



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 10:57 am BST

PDB ID : 5WDF
Title : Crystal structure of 10E8v4-5R+100cF Fab in complex with HIV-1 gp41 peptide
Authors : Kwon, Y.D.; Kwong, P.D.
Deposited on : 2017-07-05
Resolution : 3.10 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

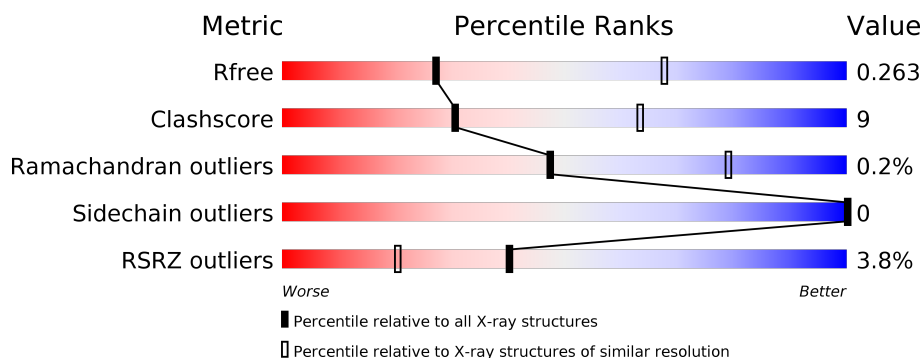
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	232	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>19%</div> <div>13%</div> </div> </div>
1	H	232	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>15%</div> <div>10%</div> </div> </div>
2	B	214	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>19%</div> <div>7%</div> </div> </div>
2	L	214	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div>•</div> </div> </div>
3	P	17	<div> <div>12%</div> <div> <div></div> <div>94%</div> <div>6%</div> </div> </div>
3	Q	17	<div> <div>6%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>6%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6558 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 10E8v4-5R+100cF Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	209	Total	C	N	O	S	0	0	0
			1615	1029	271	309	6			
1	A	202	Total	C	N	O	S	0	0	0
			1577	1004	265	303	5			

- Molecule 2 is a protein called FA10E8v4-5R+100cF FAB light chain.

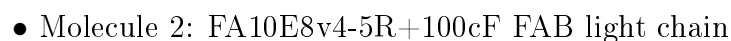
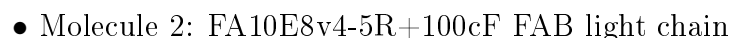
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	206	Total	C	N	O	S	0	0	0
			1554	968	268	314	4			
2	B	198	Total	C	N	O	S	0	0	0
			1496	935	257	300	4			

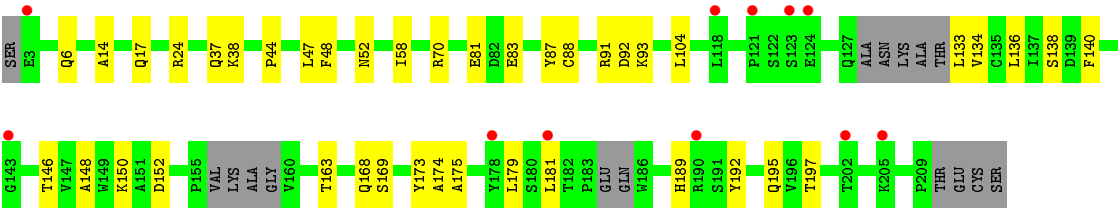
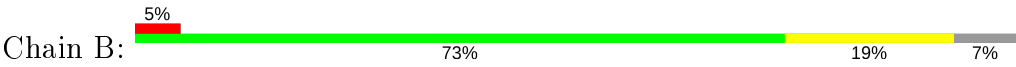
- Molecule 3 is a protein called HIV-1 gp41 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	17	Total	C	N	O	0	0	0
			167	119	25	23			
3	Q	16	Total	C	N	O	0	0	0
			149	105	23	21			



- Molecule 1: 10E8v4-5R+100cF Fab heavy chain

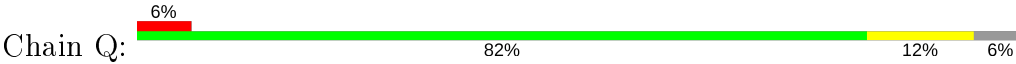




• Molecule 3: HIV-1 gp41 peptide



• Molecule 3: HIV-1 gp41 peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.28Å 60.95Å 70.15Å 103.08° 107.46° 100.05°	Depositor
Resolution (Å)	45.12 – 3.10 45.12 – 3.10	Depositor EDS
% Data completeness (in resolution range)	93.2 (45.12-3.10) 93.1 (45.12-3.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.247 , 0.281 0.249 , 0.263	Depositor DCC
R_{free} test set	751 reflections (5.22%)	wwPDB-VP
Wilson B-factor (Å ²)	92.0	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 46.3	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	0.90	EDS
Total number of atoms	6558	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.88% 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	0.26	0/1620	0.45	0/2196
1	H	0.26	0/1661	0.49	0/2258
2	B	0.27	0/1529	0.47	0/2078
2	L	0.25	0/1589	0.44	0/2162
3	P	0.22	0/176	0.30	0/240
3	Q	0.25	0/156	0.31	0/212
All	All	0.26	0/6731	0.46	0/9146

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

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	1577	0	1502	32	0
1	H	1615	0	1541	39	0
2	B	1496	0	1457	41	0
2	L	1554	0	1514	20	0
3	P	167	0	162	1	0
3	Q	149	0	140	2	0
All	All	6558	0	6316	118	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 9.

All (118) 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:H:27:PHE:CE1	1:H:29:PHE:HA	1.66	1.29
2:B:140:PHE:CE2	2:B:174:ALA:HA	1.73	1.24
2:B:140:PHE:CZ	2:B:174:ALA:HA	1.81	1.15
1:H:27:PHE:HE1	1:H:29:PHE:CA	1.64	1.09
2:B:140:PHE:CZ	2:B:174:ALA:CA	2.37	1.06
1:H:27:PHE:HE1	1:H:29:PHE:HA	0.86	1.02
1:H:27:PHE:CE1	1:H:29:PHE:CA	2.39	0.98
1:H:27:PHE:HD1	1:H:28:ASP:C	1.69	0.95
2:B:140:PHE:HZ	2:B:174:ALA:CA	1.85	0.89
1:H:27:PHE:HZ	1:H:29:PHE:HD1	1.29	0.80
1:H:27:PHE:CZ	1:H:29:PHE:HD1	2.00	0.80
2:B:140:PHE:HZ	2:B:174:ALA:C	1.85	0.79
1:H:27:PHE:CD1	1:H:28:ASP:C	2.55	0.79
2:B:140:PHE:HE2	2:B:174:ALA:HA	1.42	0.79
2:B:181:LEU:HD11	2:B:192:TYR:HE2	1.51	0.75
1:H:27:PHE:HD1	1:H:28:ASP:O	1.70	0.72
2:L:24:ARG:HG2	2:L:70:ARG:HG2	1.74	0.70
2:L:148:ALA:HB3	2:L:195:GLN:HB2	1.74	0.68
2:B:140:PHE:CZ	2:B:174:ALA:N	2.62	0.68
2:B:6:GLN:NE2	2:B:88:CYS:SG	2.65	0.67
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.77	0.67
2:L:117:THR:HB	2:L:136:LEU:HB3	1.77	0.67
2:L:146:THR:HB	2:L:197:THR:HB	1.78	0.66
1:H:27:PHE:CE1	1:H:29:PHE:CB	2.79	0.66
2:B:140:PHE:CE2	2:B:174:ALA:CA	2.64	0.65
1:H:169:VAL:HG11	2:L:161:GLU:HB3	1.79	0.64
2:B:38:LYS:HD3	2:B:44:PRO:HG3	1.83	0.61
2:B:181:LEU:HD11	2:B:192:TYR:CE2	2.34	0.61
1:H:27:PHE:CD1	1:H:28:ASP:O	2.54	0.60
1:H:87:THR:HG23	1:H:110:ILE:HA	1.85	0.59
1:A:50:ARG:HH21	3:Q:673:PHE:HZ	1.48	0.59
1:A:100(B):TRP:O	3:Q:683:LYS:NZ	2.26	0.58
2:L:38:LYS:HD3	2:L:44:PRO:HG3	1.84	0.58
2:B:148:ALA:HB3	2:B:195:GLN:HB2	1.85	0.58
1:A:66:ARG:NH1	1:A:86:ASP:OD2	2.36	0.57
1:H:38:ARG:NH1	1:H:86:ASP:OD1	2.37	0.57
1:A:29:PHE:O	1:A:71:ARG:NH2	2.39	0.56
1:A:200:HIS:CD2	1:A:202:PRO:HD2	2.41	0.56
1:A:89:TYR:HE1	1:A:108:LEU:HD13	1.70	0.56
2:B:24:ARG:HG2	2:B:70:ARG:HG2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:27:PHE:CD1	1:H:29:PHE:HA	2.34	0.56
2:B:138:SER:HA	2:B:140:PHE:HE2	1.71	0.56
1:A:169:VAL:HB	2:B:163:THR:HG22	1.88	0.55
1:H:27:PHE:CZ	1:H:29:PHE:CD1	2.90	0.54
1:A:39:GLN:HB2	1:A:45:LEU:HD23	1.90	0.53
1:A:34:MET:HB3	1:A:78:LEU:HD22	1.91	0.53
1:H:29:PHE:O	1:H:71:ARG:NH2	2.42	0.53
1:H:27:PHE:CD1	1:H:29:PHE:N	2.77	0.52
2:B:168:GLN:HG2	2:B:169:SER:H	1.75	0.51
2:B:140:PHE:HZ	2:B:175:ALA:N	2.08	0.51
2:B:189:HIS:HB2	2:B:192:TYR:HE1	1.76	0.50
2:B:6:GLN:HE22	2:B:88:CYS:H	1.59	0.50
2:L:59:PRO:HD3	2:B:81:GLU:OE2	2.11	0.50
1:A:35:THR:OG1	1:A:95:THR:OG1	2.21	0.50
1:H:27:PHE:CE1	1:H:29:PHE:HB2	2.47	0.50
1:H:34:MET:HB3	1:H:78:LEU:HD22	1.93	0.49
1:A:7:SER:OG	1:A:21:SER:OG	2.30	0.49
2:B:146:THR:HB	2:B:197:THR:HB	1.95	0.49
1:H:3:ARG:NH2	1:A:106:GLY:O	2.46	0.49
2:L:168:GLN:HG2	2:L:169:SER:H	1.78	0.48
1:H:97:LYS:HD2	3:P:672:TRP:CD2	2.48	0.48
1:H:40:PRO:HB2	1:H:43:LYS:HD2	1.95	0.48
1:A:87:THR:HG23	1:A:110:ILE:HA	1.94	0.48
1:H:171:GLN:HG2	1:H:175:LEU:O	2.13	0.48
2:B:150:LYS:HE3	2:B:195:GLN:HG3	1.96	0.48
2:B:6:GLN:NE2	2:B:88:CYS:H	2.12	0.47
1:H:50:ARG:NH1	2:L:95(B):ARG:O	2.45	0.47
1:A:89:TYR:CE1	1:A:108:LEU:HD13	2.49	0.47
2:B:47:LEU:HA	2:B:58:ILE:HD13	1.96	0.47
1:A:39:GLN:OE1	2:B:38:LYS:HE3	2.14	0.47
1:A:44:GLY:HA2	2:B:87:TYR:OH	2.15	0.46
2:L:114:PRO:HA	2:L:140:PHE:HB3	1.97	0.46
2:L:133:LEU:HD12	2:L:179:LEU:HD23	1.98	0.46
1:A:168:ALA:HB2	1:A:178:LEU:HD23	1.96	0.46
1:H:163:VAL:HG22	1:H:182:VAL:HG22	1.98	0.46
2:L:48:PHE:CZ	2:L:52:ASN:HA	2.51	0.46
1:A:100(J):GLU:HG3	2:B:91:ARG:NH2	2.31	0.45
1:H:181:VAL:HG11	2:L:136:LEU:HD13	1.99	0.45
1:H:27:PHE:HE1	1:H:29:PHE:CB	2.20	0.45
1:A:141:LEU:HD13	2:B:134:VAL:HG21	1.99	0.45
1:A:60:ALA:O	1:A:64:LYS:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:140:PHE:N	2:B:140:PHE:CD2	2.85	0.45
1:H:27:PHE:CD1	1:H:29:PHE:CA	2.95	0.45
1:H:36:TRP:CE2	1:H:80:LEU:HB2	2.52	0.45
1:A:108:LEU:HD21	1:A:110:ILE:HD11	1.98	0.45
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.99	0.45
1:A:22:CYS:HB3	1:A:78:LEU:HB3	2.00	0.44
1:A:164:HIS:ND1	2:B:168:GLN:HG3	2.33	0.44
2:B:48:PHE:CZ	2:B:52:ASN:HA	2.53	0.44
1:A:152:VAL:HA	1:A:197:ASN:O	2.18	0.43
2:B:138:SER:C	2:B:140:PHE:HD2	2.20	0.43
1:H:30:ASP:OD2	1:A:201:LYS:HE2	2.19	0.43
1:A:33:TRP:CZ2	1:A:97:LYS:HD3	2.53	0.43
2:B:133:LEU:HD12	2:B:179:LEU:HD23	2.01	0.42
1:H:146:PHE:CD1	1:H:147:PRO:HA	2.54	0.42
2:L:34:SER:OG	2:L:89:SER:OG	2.36	0.42
1:A:50:ARG:NH2	1:A:58:ASP:OD2	2.52	0.42
2:B:140:PHE:CE2	2:B:173:TYR:O	2.73	0.42
2:B:83:GLU:HG3	2:B:104:LEU:O	2.19	0.42
2:B:92:ASP:OD1	2:B:93:LYS:N	2.53	0.42
1:A:166:PHE:CE2	2:B:136:LEU:HD22	2.55	0.42
1:A:168:ALA:HA	1:A:178:LEU:HB3	2.02	0.42
1:H:124:LEU:HD13	2:L:119:PHE:CD2	2.55	0.42
2:L:109:GLN:HB2	2:L:141:TYR:CE2	2.55	0.42
2:L:133:LEU:HD21	2:L:186:TRP:CZ3	2.54	0.42
1:A:67:PHE:CE1	1:A:82:MET:HB2	2.55	0.41
1:A:63:VAL:HG13	1:A:67:PHE:CD2	2.55	0.41
1:H:152:VAL:HG22	1:H:198:VAL:HG22	2.03	0.41
1:H:30:ASP:OD1	1:H:73:ASN:HB3	2.20	0.41
1:H:27:PHE:HZ	1:H:29:PHE:CD1	2.21	0.41
2:B:14:ALA:HB3	2:B:17:GLN:HG3	2.02	0.41
1:H:20:LEU:HD22	1:H:107:THR:HG21	2.03	0.41
2:L:5:THR:N	2:L:24:ARG:O	2.38	0.41
2:B:140:PHE:CZ	2:B:175:ALA:N	2.89	0.41
1:H:33:TRP:CZ2	1:H:97:LYS:HD3	2.56	0.41
1:A:119:PRO:HB3	1:A:145:TYR:HB3	2.03	0.40
1:H:100(K):TYR:HE2	1:H:101:GLN:HE21	1.68	0.40
2:L:58:ILE:HG23	2:L:59:PRO:HD2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	192/232 (83%)	182 (95%)	10 (5%)	0	100	100
1	H	201/232 (87%)	194 (96%)	7 (4%)	0	100	100
2	B	190/214 (89%)	177 (93%)	12 (6%)	1 (0%)	29	64
2	L	202/214 (94%)	193 (96%)	8 (4%)	1 (0%)	29	64
3	P	15/17 (88%)	15 (100%)	0	0	100	100
3	Q	14/17 (82%)	14 (100%)	0	0	100	100
All	All	814/926 (88%)	775 (95%)	37 (4%)	2 (0%)	47	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	152	ASP
2	L	152	ASP

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	173/195 (89%)	173 (100%)	0	100	100
1	H	178/195 (91%)	178 (100%)	0	100	100
2	B	168/180 (93%)	168 (100%)	0	100	100
2	L	174/180 (97%)	174 (100%)	0	100	100
3	P	17/17 (100%)	17 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Q	14/17 (82%)	14 (100%)	0	100	100
All	All	724/784 (92%)	724 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some 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 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 [i](#)

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	202/232 (87%)	0.24	9 (4%)	33 16	64, 108, 165, 189	0
1	H	209/232 (90%)	0.13	4 (1%)	66 46	59, 108, 166, 194	0
2	B	198/214 (92%)	0.32	11 (5%)	24 11	62, 119, 182, 209	0
2	L	206/214 (96%)	0.19	5 (2%)	59 37	51, 111, 176, 251	0
3	P	17/17 (100%)	0.86	2 (11%)	4 2	88, 131, 184, 189	0
3	Q	16/17 (94%)	0.48	1 (6%)	20 8	97, 126, 144, 147	0
All	All	848/926 (91%)	0.24	32 (3%)	40 20	51, 113, 171, 251	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	143	GLY	4.8
1	A	163	VAL	4.8
1	A	156	SER	4.3
2	B	205	LYS	4.2
1	H	208	ASP	3.8
2	B	124	GLU	3.6
2	B	181	LEU	3.5
2	L	112	ALA	3.5
2	B	202	THR	3.4
1	H	148	GLU	3.3
1	H	59	TYR	3.3
1	A	1	GLU	3.2
3	P	668	SER	3.2
1	A	160	THR	3.0
1	A	154	TRP	3.0
2	B	123	SER	3.0
2	B	121	PRO	2.9
1	A	121	VAL	2.9
1	A	164	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
2	L	169	SER	2.7
2	B	118	LEU	2.7
2	L	121	PRO	2.7
3	P	684	LYS	2.6
2	B	178	TYR	2.4
2	B	3	GLU	2.3
1	A	98	TYR	2.3
1	A	141	LEU	2.3
2	B	190	ARG	2.2
3	Q	678	TRP	2.2
2	L	192	TYR	2.1
2	L	163	THR	2.1
1	H	100(C)	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.