



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 28, 2026 – 05:40 PM UTC

PDB ID : 4LG2 / pdb_00004lg2
Title : Crystal structure of Reston Ebola virus VP35 RNA binding domain bound to 12-bp dsRNA
Authors : Bale, S.; Julien, J.-P.; Bornholdt, Z.A.; Krois, A.S.; Wilson, I.A.; Sapphire, E.O.
Deposited on : 2013-06-27
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

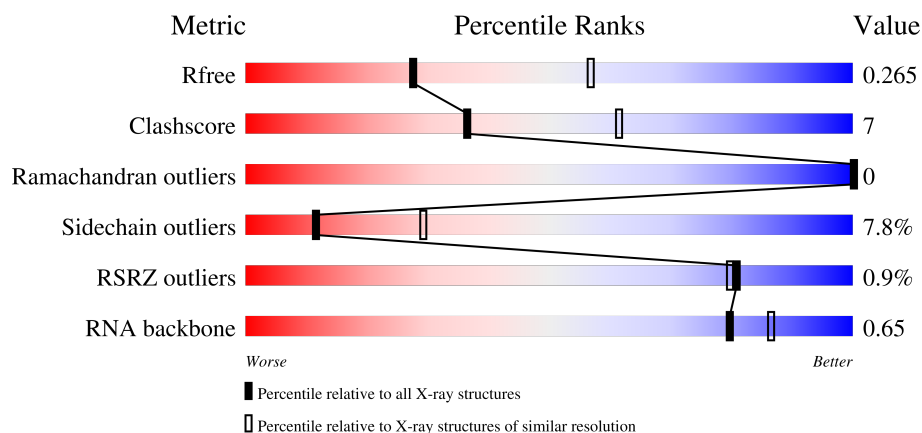
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)
RNA backbone	3983	1044 (2.90-2.50)

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 of 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	146	64% 18% • 16%
1	B	146	66% 14% • 16%
1	C	146	60% 22% • 16%
1	D	146	68% 15% • 16%

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Mol	Chain	Length	Quality of chain
2	E	12	8% 75% 25%
2	F	12	58% 17% 25%
2	I	12	75% 25%
2	J	12	8% 67% 17% 17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4703 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 Polymerase cofactor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	122	Total	C	N	O	S	0	0	0
			952	609	169	168	6			
1	B	122	Total	C	N	O	S	0	0	0
			952	609	169	168	6			
1	C	122	Total	C	N	O	S	0	0	0
			952	609	169	168	6			
1	D	122	Total	C	N	O	S	0	0	0
			952	609	169	168	6			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	184	MET	-	expression tag	UNP Q8JPY0
A	185	ALA	-	expression tag	UNP Q8JPY0
A	186	HIS	-	expression tag	UNP Q8JPY0
A	187	HIS	-	expression tag	UNP Q8JPY0
A	188	HIS	-	expression tag	UNP Q8JPY0
A	189	HIS	-	expression tag	UNP Q8JPY0
A	190	HIS	-	expression tag	UNP Q8JPY0
A	191	HIS	-	expression tag	UNP Q8JPY0
A	192	VAL	-	expression tag	UNP Q8JPY0
A	193	ASP	-	expression tag	UNP Q8JPY0
A	194	ASP	-	expression tag	UNP Q8JPY0
A	195	ASP	-	expression tag	UNP Q8JPY0
A	196	ASP	-	expression tag	UNP Q8JPY0
A	197	LYS	-	expression tag	UNP Q8JPY0
A	198	GLU	-	expression tag	UNP Q8JPY0
A	199	ASN	-	expression tag	UNP Q8JPY0
A	200	LEU	-	expression tag	UNP Q8JPY0
A	201	TYR	-	expression tag	UNP Q8JPY0
A	202	PHE	-	expression tag	UNP Q8JPY0
A	203	GLN	-	expression tag	UNP Q8JPY0
A	204	SER	-	expression tag	UNP Q8JPY0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	184	MET	-	expression tag	UNP Q8JPY0
B	185	ALA	-	expression tag	UNP Q8JPY0
B	186	HIS	-	expression tag	UNP Q8JPY0
B	187	HIS	-	expression tag	UNP Q8JPY0
B	188	HIS	-	expression tag	UNP Q8JPY0
B	189	HIS	-	expression tag	UNP Q8JPY0
B	190	HIS	-	expression tag	UNP Q8JPY0
B	191	HIS	-	expression tag	UNP Q8JPY0
B	192	VAL	-	expression tag	UNP Q8JPY0
B	193	ASP	-	expression tag	UNP Q8JPY0
B	194	ASP	-	expression tag	UNP Q8JPY0
B	195	ASP	-	expression tag	UNP Q8JPY0
B	196	ASP	-	expression tag	UNP Q8JPY0
B	197	LYS	-	expression tag	UNP Q8JPY0
B	198	GLU	-	expression tag	UNP Q8JPY0
B	199	ASN	-	expression tag	UNP Q8JPY0
B	200	LEU	-	expression tag	UNP Q8JPY0
B	201	TYR	-	expression tag	UNP Q8JPY0
B	202	PHE	-	expression tag	UNP Q8JPY0
B	203	GLN	-	expression tag	UNP Q8JPY0
B	204	SER	-	expression tag	UNP Q8JPY0
C	184	MET	-	expression tag	UNP Q8JPY0
C	185	ALA	-	expression tag	UNP Q8JPY0
C	186	HIS	-	expression tag	UNP Q8JPY0
C	187	HIS	-	expression tag	UNP Q8JPY0
C	188	HIS	-	expression tag	UNP Q8JPY0
C	189	HIS	-	expression tag	UNP Q8JPY0
C	190	HIS	-	expression tag	UNP Q8JPY0
C	191	HIS	-	expression tag	UNP Q8JPY0
C	192	VAL	-	expression tag	UNP Q8JPY0
C	193	ASP	-	expression tag	UNP Q8JPY0
C	194	ASP	-	expression tag	UNP Q8JPY0
C	195	ASP	-	expression tag	UNP Q8JPY0
C	196	ASP	-	expression tag	UNP Q8JPY0
C	197	LYS	-	expression tag	UNP Q8JPY0
C	198	GLU	-	expression tag	UNP Q8JPY0
C	199	ASN	-	expression tag	UNP Q8JPY0
C	200	LEU	-	expression tag	UNP Q8JPY0
C	201	TYR	-	expression tag	UNP Q8JPY0
C	202	PHE	-	expression tag	UNP Q8JPY0
C	203	GLN	-	expression tag	UNP Q8JPY0
C	204	SER	-	expression tag	UNP Q8JPY0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	184	MET	-	expression tag	UNP Q8JPY0
D	185	ALA	-	expression tag	UNP Q8JPY0
D	186	HIS	-	expression tag	UNP Q8JPY0
D	187	HIS	-	expression tag	UNP Q8JPY0
D	188	HIS	-	expression tag	UNP Q8JPY0
D	189	HIS	-	expression tag	UNP Q8JPY0
D	190	HIS	-	expression tag	UNP Q8JPY0
D	191	HIS	-	expression tag	UNP Q8JPY0
D	192	VAL	-	expression tag	UNP Q8JPY0
D	193	ASP	-	expression tag	UNP Q8JPY0
D	194	ASP	-	expression tag	UNP Q8JPY0
D	195	ASP	-	expression tag	UNP Q8JPY0
D	196	ASP	-	expression tag	UNP Q8JPY0
D	197	LYS	-	expression tag	UNP Q8JPY0
D	198	GLU	-	expression tag	UNP Q8JPY0
D	199	ASN	-	expression tag	UNP Q8JPY0
D	200	LEU	-	expression tag	UNP Q8JPY0
D	201	TYR	-	expression tag	UNP Q8JPY0
D	202	PHE	-	expression tag	UNP Q8JPY0
D	203	GLN	-	expression tag	UNP Q8JPY0
D	204	SER	-	expression tag	UNP Q8JPY0

- Molecule 2 is a RNA chain called dsRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	9	Total	C	N	O	P	0	0	0
			187	85	33	61	8			
2	F	9	Total	C	N	O	P	0	0	0
			193	86	35	63	9			
2	J	12	Total	C	N	O	P	0	0	0
			255	114	45	84	12			
2	I	12	Total	C	N	O	P	0	0	0
			252	114	45	82	11			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			1	1		
3	B	5	Total	O	0	0
			5	5		
3	C	1	Total	O	0	0
			1	1		

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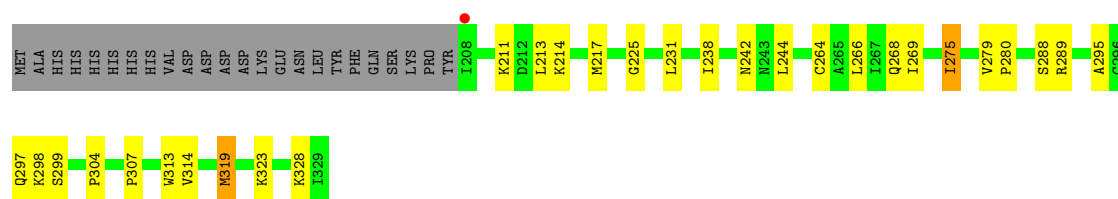
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	1	Total	O	0	0
			1	1		

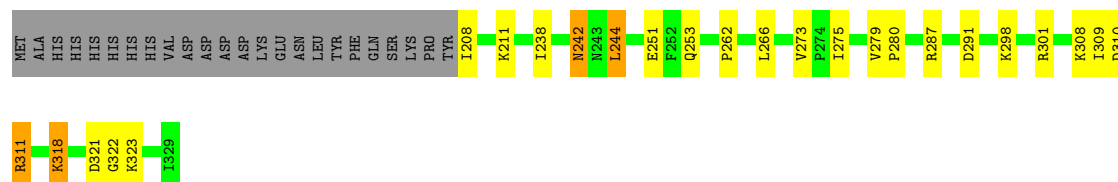
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

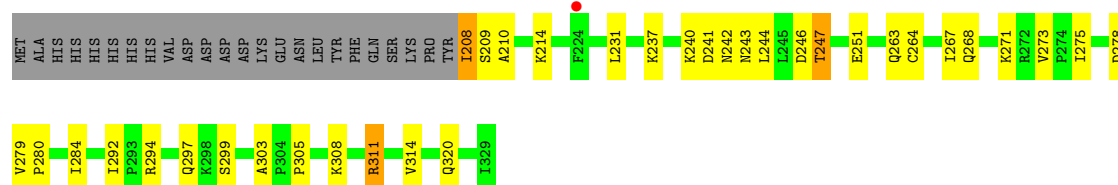
- Molecule 1: Polymerase cofactor



- Molecule 1: Polymerase cofactor



- Molecule 1: Polymerase cofactor

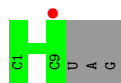
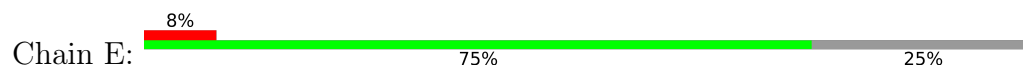


- Molecule 1: Polymerase cofactor





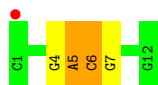
- Molecule 2: dsRNA



- Molecule 2: dsRNA



- Molecule 2: dsRNA



- Molecule 2: dsRNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.09Å 72.87Å 175.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.30 – 2.70 39.30 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.30-2.70) 99.5 (39.30-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.209 , 0.262 0.212 , 0.265	Depositor DCC
R_{free} test set	1016 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	71.1	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4703	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.52	0/974	0.88	0/1317
1	B	0.52	0/974	0.97	3/1317 (0.2%)
1	C	0.47	0/974	0.90	2/1317 (0.2%)
1	D	0.50	0/974	0.95	2/1317 (0.2%)
2	E	0.19	0/208	0.38	0/322
2	F	0.25	0/215	0.37	0/333
2	I	0.25	0/281	0.43	0/436
2	J	0.23	0/284	0.42	0/440
All	All	0.46	0/4884	0.84	7/6799 (0.1%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	242	ASN	N-CA-C	6.46	119.15	110.88
1	B	244	LEU	N-CA-C	-6.18	104.22	112.94
1	D	273	VAL	CA-C-N	6.02	125.90	119.28
1	D	273	VAL	C-N-CA	6.02	125.90	119.28
1	C	303	ALA	CA-C-N	5.90	126.45	120.38

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	952	0	984	19	0
1	B	952	0	984	17	0
1	C	952	0	984	19	0
1	D	952	0	984	8	0
2	E	187	0	99	0	0
2	F	193	0	98	1	0
2	I	252	0	131	2	0
2	J	255	0	130	3	0
3	A	1	0	0	0	0
3	B	5	0	0	0	0
3	C	1	0	0	0	0
3	J	1	0	0	0	0
All	All	4703	0	4394	65	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 7.

The worst 5 of 65 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:B:308:LYS:HB2	1:B:311:ARG:HG3	1.67	0.77
1:B:318:LYS:NZ	1:B:322:GLY:O	2.22	0.72
1:D:231:LEU:HD12	1:D:314:VAL:HG22	1.74	0.68
1:B:242:ASN:HD21	1:B:275:ILE:HG12	1.61	0.66
1:C:308:LYS:HB2	1:C:311:ARG:HG3	1.79	0.65

There are no symmetry-related clashes.

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	120/146 (82%)	120 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	120/146 (82%)	119 (99%)	1 (1%)	0	100	100
1	C	120/146 (82%)	119 (99%)	1 (1%)	0	100	100
1	D	120/146 (82%)	120 (100%)	0	0	100	100
All	All	480/584 (82%)	478 (100%)	2 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	106/129 (82%)	99 (93%)	7 (7%)	15	36
1	B	106/129 (82%)	99 (93%)	7 (7%)	15	36
1	C	106/129 (82%)	96 (91%)	10 (9%)	8	21
1	D	106/129 (82%)	97 (92%)	9 (8%)	10	25
All	All	424/516 (82%)	391 (92%)	33 (8%)	11	29

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	261	SER
1	D	273	VAL
1	D	323	LYS
1	B	311	ARG
1	B	298	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	249	HIS
1	B	242	ASN
1	B	249	HIS

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Mol	Chain	Res	Type
1	B	285	HIS
1	D	297	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	E	8/12 (66%)	0	0
2	F	8/12 (66%)	0	0
2	I	11/12 (91%)	1 (9%)	0
2	J	11/12 (91%)	3 (27%)	1 (9%)
All	All	38/48 (79%)	4 (10%)	1 (2%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	J	4	G
2	J	5	A
2	J	6	C
2	I	4	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	J	5	A

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 oligosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	122/146 (83%)	-0.58	1 (0%) 82 81	18, 29, 45, 53	0
1	B	122/146 (83%)	-0.43	0 100 100	16, 33, 54, 63	0
1	C	122/146 (83%)	-0.16	1 (0%) 82 81	33, 50, 66, 77	0
1	D	122/146 (83%)	-0.18	1 (0%) 82 81	31, 51, 64, 68	0
2	E	9/12 (75%)	-0.56	1 (11%) 10 8	27, 30, 76, 82	0
2	F	9/12 (75%)	-0.53	0 100 100	17, 44, 94, 96	0
2	I	12/12 (100%)	-0.39	0 100 100	45, 51, 83, 84	0
2	J	12/12 (100%)	-0.03	1 (8%) 17 14	37, 65, 98, 100	0
All	All	530/632 (83%)	-0.34	5 (0%) 81 80	16, 44, 66, 100	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	208	ILE	3.3
1	C	224	PHE	2.6
1	D	224	PHE	2.5
2	J	1	C	2.2
2	E	9	C	2.2

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 oligosaccharides 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.