Full wwPDB X-ray Structure Validation Report

Sep 27, 2017 – 11:25 AM EDT

PDB ID	:	5JDB
Title	:	Binding specificity of P[8] VP8* proteins of rotavirus vaccine strains with histo-blood group antigens
Authors	:	Sun, X.; Guo, N.; Li, D.; Zhou, Y.; Jin, M.; Xie, G.; Pang, L.; Zhang, Q.; Cao, Y.; Duan, Z.
Deposited on	:	unknown
Resolution	:	1.90 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

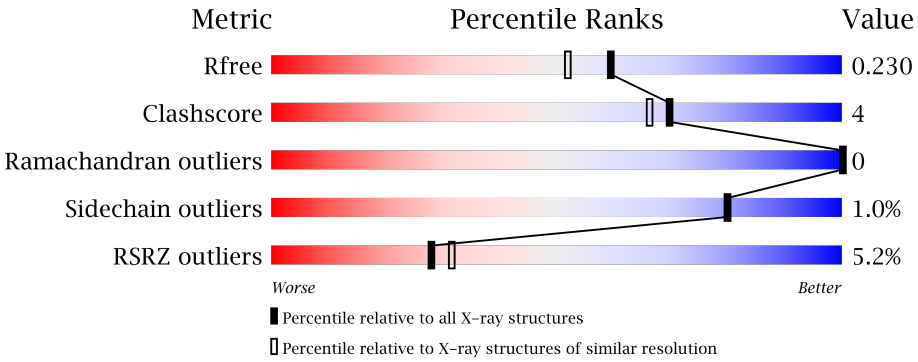
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

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 1.90 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	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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 <=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	160	9% 86% 14%
1	B	160	8% 88% 11%
1	C	160	3% 93% 6%
1	D	160	3% 93% 7%
1	E	160	4% 86% 14%

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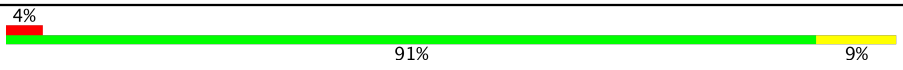
Mol	Chain	Length	Quality of chain
1	F	160	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8339 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 Outer capsid protein VP4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	S	0	0	0
			1308	828	222	256	2			
1	B	160	Total	C	N	O	S	0	0	0
			1308	828	222	256	2			
1	C	160	Total	C	N	O	S	0	1	0
			1316	832	224	258	2			
1	D	160	Total	C	N	O	S	0	0	0
			1308	828	222	256	2			
1	E	160	Total	C	N	O	S	0	0	0
			1308	828	222	256	2			
1	F	160	Total	C	N	O	S	0	0	0
			1308	828	222	256	2			

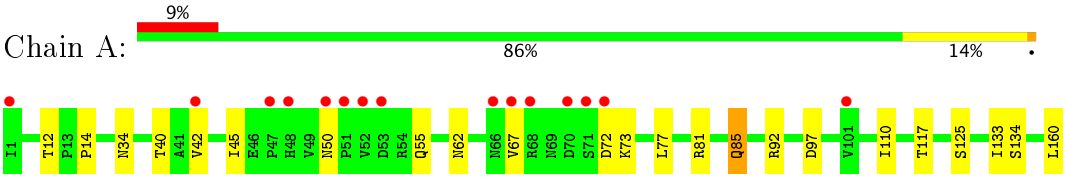
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	71	Total	O	0	0
			71	71		
2	B	76	Total	O	0	0
			76	76		
2	C	74	Total	O	0	0
			74	74		
2	D	93	Total	O	0	0
			93	93		
2	E	84	Total	O	0	0
			84	84		
2	F	85	Total	O	0	0
			85	85		

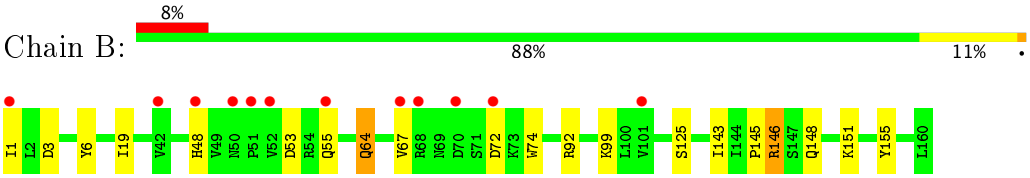
3 Residue-property plots (i)

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.

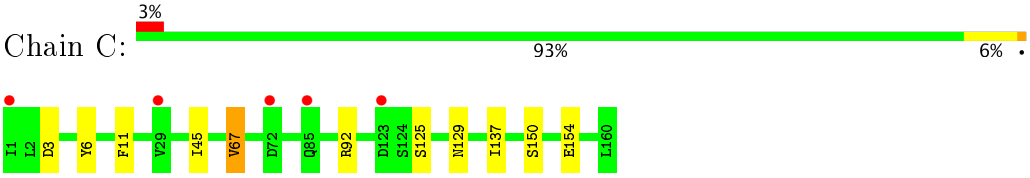
- Molecule 1: Outer capsid protein VP4



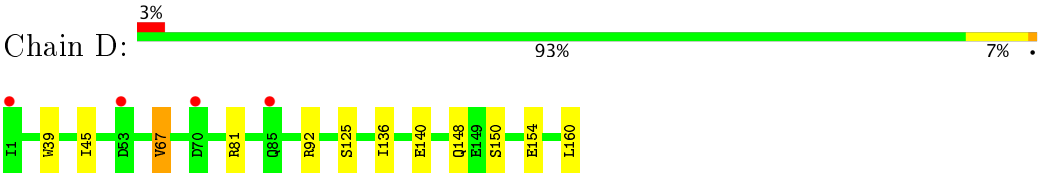
- Molecule 1: Outer capsid protein VP4



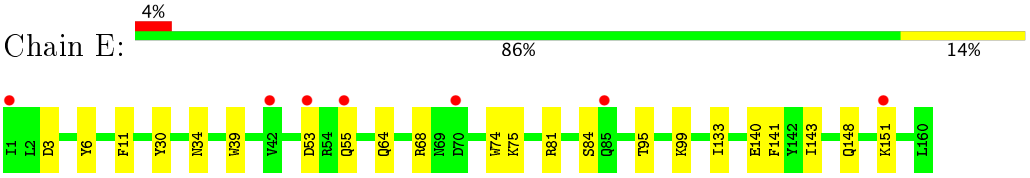
- Molecule 1: Outer capsid protein VP4



- Molecule 1: Outer capsid protein VP4

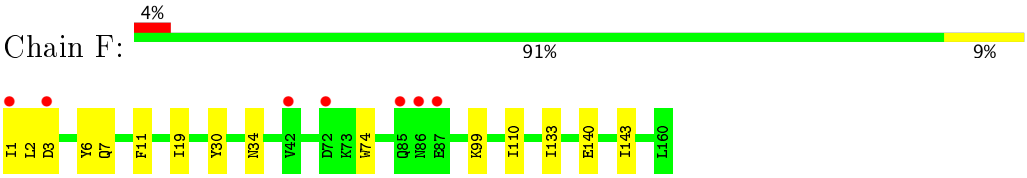


- Molecule 1: Outer capsid protein VP4



- Molecule 1: Outer capsid protein VP4

Chain F:


4%
91%
9%
I1
L2
D3
V6
Q7
F11
I19
Y30
N34
V42
D72
K73
W74
Q85
N86
E87
K99
I110
I133
E140
I143
L160

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	66.43Å 114.93Å 73.58Å 90.00° 96.05° 90.00°	Depositor
Resolution (Å)	28.98 – 1.90 28.98 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.3 (28.98-1.90) 97.4 (28.98-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.86 (at 1.91Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.202 , 0.230 0.203 , 0.230	Depositor DCC
R_{free} test set	4082 reflections (4.87%)	DCC
Wilson B-factor (Å^2)	23.5	Xtriage
Anisotropy	1.015	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 51.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8339	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.59 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.7035e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.35	0/1343	0.51	0/1830
1	B	0.34	0/1343	0.55	2/1830 (0.1%)
1	C	0.37	0/1351	0.50	0/1841
1	D	0.35	0/1343	0.50	0/1830
1	E	0.37	0/1343	0.53	0/1830
1	F	0.37	0/1343	0.51	0/1830
All	All	0.36	0/8066	0.52	2/10991 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	146	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	B	146	ARG	NE-CZ-NH1	6.48	123.54	120.30

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	1308	0	1242	20	0
1	B	1308	0	1242	11	0
1	C	1316	0	1247	6	0
1	D	1308	0	1242	9	0
1	E	1308	0	1242	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1308	0	1242	8	1
2	A	71	0	0	7	0
2	B	76	0	0	1	2
2	C	74	0	0	1	0
2	D	93	0	0	3	1
2	E	84	0	0	2	3
2	F	85	0	0	2	1
All	All	8339	0	7457	64	4

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 (64) 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:160:LEU:O	2:A:201:HOH:O	1.84	0.94
1:A:85:GLN:HE21	1:A:85:GLN:HA	1.41	0.84
1:F:140:GLU:OE2	2:F:201:HOH:O	1.96	0.84
1:E:55:GLN:HG2	1:E:64:GLN:HG3	1.65	0.78
1:A:97:ASP:OD2	2:A:202:HOH:O	2.02	0.77
1:E:148:GLN:HB3	1:E:151:LYS:HE2	1.66	0.77
1:A:85:GLN:CA	1:A:85:GLN:HE21	2.03	0.72
1:A:34:ASN:HB3	1:A:133:ILE:HG12	1.74	0.69
1:A:50:ASN:O	2:A:203:HOH:O	2.14	0.66
1:A:12:THR:HG22	1:A:134:SER:HB3	1.78	0.66
1:A:40:THR:HG21	2:A:217:HOH:O	1.96	0.64
1:D:150:SER:O	1:D:154:GLU:HG3	1.99	0.62
1:D:140:GLU:OE2	2:D:201:HOH:O	2.16	0.61
1:A:110:ILE:HD11	1:A:133:ILE:HD12	1.83	0.60
1:A:72:ASP:O	2:A:204:HOH:O	2.15	0.60
1:B:53:ASP:HB3	1:B:64:GLN:OE1	2.02	0.59
1:E:140:GLU:OE2	2:E:202:HOH:O	2.17	0.59
1:E:30:TYR:OH	2:E:201:HOH:O	2.14	0.59
1:B:48:HIS:NE2	1:B:72:ASP:OD1	2.38	0.57
1:F:110:ILE:HD11	1:F:133:ILE:HD12	1.88	0.56
1:B:146:ARG:HD2	2:B:210:HOH:O	2.06	0.55
1:B:92:ARG:NH2	1:B:125:SER:OG	2.34	0.53
1:B:151:LYS:HE2	1:B:155:TYR:HE2	1.73	0.53
1:C:150:SER:O	1:C:154:GLU:HG3	2.09	0.51
1:E:3:ASP:OD1	1:E:6:TYR:OH	2.22	0.51
1:D:92:ARG:NH2	1:D:125:SER:OG	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:GLN:NE2	1:A:85:GLN:HA	2.21	0.49
1:B:19:ILE:HD12	1:B:143:ILE:HD13	1.94	0.49
1:E:39:TRP:HB2	1:E:81:ARG:HG2	1.94	0.49
1:D:45:ILE:HD12	1:D:67:VAL:HG11	1.96	0.48
1:C:45:ILE:CD1	1:C:67:VAL:HG21	2.45	0.47
1:F:34:ASN:HB3	1:F:133:ILE:HG12	1.97	0.47
1:E:75:LYS:NZ	1:E:95:THR:OG1	2.46	0.46
1:C:92:ARG:NH2	1:C:125:SER:OG	2.38	0.46
1:A:92:ARG:NH2	1:A:125:SER:OG	2.39	0.46
1:B:55:GLN:NE2	1:B:64:GLN:HG3	2.31	0.45
1:D:92:ARG:HH22	1:D:125:SER:HG	1.62	0.45
1:F:74:TRP:NE1	1:F:99:LYS:HE2	2.31	0.45
1:B:74:TRP:NE1	1:B:99:LYS:HE2	2.31	0.45
1:C:129:ASN:ND2	2:C:208:HOH:O	2.48	0.45
1:E:74:TRP:NE1	1:E:99:LYS:HE2	2.32	0.45
1:D:148:GLN:NE2	2:D:204:HOH:O	2.41	0.45
1:E:53:ASP:HB3	1:E:64:GLN:HG2	2.00	0.44
1:B:145:PRO:HG2	1:B:148:GLN:HG3	2.00	0.44
1:F:30:TYR:OH	2:F:202:HOH:O	2.21	0.43
1:C:11:PHE:HE2	1:C:137:ILE:HD12	1.83	0.43
1:A:81:ARG:NH1	2:A:206:HOH:O	2.28	0.43
1:B:1:ILE:HG12	1:B:151:LYS:NZ	2.33	0.43
1:C:3:ASP:OD1	1:C:6:TYR:OH	2.25	0.43
1:A:42:VAL:HA	1:A:77:LEU:O	2.19	0.43
1:D:160:LEU:O	2:D:202:HOH:O	2.20	0.43
1:F:3:ASP:OD1	1:F:6:TYR:OH	2.23	0.42
1:D:39:TRP:HB2	1:D:81:ARG:HG2	2.01	0.42
1:F:1:ILE:HG13	1:F:2:LEU:N	2.34	0.42
1:A:85:GLN:CA	1:A:85:GLN:NE2	2.77	0.42
1:E:34:ASN:HB3	1:E:133:ILE:HG12	2.02	0.42
1:B:3:ASP:OD1	1:B:6:TYR:OH	2.14	0.42
1:A:73:LYS:NZ	1:A:117:THR:O	2.53	0.42
1:E:141:PHE:HE1	1:E:143:ILE:HD11	1.85	0.41
1:A:55:GLN:HG3	1:A:62:ASN:OD1	2.21	0.41
1:A:14:PRO:HG3	1:D:136:ILE:HD11	2.04	0.40
1:A:45:ILE:HD12	1:A:67:VAL:HG11	2.04	0.40
1:F:19:ILE:HD12	1:F:143:ILE:HD12	2.04	0.40
1:A:55:GLN:NE2	2:A:215:HOH:O	2.54	0.40

All (4) 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)
2:E:270:HOH:O	2:F:240:HOH:O[1_455]	2.05	0.15
2:B:263:HOH:O	2:D:215:HOH:O[1_455]	2.18	0.02
1:F:7:GLN:OE1	2:E:202:HOH:O[1_655]	2.19	0.01
2:B:270:HOH:O	2:E:220:HOH:O[2_756]	2.19	0.01

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	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
1	B	158/160 (99%)	151 (96%)	7 (4%)	0	100	100
1	C	159/160 (99%)	154 (97%)	5 (3%)	0	100	100
1	D	158/160 (99%)	154 (98%)	4 (2%)	0	100	100
1	E	158/160 (99%)	153 (97%)	5 (3%)	0	100	100
1	F	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
All	All	949/960 (99%)	916 (96%)	33 (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	148/148 (100%)	147 (99%)	1 (1%)	87	87
1	B	148/148 (100%)	146 (99%)	2 (1%)	71	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	149/148 (101%)	148 (99%)	1 (1%)	87 87
1	D	148/148 (100%)	147 (99%)	1 (1%)	87 87
1	E	148/148 (100%)	145 (98%)	3 (2%)	60 55
1	F	148/148 (100%)	147 (99%)	1 (1%)	87 87
All	All	889/888 (100%)	880 (99%)	9 (1%)	80 80

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	B	64	GLN
1	B	67	VAL
1	C	67	VAL
1	D	67	VAL
1	E	11	PHE
1	E	68	ARG
1	E	84	SER
1	F	11	PHE

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

Mol	Chain	Res	Type
1	A	85	GLN

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

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	160/160 (100%)	0.54	15 (9%) 9 10	20, 33, 64, 98	0
1	B	160/160 (100%)	0.53	12 (7%) 15 17	22, 34, 60, 82	0
1	C	160/160 (100%)	0.27	5 (3%) 49 53	22, 32, 45, 84	0
1	D	160/160 (100%)	0.26	4 (2%) 58 62	21, 30, 44, 77	0
1	E	160/160 (100%)	0.33	7 (4%) 35 38	19, 30, 51, 85	0
1	F	160/160 (100%)	0.23	7 (4%) 35 38	17, 26, 43, 80	0
All	All	960/960 (100%)	0.36	50 (5%) 28 31	17, 31, 54, 98	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	ILE	8.2
1	A	70	ASP	7.6
1	A	1	ILE	7.4
1	C	1	ILE	7.1
1	E	1	ILE	7.1
1	D	1	ILE	6.8
1	F	1	ILE	5.3
1	B	70	ASP	4.7
1	E	85	GLN	4.5
1	B	51	PRO	4.1
1	B	50	ASN	3.8
1	A	51	PRO	3.8
1	C	85	GLN	3.7
1	B	52	VAL	3.6
1	B	68	ARG	3.6
1	B	101	VAL	3.3
1	A	68	ARG	3.3
1	A	101	VAL	3.2
1	A	72	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	52	VAL	3.2
1	B	72	ASP	3.1
1	D	70	ASP	3.1
1	A	53	ASP	3.0
1	B	48	HIS	2.8
1	E	53	ASP	2.7
1	A	71	SER	2.6
1	E	70	ASP	2.6
1	F	85	GLN	2.6
1	A	50	ASN	2.5
1	A	67	VAL	2.4
1	D	85	GLN	2.3
1	E	42	VAL	2.3
1	A	42	VAL	2.3
1	F	86	ASN	2.3
1	A	66	ASN	2.2
1	D	53	ASP	2.2
1	E	151	LYS	2.2
1	A	48	HIS	2.2
1	B	42	VAL	2.2
1	C	29	VAL	2.2
1	C	72	ASP	2.2
1	F	87	GLU	2.2
1	E	55	GLN	2.1
1	A	47	PRO	2.1
1	F	42	VAL	2.1
1	B	55	GLN	2.1
1	F	3	ASP	2.1
1	C	123	ASP	2.0
1	F	72	ASP	2.0
1	B	67	VAL	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.