Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2021 – 03:43 AM EDT

PDB ID	:	2R05
Title	:	Crystal Structure of ALIX/AIP1 in complex with the HIV-1 YPLASL Late Domain
Authors	:	Hill, C.P.; Zhai, Q.; Fisher, R.D.
Deposited on	:	2007-08-17
Resolution	:	2.55 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 following versions of software and data (see references (1)) were used in the production of this report:

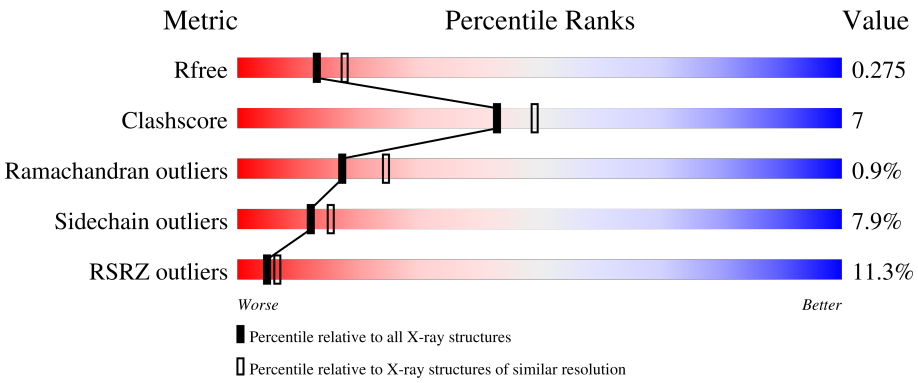
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	697	11% 80% 17% •
2	B	11	18% 82% 9% 9%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5591 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 Programmed cell death 6-interacting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	697	5486	3461	938	1069	18	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	268	TYR	LYS	engineered mutation	UNP Q8WUM4
A	269	TYR	LYS	engineered mutation	UNP Q8WUM4

- Molecule 2 is a protein called p6-Gag.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	11	88	58	14	16	0	0	0

- Molecule 3 is water.

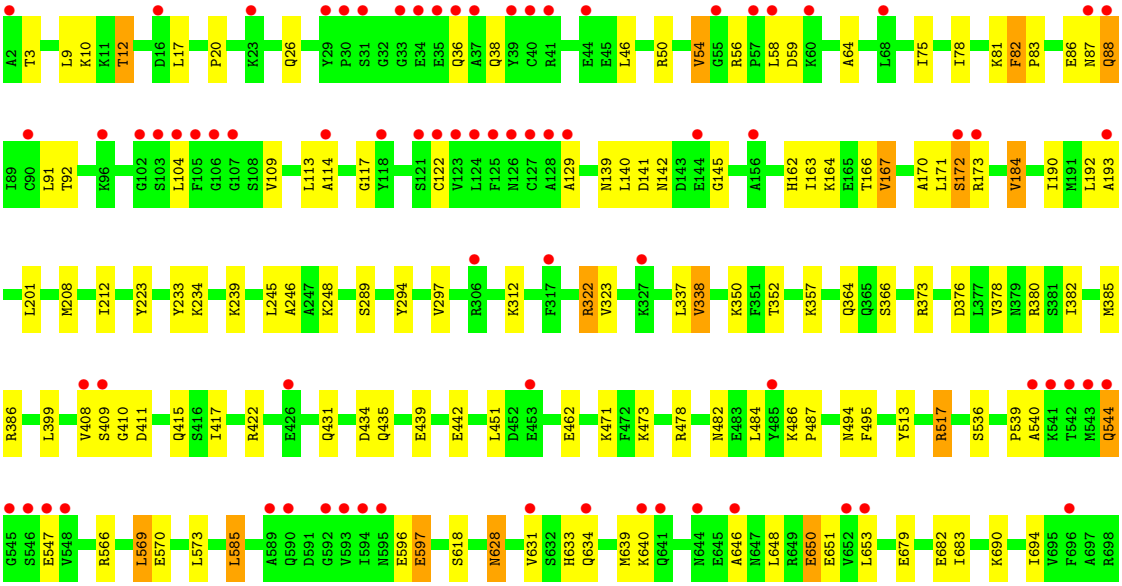
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	17	17	17	0	0

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.

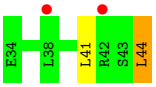
- Molecule 1: Programmed cell death 6-interacting protein

Chain A:



- Molecule 2: p6-Gag

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	146.09Å 99.44Å 73.54Å 90.00° 107.29° 90.00°	Depositor
Resolution (Å)	27.90 – 2.55 24.33 – 2.54	Depositor EDS
% Data completeness (in resolution range)	98.7 (27.90-2.55) 98.2 (24.33-2.54)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.37 (at 2.53Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.225 , 0.280 0.221 , 0.275	Depositor DCC
R_{free} test set	1622 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	69.1	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 69.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5591	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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	0.57	1/5570 (0.0%)	0.64	0/7523
2	B	2.35	1/89 (1.1%)	0.60	0/120
All	All	0.63	2/5659 (0.0%)	0.64	0/7643

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	44	LEU	C-O	21.85	1.64	1.23
1	A	246	ALA	CA-CB	5.29	1.63	1.52

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	5486	0	5532	75	0
2	B	88	0	93	2	0
3	A	17	0	0	0	0
All	All	5591	0	5625	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 7.

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)
2:B:44:LEU:O	2:B:44:LEU:C	1.64	1.35
1:A:486:LYS:HG3	1:A:487:PRO:HD3	1.45	0.97
1:A:382:ILE:HD12	1:A:570:GLU:HG3	1.46	0.94
1:A:517:ARG:HH11	1:A:517:ARG:HG3	1.39	0.87
1:A:92:THR:HG22	1:A:114:ALA:HB2	1.60	0.84
1:A:646:ALA:O	1:A:650:GLU:HB2	1.86	0.75
1:A:376:ASP:O	1:A:380:ARG:HB2	1.90	0.72
1:A:385:MET:HE1	1:A:569:LEU:HB3	1.72	0.72
1:A:486:LYS:HG3	1:A:487:PRO:CD	2.23	0.68
1:A:517:ARG:HH11	1:A:517:ARG:CG	2.08	0.66
1:A:117:GLY:HA3	1:A:170:ALA:HB1	1.80	0.64
1:A:113:LEU:HD11	1:A:173:ARG:HG3	1.83	0.60
1:A:385:MET:HE1	1:A:569:LEU:CB	2.32	0.59
1:A:192:LEU:CD1	1:A:338:VAL:HG13	2.32	0.59
1:A:415:GLN:HE22	1:A:422:ARG:NH2	2.01	0.59
1:A:386:ARG:NH2	1:A:570:GLU:OE2	2.35	0.58
1:A:142:ASN:HD22	1:A:145:GLY:H	1.50	0.58
1:A:410:GLY:O	1:A:536:SER:HA	2.04	0.58
1:A:26:GLN:HG2	1:A:36:GLN:HE21	1.69	0.57
1:A:3:THR:HG21	1:A:294:TYR:O	2.04	0.57
1:A:172:SER:O	1:A:173:ARG:HG2	2.06	0.56
1:A:517:ARG:CG	1:A:517:ARG:NH1	2.69	0.55
1:A:56:ARG:HD3	1:A:58:LEU:HD12	1.89	0.54
1:A:462:GLU:OE1	1:A:482:ASN:ND2	2.40	0.54
1:A:679:GLU:HB3	2:B:41:LEU:HD21	1.90	0.54
1:A:190:ILE:HG12	1:A:245:LEU:HD21	1.88	0.54
1:A:12:THR:HG21	1:A:50:ARG:HH22	1.72	0.53
1:A:540:ALA:HB3	1:A:640:LYS:HG2	1.90	0.53
1:A:639:MET:HB2	1:A:640:LYS:HD2	1.91	0.52
1:A:208:MET:HE2	1:A:212:ILE:HD13	1.92	0.52
1:A:17:LEU:HD13	1:A:46:LEU:HG	1.92	0.52
1:A:164:LYS:HB2	1:A:184:VAL:HG13	1.94	0.50
1:A:192:LEU:HD12	1:A:338:VAL:HG13	1.92	0.50
1:A:628:ASN:C	1:A:628:ASN:HD22	2.15	0.50
1:A:163:ILE:O	1:A:167:VAL:HG22	2.11	0.49
1:A:690:LYS:O	1:A:694:ILE:HG12	2.13	0.49
1:A:3:THR:O	1:A:248:LYS:HE2	2.14	0.48
1:A:10:LYS:HE2	1:A:122:CYS:SG	2.54	0.47
1:A:233:TYR:O	1:A:234:LYS:HG2	2.14	0.47
1:A:364:GLN:C	1:A:366:SER:H	2.17	0.47
1:A:139:ASN:OD1	1:A:141:ASP:HB2	2.15	0.47
1:A:164:LYS:HB2	1:A:184:VAL:CG1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:LEU:HD23	1:A:91:LEU:HD21	1.97	0.46
1:A:431:GLN:NE2	1:A:435:GLN:HE21	2.13	0.46
1:A:142:ASN:ND2	1:A:145:GLY:H	2.13	0.46
1:A:373:ARG:NH2	1:A:597:GLU:HG2	2.31	0.46
1:A:439:GLU:HA	1:A:442:GLU:OE2	2.15	0.45
1:A:451:LEU:HD12	1:A:495:PHE:HB3	1.97	0.45
1:A:9:LEU:HD23	1:A:129:ALA:HB3	1.98	0.45
1:A:434:ASP:OD1	1:A:513:TYR:OH	2.27	0.45
1:A:399:LEU:HD22	1:A:633:HIS:CD2	2.51	0.45
1:A:378:VAL:O	1:A:382:ILE:HG12	2.17	0.45
1:A:409:SER:OG	1:A:411:ASP:HB2	2.17	0.45
1:A:193:ALA:HB2	1:A:223:TYR:HB3	1.98	0.44
1:A:59:ASP:HB3	1:A:64:ALA:HB2	2.00	0.44
1:A:486:LYS:CG	1:A:487:PRO:HD3	2.32	0.44
1:A:162:HIS:O	1:A:166:THR:HB	2.18	0.44
1:A:386:ARG:HG2	1:A:386:ARG:HH11	1.83	0.44
1:A:385:MET:HE2	1:A:566:ARG:CB	2.47	0.43
1:A:322:ARG:NH1	1:A:323:VAL:O	2.51	0.43
1:A:233:TYR:O	1:A:234:LYS:CG	2.67	0.42
1:A:385:MET:CE	1:A:566:ARG:HA	2.50	0.42
1:A:679:GLU:O	1:A:683:ILE:HG12	2.20	0.41
1:A:540:ALA:HB3	1:A:640:LYS:CG	2.50	0.41
1:A:20:PRO:HG3	1:A:91:LEU:HD13	2.02	0.41
1:A:385:MET:HE2	1:A:566:ARG:HA	2.02	0.41
1:A:409:SER:OG	1:A:411:ASP:CB	2.68	0.41
1:A:56:ARG:HD2	1:A:56:ARG:O	2.21	0.41
1:A:171:LEU:HD23	1:A:173:ARG:HB2	2.02	0.41
1:A:192:LEU:HD11	1:A:338:VAL:HG13	2.01	0.41
1:A:208:MET:HE2	1:A:212:ILE:HG21	2.02	0.41
1:A:462:GLU:OE1	1:A:482:ASN:CG	2.59	0.41
1:A:208:MET:CE	1:A:212:ILE:HD13	2.50	0.40
1:A:409:SER:HA	1:A:539:PRO:HB3	2.03	0.40
1:A:585:LEU:HD12	1:A:585:LEU:HA	1.91	0.40
1:A:82:PHE:HA	1:A:83:PRO:HD3	1.93	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	695/697 (100%)	651 (94%)	38 (6%)	6 (1%)	17 24
2	B	9/11 (82%)	8 (89%)	1 (11%)	0	100 100
All	All	704/708 (99%)	659 (94%)	39 (6%)	6 (1%)	17 24

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	LYS
1	A	544	GLN
1	A	87	ASN
1	A	88	GLN
1	A	82	PHE
1	A	54	VAL

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	600/600 (100%)	552 (92%)	48 (8%)	12 15
2	B	10/10 (100%)	10 (100%)	0	100 100
All	All	610/610 (100%)	562 (92%)	48 (8%)	12 15

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	THR
1	A	38	GLN
1	A	54	VAL
1	A	75	ILE
1	A	78	ILE
1	A	86	GLU
1	A	88	GLN
1	A	104	LEU
1	A	109	VAL
1	A	140	LEU
1	A	167	VAL
1	A	172	SER
1	A	184	VAL
1	A	201	LEU
1	A	239	LYS
1	A	289	SER
1	A	297	VAL
1	A	312	LYS
1	A	322	ARG
1	A	337	LEU
1	A	338	VAL
1	A	350	LYS
1	A	352	THR
1	A	357	LYS
1	A	408	VAL
1	A	417	ILE
1	A	471	LYS
1	A	473	LYS
1	A	478	ARG
1	A	484	LEU
1	A	494	ASN
1	A	517	ARG
1	A	544	GLN
1	A	547	GLU
1	A	569	LEU
1	A	573	LEU
1	A	585	LEU
1	A	596	GLU
1	A	597	GLU
1	A	618	SER
1	A	628	ASN
1	A	631	VAL
1	A	634	GLN

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Mol	Chain	Res	Type
1	A	648	LEU
1	A	650	GLU
1	A	651	GLU
1	A	653	LEU
1	A	682	GLU

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	61	HIS
1	A	133	GLN
1	A	142	ASN
1	A	219	GLN
1	A	230	GLN
1	A	364	GLN
1	A	415	GLN
1	A	431	GLN
1	A	447	ASN
1	A	482	ASN
1	A	531	ASN
1	A	544	GLN
1	A	571	ASN
1	A	628	ASN
1	A	633	HIS
1	A	647	ASN
1	A	689	ASN

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	697/697 (100%)	0.76	78 (11%)	5	7	50, 93, 142, 190	2 (0%)
2	B	11/11 (100%)	1.22	2 (18%)	1	1	102, 121, 173, 182	0
All	All	708/708 (100%)	0.77	80 (11%)	5	6	50, 94, 144, 190	2 (0%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	103	SER	8.1
1	A	29	TYR	6.3
1	A	33	GLY	5.4
1	A	30	PRO	5.3
1	A	545	GLY	5.2
1	A	542	THR	5.1
1	A	593	VAL	4.9
1	A	104	LEU	4.9
1	A	88	GLN	4.5
1	A	57	PRO	4.3
1	A	696	PHE	4.3
1	A	2	ALA	4.2
1	A	543	MET	4.2
1	A	128	ALA	4.2
1	A	540	ALA	4.0
1	A	35	GLU	4.0
1	A	122	CYS	3.9
1	A	541	LYS	3.8
1	A	123	VAL	3.8
1	A	127	CYS	3.7
1	A	631	VAL	3.7
1	A	126	ASN	3.7
1	A	102	GLY	3.6
1	A	144	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	36	GLN	3.5
1	A	644	ASN	3.3
1	A	34	GLU	3.2
1	A	590	GLN	3.2
1	A	90	CYS	3.2
1	A	31	SER	3.0
1	A	58	LEU	3.0
1	A	595	ASN	3.0
1	A	426	GLU	2.9
1	A	589	ALA	2.9
1	A	107	GLY	2.9
1	A	408	VAL	2.8
1	A	592	GLY	2.8
1	A	60	LYS	2.8
1	A	125	PHE	2.8
1	A	129	ALA	2.8
1	A	641	GLN	2.8
1	A	453	GLU	2.7
1	A	124	LEU	2.7
1	A	87	ASN	2.7
1	A	37	ALA	2.6
1	A	172	SER	2.6
1	A	173	ARG	2.6
2	B	42	ARG	2.6
1	A	39	TYR	2.5
1	A	646	ALA	2.5
2	B	38	LEU	2.5
1	A	156	ALA	2.5
1	A	640	LYS	2.5
1	A	121	SER	2.4
1	A	652	VAL	2.4
1	A	485	TYR	2.4
1	A	544	GLN	2.4
1	A	634	GLN	2.4
1	A	68	LEU	2.4
1	A	41	ARG	2.4
1	A	409	SER	2.4
1	A	96	LYS	2.4
1	A	546	SER	2.3
1	A	118	TYR	2.3
1	A	653	LEU	2.3
1	A	106	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	114	ALA	2.2
1	A	16	ASP	2.2
1	A	55	GLY	2.2
1	A	327	LYS	2.2
1	A	548	VAL	2.2
1	A	44	GLU	2.2
1	A	547	GLU	2.1
1	A	40	CYS	2.1
1	A	193	ALA	2.1
1	A	306	ARG	2.1
1	A	594	ILE	2.1
1	A	317	PHE	2.1
1	A	23	LYS	2.1
1	A	105	PHE	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.