Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 01:46 am BST

PDB ID	:	6MQC
Title	:	Vaccine-elicited NHP FP-targeting neutralizing antibody 0PV-c.01 in complex with FP (residue 512-519)
Authors	:	Xu, K.; Wang, Y.; Kwong, P.D.
Deposited on	:	2018-10-09
Resolution	:	1.99 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:

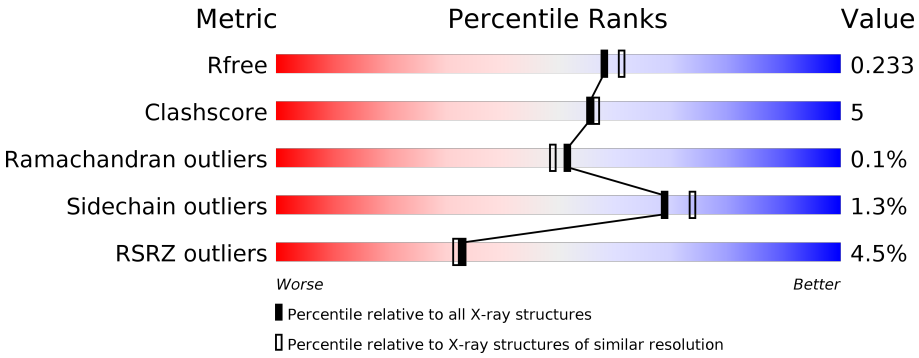
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 1.99 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	230	9% 81% 15%
1	H	230	5% 84% 10% 5%
2	B	219	% 91% 8%
2	L	219	% 86% 12%
3	C	8	13% 75% 25%
3	D	8	88% 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7169 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 0PV-C.01 antibody Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1660	1050	280	326	4			
1	H	219	Total	C	N	O	S	0	0	0
			1642	1039	277	322	4			

- Molecule 2 is a protein called 0PV-C.01 antibody Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1660	1039	275	339	7			
2	L	217	Total	C	N	O	S	0	0	0
			1660	1039	275	339	7			

- Molecule 3 is a protein called HIV fusion peptide residue 512-519.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	8	Total	C	N	O	0	0	0
			51	35	8	8			
3	D	8	Total	C	N	O	0	0	0
			51	35	8	8			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	74	Total	O	0	0
			74	74		
4	B	145	Total	O	0	0
			145	145		
4	H	96	Total	O	0	0
			96	96		
4	L	125	Total	O	0	0
			125	125		

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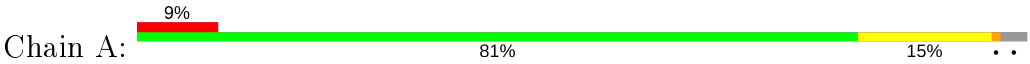
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total O 1 1	0	0
4	D	4	Total O 4 4	0	0

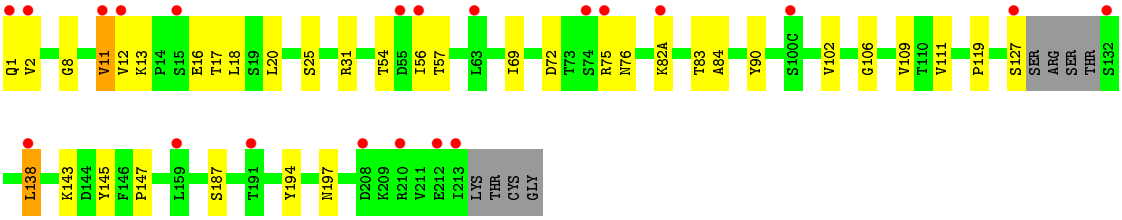
3 Residue-property plots (i)

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: 0PV-C.01 antibody Fab heavy chain

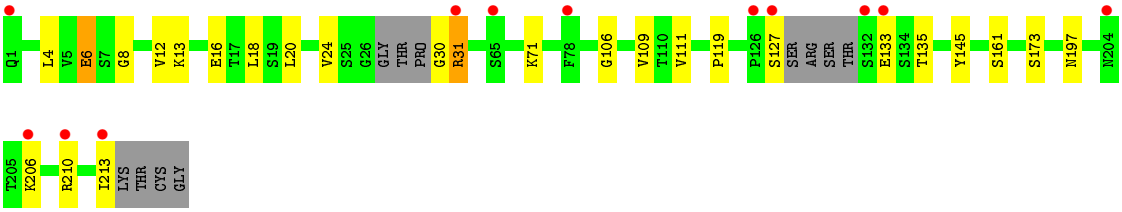
Chain A:





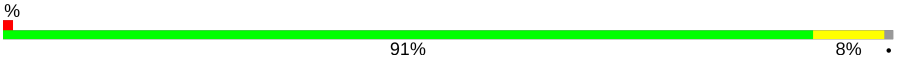
- Molecule 1: 0PV-C.01 antibody Fab heavy chain

Chain H:



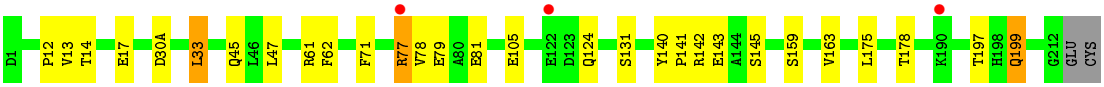
- Molecule 2: 0PV-C.01 antibody Fab light chain

Chain B:



- Molecule 2: 0PV-C.01 antibody Fab light chain

Chain L:



- Molecule 3: HIV fusion peptide residue 512-519

Chain C:

- Molecule 3: HIV fusion peptide residue 512-519

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.12Å 72.90Å 169.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.62 – 1.99 44.63 – 1.99	Depositor EDS
% Data completeness (in resolution range)	98.7 (44.62-1.99) 98.7 (44.63-1.99)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.199 , 0.234 0.198 , 0.233	Depositor DCC
R_{free} test set	3061 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	33.6	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 46.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.020 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7169	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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

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	0.33	0/1701	0.66	4/2327 (0.2%)
1	H	0.35	0/1681	0.68	5/2297 (0.2%)
2	B	0.40	0/1695	0.67	5/2306 (0.2%)
2	L	0.59	0/1695	0.67	4/2306 (0.2%)
3	C	0.88	0/51	0.48	0/68
3	D	0.25	0/51	0.44	0/68
All	All	0.43	0/6874	0.67	18/9372 (0.2%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	24	ARG	NE-CZ-NH1	-11.85	114.38	120.30
2	L	77	ARG	CG-CD-NE	10.72	134.32	111.80
1	H	210	ARG	CB-CG-CD	-9.98	85.66	111.60
1	A	138	LEU	CB-CG-CD1	-9.37	95.08	111.00
1	H	210	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	A	138	LEU	CA-CB-CG	7.84	133.34	115.30
1	H	206	LYS	CB-CG-CD	7.82	131.93	111.60
2	B	24	ARG	NE-CZ-NH2	6.85	123.73	120.30
2	L	77	ARG	NE-CZ-NH1	6.82	123.71	120.30
2	B	24	ARG	CB-CA-C	-6.57	97.27	110.40
2	L	77	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	11	VAL	CG1-CB-CG2	6.21	120.84	110.90
1	A	138	LEU	CB-CA-C	-6.01	98.79	110.20
2	B	24	ARG	CD-NE-CZ	5.76	131.67	123.60
2	L	30(A)	ASP	CB-CG-OD2	5.59	123.34	118.30
1	H	206	LYS	CD-CE-NZ	5.38	124.08	111.70
2	B	24	ARG	N-CA-CB	5.36	120.26	110.60
1	H	206	LYS	CA-CB-CG	5.25	124.94	113.40

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	1660	0	1648	21	1
1	H	1642	0	1630	15	1
2	B	1660	0	1613	13	0
2	L	1660	0	1613	19	0
3	C	51	0	53	2	0
3	D	51	0	53	1	0
4	A	74	0	0	1	0
4	B	145	0	0	7	0
4	C	1	0	0	0	0
4	D	4	0	0	0	0
4	H	96	0	0	5	0
4	L	125	0	0	4	0
All	All	7169	0	6610	68	1

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 5.

All (68) 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:54:ARG:NH2	4:B:302:HOH:O	1.83	1.12
2:B:79:GLU:OE2	4:B:301:HOH:O	1.82	0.95
1:H:213:ILE:O	4:H:301:HOH:O	1.98	0.80
1:H:30:GLY:N	4:H:303:HOH:O	2.23	0.70
2:L:13:VAL:HG11	2:L:78:VAL:HG21	1.73	0.70
1:A:187:SER:O	4:A:301:HOH:O	2.10	0.69
2:B:124:GLN:OE1	2:B:131:SER:N	2.25	0.69
1:A:18:LEU:HD13	1:A:109:VAL:HG11	1.75	0.67
1:A:11:VAL:HG21	1:A:147:PRO:HG3	1.81	0.63
2:L:105:GLU:HB3	4:L:406:HOH:O	2.01	0.61
2:B:14:THR:HG22	2:B:107:ARG:HD2	1.84	0.58
2:B:72:THR:HG21	2:B:74:LYS:HE3	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:THR:OG1	1:A:56:ILE:HG13	2.02	0.58
1:H:31:ARG:NH2	4:H:306:HOH:O	2.37	0.57
1:H:119:PRO:HB3	1:H:145:TYR:HB3	1.87	0.57
1:A:83:THR:O	1:A:111:VAL:HG21	2.05	0.56
2:L:45:GLN:HB2	4:L:417:HOH:O	2.06	0.55
2:L:143:GLU:OE1	4:L:301:HOH:O	2.18	0.55
2:L:124:GLN:OE1	2:L:131:SER:N	2.34	0.55
1:H:173:SER:OG	4:H:302:HOH:O	2.04	0.54
1:H:133:GLU:HG3	1:H:135:THR:H	1.72	0.54
1:A:12:VAL:HG23	1:A:111:VAL:HG12	1.90	0.53
1:A:84:ALA:HA	1:A:111:VAL:HG23	1.91	0.53
1:H:8:GLY:HA3	1:H:20:LEU:HD23	1.90	0.53
2:B:54:ARG:NH2	4:B:307:HOH:O	2.43	0.52
2:B:45:GLN:HB2	4:B:335:HOH:O	2.11	0.51
1:A:12:VAL:CG2	1:A:111:VAL:HG12	2.41	0.51
1:A:8:GLY:HA3	1:A:20:LEU:HD23	1.94	0.49
1:H:6:GLU:OE2	1:H:106:GLY:N	2.45	0.48
2:L:47:LEU:HD21	2:L:62:PHE:CD1	2.48	0.48
2:L:199:GLN:NE2	4:L:303:HOH:O	2.34	0.48
1:A:13:LYS:HB2	1:A:16:GLU:HG3	1.96	0.47
1:A:57:THR:HG21	1:A:69:ILE:HB	1.95	0.47
2:L:12:PRO:HA	2:L:105:GLU:HG3	1.96	0.46
1:H:31:ARG:HG2	3:C:519:PHE:CE1	2.51	0.46
1:A:138:LEU:HD11	1:A:194:TYR:CB	2.46	0.46
1:H:18:LEU:HD13	1:H:109:VAL:HG11	1.96	0.46
2:L:81:GLU:CD	2:L:81:GLU:H	2.19	0.45
1:A:17:THR:OG1	1:A:82(A):LYS:HD2	2.17	0.45
2:L:145:SER:HB2	2:L:197:THR:HB	1.97	0.45
2:L:77:ARG:HH21	2:L:77:ARG:HD2	1.56	0.45
1:H:4:LEU:HD22	1:H:24:VAL:HG22	1.99	0.45
2:L:61:ARG:CZ	2:L:79:GLU:HG3	2.47	0.45
2:L:159:SER:HA	2:L:178:THR:O	2.17	0.44
1:A:119:PRO:HB3	1:A:145:TYR:HB3	2.00	0.44
1:A:2:VAL:HG12	1:A:25:SER:O	2.16	0.44
2:B:45:GLN:NE2	4:B:309:HOH:O	2.50	0.44
1:H:31:ARG:O	3:C:518:VAL:HA	2.17	0.44
2:L:163:VAL:HG22	2:L:175:LEU:HD12	2.00	0.44
2:B:122:GLU:O	2:B:126:LYS:HG3	2.18	0.44
2:B:140:TYR:CG	2:B:141:PRO:HA	2.53	0.44
2:L:142:ARG:CZ	2:L:163:VAL:HG21	2.47	0.44
2:B:45:GLN:NE2	4:B:304:HOH:O	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:TRP:HB2	2:B:48:ILE:HB	2.02	0.42
1:A:143:LYS:HB2	1:A:143:LYS:HE2	1.75	0.42
2:L:142:ARG:NH2	2:L:163:VAL:HG21	2.35	0.42
2:L:14:THR:HB	2:L:17:GLU:HG3	2.01	0.42
2:B:74:LYS:HD2	4:B:336:HOH:O	2.20	0.42
1:H:13:LYS:HB2	1:H:16:GLU:HG3	2.02	0.42
1:H:12:VAL:O	1:H:111:VAL:HA	2.20	0.41
2:L:140:TYR:CG	2:L:141:PRO:HA	2.55	0.41
1:A:1:GLN:O	1:A:102:VAL:HG21	2.20	0.41
1:A:72:ASP:HB3	1:A:75:ARG:HB2	2.02	0.41
1:A:90:TYR:O	1:A:106:GLY:HA2	2.22	0.41
1:H:31:ARG:CZ	4:H:306:HOH:O	2.68	0.40
2:L:33:LEU:HD13	2:L:71:PHE:CD1	2.56	0.40
1:A:138:LEU:HD11	1:A:194:TYR:CG	2.56	0.40
1:A:31:ARG:O	3:D:518:VAL:HA	2.22	0.40

All (1) 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:75:ARG:NH1	1:H:161:SER:OG[1_545]	1.98	0.22

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	218/230 (95%)	214 (98%)	3 (1%)	1 (0%)	29 23
1	H	213/230 (93%)	212 (100%)	1 (0%)	0	100 100
2	B	215/219 (98%)	211 (98%)	4 (2%)	0	100 100
2	L	215/219 (98%)	211 (98%)	4 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C	6/8 (75%)	6 (100%)	0	0	100 100
3	D	6/8 (75%)	6 (100%)	0	0	100 100
All	All	873/914 (96%)	860 (98%)	12 (1%)	1 (0%)	51 49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	ASN

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	191/198 (96%)	189 (99%)	2 (1%)	76 81
1	H	189/198 (96%)	184 (97%)	5 (3%)	46 48
2	B	195/197 (99%)	194 (100%)	1 (0%)	88 92
2	L	195/197 (99%)	193 (99%)	2 (1%)	76 81
3	C	4/4 (100%)	4 (100%)	0	100 100
3	D	4/4 (100%)	4 (100%)	0	100 100
All	All	778/798 (98%)	768 (99%)	10 (1%)	69 74

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	SER
1	A	197	ASN
2	B	154	LEU
1	H	6	GLU
1	H	31	ARG
1	H	71	LYS
1	H	127	SER
1	H	197	ASN
2	L	33	LEU

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Mol	Chain	Res	Type
2	L	199	GLN

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

Mol	Chain	Res	Type
2	L	42	GLN

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

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, 95^{th} 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	222/230 (96%)	0.83	21 (9%) 8 7	28, 46, 64, 74	0
1	H	219/230 (95%)	0.40	12 (5%) 25 24	26, 39, 61, 79	0
2	B	217/219 (99%)	0.25	3 (1%) 75 74	23, 33, 49, 59	0
2	L	217/219 (99%)	0.37	3 (1%) 75 74	22, 33, 49, 64	0
3	C	8/8 (100%)	0.63	1 (12%) 3 3	26, 29, 43, 54	0
3	D	8/8 (100%)	0.39	0 100 100	29, 33, 39, 39	0
All	All	891/914 (97%)	0.46	40 (4%) 33 32	22, 37, 59, 79	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	75	ARG	7.0
1	H	127	SER	6.6
1	A	213	ILE	5.3
1	A	132	SER	5.2
1	H	1	GLN	4.9
1	A	15	SER	4.1
1	A	63	LEU	3.9
3	C	519	PHE	3.5
2	L	77	ARG	3.3
1	H	126	PRO	3.3
1	A	82(A)	LYS	3.2
1	A	100(C)	SER	3.1
1	H	210	ARG	3.1
1	A	1	GLN	3.0
1	H	31	ARG	3.0
2	B	45	GLN	3.0
1	A	55	ASP	2.9
1	H	133	GLU	2.8
1	A	11	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	212	GLU	2.8
2	L	190	LYS	2.7
2	L	122	GLU	2.6
1	H	206	LYS	2.5
1	A	127	SER	2.5
1	A	138	LEU	2.4
1	A	74	SER	2.4
1	A	12	VAL	2.4
1	H	204	ASN	2.4
1	A	191	THR	2.3
1	H	132	SER	2.3
1	H	65	SER	2.2
1	A	56	ILE	2.2
1	H	78	PHE	2.2
1	A	2	VAL	2.2
1	A	159	LEU	2.1
1	H	213	ILE	2.1
1	A	210	ARG	2.1
1	A	208	ASP	2.1
2	B	123	ASP	2.0
2	B	185	GLU	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.