



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 06:51 am BST

PDB ID : 6IG5
Title : Crystal structure of argininosuccinate lyase from Mycobacterium tuberculosis
Authors : Chen, X.B.; Liu, X.
Deposited on : 2018-09-24
Resolution : 2.08 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 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 : 2.11
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) : 2.11

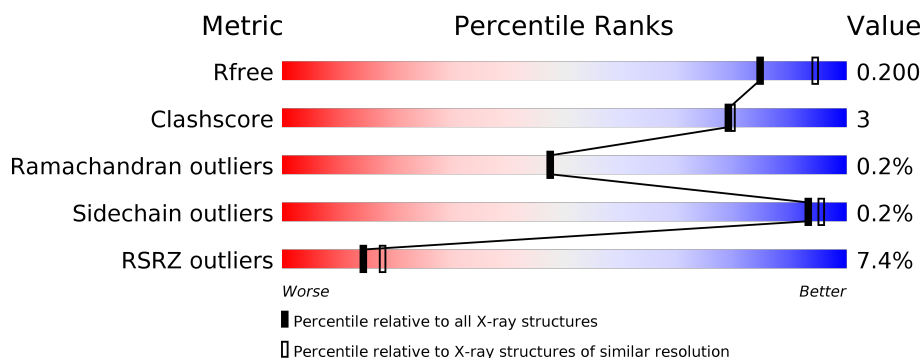
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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 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	470	<div> <div>6%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div>.</div> </div> </div>
1	B	470	<div> <div>10%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div>.</div> </div> </div>
1	C	470	<div> <div>7%</div> <div> <div></div> <div>92%</div> <div>.</div> <div>.</div> </div> </div>
1	D	470	<div> <div>6%</div> <div> <div></div> <div>92%</div> <div>.</div> <div>.</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14705 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 Argininosuccinate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3397	2122	616	651	8			
1	B	455	Total	C	N	O	S	0	0	0
			3397	2122	616	651	8			
1	C	455	Total	C	N	O	S	0	0	0
			3397	2122	616	651	8			
1	D	455	Total	C	N	O	S	0	0	0
			3397	2122	616	651	8			

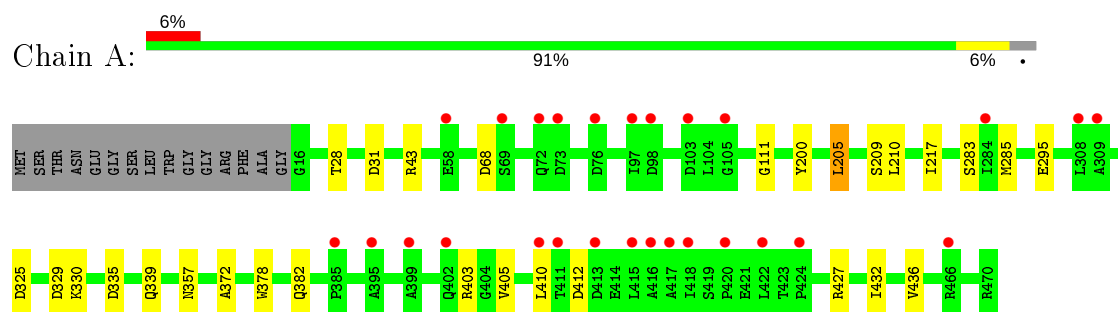
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	259	Total	O	0	0
			259	259		
2	B	253	Total	O	0	0
			253	253		
2	C	305	Total	O	0	0
			305	305		
2	D	300	Total	O	0	0
			300	300		

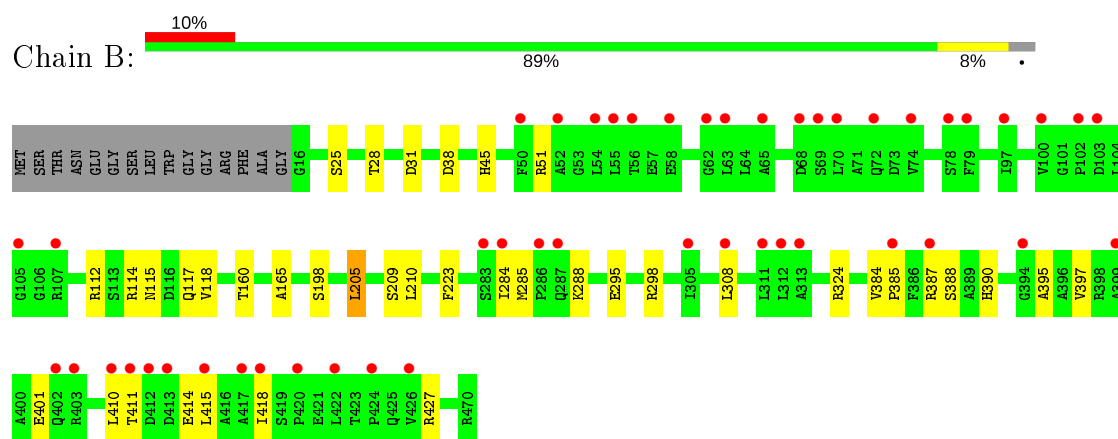
3 Residue-property plots [i](#)

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

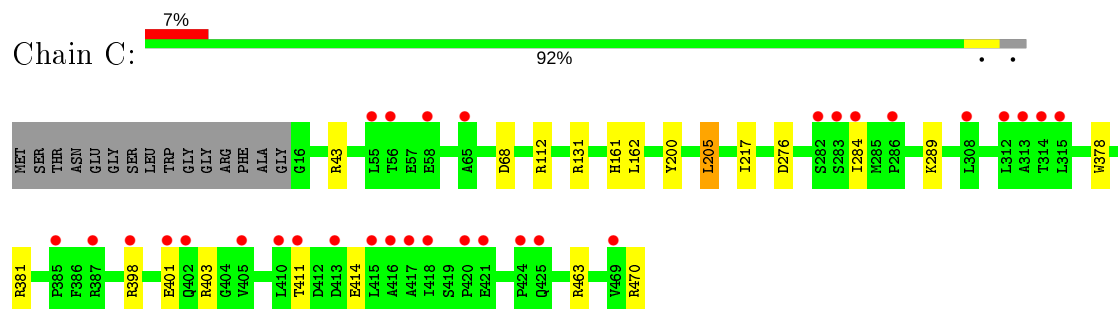
- Molecule 1: Argininosuccinate lyase



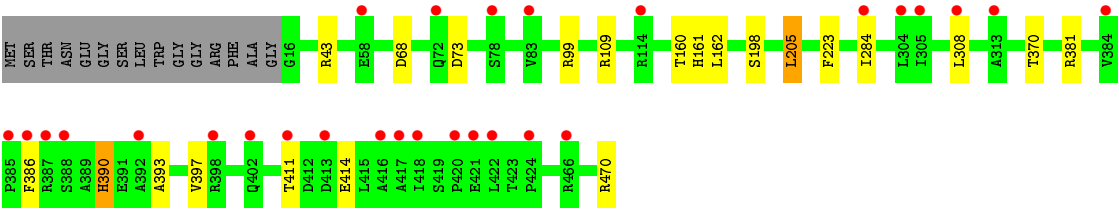
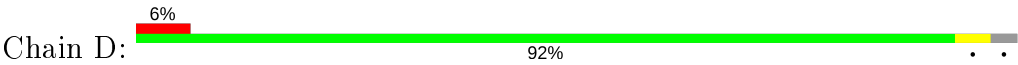
- Molecule 1: Argininosuccinate lyase



- Molecule 1: Argininosuccinate lyase



- Molecule 1: Argininosuccinate lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	115.35Å 120.35Å 155.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.59 – 2.08 47.59 – 2.08	Depositor EDS
% Data completeness (in resolution range)	98.5 (47.59-2.08) 98.5 (47.59-2.08)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.166 , 0.200 0.170 , 0.200	Depositor DCC
R_{free} test set	6249 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14705	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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	0.49	0/3455	0.53	0/4697
1	B	0.43	0/3455	0.53	0/4697
1	C	0.48	0/3455	0.56	0/4697
1	D	0.41	0/3455	0.52	0/4697
All	All	0.45	0/13820	0.53	0/18788

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 [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	3397	0	3388	19	0
1	B	3397	0	3388	35	0
1	C	3397	0	3388	18	0
1	D	3397	0	3388	23	0
2	A	259	0	0	1	0
2	B	253	0	0	3	0
2	C	305	0	0	2	0
2	D	300	0	0	1	0
All	All	14705	0	13552	76	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 (76) 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:385:PRO:HG2	1:B:388:SER:HB2	1.53	0.90
1:B:385:PRO:HG2	1:B:388:SER:CB	2.14	0.78
1:B:384:VAL:HG13	1:B:385:PRO:HD2	1.69	0.74
1:B:284:ILE:HG22	1:B:285:MET:HG3	1.77	0.65
1:B:384:VAL:CG1	1:B:385:PRO:HD2	2.25	0.65
1:B:390:HIS:CD2	1:C:284:ILE:HD11	2.33	0.64
1:D:43:ARG:NH1	1:D:68:ASP:OD1	2.32	0.62
1:B:410:LEU:O	1:B:427:ARG:NH2	2.33	0.59
1:C:398:ARG:HA	1:C:401:GLU:HB2	1.84	0.58
1:A:283:SER:OG	1:D:390:HIS:HE1	1.88	0.57
1:D:411:THR:OG1	1:D:414:GLU:HG3	2.04	0.57
1:B:51:ARG:NH1	2:B:504:HOH:O	2.37	0.57
1:D:393:ALA:O	1:D:397:VAL:HG23	2.04	0.57
2:B:706:HOH:O	1:D:381:ARG:HD2	2.04	0.57
1:C:43:ARG:NH1	1:C:68:ASP:OD1	2.38	0.56
1:B:387:ARG:HD3	1:D:109:ARG:HH22	1.71	0.56
1:C:463:ARG:HG2	1:C:463:ARG:HH11	1.70	0.55
1:A:410:LEU:O	1:A:427:ARG:NH2	2.34	0.55
1:A:357:ASN:HB3	2:A:676:HOH:O	2.07	0.54
1:C:403:ARG:NH1	1:C:414:GLU:OE1	2.41	0.54
1:A:209:SER:O	1:C:381:ARG:HD3	2.07	0.53
1:A:28:THR:HA	1:A:31:ASP:OD1	2.09	0.53
1:A:43:ARG:NH1	1:A:68:ASP:OD1	2.43	0.52
1:A:378:TRP:O	1:A:382:GLN:HG2	2.09	0.52
1:C:131:ARG:CZ	1:C:470:ARG:HD2	2.40	0.51
1:B:114:ARG:NH2	1:B:115:ASN:OD1	2.41	0.51
1:C:378:TRP:HD1	1:C:381:ARG:HH21	1.59	0.51
1:B:205:LEU:CD2	1:D:160:THR:HG23	2.41	0.51
1:D:470:ARG:NH1	2:D:502:HOH:O	2.27	0.50
1:B:387:ARG:HG3	1:D:109:ARG:NH2	2.27	0.50
1:B:308:LEU:HD21	1:D:308:LEU:HD21	1.94	0.49
1:B:385:PRO:HG2	1:B:388:SER:OG	2.12	0.49
1:B:288:LYS:NZ	2:B:505:HOH:O	2.40	0.49
1:B:397:VAL:O	1:B:401:GLU:HB2	2.13	0.48
1:B:387:ARG:CD	1:D:109:ARG:HH22	2.26	0.48
1:A:200:TYR:CD1	1:A:217:ILE:HG21	2.50	0.47
1:C:276:ASP:OD1	1:C:289:LYS:HE2	2.14	0.47
1:B:38:ASP:OD2	1:B:117:GLN:NE2	2.44	0.47
1:C:112:ARG:NH1	2:C:504:HOH:O	2.39	0.47
1:B:114:ARG:O	1:B:118:VAL:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:SER:HB2	1:B:223:PHE:CG	2.49	0.47
1:B:395:ALA:CB	1:B:418:ILE:HG23	2.45	0.46
1:C:200:TYR:CD1	1:C:217:ILE:HG21	2.50	0.46
1:A:325:ASP:OD1	1:B:298:ARG:HB3	2.16	0.46
1:C:463:ARG:HG2	1:C:463:ARG:NH1	2.31	0.45
1:B:45:HIS:CE1	1:B:112:ARG:HG2	2.51	0.45
1:C:411:THR:OG1	1:C:414:GLU:HG3	2.16	0.45
1:B:411:THR:OG1	1:B:414:GLU:HG3	2.16	0.44
1:A:209:SER:HB2	1:C:381:ARG:NH1	2.32	0.44
1:A:403:ARG:HB2	1:A:405:VAL:HG22	1.99	0.44
1:A:412:ASP:OD1	1:A:427:ARG:NH1	2.46	0.43
1:B:395:ALA:HB3	1:B:418:ILE:CG2	2.48	0.43
1:A:295:GLU:OE1	1:D:161:HIS:HA	2.18	0.43
1:B:165:ALA:HB3	1:D:205:LEU:HD21	2.01	0.43
1:A:432:ILE:O	1:A:436:VAL:HG13	2.18	0.43
1:B:28:THR:HA	1:B:31:ASP:OD1	2.19	0.43
1:A:285:MET:HG2	1:D:370:THR:HA	2.00	0.43
1:A:335:ASP:O	1:A:339:GLN:HG2	2.18	0.43
1:D:198:SER:HB2	1:D:223:PHE:CG	2.54	0.43
1:B:410:LEU:HB2	1:B:415:LEU:HD21	2.00	0.43
1:B:387:ARG:CG	1:D:109:ARG:HH22	2.32	0.42
1:B:209:SER:O	1:D:381:ARG:HD3	2.19	0.42
1:B:25:SER:HB2	1:B:324:ARG:NH2	2.34	0.42
1:A:111:GLY:HA3	1:A:210:LEU:HD22	2.02	0.41
1:B:295:GLU:OE1	1:C:161:HIS:HA	2.21	0.41
1:D:386:PHE:CD2	1:D:386:PHE:C	2.93	0.41
1:C:162:LEU:HD12	1:C:162:LEU:HA	1.93	0.41
1:D:73:ASP:OD2	1:D:99:ARG:NH2	2.35	0.41
1:B:209:SER:O	1:D:381:ARG:NH1	2.54	0.41
1:C:131:ARG:NE	1:C:470:ARG:HD2	2.35	0.41
1:B:210:LEU:HD12	1:D:381:ARG:HG2	2.02	0.41
1:A:372:ALA:CB	1:D:284:ILE:HG21	2.52	0.40
1:B:160:THR:HG23	2:C:598:HOH:O	2.21	0.40
1:D:162:LEU:HA	1:D:162:LEU:HD12	1.95	0.40
1:A:329:ASP:OD1	1:A:330:LYS:N	2.54	0.40
1:C:403:ARG:HE	1:C:403:ARG:HB3	1.63	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	453/470 (96%)	443 (98%)	9 (2%)	1 (0%)	47	47
1	B	453/470 (96%)	445 (98%)	7 (2%)	1 (0%)	47	47
1	C	453/470 (96%)	445 (98%)	7 (2%)	1 (0%)	47	47
1	D	453/470 (96%)	446 (98%)	6 (1%)	1 (0%)	47	47
All	All	1812/1880 (96%)	1779 (98%)	29 (2%)	4 (0%)	47	47

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	205	LEU
1	D	205	LEU
1	C	205	LEU
1	B	205	LEU

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	342/352 (97%)	341 (100%)	1 (0%)	92	95
1	B	342/352 (97%)	342 (100%)	0	100	100
1	C	342/352 (97%)	341 (100%)	1 (0%)	92	95
1	D	342/352 (97%)	341 (100%)	1 (0%)	92	95
All	All	1368/1408 (97%)	1365 (100%)	3 (0%)	93	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	LEU
1	C	205	LEU
1	D	390	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	390	HIS
1	D	390	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](#)

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	455/470 (96%)	0.29	27 (5%) 22 26	21, 34, 65, 79	0
1	B	455/470 (96%)	0.42	48 (10%) 6 7	21, 34, 70, 87	0
1	C	455/470 (96%)	0.30	31 (6%) 17 21	20, 33, 70, 93	0
1	D	455/470 (96%)	0.28	28 (6%) 20 24	21, 33, 61, 85	0
All	All	1820/1880 (96%)	0.32	134 (7%) 14 18	20, 34, 66, 93	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	284	ILE	6.7
1	A	418	ILE	6.0
1	B	402	GLN	5.5
1	C	417	ALA	5.4
1	B	387	ARG	5.2
1	D	402	GLN	5.1
1	C	418	ILE	4.6
1	A	417	ALA	4.5
1	C	420	PRO	4.2
1	B	418	ILE	4.2
1	A	411	THR	4.1
1	C	424	PRO	4.1
1	D	385	PRO	4.1
1	B	413	ASP	4.1
1	C	398	ARG	4.1
1	A	415	LEU	3.9
1	B	286	PRO	3.8
1	D	418	ILE	3.8
1	A	284	ILE	3.7
1	B	415	LEU	3.6
1	B	417	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	402	GLN	3.6
1	D	416	ALA	3.5
1	D	417	ALA	3.5
1	B	410	LEU	3.5
1	B	283	SER	3.5
1	B	72	GLN	3.4
1	A	420	PRO	3.4
1	C	425	GLN	3.4
1	B	411	THR	3.3
1	C	312	LEU	3.3
1	A	424	PRO	3.3
1	B	74	VAL	3.3
1	D	413	ASP	3.3
1	D	387	ARG	3.3
1	A	410	LEU	3.3
1	D	420	PRO	3.3
1	C	416	ALA	3.2
1	A	395	ALA	3.2
1	C	55	LEU	3.1
1	C	387	ARG	3.1
1	A	416	ALA	3.1
1	C	415	LEU	3.1
1	C	411	THR	3.1
1	A	413	ASP	3.1
1	C	402	GLN	3.0
1	D	386	PHE	3.0
1	D	392	ALA	3.0
1	B	50	PHE	2.9
1	B	284	ILE	2.9
1	B	420	PRO	2.9
1	B	58	GLU	2.8
1	B	103	ASP	2.8
1	A	385	PRO	2.8
1	A	308	LEU	2.8
1	B	97	ILE	2.8
1	B	79	PHE	2.8
1	B	65	ALA	2.8
1	B	424	PRO	2.8
1	C	385	PRO	2.8
1	B	385	PRO	2.8
1	B	54	LEU	2.7
1	B	62	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	114	ARG	2.7
1	B	52	ALA	2.7
1	B	70	LEU	2.7
1	B	312	LEU	2.7
1	C	410	LEU	2.7
1	C	286	PRO	2.7
1	C	421	GLU	2.7
1	C	413	ASP	2.6
1	C	308	LEU	2.6
1	A	399	ALA	2.6
1	B	56	THR	2.6
1	B	55	LEU	2.6
1	C	469	VAL	2.6
1	C	315	LEU	2.6
1	C	283	SER	2.5
1	B	105	GLY	2.5
1	D	422	LEU	2.5
1	D	384	VAL	2.5
1	B	412	ASP	2.5
1	A	58	GLU	2.5
1	B	403	ARG	2.5
1	D	466	ARG	2.5
1	D	421	GLU	2.4
1	B	399	ALA	2.4
1	B	63	LEU	2.4
1	B	308	LEU	2.4
1	A	103	ASP	2.4
1	A	69	SER	2.4
1	A	98	ASP	2.4
1	B	313	ALA	2.4
1	B	78	SER	2.4
1	D	305	ILE	2.4
1	C	58	GLU	2.4
1	B	287	GLN	2.4
1	D	72	GLN	2.3
1	D	398	ARG	2.3
1	D	78	SER	2.3
1	C	314	THR	2.3
1	C	405	VAL	2.3
1	B	107	ARG	2.3
1	A	422	LEU	2.3
1	B	68	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	284	ILE	2.3
1	D	304	LEU	2.3
1	D	411	THR	2.3
1	A	105	GLY	2.2
1	D	308	LEU	2.2
1	D	388	SER	2.2
1	A	76	ASP	2.2
1	B	311	LEU	2.2
1	B	426	VAL	2.2
1	D	424	PRO	2.2
1	A	72	GLN	2.2
1	B	422	LEU	2.2
1	B	100	VAL	2.2
1	A	73	ASP	2.1
1	C	313	ALA	2.1
1	C	282	SER	2.1
1	B	305	ILE	2.1
1	C	65	ALA	2.1
1	C	401	GLU	2.0
1	D	58	GLU	2.0
1	A	466	ARG	2.0
1	B	102	PRO	2.0
1	A	309	ALA	2.0
1	B	69	SER	2.0
1	D	313	ALA	2.0
1	D	83	VAL	2.0
1	B	394	GLY	2.0
1	A	97	ILE	2.0
1	C	56	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.