



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 07:59 am GMT

PDB ID : 1U95
Title : Crystal structure of the HIV-1 Cross Neutralizing Monoclonal Antibody 2F5
in complex with gp41 Peptide ELDHWAS
Authors : Bryson, S.; Julien, J.-P.; Hynes, R.C.; Pai, E.F.
Deposited on : 2004-08-09
Resolution : 2.24 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

<http://wwpdb.org/validation/2016/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) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

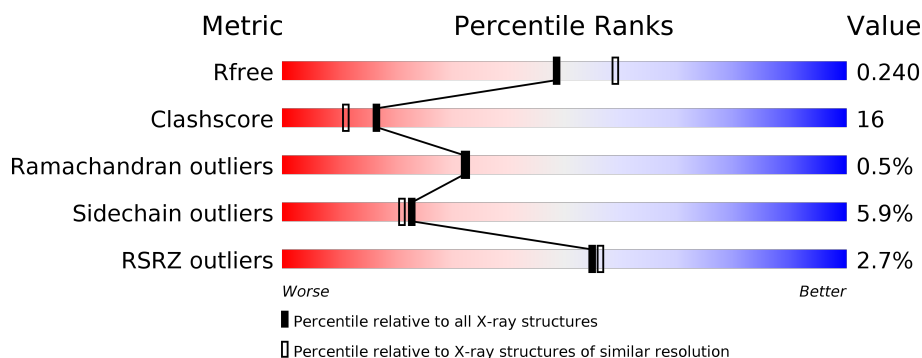
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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}	100719	1804 (2.26-2.22)
Clashscore	112137	1957 (2.26-2.22)
Ramachandran outliers	110173	1916 (2.26-2.22)
Sidechain outliers	110143	1917 (2.26-2.22)
RSRZ outliers	101464	1809 (2.26-2.22)

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	214	<div> <div>71%</div> <div>26%</div> <div>.</div> </div>
2	B	235	<div> <div>5%</div> <div>69%</div> <div>24%</div> <div>...</div> </div>
3	C	7	<div> <div>100%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3591 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 ANTIBODY 2F5 (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1644	1025	281	333	5			

- Molecule 2 is a protein called ANTIBODY 2F5 (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	0	0
			1705	1084	289	325	7			

- Molecule 3 is a protein called GP41 PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	7	Total	C	N	O	0	0	0
			61	38	10	13			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	86	Total	O	0	0
			86	86		
4	B	91	Total	O	0	0
			91	91		
4	C	4	Total	O	0	0
			4	4		

- Molecule 1: ANTIBODY 2F5 (LIGHT CHAIN)

- Molecule 2: ANTIBODY 2F5 (HEAVY CHAIN)

- Molecule 3: GP41 PEPTIDE

100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.70Å 64.90Å 175.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.00 – 2.24 60.89 – 2.22	Depositor EDS
% Data completeness (in resolution range)	95.7 (80.00-2.24) 94.5 (60.89-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.39 (at 2.22Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.210 , 0.238 0.212 , 0.240	Depositor DCC
R_{free} test set	1532 reflections (4.91%)	DCC
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 41.2	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	0.95	EDS
Total number of atoms	3591	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% 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

5.1 Standard geometry

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	0.90	2/1681 (0.1%)	0.94	2/2284 (0.1%)
2	B	0.94	2/1746 (0.1%)	1.07	8/2385 (0.3%)
3	C	0.84	0/63	0.76	0/84
All	All	0.92	4/3490 (0.1%)	1.01	10/4753 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	216	CYS	CB-SG	10.04	1.99	1.82
1	A	193	GLU	CG-CD	8.57	1.64	1.51
2	B	59	TYR	CD1-CE1	5.32	1.47	1.39
1	A	193	GLU	CB-CG	5.00	1.61	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	38	ARG	NE-CZ-NH2	-12.84	113.88	120.30
2	B	38	ARG	NE-CZ-NH1	12.79	126.70	120.30
2	B	66	ARG	NE-CZ-NH1	8.84	124.72	120.30
2	B	66	ARG	NE-CZ-NH2	-6.40	117.10	120.30
2	B	216	CYS	CA-CB-SG	6.01	124.82	114.00
2	B	178	LEU	CA-CB-CG	5.82	128.68	115.30
2	B	100(N)	MET	N-CA-C	-5.74	95.50	111.00
1	A	37	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	A	114	SER	N-CA-C	-5.20	96.95	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	38	ARG	CB-CG-CD	5.12	124.91	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	86	TYR	Sidechain

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	1644	0	1588	56	0
2	B	1705	0	1721	58	0
3	C	61	0	50	0	0
4	A	86	0	0	1	0
4	B	91	0	0	1	0
4	C	4	0	0	0	0
All	All	3591	0	3359	107	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 16.

All (107) 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:84:PRO:O	2:B:87:THR:HG23	1.65	0.96
1:A:90:GLN:HE22	1:A:93:PHE:H	1.01	0.93
1:A:20:THR:HG22	1:A:74:THR:HB	1.50	0.91
2:B:86:ASP:HB2	2:B:111:ILE:HD12	1.59	0.84
1:A:106:VAL:H	1:A:166:GLN:HE22	1.26	0.81
2:B:38:ARG:HD2	2:B:48:LEU:HD21	1.60	0.80
1:A:90:GLN:NE2	1:A:93:PHE:H	1.81	0.76
1:A:90:GLN:NE2	1:A:92:HIS:H	1.84	0.75
1:A:162:SER:HB2	2:B:167:PRO:HG2	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:ARG:NH1	2:B:212:GLU:OE1	2.25	0.70
2:B:29:LEU:O	2:B:53:SER:HB2	1.93	0.69
1:A:133:VAL:HG21	2:B:124:LEU:HD22	1.75	0.67
1:A:118:PHE:HB2	1:A:133:VAL:HG22	1.77	0.67
1:A:90:GLN:HE21	1:A:92:HIS:H	1.42	0.64
1:A:190:LYS:HG3	1:A:191:VAL:HG23	1.77	0.64
1:A:118:PHE:HD2	1:A:133:VAL:HG23	1.61	0.64
2:B:214:LYS:N	2:B:214:LYS:HE3	2.13	0.64
2:B:82(C):VAL:HB	2:B:111:ILE:HD13	1.79	0.63
1:A:8:PRO:O	1:A:102:THR:HB	2.01	0.61
1:A:79:ARG:HB3	1:A:81:GLU:OE2	2.01	0.60
1:A:167:ASP:HB3	1:A:170:ASP:HB2	1.84	0.60
2:B:82(C):VAL:CG2	2:B:111:ILE:HD13	2.33	0.59
2:B:213:PRO:C	2:B:214:LYS:HE3	2.23	0.59
1:A:29:VAL:HG11	1:A:90:GLN:HG3	1.84	0.59
2:B:213:PRO:HA	2:B:214:LYS:HE3	1.84	0.58
1:A:12:SER:HB3	1:A:140:TYR:OH	2.04	0.58
1:A:29:VAL:HG11	1:A:90:GLN:CG	2.35	0.57
1:A:90:GLN:NE2	1:A:92:HIS:N	2.51	0.57
1:A:183:LYS:O	1:A:187:GLU:HG2	2.05	0.56
2:B:135:ALA:HB1	2:B:183:THR:HG23	1.88	0.56
2:B:38:ARG:HD3	2:B:46:GLU:OE1	2.06	0.55
1:A:133:VAL:CG2	2:B:124:LEU:HD22	2.37	0.55
2:B:121:VAL:O	2:B:209:LYS:HE3	2.07	0.55
2:B:86:ASP:HB2	2:B:111:ILE:CD1	2.34	0.55
2:B:96:ARG:HD3	2:B:101:ASP:OD2	2.06	0.54
2:B:38:ARG:HB3	2:B:48:LEU:HD11	1.87	0.54
1:A:4:LEU:HD11	1:A:90:GLN:HB2	1.89	0.54
2:B:185:PRO:O	2:B:187:SER:N	2.40	0.54
1:A:21:ILE:HG23	1:A:102:THR:HG21	1.90	0.53
2:B:100(B):PHE:O	2:B:100(D):VAL:HG23	2.08	0.53
1:A:6:GLN:HE21	1:A:99:GLY:HA3	1.73	0.53
1:A:124:GLN:HE22	1:A:131:SER:HB2	1.75	0.52
1:A:81:GLU:CD	1:A:81:GLU:H	2.13	0.52
2:B:185:PRO:C	2:B:187:SER:H	2.13	0.52
1:A:124:GLN:NE2	1:A:131:SER:H	2.07	0.52
1:A:147:GLN:NE2	1:A:154:LEU:HG	2.25	0.52
1:A:39:LYS:HE3	4:A:248:HOH:O	2.09	0.52
2:B:188:SER:HB3	2:B:194:TYR:OH	2.10	0.51
2:B:213:PRO:C	2:B:214:LYS:HZ2	2.13	0.51
1:A:94:TYR:CZ	2:B:58:ARG:HG3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ASN:ND2	1:A:158:ASN:H	2.09	0.51
2:B:87:THR:HG22	2:B:111:ILE:H	1.75	0.51
2:B:193:THR:HG22	2:B:210:ARG:HH21	1.76	0.51
1:A:9:SER:O	1:A:102:THR:HA	2.10	0.51
1:A:155:GLN:HB3	1:A:158:ASN:HD21	1.76	0.51
1:A:118:PHE:HB2	1:A:133:VAL:CG2	2.41	0.50
2:B:84:PRO:O	2:B:87:THR:CG2	2.51	0.50
2:B:12:VAL:O	2:B:111:ILE:HA	2.13	0.49
2:B:114:THR:HG21	2:B:146:PHE:CB	2.43	0.49
2:B:87:THR:HB	2:B:110:THR:HA	1.95	0.48
1:A:170:ASP:HB3	1:A:172:THR:HG23	1.95	0.48
2:B:82(C):VAL:CB	2:B:111:ILE:HD13	2.43	0.48
1:A:147:GLN:CD	1:A:154:LEU:HD11	2.34	0.48
2:B:82(C):VAL:HB	2:B:111:ILE:CD1	2.42	0.48
2:B:201:LYS:HB2	2:B:202:PRO:HD3	1.96	0.47
1:A:2:LEU:C	1:A:2:LEU:HD23	2.34	0.47
1:A:158:ASN:H	1:A:158:ASN:HD22	1.62	0.47
1:A:37:ARG:HB2	1:A:47:LEU:HD11	1.96	0.47
1:A:118:PHE:CD2	1:A:133:VAL:HG23	2.47	0.47
1:A:90:GLN:HE22	1:A:93:PHE:N	1.87	0.46
2:B:29:LEU:O	2:B:53:SER:CB	2.62	0.46
1:A:138:ASN:OD1	2:B:164:HIS:HE1	1.97	0.46
2:B:13:LYS:H	2:B:16:GLN:NE2	2.13	0.46
2:B:213:PRO:C	2:B:214:LYS:NZ	2.69	0.45
1:A:143:GLU:H	1:A:143:GLU:CD	2.20	0.45
1:A:147:GLN:CG	1:A:154:LEU:HD11	2.47	0.45
2:B:35(B):GLY:HA2	2:B:50:ILE:HA	1.98	0.45
2:B:213:PRO:C	2:B:214:LYS:CE	2.85	0.45
1:A:44:PRO:HD2	2:B:103:TRP:CE3	2.52	0.44
2:B:114:THR:CG2	2:B:115:SER:N	2.81	0.44
2:B:114:THR:CG2	2:B:115:SER:O	2.65	0.44
1:A:124:GLN:HG2	1:A:129:THR:O	2.16	0.44
1:A:201:LEU:HD13	1:A:205:VAL:HG12	1.99	0.44
1:A:206:THR:O	1:A:207:LYS:HD2	2.18	0.44
2:B:114:THR:HG21	2:B:175:LEU:HD23	1.99	0.43
1:A:175:LEU:HD23	1:A:175:LEU:C	2.38	0.43
1:A:201:LEU:CD1	1:A:205:VAL:HG12	2.49	0.43
1:A:133:VAL:HG21	2:B:124:LEU:CD2	2.44	0.43
1:A:158:ASN:N	1:A:158:ASN:ND2	2.66	0.43
2:B:178:LEU:HD12	2:B:178:LEU:C	2.39	0.43
2:B:114:THR:HG22	2:B:115:SER:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100(H):ARG:O	2:B:100(K):VAL:HG22	2.20	0.42
2:B:70:THR:CG2	2:B:79:VAL:HB	2.50	0.42
2:B:100(A):LEU:HG	2:B:100(B):PHE:CD1	2.55	0.41
1:A:6:GLN:NE2	1:A:88:CYS:H	2.18	0.41
2:B:138:LEU:N	2:B:138:LEU:CD2	2.83	0.41
1:A:159:SER:HA	1:A:178:THR:O	2.21	0.41
2:B:100:THR:HA	2:B:100(D):VAL:O	2.21	0.41
2:B:185:PRO:C	2:B:187:SER:N	2.73	0.41
2:B:87:THR:CG2	2:B:111:ILE:H	2.34	0.41
2:B:138:LEU:N	2:B:138:LEU:HD23	2.36	0.41
2:B:76:ASN:ND2	4:B:217:HOH:O	2.51	0.41
1:A:150:VAL:O	1:A:151:ASP:C	2.60	0.41
1:A:29:VAL:HG11	1:A:90:GLN:HG2	2.03	0.41
2:B:66:ARG:NH2	2:B:86:ASP:OD2	2.53	0.41
1:A:24:ARG:HA	1:A:69:THR:O	2.21	0.40
2:B:213:PRO:CA	2:B:214:LYS:HE3	2.48	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	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
2	B	221/235 (94%)	212 (96%)	7 (3%)	2 (1%)	20	16
3	C	5/7 (71%)	5 (100%)	0	0	100	100
All	All	438/456 (96%)	421 (96%)	15 (3%)	2 (0%)	32	32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	214	LYS

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Mol	Chain	Res	Type
2	B	186	SER

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	187/187 (100%)	177 (95%)	10 (5%)	26	26
2	B	197/203 (97%)	184 (93%)	13 (7%)	19	17
3	C	6/6 (100%)	6 (100%)	0	100	100
All	All	390/396 (98%)	367 (94%)	23 (6%)	23	21

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	A	24	ARG
1	A	54	LEU
1	A	74	THR
1	A	97	THR
1	A	102	THR
1	A	143	GLU
1	A	158	ASN
1	A	170	ASP
1	A	202	SER
2	B	29	LEU
2	B	38	ARG
2	B	87	THR
2	B	96	ARG
2	B	138	LEU
2	B	149	PRO
2	B	159	LEU
2	B	170	LEU
2	B	178	LEU
2	B	195	THR
2	B	197	ASN

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Mol	Chain	Res	Type
2	B	199	ASN
2	B	214	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	38	GLN
1	A	90	GLN
1	A	124	GLN
1	A	137	ASN
1	A	147	GLN
1	A	155	GLN
1	A	158	ASN
1	A	166	GLN
1	A	199	GLN
2	B	16	GLN
2	B	39	GLN
2	B	76	ASN
2	B	164	HIS
2	B	192	GLN
2	B	199	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	214/214 (100%)	0.14	1 (0%) 90 91	25, 37, 52, 58	0
2	B	227/235 (96%)	0.27	11 (4%) 31 31	23, 35, 57, 78	0
3	C	7/7 (100%)	0.10	0 100 100	30, 33, 43, 58	0
All	All	448/456 (98%)	0.21	12 (2%) 55 56	23, 36, 56, 78	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	216	CYS	12.5
2	B	133	GLY	5.1
2	B	215	SER	4.7
2	B	126	PRO	4.4
2	B	134	ALA	4.2
2	B	100(B)	PHE	3.1
2	B	114	THR	2.8
2	B	214	LYS	2.6
2	B	187	SER	2.5
2	B	186	SER	2.4
2	B	213	PRO	2.2
1	A	170	ASP	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.