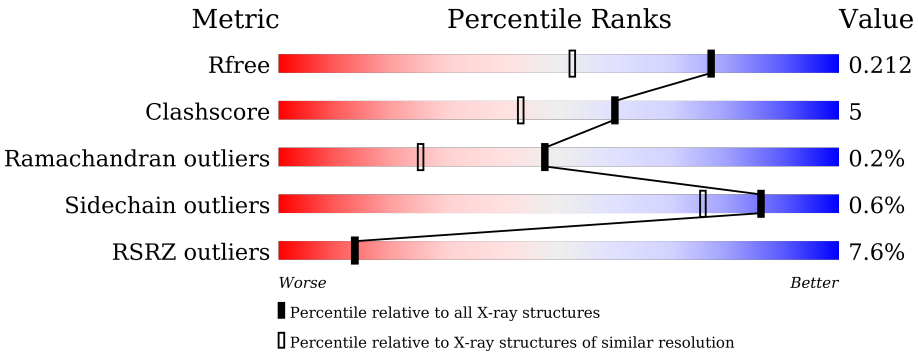
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.57 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	5534 (1.60-1.56)
Clashscore	141614	5861 (1.60-1.56)
Ramachandran outliers	138981	5708 (1.60-1.56)
Sidechain outliers	138945	5703 (1.60-1.56)
RSRZ outliers	127900	5431 (1.60-1.56)

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 <=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	524	5% 90% 8%
1	B	524	10% 90% 9%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9008 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 Benzoate-coenzyme A ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	518	Total	C	N	O	S	0	3	0
			3914	2508	676	721	9			
1	B	518	Total	C	N	O	S	1	3	0
			3914	2508	676	721	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q93TK0
A	83	ALA	THR	engineered mutation	UNP Q93TK0
A	333	ALA	HIS	engineered mutation	UNP Q93TK0
A	334	ALA	ILE	engineered mutation	UNP Q93TK0
A	341	ASP	GLY	engineered mutation	UNP Q93TK0
A	524	GLY	-	expression tag	UNP Q93TK0
B	1	MET	-	initiating methionine	UNP Q93TK0
B	83	ALA	THR	engineered mutation	UNP Q93TK0
B	333	ALA	HIS	engineered mutation	UNP Q93TK0
B	334	ALA	ILE	engineered mutation	UNP Q93TK0
B	341	ASP	GLY	engineered mutation	UNP Q93TK0
B	524	GLY	-	expression tag	UNP Q93TK0

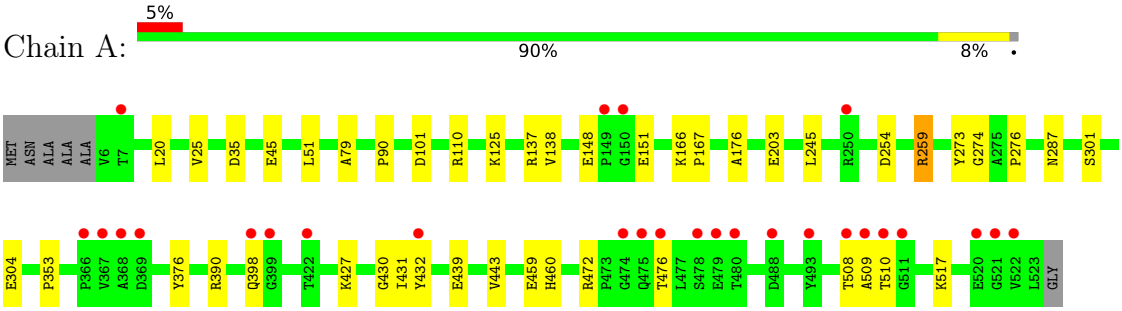
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	594	Total	O	0	0
			594	594		
2	B	586	Total	O	0	0
			586	586		

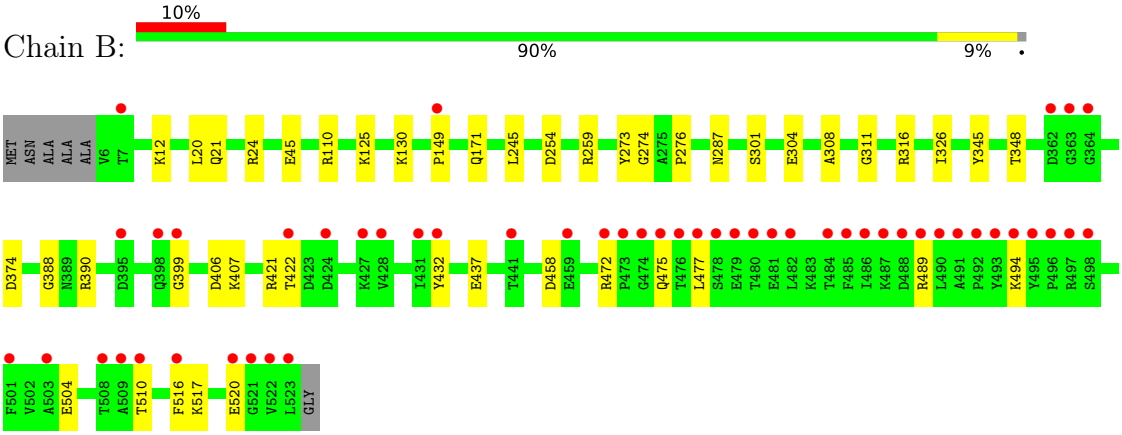
3 Residue-property plots (i)

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: Benzoate-coenzyme A ligase



• Molecule 1: Benzoate-coenzyme A ligase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.12Å 95.38Å 94.99Å 90.00° 105.05° 90.00°	Depositor
Resolution (Å)	29.52 – 1.57 29.52 – 1.57	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.52-1.57) 99.1 (29.52-1.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.58 (at 1.57Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.187 , 0.212 0.187 , 0.212	Depositor DCC
R_{free} test set	2006 reflections (1.43%)	wwPDB-VP
Wilson B-factor (Å^2)	12.4	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9008	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.39	0/4026	0.60	0/5494
1	B	0.40	0/4026	0.60	0/5494
All	All	0.39	0/8052	0.60	0/10988

There are no bond length outliers.

There are no bond angle outliers.

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	3914	0	3835	34	0
1	B	3914	0	3835	38	0
2	A	594	0	0	15	2
2	B	586	0	0	16	2
All	All	9008	0	7670	71	2

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 5.

All (71) 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:388:GLY:H	1:B:390:ARG:HH22	1.19	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ASP:OD2	2:A:601:HOH:O	1.97	0.82
1:A:245:LEU:HD21	1:A:259:ARG:HG2	1.66	0.78
1:A:476:THR:O	2:A:602:HOH:O	2.06	0.72
1:B:520:GLU:O	2:B:601:HOH:O	2.06	0.71
1:A:510:THR:HG22	1:B:149:PRO:HG3	1.74	0.68
1:B:504:GLU:OE2	2:B:602:HOH:O	2.12	0.67
1:A:203:GLU:OE2	2:A:603:HOH:O	2.13	0.67
1:A:137:ARG:NH1	2:A:610:HOH:O	2.27	0.66
1:A:431:ILE:HA	2:A:605:HOH:O	1.94	0.66
1:B:494:LYS:NZ	2:B:603:HOH:O	2.13	0.66
1:B:517:LYS:HA	1:B:520:GLU:HB2	1.81	0.62
1:A:376:TYR:HE2	1:A:398:GLN:HE22	1.47	0.62
1:B:130:LYS:NZ	2:B:607:HOH:O	2.24	0.61
1:B:458:ASP:O	2:B:606:HOH:O	2.16	0.59
1:B:437:GLU:OE2	2:B:605:HOH:O	2.15	0.59
1:B:520:GLU:HB3	2:B:601:HOH:O	2.02	0.58
1:A:430:GLY:O	2:A:605:HOH:O	2.17	0.57
1:B:276:PRO:HD2	1:B:304:GLU:HG2	1.85	0.57
1:A:110:ARG:NH2	2:A:615:HOH:O	2.36	0.57
1:B:388:GLY:N	1:B:390:ARG:HH22	1.96	0.57
1:B:308:ALA:CB	2:B:868:HOH:O	2.56	0.54
1:A:25:VAL:HG13	2:A:666:HOH:O	2.08	0.54
1:B:245:LEU:HD21	1:B:259:ARG:HG2	1.90	0.54
1:A:472:ARG:NH1	2:A:619:HOH:O	2.41	0.53
1:B:477:LEU:N	2:B:615:HOH:O	2.41	0.52
1:A:51:LEU:CD2	1:A:79:ALA:HA	2.40	0.52
1:A:125:LYS:HG3	2:A:827:HOH:O	2.10	0.51
1:B:308:ALA:HA	1:B:345:TYR:HB3	1.92	0.51
1:B:472:ARG:HB3	1:B:475:GLN:HG3	1.93	0.51
1:B:110:ARG:NH2	2:B:620:HOH:O	2.43	0.51
1:B:326:ILE:HG22	1:B:348:THR:HG21	1.92	0.50
1:B:21:GLN:OE1	1:B:24:ARG:NH1	2.39	0.50
1:B:406:ASP:OD1	1:B:421:ARG:NH1	2.42	0.50
1:B:388:GLY:H	1:B:390:ARG:NH2	1.97	0.50
1:A:508:THR:C	1:A:510:THR:H	2.16	0.48
1:B:20:LEU:HD13	1:B:45:GLU:HG3	1.95	0.48
1:A:276:PRO:HD2	1:A:304:GLU:HG2	1.94	0.48
1:B:12:LYS:HE3	1:B:171:GLN:OE1	2.15	0.47
1:B:311:GLY:HA3	1:B:345:TYR:CE1	2.50	0.47
1:B:390:ARG:NH2	2:B:626:HOH:O	2.48	0.46
1:B:316:ARG:NH2	2:B:613:HOH:O	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:ARG:NH2	2:A:625:HOH:O	2.48	0.46
1:A:148:GLU:O	1:A:151:GLU:HB2	2.17	0.45
1:A:443[A]:VAL:HG21	1:B:125:LYS:HD3	1.99	0.45
1:B:254:ASP:OD1	1:B:287:ASN:ND2	2.43	0.44
1:B:308:ALA:HB3	2:B:868:HOH:O	2.16	0.44
1:A:138:VAL:HB	1:A:151:GLU:HG2	1.98	0.44
1:A:254:ASP:OD1	1:A:287:ASN:ND2	2.36	0.44
1:B:407:LYS:HZ3	1:B:422:THR:HG22	1.83	0.44
1:A:166:LYS:HG3	1:A:167:PRO:HD2	2.00	0.43
1:A:90:PRO:HD2	1:A:176:ALA:O	2.19	0.43
1:B:245:LEU:HD21	1:B:259:ARG:CG	2.48	0.43
1:A:20:LEU:HD13	1:A:45:GLU:HG3	2.01	0.42
1:A:101:ASP:HA	2:A:942:HOH:O	2.19	0.42
1:A:274:GLY:O	1:A:301[A]:SER:HA	2.20	0.42
1:B:274:GLY:O	1:B:301[B]:SER:HA	2.20	0.42
1:B:510:THR:HG21	2:B:1144:HOH:O	2.19	0.42
1:A:398:GLN:NE2	2:A:632:HOH:O	2.52	0.42
1:B:374:ASP:OD1	1:B:407:LYS:NZ	2.43	0.42
1:A:439:GLU:O	1:A:443[B]:VAL:HG23	2.20	0.41
1:A:274:GLY:O	1:A:301[B]:SER:HA	2.20	0.41
1:A:427:LYS:HE3	1:A:432:TYR:CD1	2.55	0.41
1:A:517:LYS:NZ	2:A:633:HOH:O	2.53	0.41
1:B:316:ARG:NE	2:B:613:HOH:O	2.35	0.41
1:A:353:PRO:HD2	2:A:910:HOH:O	2.21	0.41
1:A:427:LYS:HD3	1:A:427:LYS:HA	1.86	0.41
1:B:516:PHE:CE2	1:B:517:LYS:HG3	2.56	0.40
1:B:326:ILE:CG2	1:B:348:THR:HG21	2.52	0.40
1:A:459:GLU:HG2	1:A:460:HIS:CD2	2.56	0.40

All (2) 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)
2:A:966:HOH:O	2:B:963:HOH:O[1_554]	1.86	0.34
2:A:1066:HOH:O	2:B:833:HOH:O[1_554]	2.17	0.03

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	519/524 (99%)	510 (98%)	8 (2%)	1 (0%)	47 25
1	B	519/524 (99%)	510 (98%)	8 (2%)	1 (0%)	47 25
All	All	1038/1048 (99%)	1020 (98%)	16 (2%)	2 (0%)	47 25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	509	ALA
1	B	399	GLY

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	A	395/412 (96%)	393 (100%)	2 (0%)	88 80
1	B	395/412 (96%)	392 (99%)	3 (1%)	81 68
All	All	790/824 (96%)	785 (99%)	5 (1%)	86 76

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	259	ARG
1	A	273	TYR
1	B	273	TYR
1	B	432	TYR

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Mol	Chain	Res	Type
1	B	489	ARG

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

Mol	Chain	Res	Type
1	A	50	GLN
1	A	398	GLN
1	B	211	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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^{th} 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	518/524 (98%)	0.17	27 (5%) 27 27	6, 16, 35, 53	1 (0%)
1	B	518/524 (98%)	0.53	52 (10%) 7 7	6, 16, 49, 64	1 (0%)
All	All	1036/1048 (98%)	0.35	79 (7%) 13 13	6, 16, 41, 64	2 (0%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	486	ILE	14.8
1	B	522	VAL	14.5
1	B	490	LEU	12.7
1	A	509	ALA	12.1
1	B	476	THR	11.5
1	B	492	PRO	9.9
1	B	480	THR	9.5
1	B	474	GLY	9.1
1	B	484	THR	9.0
1	A	150	GLY	8.8
1	B	493	TYR	8.5
1	B	495	TYR	8.2
1	B	509	ALA	7.9
1	B	485	PHE	7.8
1	B	478	SER	7.1
1	B	477	LEU	7.1
1	B	520	GLU	6.8
1	A	522	VAL	6.7
1	B	523	LEU	6.5
1	B	481	GLU	6.4
1	B	482	LEU	6.3
1	B	362	ASP	6.1
1	B	475	GLN	5.8
1	B	510	THR	5.8

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Mol	Chain	Res	Type	RSRZ
1	B	479	GLU	5.7
1	B	422	THR	5.4
1	A	508	THR	5.3
1	A	476	THR	4.9
1	B	432	TYR	4.8
1	B	488	ASP	4.8
1	B	473	PRO	4.5
1	A	474	GLY	4.4
1	B	521	GLY	4.2
1	B	398	GLN	4.0
1	A	368	ALA	4.0
1	A	510	THR	4.0
1	B	431	ILE	3.9
1	B	428	VAL	3.8
1	A	149	PRO	3.7
1	B	487	LYS	3.6
1	B	496	PRO	3.5
1	B	427	LYS	3.5
1	B	497	ARG	3.4
1	B	491	ALA	3.4
1	A	520	GLU	3.3
1	B	424	ASP	3.2
1	B	498	SER	3.2
1	B	508	THR	3.1
1	A	398	GLN	3.1
1	A	399	GLY	3.0
1	A	366	PRO	2.8
1	B	459	GLU	2.8
1	A	478	SER	2.7
1	B	503	ALA	2.6
1	A	432	TYR	2.6
1	A	7	THR	2.6
1	B	516	PHE	2.6
1	B	489	ARG	2.6
1	B	7	THR	2.5
1	A	250	ARG	2.5
1	A	511	GLY	2.4
1	B	399	GLY	2.4
1	A	369	ASP	2.4
1	A	488	ASP	2.4
1	A	480	THR	2.3
1	A	521	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	395	ASP	2.3
1	B	363	GLY	2.3
1	B	501	PHE	2.2
1	A	475	GLN	2.2
1	A	479	GLU	2.2
1	A	493	TYR	2.2
1	B	472	ARG	2.1
1	B	364	GLY	2.1
1	B	494	LYS	2.1
1	B	441	THR	2.1
1	B	149	PRO	2.0
1	A	367	VAL	2.0
1	A	422	THR	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 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.