



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 01:11 pm GMT

PDB ID : 5V4L
Title : Cryptococcus neoformans adenylosuccinate lyase
Authors : Chitty, J.; Williams, S.J.; Kobe, B.; Fraser, J.A.
Deposited on : 2017-03-09
Resolution : 2.10 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	:	trunk31020
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk31020

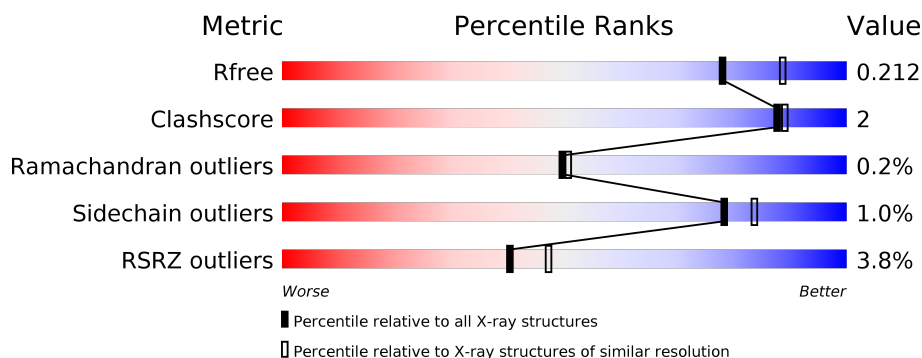
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	111664	4608 (2.10-2.10)
Clashscore	122126	5109 (2.10-2.10)
Ramachandran outliers	120053	5059 (2.10-2.10)
Sidechain outliers	120020	5060 (2.10-2.10)
RSRZ outliers	108989	4497 (2.10-2.10)

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. 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	479	<div> <div style="width: 91%;"></div> <div>91% 5%</div> </div>
1	B	479	<div> <div style="width: 90%;"></div> <div>90% 5% 5%</div> </div>
1	C	479	<div> <div style="width: 90%;"></div> <div>90% 6% . .</div> </div>
1	D	479	<div> <div style="width: 88%;"></div> <div>88% 6% 6%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15996 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 Adenylosuccinate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	0	0
			3606	2291	630	671	14			
1	B	454	Total	C	N	O	S	0	1	0
			3578	2274	620	669	15			
1	C	467	Total	C	N	O	S	0	0	0
			3678	2333	642	688	15			
1	D	451	Total	C	N	O	S	0	1	0
			3556	2260	616	666	14			

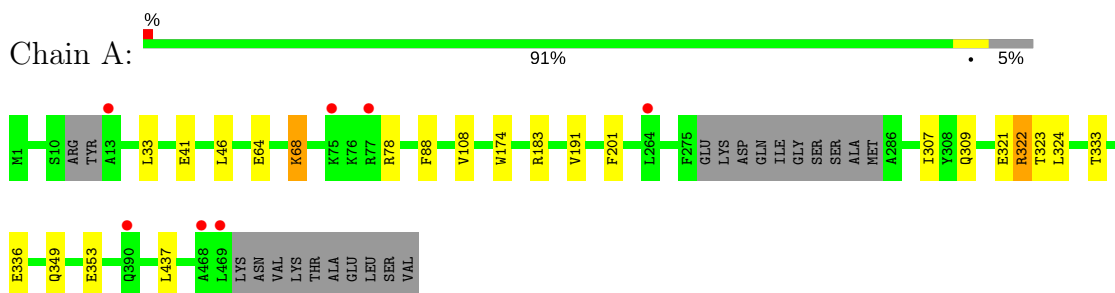
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	486	Total	O	0	0
			486	486		
2	B	402	Total	O	0	0
			402	402		
2	C	385	Total	O	0	0
			385	385		
2	D	305	Total	O	0	0
			305	305		

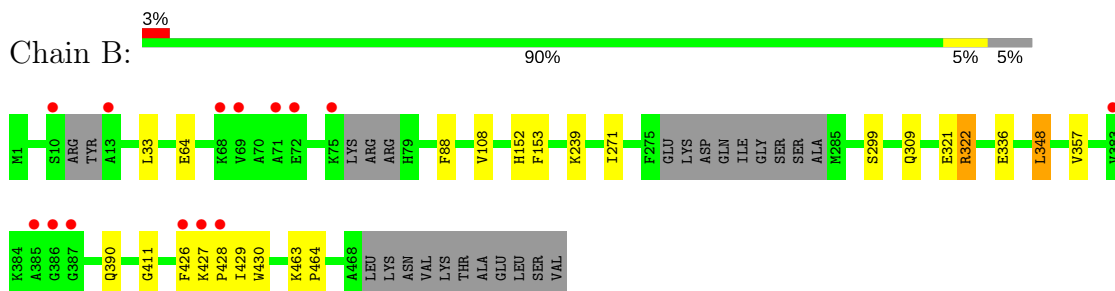
3 Residue-property plots [i](#)

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.

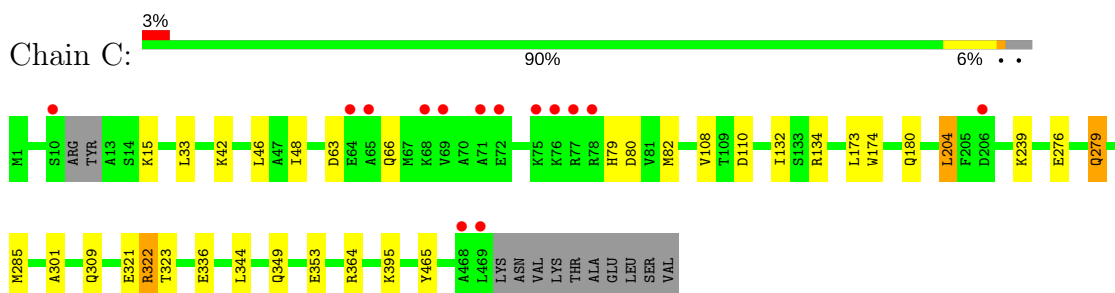
- Molecule 1: Adenylosuccinate lyase



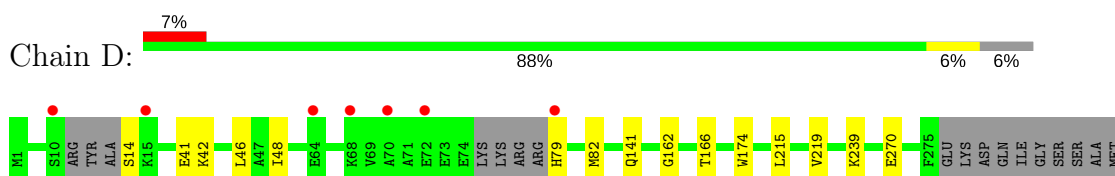
- Molecule 1: Adenylosuccinate lyase

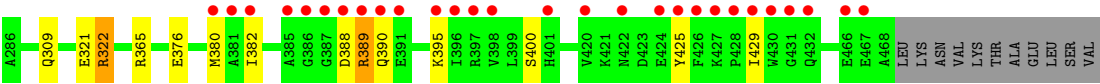


- Molecule 1: Adenylosuccinate lyase



- Molecule 1: Adenylosuccinate lyase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.11Å 93.50Å 159.25Å 90.00° 97.54° 90.00°	Depositor
Resolution (Å)	39.44 – 2.10 39.44 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.6 (39.44-2.10) 98.6 (39.44-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.157 , 0.211 0.158 , 0.212	Depositor DCC
R_{free} test set	6478 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 61.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15996	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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	0.39	0/3675	0.51	0/4973
1	B	0.40	0/3649	0.52	0/4938
1	C	0.38	0/3748	0.50	0/5071
1	D	0.35	0/3627	0.48	0/4910
All	All	0.38	0/14699	0.50	0/19892

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	3606	0	3628	16	0
1	B	3578	0	3591	15	0
1	C	3678	0	3698	24	0
1	D	3556	0	3564	18	0
2	A	486	0	0	1	0
2	B	402	0	0	3	0
2	C	385	0	0	1	0
2	D	305	0	0	2	0
All	All	15996	0	14481	64	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 2.

All (64) 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:C:79:HIS:HD2	1:C:82:MET:H	1.33	0.77
1:B:336:GLU:OE2	2:B:501:HOH:O	2.06	0.74
1:D:376:GLU:OE2	1:D:389:ARG:NH2	2.23	0.70
1:D:141:GLN:NE2	2:D:501:HOH:O	2.27	0.68
1:C:79:HIS:CD2	1:C:82:MET:HG2	2.36	0.61
1:D:380:MET:SD	1:D:389:ARG:NH2	2.79	0.55
1:C:79:HIS:CD2	1:C:82:MET:H	2.18	0.55
1:A:78:ARG:NH2	1:C:276:GLU:OE2	2.41	0.54
1:A:68:LYS:N	1:A:68:LYS:HD3	2.21	0.54
1:A:309:GLN:NE2	1:B:309:GLN:OE1	2.41	0.53
1:C:134:ARG:NH1	1:C:353:GLU:OE2	2.41	0.53
1:A:336:GLU:OE1	2:A:501:HOH:O	2.19	0.53
1:A:321:GLU:O	1:A:322:ARG:HB2	2.09	0.53
1:C:46:LEU:HD21	1:C:204:LEU:HD12	1.92	0.52
1:B:390:GLN:NE2	2:B:513:HOH:O	2.44	0.51
1:D:42:LYS:NZ	1:D:48:ILE:O	2.42	0.49
1:A:307:ILE:HG12	1:A:333:THR:HG23	1.95	0.49
1:A:322:ARG:HG2	1:A:323:THR:N	2.27	0.48
1:B:64:GLU:HG2	2:B:746:HOH:O	2.11	0.48
1:C:239:LYS:HD3	1:D:174:TRP:HE3	1.79	0.47
1:C:276:GLU:O	1:C:279:GLN:NE2	2.47	0.47
1:D:41:GLU:HB3	1:D:46:LEU:HD12	1.97	0.47
1:A:191:VAL:HB	1:A:201:PHE:CE2	2.50	0.47
1:A:64:GLU:OE1	1:A:68:LYS:NZ	2.42	0.47
1:C:180:GLN:OE1	1:C:465:TYR:OH	2.10	0.46
1:C:174:TRP:HE3	1:D:239:LYS:HD3	1.81	0.46
1:B:271:ILE:HD13	1:B:357:VAL:HG22	1.98	0.46
1:D:388:ASP:HB3	1:D:390:GLN:OE1	2.15	0.46
1:B:426:PHE:O	1:B:429:ILE:HG13	2.16	0.45
1:C:321:GLU:O	1:C:322:ARG:HB2	2.17	0.45
1:D:215:LEU:O	1:D:219:VAL:HG22	2.16	0.44
1:C:33:LEU:HD13	1:C:108:VAL:HA	1.98	0.44
1:D:309:GLN:NE2	2:D:506:HOH:O	2.41	0.44
1:D:79:HIS:CE1	1:D:82:MET:HG2	2.52	0.44
1:D:395:LYS:HD2	1:D:425:TYR:CD2	2.53	0.44
1:B:427:LYS:HA	1:B:430:TRP:CD2	2.53	0.44
1:B:321:GLU:O	1:B:322:ARG:HB2	2.18	0.43
1:C:309:GLN:NE2	1:D:309:GLN:OE1	2.51	0.43
1:C:132:ILE:HD13	1:C:173:LEU:HD23	2.00	0.43
1:C:63:ASP:OD1	1:C:66:GLN:HG3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:GLU:HB3	1:A:46:LEU:HD12	1.99	0.43
1:C:349:GLN:O	1:C:353:GLU:HG3	2.19	0.43
1:A:336:GLU:OE2	1:C:336:GLU:OE2	2.36	0.42
1:C:42:LYS:HE2	1:C:48:ILE:O	2.19	0.42
1:C:322:ARG:HG2	1:C:323:THR:N	2.35	0.42
1:C:80:ASP:OD1	1:C:80:ASP:N	2.53	0.42
1:A:307:ILE:HD11	1:A:333:THR:HA	2.02	0.42
1:B:411:GLY:O	1:C:364:ARG:HD2	2.20	0.42
1:D:321:GLU:O	1:D:322:ARG:HB2	2.20	0.42
1:B:348:LEU:HA	1:B:348:LEU:HD12	1.87	0.42
1:C:301:ALA:HA	1:C:344:LEU:HD11	2.02	0.41
1:A:174:TRP:HE3	1:B:239:LYS:HD3	1.85	0.41
1:D:162:GLY:O	1:D:166:THR:HG23	2.20	0.41
1:D:390:GLN:N	1:D:390:GLN:OE1	2.53	0.41
1:A:33:LEU:HD13	1:A:108:VAL:HA	2.02	0.41
1:B:33:LEU:HD13	1:B:108:VAL:HA	2.03	0.41
1:D:382:ILE:HG12	1:D:429:ILE:HD13	2.02	0.41
1:B:463:LYS:HB3	1:B:464:PRO:HD3	2.03	0.41
1:A:324:LEU:HD23	1:B:152:HIS:CE1	2.56	0.41
1:D:270:GLU:OE1	1:D:365:ARG:HD2	2.20	0.41
1:C:395:LYS:HD3	2:C:742:HOH:O	2.20	0.40
1:A:349:GLN:O	1:A:353:GLU:HG2	2.21	0.40
1:C:15:LYS:HB3	1:C:15:LYS:HE3	1.74	0.40
1:B:427:LYS:N	1:B:428:PRO:HD2	2.37	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	451/479 (94%)	447 (99%)	3 (1%)	1 (0%)	49 51

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	447/479 (93%)	443 (99%)	3 (1%)	1 (0%)	49	51
1	C	463/479 (97%)	453 (98%)	9 (2%)	1 (0%)	49	51
1	D	444/479 (93%)	435 (98%)	8 (2%)	1 (0%)	49	51
All	All	1805/1916 (94%)	1778 (98%)	23 (1%)	4 (0%)	49	51

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	322	ARG
1	B	322	ARG
1	D	322	ARG
1	C	322	ARG

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	381/400 (95%)	377 (99%)	4 (1%)	78	83
1	B	379/400 (95%)	375 (99%)	4 (1%)	76	81
1	C	389/400 (97%)	385 (99%)	4 (1%)	78	83
1	D	377/400 (94%)	374 (99%)	3 (1%)	83	88
All	All	1526/1600 (95%)	1511 (99%)	15 (1%)	78	83

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	LYS
1	A	88	PHE
1	A	183	ARG
1	A	437	LEU
1	B	88	PHE
1	B	153	PHE
1	B	299	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	348	LEU
1	C	110	ASP
1	C	204	LEU
1	C	279	GLN
1	C	285	MET
1	D	14	SER
1	D	389	ARG
1	D	400	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	79	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	457/479 (95%)	-0.33	7 (1%) 73 77	9, 20, 47, 85	0
1	B	454/479 (94%)	-0.21	14 (3%) 49 56	9, 19, 58, 83	0
1	C	467/479 (97%)	-0.18	14 (2%) 50 57	11, 23, 52, 109	0
1	D	451/479 (94%)	0.04	35 (7%) 13 17	10, 25, 72, 110	0
All	All	1829/1916 (95%)	-0.17	70 (3%) 40 47	9, 22, 60, 110	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	76	LYS	5.4
1	A	469	LEU	5.1
1	C	10	SER	4.3
1	D	425	TYR	4.3
1	D	382	ILE	4.2
1	C	71	ALA	4.0
1	D	68	LYS	3.8
1	D	431	GLY	3.7
1	C	75	LYS	3.7
1	D	64	GLU	3.5
1	C	72	GLU	3.3
1	B	385	ALA	3.3
1	B	383	VAL	3.3
1	C	77	ARG	3.3
1	B	72	GLU	3.2
1	D	388	ASP	3.2
1	D	432	GLN	3.2
1	D	15	LYS	3.2
1	D	389	ARG	3.1
1	A	13	ALA	3.1
1	D	385	ALA	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	430	TRP	3.1
1	C	68	LYS	3.1
1	A	77	ARG	3.0
1	C	69	VAL	3.0
1	C	78	ARG	3.0
1	B	75	LYS	3.0
1	D	390	GLN	3.0
1	B	386	GLY	2.9
1	D	391	GLU	2.9
1	D	427	LYS	2.9
1	B	10	SER	2.8
1	C	469	LEU	2.8
1	D	428	PRO	2.7
1	D	429	ILE	2.7
1	C	64	GLU	2.7
1	D	426	PHE	2.7
1	D	395	LYS	2.7
1	D	79	HIS	2.6
1	D	398	VAL	2.6
1	D	396	ILE	2.6
1	D	72	GLU	2.6
1	D	466	GLU	2.6
1	D	386	GLY	2.5
1	D	387	GLY	2.5
1	B	426	PHE	2.4
1	A	390	GLN	2.4
1	A	264	LEU	2.4
1	B	68	LYS	2.4
1	D	467	GLU	2.4
1	D	424	GLU	2.4
1	B	427	LYS	2.3
1	B	13	ALA	2.3
1	B	428	PRO	2.3
1	D	401	HIS	2.2
1	D	422	ASN	2.2
1	C	65	ALA	2.2
1	B	69	VAL	2.2
1	A	468	ALA	2.2
1	B	71	ALA	2.2
1	A	75	LYS	2.2
1	B	387	GLY	2.1
1	D	420	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	468	ALA	2.1
1	D	70	ALA	2.1
1	D	397	ARG	2.1
1	C	206	ASP	2.1
1	D	10	SER	2.0
1	D	380	MET	2.0
1	D	381	ALA	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 carbohydrates 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.