Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 03:19 AM EDT

PDB ID	:	6UC6
Title	:	Crystal structure of BoNT/B receptor-binding domain in complex with VHH JLI-H11
Authors	:	Lam, K.; Jin, R.
Deposited on	:	2019-09-15
Resolution	:	2.32 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:

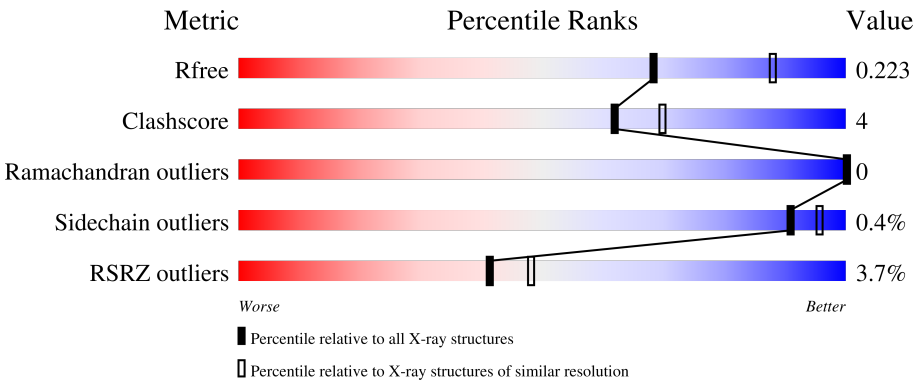
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.32 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	438	5%, 81%, 14%, 5%
1	B	438	3%, 86%, 8%, 6%
2	C	154	2%, 74%, 8%, 18%
2	D	154	2%, 74%, 9%, 17%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9263 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 Botulinum neurotoxin type B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	414	3521	2272	577	664	8	0	0	0
1	B	412	3533	2285	580	660	8	0	2	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	854	GLY	-	expression tag	UNP P10844
A	855	PRO	-	expression tag	UNP P10844
A	856	LEU	-	expression tag	UNP P10844
A	857	GLY	-	expression tag	UNP P10844
A	858	SER	-	expression tag	UNP P10844
B	854	GLY	-	expression tag	UNP P10844
B	855	PRO	-	expression tag	UNP P10844
B	856	LEU	-	expression tag	UNP P10844
B	857	GLY	-	expression tag	UNP P10844
B	858	SER	-	expression tag	UNP P10844

- Molecule 2 is a protein called JLI-H11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	126	934	582	156	190	6	0	0	0
2	D	128	950	591	160	193	6	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	111	111	111	0	0

Continued on next page...

Continued from previous page...

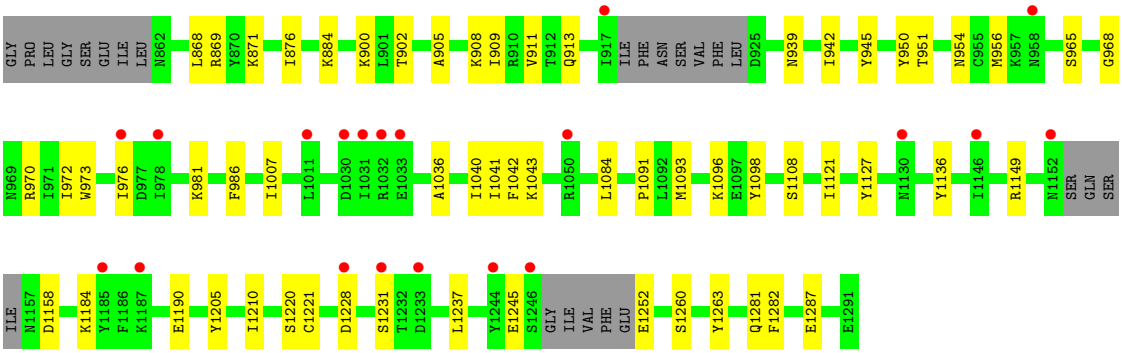
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	C	40	40	40	0	0
			Total	O		
3	B	133	133	133	0	0
			Total	O		
3	D	41	41	41	0	0

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.

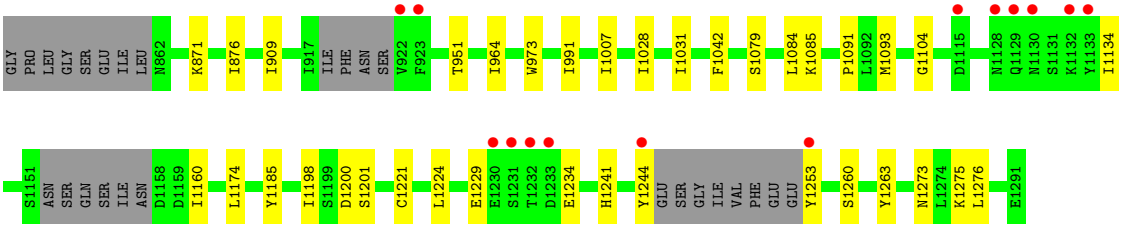
• Molecule 1: Botulinum neurotoxin type B

Chain A:



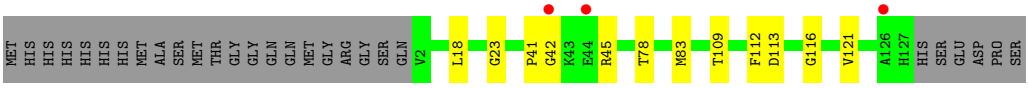
• Molecule 1: Botulinum neurotoxin type B

Chain B:



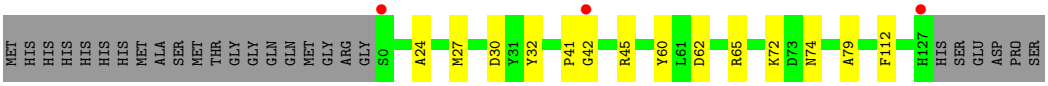
• Molecule 2: JLI-H11

Chain C:



• Molecule 2: JLI-H11

Chain D:


MET
HIS
HIS
HIS
HIS
HIS
HIS
MET
ALA
SER
MET
THR
GLY
GLY
GLN
GLN
MET
GLY
ARG
GLY
S0
A24
M27
D30
Y31
Y32
P41
G42
R45
Y60
L61
D62
R65
K72
D73
N74
A79
F112
H127
HIS
SER
GLU
ASP
PRO
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	71.21Å 73.28Å 76.37Å 87.83° 65.75° 66.55°	Depositor
Resolution (Å)	37.48 – 2.32 37.48 – 2.32	Depositor EDS
% Data completeness (in resolution range)	98.5 (37.48-2.32) 98.5 (37.48-2.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 2.31Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.170 , 0.222 0.172 , 0.223	Depositor DCC
R_{free} test set	2764 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	39.7	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 42.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.033 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9263	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% 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	0.40	0/3603	0.53	0/4856
1	B	0.42	0/3616	0.54	0/4871
2	C	0.46	0/951	0.53	0/1288
2	D	0.55	0/968	0.54	0/1311
All	All	0.43	0/9138	0.53	0/12326

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	3521	0	3414	46	0
1	B	3533	0	3441	19	0
2	C	934	0	887	6	0
2	D	950	0	902	8	0
3	A	111	0	0	1	0
3	B	133	0	0	1	0
3	C	40	0	0	0	0
3	D	41	0	0	0	0
All	All	9263	0	8644	78	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 4.

All (78) 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:A:1228:ASP:OD1	1:A:1231:SER:HB2	1.63	0.98
1:A:1228:ASP:OD1	1:A:1231:SER:CB	2.20	0.90
1:B:1028:ILE:O	1:B:1031:ILE:HG22	1.78	0.83
1:A:871:LYS:HB3	1:A:876:ILE:HD12	1.74	0.69
1:A:1084:LEU:HD22	1:A:1221:CYS:CB	2.22	0.69
1:B:1104:GLY:HA2	1:B:1275:LYS:HD3	1.75	0.68
1:A:1084:LEU:HD13	1:A:1210:ILE:CD1	2.24	0.67
1:A:1084:LEU:HD13	1:A:1210:ILE:HD13	1.79	0.64
1:A:1084:LEU:HD22	1:A:1221:CYS:HB3	1.82	0.62
1:A:976:ILE:O	1:A:976:ILE:HG13	1.97	0.62
1:A:1237:LEU:HD12	1:A:1263:TYR:HB3	1.81	0.61
1:A:913:GLN:NE2	1:A:1036:ALA:O	2.32	0.61
1:A:911:VAL:HG22	1:A:1040:ILE:HB	1.84	0.60
1:B:951:THR:HG23	1:B:964:ILE:O	2.01	0.59
1:A:905:ALA:O	1:A:1043:LYS:NZ	2.36	0.58
1:A:1091:PRO:HB2	1:A:1093:MET:CE	2.33	0.58
2:C:23:GLY:HA2	2:C:78:THR:HG22	1.86	0.57
1:B:991:ILE:HD12	1:B:1134:ILE:HG22	1.87	0.56
1:B:1079:SER:O	1:B:1085:LYS:NZ	2.40	0.54
1:A:965:SER:OG	1:A:972:ILE:HD11	2.07	0.54
2:D:60:TYR:O	2:D:65:ARG:NH2	2.41	0.53
1:B:909:ILE:HB	1:B:1042:PHE:HB2	1.91	0.53
1:A:1149:ARG:NH2	1:A:1158:ASP:O	2.39	0.53
1:B:1224:LEU:HD11	1:B:1234:GLU:HB3	1.89	0.52
1:B:1093:MET:HE2	1:B:1160:ILE:HA	1.90	0.51
1:A:970:ARG:HD2	1:A:986:PHE:CD1	2.46	0.51
1:A:1084:LEU:HD22	1:A:1221:CYS:HB2	1.92	0.51
1:A:1084:LEU:CD2	1:A:1221:CYS:CB	2.88	0.51
2:D:62:ASP:OD1	2:D:65:ARG:NH1	2.35	0.51
1:A:1084:LEU:CD2	1:A:1221:CYS:HB3	2.41	0.50
2:D:45:ARG:HD3	2:D:112:PHE:HD2	1.76	0.50
1:A:909:ILE:HB	1:A:1042:PHE:HB2	1.93	0.50
1:B:1200:ASP:OD1	1:B:1201:SER:N	2.45	0.50
2:D:24:ALA:HB1	2:D:27:MET:HB2	1.94	0.49
1:A:1190:GLU:HG3	1:A:1260:SER:CB	2.42	0.49
1:A:908:LYS:HE3	1:A:1041:ILE:HG23	1.94	0.49
1:A:1084:LEU:HD11	1:A:1210:ILE:HG12	1.96	0.48
2:D:41:PRO:HA	2:D:42:GLY:HA2	1.64	0.48
2:C:83:MET:HE1	2:C:121:VAL:HG21	1.95	0.48
1:A:1096:LYS:NZ	3:A:1307:HOH:O	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:41:PRO:HA	2:C:42:GLY:HA2	1.57	0.47
1:A:951:THR:HA	1:A:965:SER:HB3	1.97	0.47
1:A:1228:ASP:OD1	1:A:1231:SER:OG	2.32	0.47
1:A:1184:LYS:HE2	1:A:1205:TYR:CE1	2.49	0.47
1:A:945:TYR:CE2	1:A:968:GLY:HA2	2.49	0.47
1:A:950:TYR:O	1:A:965:SER:HB2	2.15	0.46
2:C:112:PHE:O	2:C:116:GLY:N	2.44	0.46
1:B:1198:ILE:HD12	2:D:32:TYR:CE1	2.51	0.45
1:B:1084:LEU:HD22	1:B:1221:CYS:HB3	1.99	0.45
1:B:1244:TYR:HA	1:B:1253:TYR:CD2	2.52	0.45
1:A:1084:LEU:CD2	1:A:1221:CYS:HB2	2.47	0.45
2:C:18:LEU:HB3	2:C:83:MET:CE	2.47	0.44
1:A:1091:PRO:HB2	1:A:1093:MET:HE3	1.98	0.44
2:D:30:ASP:OD1	2:D:74:ASN:HB3	2.17	0.44
1:A:1220:SER:HA	1:A:1281:GLN:HG2	1.99	0.44
1:A:1127:TYR:HB2	1:A:1136:TYR:CE2	2.53	0.44
1:B:1273:ASN:HB3	1:B:1276:LEU:HG	1.99	0.43
1:A:1108:SER:HB3	1:A:1121:ILE:CG2	2.49	0.43
1:A:1245:GLU:O	1:A:1252:GLU:N	2.52	0.43
1:A:900:LYS:HE2	1:A:902:THR:HG22	2.00	0.43
1:B:871:LYS:HB3	1:B:876:ILE:HD12	2.01	0.43
1:A:1098:TYR:CG	1:A:1282:PHE:HB3	2.54	0.43
1:A:939:ASN:HA	1:A:942:ILE:HD11	2.01	0.43
1:A:1190:GLU:HG3	1:A:1260:SER:HB2	2.01	0.42
1:B:973:TRP:CD2	1:B:1007:ILE:HG21	2.54	0.42
1:A:868:LEU:O	1:A:869:ARG:HD3	2.20	0.42
1:B:1241:HIS:HD2	3:B:1423:HOH:O	2.03	0.42
2:D:72:LYS:HA	2:D:79:ALA:HA	2.02	0.41
1:B:1091:PRO:HB2	1:B:1093:MET:CE	2.51	0.41
1:A:1228:ASP:OD1	1:A:1231:SER:N	2.49	0.41
1:A:954:ASN:HD21	1:A:956:MET:HG2	1.86	0.41
2:C:45:ARG:HH22	2:C:109:THR:HA	1.86	0.41
1:A:976:ILE:HA	1:A:981:LYS:O	2.20	0.41
1:A:884:LYS:O	1:A:911:VAL:HA	2.21	0.41
1:A:973:TRP:CD2	1:A:1007:ILE:HG21	2.56	0.41
1:B:1260:SER:HB3	1:B:1263:TYR:CD2	2.57	0.40
1:A:954:ASN:ND2	1:A:956:MET:HG2	2.37	0.40
1:B:1229:GLU:OE1	1:B:1229:GLU:N	2.52	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	406/438 (93%)	390 (96%)	16 (4%)	0	100	100
1	B	406/438 (93%)	390 (96%)	16 (4%)	0	100	100
2	C	124/154 (80%)	121 (98%)	3 (2%)	0	100	100
2	D	126/154 (82%)	121 (96%)	5 (4%)	0	100	100
All	All	1062/1184 (90%)	1022 (96%)	40 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	387/411 (94%)	386 (100%)	1 (0%)	92	96
1	B	388/411 (94%)	386 (100%)	2 (0%)	88	95
2	C	98/122 (80%)	97 (99%)	1 (1%)	76	87
2	D	100/122 (82%)	100 (100%)	0	100	100
All	All	973/1066 (91%)	969 (100%)	4 (0%)	91	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1287	GLU
2	C	113	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1174	LEU
1	B	1185	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	414/438 (94%)	-0.06	20 (4%)	30	38	29, 53, 104, 136	0
1	B	412/438 (94%)	-0.19	14 (3%)	45	52	25, 44, 87, 121	0
2	C	126/154 (81%)	-0.55	3 (2%)	59	66	33, 44, 67, 86	0
2	D	128/154 (83%)	-0.52	3 (2%)	60	67	30, 44, 73, 125	0
All	All	1080/1184 (91%)	-0.22	40 (3%)	41	48	25, 46, 95, 136	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1185	TYR	6.2
1	B	1130	ASN	5.5
1	B	1128	ASN	4.8
1	B	1230	GLU	4.8
1	B	1244	TYR	4.5
1	A	1130	ASN	4.2
1	A	1246	SER	4.2
1	B	1133	TYR	4.0
1	B	1253	TYR	3.7
2	D	127	HIS	3.7
1	A	1231	SER	3.5
1	B	923	PHE	3.4
1	B	1115	ASP	3.4
1	B	1231	SER	3.4
1	A	917	ILE	3.1
2	D	0	SER	3.1
1	A	1244	TYR	3.1
1	A	1011	LEU	3.1
1	A	1030	ASP	2.9
1	B	1232	THR	2.8
1	A	1228	ASP	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1033	GLU	2.7
2	C	44	GLU	2.7
1	A	1050	ARG	2.7
1	A	1031	ILE	2.7
1	A	1146	ILE	2.7
2	D	42	GLY	2.5
1	B	922	VAL	2.5
1	B	1233	ASP	2.4
1	B	1129	GLN	2.4
1	A	978	ILE	2.3
1	B	1132	LYS	2.3
1	A	958	ASN	2.3
1	A	1233	ASP	2.2
1	A	1032	ARG	2.2
2	C	126	ALA	2.1
1	A	1152	ASN	2.1
1	A	976	ILE	2.1
1	A	1187	LYS	2.1
2	C	42	GLY	2.1

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.