



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 16, 2018 – 12:04 AM EST

PDB ID : 6F5F
Title : Structure of ARTD2/PARP2 WGR domain bound to double strand DNA with
5 nucleotide overhang and 5'phosphate
Authors : Obaji, E.; Haikarainen, T.; Lehtio, L.
Deposited on : 2017-12-01
Resolution : 2.98 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:

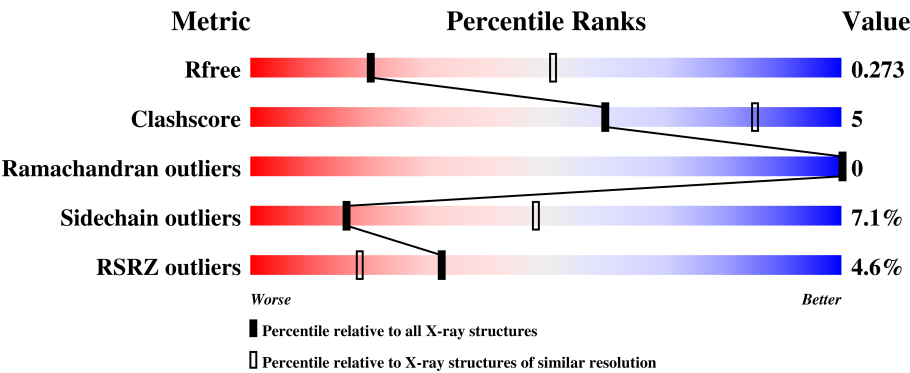
MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : rb-20031633
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

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 2.98 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.




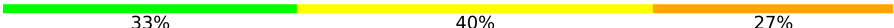
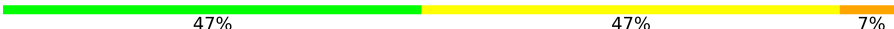
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	111664	2374 (3.00-2.96)
Clashscore	122126	2712 (3.00-2.96)
Ramachandran outliers	120053	2626 (3.00-2.96)
Sidechain outliers	120020	2629 (3.00-2.96)
RSRZ outliers	108989	2268 (3.00-2.96)

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	131	<div><div>3%</div><div><div></div><div>76%</div><div>12%</div><div>11%</div></div></div>
1	B	131	<div><div>2%</div><div><div></div><div>79%</div><div>7%</div><div>•</div><div>11%</div></div></div>
1	C	131	<div><div>2%</div><div><div></div><div>73%</div><div>11%</div><div>•</div><div>12%</div></div></div>
1	D	131	<div><div>11%</div><div><div></div><div>70%</div><div>15%</div><div>•</div><div>13%</div></div></div>
2	E	15	<div><div></div><div><div></div><div>47%</div><div>47%</div><div>7%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	F	15	 53% 47%
2	G	15	 33% 40% 27%
2	H	15	 47% 47% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5012 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 Poly [ADP-ribose] polymerase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	116	Total	C	N	O	S	0	0	0
			951	600	166	177	8			
1	B	116	Total	C	N	O	S	0	0	0
			951	600	166	177	8			
1	C	115	Total	C	N	O	S	0	0	0
			943	596	165	174	8			
1	D	114	Total	C	N	O	S	0	0	0
			935	591	164	173	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	88	SER	-	expression tag	UNP Q9UGN5
A	89	MET	-	expression tag	UNP Q9UGN5
B	88	SER	-	expression tag	UNP Q9UGN5
B	89	MET	-	expression tag	UNP Q9UGN5
C	88	SER	-	expression tag	UNP Q9UGN5
C	89	MET	-	expression tag	UNP Q9UGN5
D	88	SER	-	expression tag	UNP Q9UGN5
D	89	MET	-	expression tag	UNP Q9UGN5

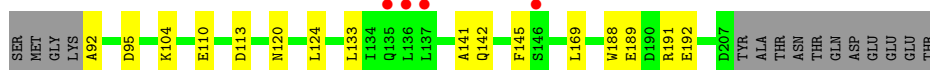
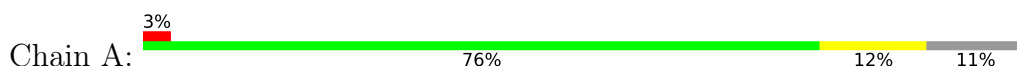
- Molecule 2 is a DNA chain called DNA (5'-D(P*CP*GP*GP*TP*CP*GP*CP*CP*TP*AP*TP*AP*GP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	15	Total	C	N	O	P	0	0	0
			308	145	56	92	15			
2	F	15	Total	C	N	O	P	0	0	0
			308	145	56	92	15			
2	G	15	Total	C	N	O	P	0	0	0
			308	145	56	92	15			
2	H	15	Total	C	N	O	P	0	0	0
			308	145	56	92	15			

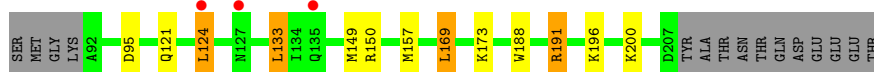
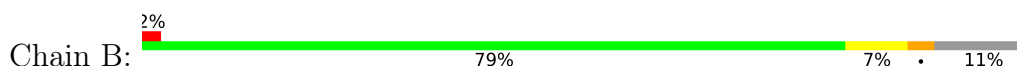
3 Residue-property plots [i](#)

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.

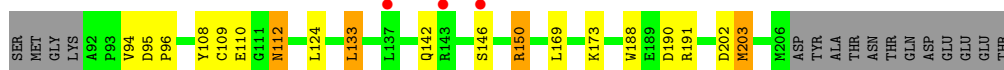
- Molecule 1: Poly [ADP-ribose] polymerase 2



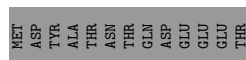
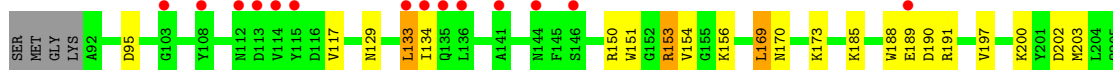
- Molecule 1: Poly [ADP-ribose] polymerase 2



- Molecule 1: Poly [ADP-ribose] polymerase 2



- Molecule 1: Poly [ADP-ribose] polymerase 2



- Molecule 2: DNA (5'-D(P*CP*GP*GP*TP*CP*GP*CP*CP*TP*AP*TP*AP*GP*GP*C)-3')



- Molecule 2: DNA (5'-D(P*CP*GP*GP*TP*CP*GP*CP*CP*TP*AP*TP*AP*GP*GP*C)-3')

Chain F:  53% 47%



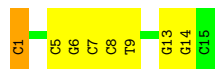
- Molecule 2: DNA (5'-D(P*CP*GP*GP*TP*CP*GP*CP*CP*TP*AP*TP*AP*GP*GP*C)-3')

Chain G:  33% 40% 27%



- Molecule 2: DNA (5'-D(P*CP*GP*GP*TP*CP*GP*CP*CP*TP*AP*TP*AP*GP*GP*C)-3')

Chain H:  47% 47% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.15Å 87.15Å 185.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.86 – 2.98 19.86 – 2.98	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.86-2.98) 99.7 (19.86-2.98)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.228 , 0.275 0.233 , 0.273	Depositor DCC
R_{free} test set	1155 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	102.3	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 59.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5012	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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	0.59	1/971 (0.1%)	0.82	0/1305
1	B	0.58	0/971	0.91	3/1305 (0.2%)
1	C	0.55	0/963	0.90	1/1294 (0.1%)
1	D	0.56	0/955	0.85	0/1284
2	E	0.97	1/344 (0.3%)	1.29	2/527 (0.4%)
2	F	0.87	1/344 (0.3%)	1.09	0/527
2	G	0.93	2/344 (0.6%)	1.26	6/527 (1.1%)
2	H	1.06	3/344 (0.9%)	1.32	4/527 (0.8%)
All	All	0.69	8/5236 (0.2%)	0.99	16/7296 (0.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	DC	OP3-P	-11.00	1.48	1.61
2	E	1	DC	OP3-P	-10.22	1.48	1.61
2	F	1	DC	OP3-P	-9.71	1.49	1.61
2	G	1	DC	OP3-P	-8.74	1.50	1.61
1	A	92	ALA	N-CA	5.23	1.56	1.46
2	H	13	DG	O3'-P	-5.15	1.54	1.61
2	H	14	DG	O3'-P	-5.12	1.55	1.61
2	G	6	DG	O3'-P	-5.07	1.55	1.61

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	8	DC	O5'-P-OP2	-10.47	96.28	105.70
2	G	2	DG	O5'-P-OP1	-9.51	97.14	105.70
1	B	191	ARG	CG-CD-NE	8.71	130.08	111.80
2	E	2	DG	O4'-C4'-C3'	-8.63	100.82	106.00
2	E	2	DG	C1'-O4'-C4'	-7.83	102.27	110.10
2	H	13	DG	C5'-C4'-C3'	-7.11	101.30	114.10
1	B	157	MET	CG-SD-CE	6.75	110.99	100.20
2	H	14	DG	C5'-C4'-C3'	-6.08	103.16	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	14	DG	O5'-P-OP1	5.79	117.65	110.70
2	G	13	DG	C1'-O4'-C4'	-5.62	104.48	110.10
2	H	7	DC	O4'-C4'-C3'	-5.51	102.29	104.50
2	G	5	DC	O5'-P-OP1	-5.44	100.80	105.70
2	G	5	DC	C5'-C4'-C3'	5.43	123.88	114.10
1	C	150	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	124	LEU	CA-CB-CG	5.32	127.53	115.30
2	G	8	DC	C5'-C4'-C3'	5.16	123.38	114.10

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	951	0	924	7	0
1	B	951	0	924	6	0
1	C	943	0	920	9	0
1	D	935	0	911	13	0
2	E	308	0	169	4	2
2	F	308	0	169	4	0
2	G	308	0	169	4	2
2	H	308	0	169	4	0
All	All	5012	0	4355	47	2

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 (47) 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:G:4:DT:H2''	2:G:5:DC:H5'	1.48	0.92
1:B:169:LEU:HD13	1:B:173:LYS:HD2	1.64	0.78
1:D:169:LEU:HD13	1:D:173:LYS:HD2	1.67	0.75
2:F:4:DT:H6	2:F:4:DT:H5''	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1:DC:H2'	2:H:1:DC:O2	1.90	0.71
1:B:121:GLN:HE22	1:B:196:LYS:HE2	1.59	0.67
1:A:145:PHE:CZ	1:A:169:LEU:HD13	2.28	0.67
1:B:121:GLN:NE2	1:B:200:LYS:O	2.27	0.67
2:G:7:DC:H2''	2:G:8:DC:H5'	1.83	0.61
1:D:117:VAL:CG1	1:D:134:ILE:HG22	2.33	0.58
1:D:197:VAL:HG13	1:D:200:LYS:HB2	1.88	0.56
1:C:112:ASN:HD22	1:C:112:ASN:N	2.05	0.55
1:A:141:ALA:HB3	1:A:142:GLN:OE1	2.07	0.55
1:A:110:GLU:HG2	1:C:96:PRO:CB	2.38	0.53
2:H:8:DC:H2'	2:H:9:DT:C6	2.44	0.53
1:A:110:GLU:HG2	1:C:96:PRO:HB3	1.91	0.53
1:B:188:TRP:O	1:B:191:ARG:CD	2.58	0.52
2:F:5:DC:H2''	2:F:6:DG:H5'	1.93	0.50
1:C:188:TRP:O	1:C:191:ARG:HD3	2.12	0.49
1:A:188:TRP:O	1:A:191:ARG:HD3	2.12	0.49
1:D:188:TRP:O	1:D:191:ARG:HD3	2.13	0.49
1:D:117:VAL:HG12	1:D:134:ILE:HG22	1.94	0.49
1:D:133:LEU:HD23	1:D:150:ARG:HB3	1.94	0.49
2:H:1:DC:C2'	2:H:1:DC:O2	2.57	0.48
1:C:133:LEU:HD23	1:C:150:ARG:HB3	1.95	0.48
2:E:7:DC:H2'	2:E:8:DC:C6	2.49	0.48
1:B:133:LEU:HD23	1:B:150:ARG:HB3	1.94	0.48
2:E:4:DT:O2	2:E:4:DT:O5'	2.32	0.48
1:C:169:LEU:HG	1:C:173:LYS:HD2	1.96	0.47
1:C:202:ASP:OD1	1:C:203:MET:N	2.47	0.47
2:H:5:DC:H2''	2:H:6:DG:H5'	1.95	0.47
1:D:117:VAL:HG12	1:D:134:ILE:CG2	2.45	0.46
1:C:108:TYR:OH	1:C:110:GLU:OE2	2.25	0.46
1:B:188:TRP:O	1:B:191:ARG:HD3	2.16	0.46
1:D:202:ASP:OD1	1:D:203:MET:N	2.48	0.46
2:E:12:DA:C2	2:F:10:DA:C2	3.04	0.45
1:A:145:PHE:CE1	1:A:169:LEU:HD13	2.52	0.45
1:D:169:LEU:HD13	1:D:173:LYS:CD	2.44	0.45
1:D:169:LEU:CD1	1:D:173:LYS:HD2	2.41	0.44
2:E:10:DA:H2''	2:E:11:DT:H5''	2.00	0.44
1:D:153:ARG:HB3	1:D:156:LYS:HG2	2.00	0.44
2:F:7:DC:H2'	2:F:8:DC:C6	2.52	0.44
2:G:13:DG:H2''	2:G:14:DG:C8	2.53	0.44
1:A:113:ASP:HA	1:A:191:ARG:HH22	1.85	0.42
1:C:124:LEU:HD12	1:C:124:LEU:HA	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:TRP:CD1	2:G:2:DG:H4'	2.56	0.41
1:D:129:ASN:O	1:D:154:VAL:HG23	2.21	0.40

All (2) 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:4:DT:C7	2:G:3:DG:O6[4_555]	1.66	0.54
2:E:2:DG:O6	2:G:5:DC:N3[4_555]	2.06	0.14

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	114/131 (87%)	106 (93%)	8 (7%)	0	100	100
1	B	114/131 (87%)	106 (93%)	8 (7%)	0	100	100
1	C	113/131 (86%)	105 (93%)	8 (7%)	0	100	100
1	D	112/131 (86%)	104 (93%)	8 (7%)	0	100	100
All	All	453/524 (86%)	421 (93%)	32 (7%)	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	103/116 (89%)	96 (93%)	7 (7%)	17	50
1	B	103/116 (89%)	98 (95%)	5 (5%)	27	64
1	C	102/116 (88%)	93 (91%)	9 (9%)	11	37
1	D	101/116 (87%)	93 (92%)	8 (8%)	13	42
All	All	409/464 (88%)	380 (93%)	29 (7%)	16	48

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	ASP
1	A	104	LYS
1	A	120	ASN
1	A	124	LEU
1	A	133	LEU
1	A	189	GLU
1	A	192	GLU
1	B	95	ASP
1	B	124	LEU
1	B	133	LEU
1	B	149	MET
1	B	169	LEU
1	C	94	VAL
1	C	95	ASP
1	C	109	CYS
1	C	112	ASN
1	C	133	LEU
1	C	142	GLN
1	C	146	SER
1	C	190	ASP
1	C	203	MET
1	D	95	ASP
1	D	133	LEU
1	D	153	ARG
1	D	169	LEU
1	D	170	ASN
1	D	185	LYS
1	D	189	GLU
1	D	190	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
1	B	112	ASN
1	B	121	GLN
1	B	142	GLN
1	C	112	ASN
1	D	142	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 [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	116/131 (88%)	-0.05	4 (3%)	45	27	82, 103, 143, 176	0
1	B	116/131 (88%)	0.07	3 (2%)	56	35	79, 123, 163, 172	0
1	C	115/131 (87%)	-0.01	3 (2%)	56	35	94, 125, 159, 181	0
1	D	114/131 (87%)	0.60	14 (12%)	4	2	102, 159, 197, 230	0
2	E	15/15 (100%)	-0.76	0	100	100	102, 123, 132, 152	0
2	F	15/15 (100%)	-0.65	0	100	100	84, 111, 135, 140	0
2	G	15/15 (100%)	-0.81	0	100	100	84, 107, 125, 170	0
2	H	15/15 (100%)	-0.87	0	100	100	90, 98, 118, 123	0
All	All	521/584 (89%)	0.04	24 (4%)	32	18	79, 123, 180, 230	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	135	GLN	5.0
1	D	114	VAL	4.9
1	D	136	LEU	4.8
1	D	144	ASN	4.1
1	D	146	SER	3.9
1	D	115	TYR	3.5
1	D	141	ALA	3.5
1	D	134	ILE	3.4
1	C	146	SER	3.1
1	A	136	LEU	3.1
1	B	135	GLN	2.6
1	C	143	ARG	2.6
1	D	112	ASN	2.6
1	D	133	LEU	2.5
1	A	146	SER	2.5
1	C	137	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	124	LEU	2.3
1	A	137	LEU	2.2
1	D	189	GLU	2.2
1	B	127	ASN	2.1
1	D	108	TYR	2.1
1	D	103	GLY	2.1
1	D	113	ASP	2.1
1	A	135	GLN	2.1

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.