



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 03:10 pm BST

PDB ID : 5JQD
Title : Antibody Fab Fragment
Authors : Zhang, Z.; Prachanronarong, K.; Gellatly, K.; Marasco, W.A.; Schiffer, C.A.
Deposited on : 2016-05-04
Resolution : 2.59 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

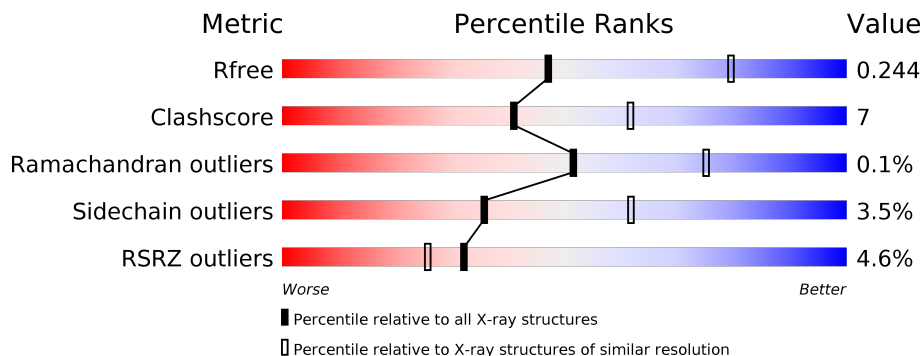
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	215	 85% 14%
1	B	215	 89% 10%
2	C	228	 77% 13% 6% 8%
2	D	228	 69% 23% 10% 6%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6431 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 D80 Fab Fragment Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	214	Total 1628	C 1013	N 278	O 333	S 4	0	0	0
1	B	214	Total 1640	C 1022	N 280	O 334	S 4	0	1	0

- Molecule 2 is a protein called D80 Fab Fragment Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	209	Total 1530	C 973	N 247	O 303	S 7	0	0	0
2	D	214	Total 1540	C 974	N 251	O 308	S 7	0	0	0


- Molecule 3 is water.

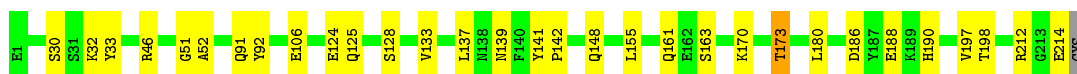
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total 18	O 18	0	0
3	B	40	Total 40	O 40	0	0
3	C	17	Total 17	O 17	0	0
3	D	18	Total 18	O 18	0	0

3 Residue-property plots


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: D80 Fab Fragment Light Chain

Chain A: 




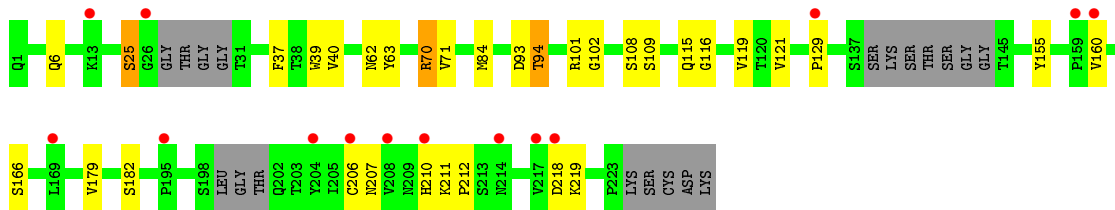
- Molecule 1: D80 Fab Fragment Light Chain

Chain B: 



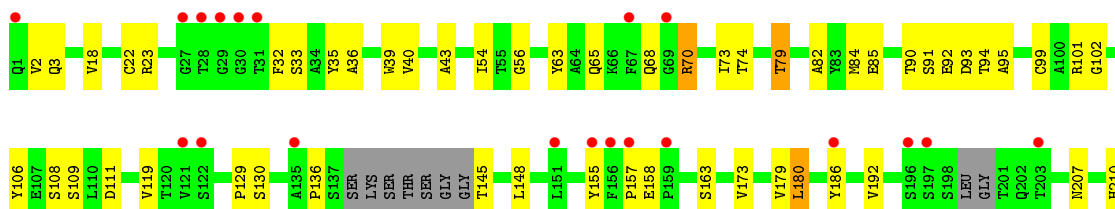
- Molecule 2: D80 Fab Fragment Heavy Chain

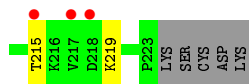
Chain C: 



- Molecule 2: D80 Fab Fragment Heavy Chain

Chain D: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.06Å 91.58Å 106.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.12 – 2.59 46.12 – 2.59	Depositor EDS
% Data completeness (in resolution range)	95.0 (46.12-2.59) 95.0 (46.12-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.58Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.211 , 0.242 0.215 , 0.244	Depositor DCC
R_{free} test set	1273 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtrriage
Anisotropy	0.089	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.023 for k,h,-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6431	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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	0.32	0/1662	0.51	0/2259
1	B	0.31	0/1674	0.51	0/2274
2	C	0.32	0/1566	0.52	0/2138
2	D	0.36	0/1576	0.53	1/2154 (0.0%)
All	All	0.33	0/6478	0.52	1/8825 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	180	LEU	CB-CG-CD2	5.75	120.77	111.00

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	1628	0	1567	16	2
1	B	1640	0	1588	13	1
2	C	1530	0	1445	21	1
2	D	1540	0	1434	44	2
3	A	18	0	0	2	0
3	B	40	0	0	2	0
3	C	17	0	0	3	0
3	D	18	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6431	0	6034	88	3

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 (88) 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:54:SER:OG	3:B:301:HOH:O	1.85	0.95
2:C:70:ARG:NH2	2:C:93:ASP:OD2	2.06	0.89
2:D:163:SER:OG	2:D:207:ASN:OD1	1.93	0.87
1:A:124:GLU:OE1	2:D:219:LYS:NZ	2.13	0.82
1:A:161:GLN:NE2	2:D:180:LEU:O	2.12	0.81
1:A:46:ARG:NH1	3:A:302:HOH:O	2.14	0.80
2:C:115:GLN:O	3:C:301:HOH:O	2.04	0.74
2:D:180:LEU:HD11	2:D:186:TYR:CE2	2.23	0.74
2:C:62:ASN:OD1	3:C:302:HOH:O	2.09	0.70
1:B:125:GLN:O	1:B:128:SER:OG	2.09	0.69
1:B:91:GLN:OE1	1:B:98:THR:OG1	2.08	0.69
1:B:209:SER:OG	3:B:302:HOH:O	2.11	0.69
1:A:106:GLU:OE2	3:A:301:HOH:O	2.11	0.69
2:C:101:ARG:NH1	2:C:102:GLY:O	2.27	0.68
2:C:116:GLY:O	3:C:303:HOH:O	2.13	0.65
2:D:157:PRO:HA	2:D:186:TYR:CE1	2.32	0.64
2:D:63:TYR:O	3:D:301:HOH:O	2.15	0.63
2:D:180:LEU:CD1	2:D:186:TYR:CE2	2.82	0.63
2:D:70:ARG:NH2	2:D:93:ASP:OD2	2.33	0.62
2:D:180:LEU:CD1	2:D:186:TYR:CD2	2.84	0.61
1:A:161:GLN:HB3	2:D:179:VAL:HG11	1.84	0.59
2:D:23:ARG:NH2	2:D:79:THR:O	2.34	0.59
2:D:157:PRO:HA	2:D:186:TYR:HE1	1.67	0.58
2:D:90:THR:HG22	2:D:92:GLU:H	1.71	0.56
2:D:54:ILE:HD11	2:D:73:ILE:O	2.06	0.56
1:B:34:LEU:O	1:B:51:GLY:O	2.24	0.55
1:B:161:GLN:HB3	2:C:179:VAL:HG21	1.88	0.55
2:C:94:THR:HG22	2:C:121:VAL:H	1.74	0.53
1:A:125:GLN:O	1:A:128:SER:OG	2.18	0.53
2:D:158:GLU:N	2:D:186:TYR:CE1	2.77	0.53
2:D:158:GLU:N	2:D:186:TYR:HE1	2.08	0.51
2:D:70:ARG:NH2	2:D:93:ASP:OD1	2.39	0.51
2:C:166:SER:H	2:C:207:ASN:HD21	1.58	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:25:SER:OG	2:C:25:SER:O	2.29	0.51
2:C:206:CYS:O	2:C:218:ASP:HA	2.13	0.48
2:D:180:LEU:HD11	2:D:186:TYR:CD2	2.47	0.48
1:A:30:SER:O	1:A:32:LYS:O	2.32	0.48
2:D:129:PRO:HB3	2:D:155:TYR:HB3	1.96	0.48
2:D:65:GLN:HA	2:D:68:GLN:HG2	1.96	0.48
1:B:133:VAL:HG13	1:B:180:LEU:HB3	1.96	0.47
1:B:133:VAL:CG1	1:B:180:LEU:HB3	2.45	0.47
2:D:157:PRO:CA	2:D:186:TYR:HE1	2.27	0.47
2:D:101:ARG:NH1	2:D:102:GLY:O	2.47	0.47
2:D:33:SER:O	2:D:56:GLY:O	2.32	0.47
2:D:108:SER:OG	2:D:109:SER:N	2.48	0.47
2:C:39:TRP:CE2	2:C:84:MET:HB2	2.49	0.47
2:D:108:SER:N	3:D:303:HOH:O	2.33	0.47
2:D:22:CYS:HB3	2:D:82:ALA:HB3	1.97	0.47
2:D:70:ARG:NH2	2:D:93:ASP:CG	2.68	0.46
1:B:182:LEU:HD22	1:B:186:ASP:HB2	1.98	0.46
1:A:32:LYS:O	1:A:33:TYR:HB2	2.16	0.46
1:A:139:ASN:HA	1:A:173:THR:CG2	2.45	0.46
2:D:210:HIS:HB3	2:D:215:THR:OG1	2.16	0.46
1:A:137:LEU:HD21	1:A:197:VAL:HG13	1.97	0.45
2:C:129:PRO:HB3	2:C:155:TYR:HB3	1.97	0.45
2:D:94:THR:HA	2:D:119:VAL:O	2.17	0.45
2:D:91:SER:O	2:D:94:THR:HG22	2.17	0.45
2:D:94:THR:O	2:D:94:THR:HG23	2.16	0.45
2:C:37:PHE:CZ	2:C:101:ARG:HD3	2.52	0.45
2:C:63:TYR:CD1	2:C:71:VAL:HG13	2.53	0.44
2:D:18:VAL:O	2:D:85:GLU:HA	2.17	0.44
2:C:160:VAL:HG12	2:C:210:HIS:CD2	2.53	0.44
2:C:108:SER:OG	2:C:109:SER:N	2.50	0.44
2:D:43:ALA:HA	2:D:95:ALA:HB2	2.00	0.44
2:C:211:LYS:N	2:C:212:PRO:CD	2.81	0.43
2:D:2:VAL:HG21	2:D:101:ARG:NH2	2.33	0.43
2:D:39:TRP:CE2	2:D:84:MET:HB2	2.52	0.43
2:C:70:ARG:NH2	2:C:93:ASP:CG	2.72	0.43
2:D:36:ALA:HA	2:D:54:ILE:O	2.19	0.43
2:D:54:ILE:HD12	2:D:73:ILE:HG22	2.01	0.43
1:A:190:HIS:O	1:A:212:ARG:NH1	2.47	0.43
2:D:173:VAL:HG22	2:D:192:VAL:HB	2.01	0.43
2:D:136:PRO:HG3	2:D:148:LEU:HB3	2.01	0.42
1:A:133:VAL:HG13	1:A:180:LEU:HB3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:73:ILE:O	2:D:74:THR:HG23	2.20	0.42
1:A:51:GLY:O	1:A:52:ALA:HB3	2.20	0.42
2:C:94:THR:HA	2:C:119:VAL:O	2.20	0.42
1:B:13:LEU:O	1:B:107:ILE:HA	2.20	0.41
2:D:180:LEU:CD1	2:D:186:TYR:HE2	2.32	0.41
1:B:19:ALA:O	1:B:75:THR:HA	2.20	0.41
2:D:54:ILE:HD11	2:D:73:ILE:C	2.41	0.41
1:A:188:GLU:HA	1:A:212:ARG:HD2	2.03	0.41
1:A:33:TYR:HA	1:A:92:TYR:CE2	2.55	0.41
1:B:124:GLU:CD	2:C:219:LYS:NZ	2.74	0.41
2:D:210:HIS:HB3	2:D:215:THR:HG1	1.85	0.41
1:A:141:TYR:CG	1:A:142:PRO:HA	2.56	0.41
2:D:180:LEU:HA	2:D:180:LEU:HD12	1.76	0.41
1:B:124:GLU:OE2	2:C:219:LYS:NZ	2.52	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ASP:OD1	2:D:106:TYR:OH[3_544]	1.92	0.28
1:B:55:ARG:NH1	2:C:182:SER:O[4_544]	1.97	0.23
1:A:155:LEU:O	2:D:35:TYR:OH[3_544]	2.05	0.15

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	212/215 (99%)	205 (97%)	7 (3%)	0	100	100
1	B	213/215 (99%)	206 (97%)	5 (2%)	2 (1%)	17	35
2	C	201/228 (88%)	194 (96%)	7 (4%)	0	100	100
2	D	208/228 (91%)	200 (96%)	8 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	834/886 (94%)	805 (96%)	27 (3%)	2 (0%)	51 71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	166[A]	GLU
1	B	166[B]	GLU

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	182/186 (98%)	175 (96%)	7 (4%)	33 59
1	B	184/186 (99%)	181 (98%)	3 (2%)	62 82
2	C	162/187 (87%)	157 (97%)	5 (3%)	40 66
2	D	159/187 (85%)	150 (94%)	9 (6%)	20 41
All	All	687/746 (92%)	663 (96%)	24 (4%)	36 62

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	148	GLN
1	A	163	SER
1	A	170	LYS
1	A	173	THR
1	A	198	THR
1	A	214	GLU
1	B	12	SER
1	B	34	LEU
1	B	73	THR
2	C	6	GLN
2	C	25	SER
2	C	40	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	70	ARG
2	C	94	THR
2	D	3	GLN
2	D	32	PHE
2	D	40	VAL
2	D	70	ARG
2	D	79	THR
2	D	99	CYS
2	D	111	ASP
2	D	130	SER
2	D	145	THR

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

Mol	Chain	Res	Type
1	B	138	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 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

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	214/215 (99%)	0.04	0 100 100	23, 46, 66, 86	0
1	B	214/215 (99%)	0.08	2 (0%) 84 82	22, 40, 63, 86	0
2	C	209/228 (91%)	0.38	14 (6%) 17 13	24, 50, 81, 100	0
2	D	214/228 (93%)	0.50	23 (10%) 6 3	28, 54, 84, 111	0
All	All	851/886 (96%)	0.25	39 (4%) 32 26	22, 47, 76, 111	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	214	ASN	4.7
2	C	160	VAL	4.3
2	C	208	VAL	4.3
2	C	217	VAL	4.2
2	C	218	ASP	4.1
2	D	27	GLY	3.6
2	D	122	SER	3.5
2	C	204	TYR	3.4
2	D	69	GLY	3.2
2	D	28	THR	3.2
2	C	26	GLY	3.2
2	D	197	SER	3.1
2	D	135	ALA	3.0
2	C	159	PRO	2.9
2	C	195	PRO	2.9
1	B	213	GLY	2.9
2	D	203	THR	2.7
2	C	206	CYS	2.7
2	D	155	TYR	2.7
2	D	215	THR	2.7
2	C	169	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	210	HIS	2.6
2	D	157	PRO	2.6
2	D	1	GLN	2.6
2	D	196	SER	2.5
2	C	129	PRO	2.5
2	D	218	ASP	2.5
2	D	159	PRO	2.3
2	D	31	THR	2.3
2	D	151	LEU	2.3
2	D	29	GLY	2.3
2	D	30	GLY	2.2
2	D	121	VAL	2.1
2	D	186	TYR	2.1
2	C	13	LYS	2.1
2	D	217	VAL	2.0
1	B	30	SER	2.0
2	D	67	PHE	2.0
2	D	156	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 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.