



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 07:49 AM GMT

PDB ID : 1WCE
Title : Crystal structure of the T13 IBDV viral particle reveals a missing link in icosahedral viruses evolution
Authors : Coulibaly, F.; Chevalier, C.; Gutsche, I.; Pous, J.; Bressanelli, S.; Navaza, J.; Delmas, B.; Rey, F.A.
Deposited on : 2004-11-12
Resolution : 7.00 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

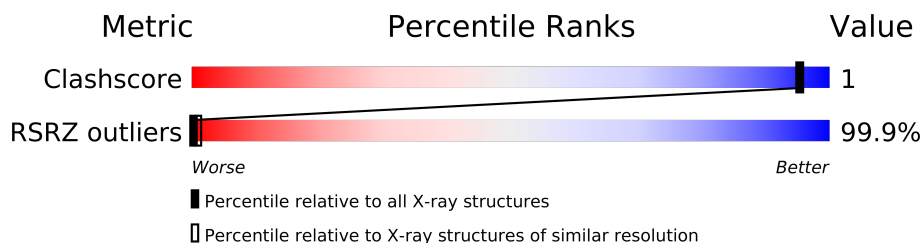
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance














The reported resolution of this entry is 7.00 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))
Clashscore	79885	1039 (10.00-3.52)
RSRZ outliers	66119	1097 (10.00-3.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	441	
1	B	441	
1	C	441	
1	D	441	
1	E	441	
1	F	441	
1	G	441	
1	H	441	
1	I	441	
1	J	441	
1	K	441	
1	L	441	
1	M	441	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5533 atoms, of which 0 are hydrogen and 0 are deuterium.

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 MAJOR STRUCTURAL PROTEIN VP2.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	425	Total C 425 425	0	0	425
1	B	430	Total C 430 430	0	0	430
1	C	430	Total C 430 430	0	0	430
1	D	424	Total C 424 424	0	0	424
1	E	429	Total C 429 429	0	0	429
1	F	436	Total C 436 436	0	0	436
1	G	426	Total C 426 426	0	0	426
1	H	423	Total C 423 423	0	0	423
1	I	417	Total C 417 417	0	0	417
1	J	423	Total C 423 423	0	0	423
1	K	416	Total C 416 416	0	0	416
1	L	429	Total C 429 429	0	0	429
1	M	425	Total C 425 425	0	0	425

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

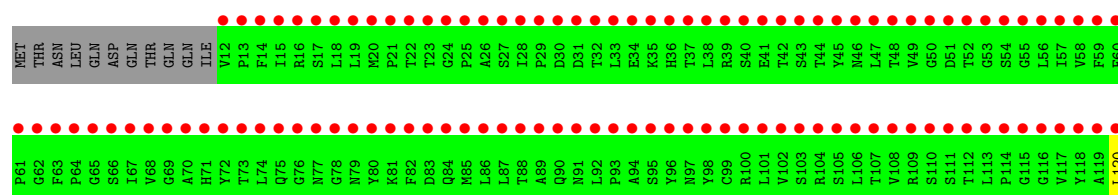
• Molecule 1: MAJOR STRUCTURAL PROTEIN VP2

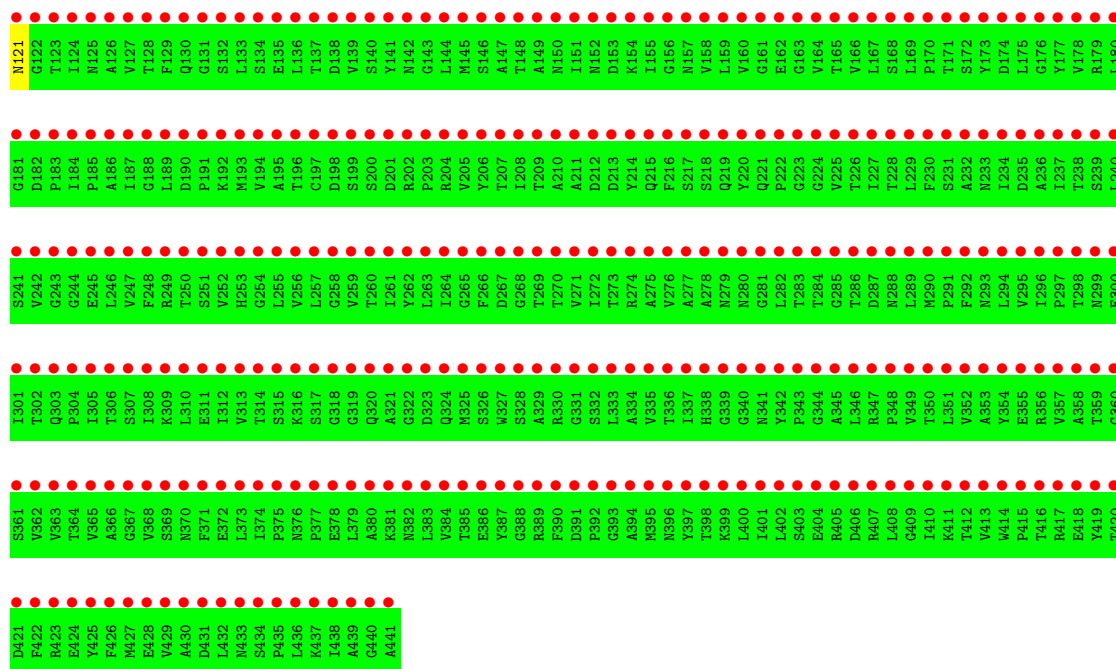
Chain A: 



• Molecule 1: MAJOR STRUCTURAL PROTEIN VP2

Chain B: 





• Molecule 1: MAJOR STRUCTURAL PROTEIN VP2

Chain C: 



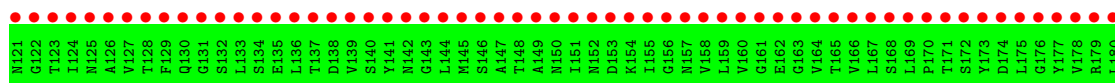
• Molecule 1: MAJOR STRUCTURAL PROTEIN VP2

Chain D:

MET	THR	ASN	LEU	GLN	ASP	GLN	THR	GLN	ILE	VAL	P13	F14	I15	R16	S17	L18	L19	M20	P21	T22	T23	G24	P25	A26	S27	L28	P29	D30	D31	T32	L33	E34	K35	H36	T37	L38	R39	S40	E41	V102	T42	T43	S43	T44	Y45	M46	L47	T48	V49	G50	D51	T52	G53	S54	G55	L56	I57	V58	R59	F60
P61	G62	F63	P64	G65	S66	T67	V68	G69	A70	H71	I72	T73	L74	G75	N77	D78	V79	T80	K81	F82	D83	O84	N85	L86	L87	T88	A89	D90	N91	L92	P93	A94	S95	Y96	N97	Y98	C99	R100	L101	V102	S103	R104	S105	L106	T107	V108	R109	S110	S111	T112	L113	P114	G115	L116	V117	I118	A119	L120		
H121	G122	T123	I124	N125	A126	V127	T128	F129	Q130	G131	S132	L133	S134	E135	L136	T137	D138	V139	S140	Y141	N142	G143	L144	M145	S146	A147	T148	A149	N150	N151	N152	D153	K154	I155	G156	N157	V158	L159	V160	G161	E162	G163	V164	T165	V166	L167	S168	L169	P170	T171	S172	Y173	D174	L175	A236	I237	T238	R239	M299	E300
G181	D182	P183	I184	P185	A186	I187	G188	L189	D190	P191	K192	M193	V194	A195	T196	C197	D198	S199	S200	D201	F202	P203	R204	V205	Y206	T207	L208	T209	A210	A211	D212	D213	Y214	Q215	F216	S217	S218	Q219	Y220	Q221	P222	E223	G224	V225	T226	I227	T228	L229	F230	S231	A232	N233	I234	D235	L236	P237	T238	S239	E300	
S241	V242	G243	G244	E245	L246	V247	F248	R249	T250	S251	V252	H253	G254	L255	V256	L257	G258	V259	T260	I261	F262	P263	L264	G265	F266	D267	G268	T269	T270	V271	L272	T273	A274	A275	V276	A277	A278	N279	N280	G281	L282	T283	T284	G285	T286	D287	N288	L289	M290	F291	F292	N293	L294	V295	L296	P297	T298	N299	E300	
I301	T302	Q303	P304	L305	T306	S307	L308	K309	L310	E311	L312	V313	T314	S315	K316	S317	G318	C319	Q320	A321	G322	D323	Q324	K325	S326	W327	S328	A329	R330	G331	S332	L333	A334	M335	T336	I337	H338	G339	G340	L341	Y342	N343	E344	A345	L346	R347	P348	V349	T350	L351	V352	A353	Y354	E355	R356	V357	A358	T359	G360	
S361	V362	V363	L364	V365	A366	G367	V368	S369	N370	F371	L372	L373	I374	P375	N376	P377	G378	L379	A380	K381	G382	L383	V384	T385	E386	T387	G388	R389	F390	D391	P392	G393	A394	M395	N396	Y397	T398	K399	L400	L401	L402	S403	E404	R405	D406	R407	L408	G409	I410	K411	T412	V413	W414	P415	T416	R417	E418	Y419	T420	
D421	F422	E423	E424	Y425	F426	M427	E428	V429	A430	D431	L432	M433	S434	P435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	
D421	F422	E423	E424	Y425	F426	M427	E428	V429	A430	D431	L432	M433	S434	P435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	
D421	F422	E423	E424	Y425	F426	M427	E428	V429	A430	D431	L432	M433	S434	P435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	
D421	F422	E423	E424	Y425	F426	M427	E428	V429	A430	D431	L432	M433	S434	P435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	
D421	F422	E423	E424	Y425	F426	M427	E428	V429	A430	D431	L432	M433	S434	P435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	
D421	F422	E423	E424	Y425	F426	M427	E428	V429	A430	D431	L432	M433	S434	P435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	
D421	F422	E423	E424	Y425	F426	M427	E428	V429	A430	D431	L432	M433	S434	P435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	
D421	F422	E423	E424	Y425	F426	M427	E428	V429	A430	D431	L432	M433	S434	P435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	
D421	F422	E423	E424	Y425	F426	M427	E428	V429	A430	D431	L432	M433	S434	P435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	
D421	F422	E423	E424	Y425	F426	M427	E428	V429	A430	D431	L432	M433	S434	P435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	
D421	F422	E423	E424	Y425	F426	M427	E428	V429	A430	D431	L432	M433	S434	P435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	
D421	F422	E423	E424	Y425	F426	M427	E428	V429	A430	D431	L432	M433	S434	P435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	
D421	F422	E423	E424	Y425	F426	M427	E428	V429	A430	D431	L432	M433	S434	P435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	
D421	F422	E423	E424	Y425	F426	M427	E428	V429	A430	D431	L432	M433	S434	P435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	
D421	F422	E423	E424	Y425	F426	M427	E428	V429	A430	D431	L432	M433	S434	P435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	
D421	F422	E423	E424	Y425	F426	M427	E428	V429	A430	D431	L432	M433	S434	P435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	
D421	F422	E423	E424	Y425	F426	M427	E428	V429	A430	D431	L432	M433	S434	P435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	
D421	F422	E423	E424	Y425	F426	M427	E428	V429	A430	D431	L432	M433	S434	P435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	
D421	F422	E423	E424	Y425	F426	M427	E428	V429	A430	D431	L432	M433	S434	P435	L43																																													







4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	854.01Å 692.23Å 792.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 7.00 49.86 – 6.97	Depositor EDS
% Data completeness (in resolution range)	75.1 (50.00-7.00) 59.9 (49.86-6.97)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 6.68Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	(Not available) , (Not available) 0.369 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	190.2	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.7	EDS
Estimated twinning fraction	0.327 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	2 of 1089556 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.52	EDS
Total number of atoms	5533	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	$\# Z > 5$

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	425	0	0	2	0
1	B	430	0	0	2	0
1	C	430	0	0	0	0
1	D	424	0	0	1	0
1	E	429	0	0	1	0
1	F	436	0	0	1	0
1	G	426	0	0	1	0
1	H	423	0	0	0	0
1	I	417	0	0	0	0
1	J	423	0	0	1	0
1	K	416	0	0	1	0
1	L	429	0	0	1	0
1	M	425	0	0	1	0
All	All	5533	0	0	7	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 1.

The worst 5 of 7 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:111:SER:CA	1:D:112:THR:CA	1.85	1.51
1:E:117:VAL:CA	1:M:115:GLY:CA	2.26	1.13
1:A:112:THR:CA	1:B:121:ASN:CA	2.64	0.76
1:K:118:TYR:CA	1:L:115:GLY:CA	2.82	0.58
1:A:112:THR:CA	1:B:120:LEU:CA	2.96	0.43

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains ⓘ

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

5.3.3 RNA ⓘ

There are no RNA chains 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, 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	425/441 (96%)	18.89	424 (99%) 0 1	20, 47, 95, 99	0
1	B	430/441 (97%)	19.18	430 (100%) 0 1	20, 47, 95, 99	0
1	C	430/441 (97%)	20.59	430 (100%) 0 1	20, 47, 95, 99	0
1	D	424/441 (96%)	19.45	423 (99%) 0 1	20, 47, 95, 99	0
1	E	429/441 (97%)	20.66	428 (99%) 0 1	20, 47, 95, 99	0
1	F	436/441 (98%)	18.32	434 (99%) 0 1	20, 46, 95, 99	0
1	G	426/441 (96%)	20.98	426 (100%) 0 1	20, 47, 95, 99	0
1	H	423/441 (95%)	20.05	423 (100%) 0 1	20, 47, 95, 99	0
1	I	417/441 (94%)	20.57	417 (100%) 0 1	20, 47, 96, 99	0
1	J	423/441 (95%)	19.69	423 (100%) 0 1	20, 47, 95, 99	0
1	K	416/441 (94%)	19.88	416 (100%) 0 1	20, 47, 96, 99	0
1	L	429/441 (97%)	19.18	429 (100%) 0 1	20, 47, 95, 99	0
1	M	425/441 (96%)	18.81	425 (100%) 0 1	20, 47, 95, 99	0
All	All	5533/5733 (96%)	19.71	5528 (99%) 0 1	20, 47, 96, 99	0

The worst 5 of 5528 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	330	ARG	85.3
1	C	150	ASN	73.5
1	H	150	ASN	70.6
1	E	344	GLY	67.7
1	J	203	PRO	66.8

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

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

6.3 Carbohydrates ⓘ

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.