Full wwPDB X-ray Structure Validation Report (i)

Apr 29, 2024 – 09:47 am BST

PDB ID	:	2IY1
Title	:	SENP1 (mutant) full length SUMO1
Authors	:	Shen, L.; Dong, C.; Naismith, J.H.
Deposited on	:	2006-07-11
Resolution	:	2.46 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 (i) 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 (1)) were used in the production of this report:

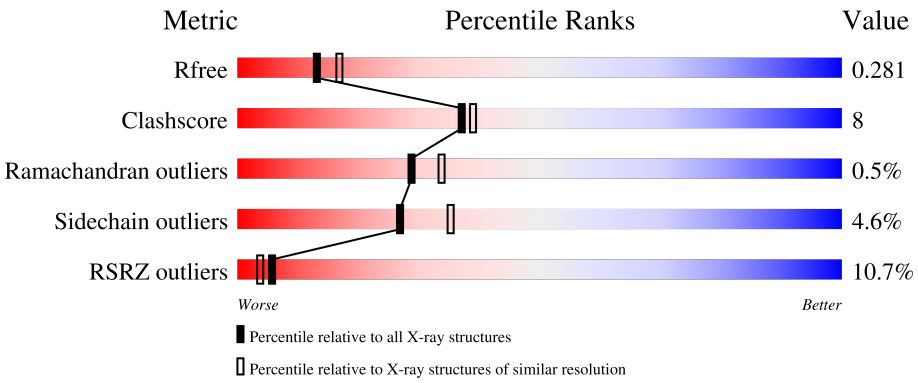
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.46 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	226	11% 85% 14% •
1	C	226	7% 82% 17%
2	B	83	16% 70% 27% • •
2	D	83	14% 63% 35% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5239 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 SENTRIN-SPECIFIC PROTEASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	226	1890	1213	327	337	13	0	0	0
1	C	226	1890	1213	327	337	13	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	603	ALA	CYS	engineered mutation	UNP Q9P0U3
C	603	ALA	CYS	engineered mutation	UNP Q9P0U3

- Molecule 2 is a protein called SMALL UBIQUITIN-RELATED MODIFIER 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	83	673	421	116	131	5	0	0	0
2	D	83	673	421	116	131	5	0	0	0

- Molecule 3 is water.

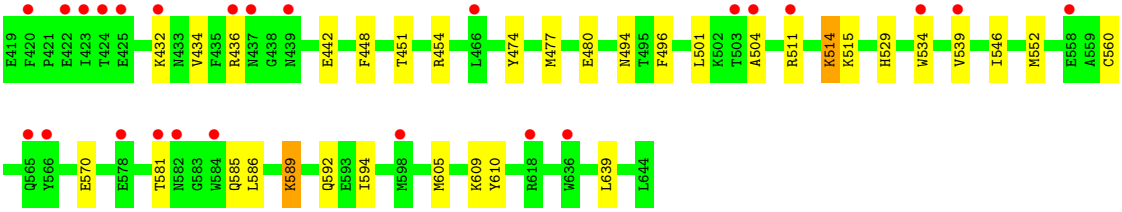
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	38	38	38	0	0
3	B	13	13	13	0	0
3	C	48	48	48	0	0
3	D	14	14	14	0	0

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.

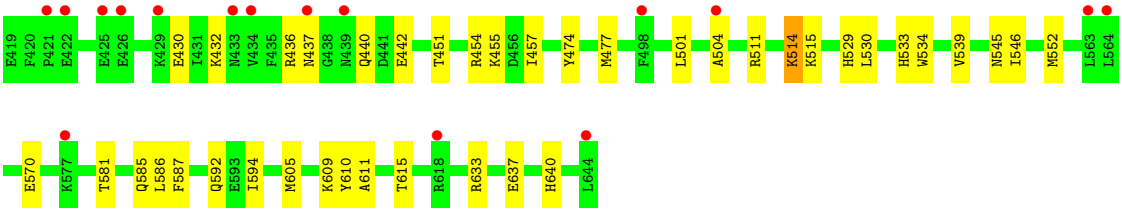
- Molecule 1: SENTRIN-SPECIFIC PROTEASE 1

Chain A:



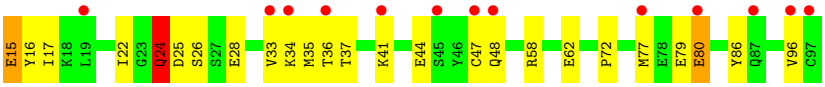
- Molecule 1: SENTRIN-SPECIFIC PROTEASE 1

Chain C:



- Molecule 2: SMALL UBIQUITIN-RELATED MODIFIER 1

Chain B:



- Molecule 2: SMALL UBIQUITIN-RELATED MODIFIER 1

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	141.23Å 141.23Å 98.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.72 – 2.46 40.71 – 2.46	Depositor EDS
% Data completeness (in resolution range)	97.9 (40.72-2.46) 97.9 (40.71-2.46)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.249 , 0.281 0.250 , 0.281	Depositor DCC
R_{free} test set	1810 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	46.2	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 47.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5239	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.85% 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 (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	0.70	2/1933 (0.1%)	0.69	1/2598 (0.0%)
1	C	0.72	2/1933 (0.1%)	0.72	1/2598 (0.0%)
2	B	0.60	0/684	0.77	1/914 (0.1%)
2	D	0.62	0/684	0.74	0/914
All	All	0.68	4/5234 (0.1%)	0.72	3/7024 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	570	GLU	CD-OE2	-6.14	1.18	1.25
1	A	570	GLU	CD-OE2	-5.40	1.19	1.25
1	C	570	GLU	CD-OE1	-5.30	1.19	1.25
1	A	570	GLU	CD-OE1	-5.26	1.19	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	570	GLU	OE1-CD-OE2	-7.21	114.65	123.30
1	A	570	GLU	OE1-CD-OE2	-6.33	115.71	123.30
2	B	24	GLN	CA-CB-CG	5.23	124.91	113.40

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	1890	0	1890	21	0
1	C	1890	0	1890	23	0
2	B	673	0	665	16	0
2	D	673	0	665	24	0
3	A	38	0	0	1	0
3	B	13	0	0	1	0
3	C	48	0	0	2	0
3	D	14	0	0	2	0
All	All	5239	0	5110	80	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 8.

All (80) 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:530:LEU:HB2	3:C:2024:HOH:O	1.40	1.18
1:C:533:HIS:HB3	3:C:2024:HOH:O	1.44	1.15
2:D:72:PRO:HA	2:D:77:MET:HE2	1.52	0.91
2:B:79:GLU:O	2:B:80:GLU:HG3	1.72	0.88
1:C:511:ARG:HD3	2:D:62:GLU:OE2	1.74	0.87
2:D:72:PRO:HA	2:D:77:MET:CE	2.04	0.87
2:D:96:VAL:O	2:D:97:CYS:HB2	1.72	0.86
2:D:80:GLU:HB3	3:D:2003:HOH:O	1.76	0.84
1:A:511:ARG:HD3	2:B:62:GLU:OE2	1.80	0.81
2:B:72:PRO:HA	2:B:77:MET:CE	2.14	0.78
2:B:72:PRO:HA	2:B:77:MET:HE2	1.66	0.77
2:D:79:GLU:O	2:D:80:GLU:HG3	1.89	0.73
1:C:440:GLN:HG3	1:C:455:LYS:HB2	1.78	0.66
2:D:16:TYR:HB3	2:D:35:MET:HE1	1.77	0.65
2:D:16:TYR:HB3	2:D:35:MET:CE	2.28	0.64
2:B:47:CYS:SG	2:B:48:GLN:N	2.73	0.62
1:A:448:PHE:HE2	1:A:480:GLU:HG2	1.62	0.62
1:A:546:ILE:HB	1:A:586:LEU:HD22	1.82	0.62
1:C:514:LYS:O	1:C:515:LYS:HG2	1.99	0.62
1:A:585:GLN:HB2	3:A:2027:HOH:O	2.02	0.59
1:A:594:ILE:HD12	1:A:610:TYR:CZ	2.38	0.58
1:C:546:ILE:HB	1:C:586:LEU:HD22	1.86	0.57
2:B:17:ILE:HG23	2:B:35:MET:HE1	1.87	0.56
1:A:514:LYS:O	1:A:515:LYS:HG2	2.06	0.56
2:D:96:VAL:O	2:D:97:CYS:CB	2.49	0.54
2:D:25:ASP:O	2:D:26:SER:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:43:LYS:HG2	2:D:59:PHE:CD1	2.44	0.53
1:A:501:LEU:O	1:A:504:ALA:O	2.26	0.53
1:A:494:ASN:OD1	1:A:494:ASN:C	2.47	0.53
1:A:539:VAL:HG22	1:A:546:ILE:HG12	1.90	0.53
2:B:22:ILE:HG12	2:B:28:GLU:HG2	1.91	0.53
1:A:589:LYS:HG2	1:A:594:ILE:CG2	2.39	0.52
2:D:72:PRO:CA	2:D:77:MET:CE	2.82	0.52
2:B:15:GLU:OE1	2:B:34:LYS:HD2	2.09	0.52
2:D:80:GLU:CB	3:D:2003:HOH:O	2.48	0.52
2:B:72:PRO:HA	2:B:77:MET:HE3	1.91	0.52
2:D:44:GLU:O	2:D:48:GLN:HB2	2.09	0.52
1:C:533:HIS:CD2	2:D:94:SER:HB3	2.45	0.51
1:C:539:VAL:HG22	1:C:546:ILE:HG12	1.92	0.51
2:D:22:ILE:HG12	2:D:28:GLU:HG2	1.92	0.51
2:D:72:PRO:CB	2:D:77:MET:HE3	2.41	0.51
1:C:545:ASN:HB3	1:C:585:GLN:HB3	1.93	0.51
1:A:442:GLU:OE1	1:A:454:ARG:NH1	2.44	0.51
2:B:25:ASP:O	2:B:26:SER:HB3	2.11	0.49
2:B:16:TYR:HB2	3:B:2002:HOH:O	2.12	0.49
2:D:17:ILE:HG23	2:D:35:MET:HE3	1.94	0.49
2:D:72:PRO:HA	2:D:77:MET:HE3	1.88	0.49
2:B:79:GLU:C	2:B:80:GLU:HG3	2.32	0.48
1:C:474:TYR:HA	1:C:477:MET:CE	2.43	0.48
2:B:44:GLU:O	2:B:48:GLN:HB2	2.13	0.47
1:A:514:LYS:HB3	1:A:514:LYS:HE2	1.40	0.47
1:A:589:LYS:HG2	1:A:594:ILE:HG23	1.95	0.47
2:D:72:PRO:HB3	2:D:77:MET:HE3	1.96	0.47
1:C:605:MET:O	1:C:609:LYS:HG2	2.14	0.47
1:A:605:MET:O	1:A:609:LYS:HG2	2.15	0.47
2:D:34:LYS:HB3	2:D:37:THR:OG1	2.15	0.46
1:C:529:HIS:HB2	1:C:534:TRP:CZ3	2.52	0.45
1:C:430:GLU:OE2	1:C:640:HIS:NE2	2.50	0.45
1:C:511:ARG:O	1:C:514:LYS:HG2	2.18	0.44
2:D:72:PRO:CA	2:D:77:MET:HE3	2.44	0.44
1:A:434:VAL:HG21	1:A:639:LEU:HD11	2.00	0.44
1:C:611:ALA:O	1:C:615:THR:HG23	2.17	0.44
1:A:529:HIS:HB2	1:A:534:TRP:CZ3	2.53	0.44
1:C:594:ILE:HD12	1:C:610:TYR:CZ	2.53	0.44
1:A:474:TYR:HA	1:A:477:MET:CE	2.47	0.43
1:C:514:LYS:O	1:C:515:LYS:CG	2.65	0.43
2:D:52:VAL:HB	2:D:53:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:LYS:HB3	2:B:37:THR:OG1	2.20	0.42
1:C:514:LYS:HB3	1:C:514:LYS:HE2	1.51	0.42
1:C:442:GLU:OE1	1:C:454:ARG:NH1	2.53	0.41
2:B:24:GLN:OE1	2:B:86:TYR:HA	2.20	0.41
1:A:432:LYS:O	1:A:436:ARG:HG2	2.21	0.41
1:C:501:LEU:O	1:C:504:ALA:O	2.39	0.41
1:C:633:ARG:O	1:C:637:GLU:HG3	2.20	0.41
1:A:496:PHE:CZ	2:B:58:ARG:HG3	2.56	0.41
1:A:560:CYS:HB3	1:A:586:LEU:HB3	2.01	0.41
1:A:448:PHE:CE2	1:A:480:GLU:HG2	2.50	0.41
2:D:20:LYS:HG2	2:D:30:HIS:CD2	2.56	0.40
1:C:432:LYS:O	1:C:436:ARG:HG2	2.22	0.40
1:C:474:TYR:HA	1:C:477:MET:HE2	2.03	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	224/226 (99%)	217 (97%)	7 (3%)	0	100	100
1	C	224/226 (99%)	216 (96%)	7 (3%)	1 (0%)	34	41
2	B	81/83 (98%)	78 (96%)	2 (2%)	1 (1%)	13	12
2	D	81/83 (98%)	77 (95%)	3 (4%)	1 (1%)	13	12
All	All	610/618 (99%)	588 (96%)	19 (3%)	3 (0%)	29	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	96	VAL
1	C	437	ASN

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Mol	Chain	Res	Type
2	D	92	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	208/208 (100%)	202 (97%)	6 (3%)	42	53
1	C	208/208 (100%)	201 (97%)	7 (3%)	37	48
2	B	76/76 (100%)	70 (92%)	6 (8%)	12	14
2	D	76/76 (100%)	69 (91%)	7 (9%)	9	9
All	All	568/568 (100%)	542 (95%)	26 (5%)	27	35

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	451	THR
1	A	514	LYS
1	A	552	MET
1	A	581	THR
1	A	589	LYS
1	A	592	GLN
2	B	15	GLU
2	B	24	GLN
2	B	33	VAL
2	B	36	THR
2	B	41	LYS
2	B	80	GLU
1	C	451	THR
1	C	457	ILE
1	C	514	LYS
1	C	552	MET
1	C	581	THR
1	C	587	PHE
1	C	592	GLN
2	D	15	GLU

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Mol	Chain	Res	Type
2	D	33	VAL
2	D	36	THR
2	D	73	LYS
2	D	80	GLU
2	D	95	THR
2	D	97	CYS

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

Mol	Chain	Res	Type
2	B	87	GLN

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 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 (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	226/226 (100%)	0.83	25 (11%)	5	3	49, 59, 67, 72	0
1	C	226/226 (100%)	0.66	16 (7%)	16	12	49, 59, 67, 73	0
2	B	83/83 (100%)	1.12	13 (15%)	2	1	53, 58, 66, 80	0
2	D	83/83 (100%)	1.08	12 (14%)	2	1	53, 58, 67, 80	0
All	All	618/618 (100%)	0.84	66 (10%)	6	4	49, 59, 67, 80	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	97	CYS	7.0
2	D	26	SER	6.0
2	B	96	VAL	5.8
2	B	97	CYS	5.5
1	C	434	VAL	5.3
1	A	636	TRP	4.4
1	A	584	TRP	4.4
2	D	47	CYS	4.4
2	B	48	GLN	4.4
1	A	425	GLU	4.4
1	C	433	ASN	4.1
2	D	96	VAL	4.1
1	C	437	ASN	3.8
2	B	33	VAL	3.7
2	D	41	LYS	3.7
2	D	30	HIS	3.7
2	B	87	GLN	3.6
1	C	429	LYS	3.5
1	C	421	PRO	3.5
2	B	80	GLU	3.5
1	C	425	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	432	LYS	3.4
2	D	52	VAL	3.4
1	A	581	THR	3.4
1	C	498	PHE	3.3
1	A	558	GLU	3.3
2	B	45	SER	3.3
1	C	422	GLU	3.2
1	A	437	ASN	3.2
2	B	34	LYS	3.2
1	A	423	ILE	3.1
2	B	47	CYS	3.1
1	C	426	GLU	3.1
2	D	42	LEU	2.9
1	A	565	GLN	2.9
1	A	436	ARG	2.8
1	A	566	TYR	2.8
1	C	618	ARG	2.8
2	B	19	LEU	2.7
2	D	15	GLU	2.7
1	A	578	GLU	2.6
2	B	41	LYS	2.6
1	A	504	ALA	2.6
1	A	424	THR	2.5
1	A	503	THR	2.4
1	A	511	ARG	2.4
1	A	420	PHE	2.4
1	A	422	GLU	2.4
1	C	577	LYS	2.3
2	D	46	TYR	2.3
1	C	504	ALA	2.3
1	C	563	LEU	2.3
1	A	439	ASN	2.3
1	A	618	ARG	2.3
1	C	439	ASN	2.3
1	C	644	LEU	2.2
2	D	50	GLN	2.2
1	C	564	LEU	2.1
2	D	16	TYR	2.1
2	B	36	THR	2.1
1	A	539	VAL	2.0
1	A	582	ASN	2.0
1	A	534	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	466	LEU	2.0
1	A	598	MET	2.0
2	B	77	MET	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.