



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2016 – 10:52 PM EDT

PDB ID : 5D8D
Title : Crystal structure of D-alanine-D-alanine ligase from *Acinetobacter baumannii*
Authors : Huynh, K.H.; Hong, M.K.; Kang, L.W.
Deposited on : 2015-08-17
Resolution : 2.19 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

<http://wwpdb.org/validation/2016/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
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
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-20027939

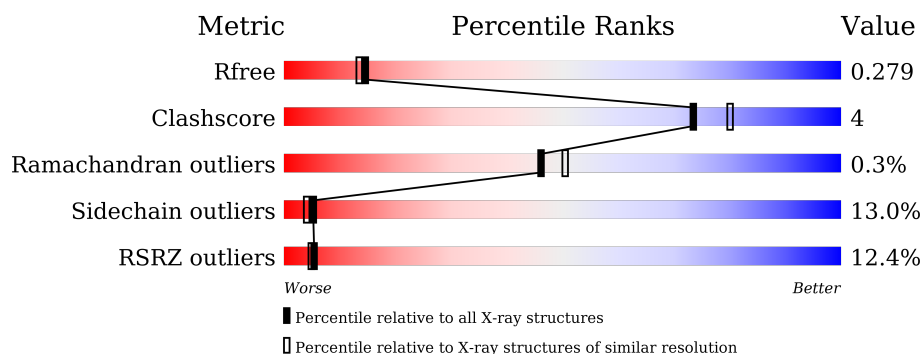
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	308	<div> <div>7%</div> <div> <div></div> <div>77%</div> <div>12%</div> <div>•</div> <div>8%</div> </div> </div>
1	B	308	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>13%</div> <div>5%</div> <div>8%</div> </div> </div>
1	C	308	<div> <div>16%</div> <div> <div></div> <div>74%</div> <div>12%</div> <div>•</div> <div>11%</div> </div> </div>
1	D	308	<div> <div>8%</div> <div> <div></div> <div>74%</div> <div>16%</div> <div>••</div> <div>8%</div> </div> </div>
1	E	308	<div> <div>10%</div> <div> <div></div> <div>75%</div> <div>12%</div> <div>•</div> <div>10%</div> </div> </div>
1	F	308	<div> <div>21%</div> <div> <div></div> <div>74%</div> <div>14%</div> <div>••</div> <div>10%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12910 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 D-alanine–D-alanine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	0	0
			2139	1356	363	412	8			
1	B	282	Total	C	N	O	S	0	0	0
			2141	1357	363	413	8			
1	C	274	Total	C	N	O	S	0	0	0
			2082	1323	354	397	8			
1	D	284	Total	C	N	O	S	0	0	0
			2154	1364	365	417	8			
1	E	276	Total	C	N	O	S	0	0	0
			2083	1322	353	400	8			
1	F	278	Total	C	N	O	S	0	0	0
			2112	1336	358	410	8			

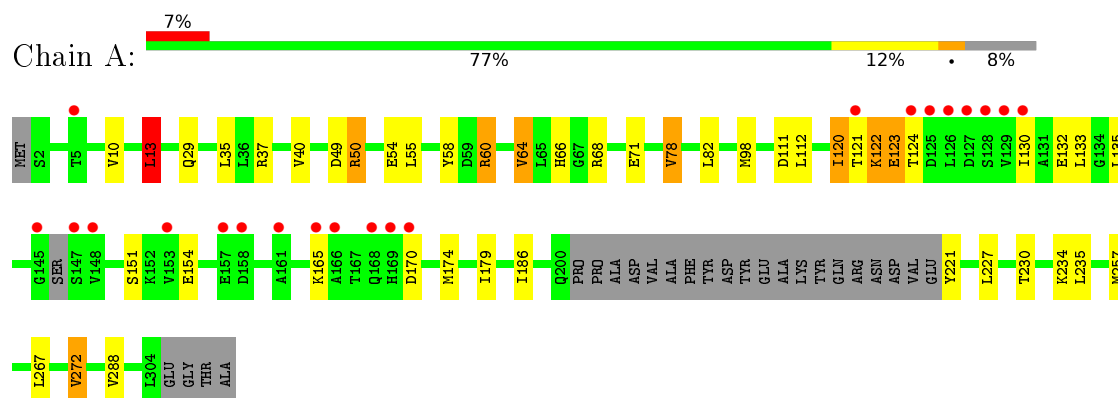
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	33	Total	O	0	0
			33	33		
2	B	30	Total	O	0	0
			30	30		
2	C	29	Total	O	0	0
			29	29		
2	D	36	Total	O	0	0
			36	36		
2	E	37	Total	O	0	0
			37	37		
2	F	34	Total	O	0	0
			34	34		

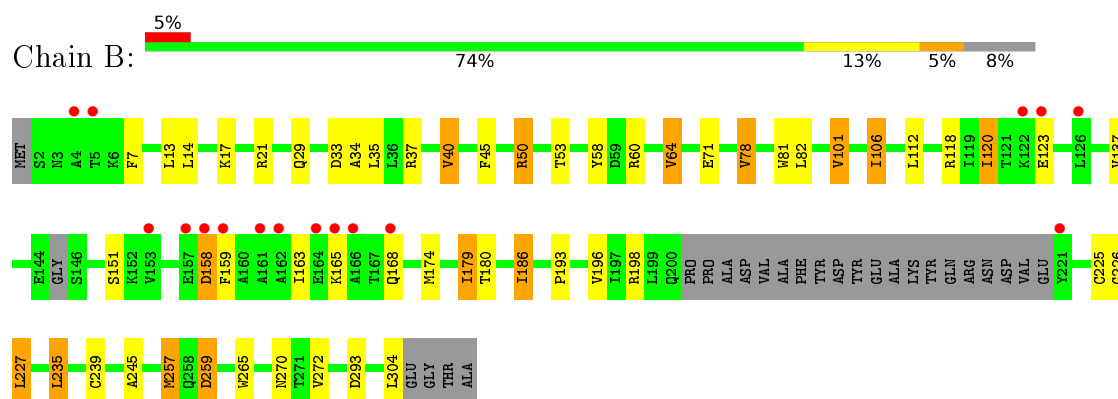
3 Residue-property plots [i](#)

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

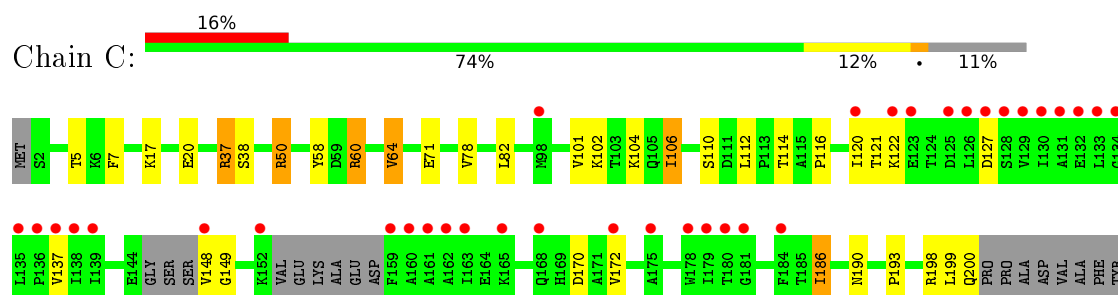
• Molecule 1: D-alanine-D-alanine ligase

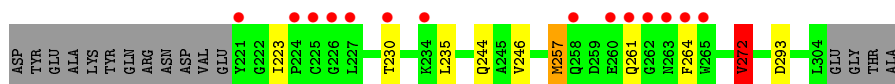


• Molecule 1: D-alanine-D-alanine ligase

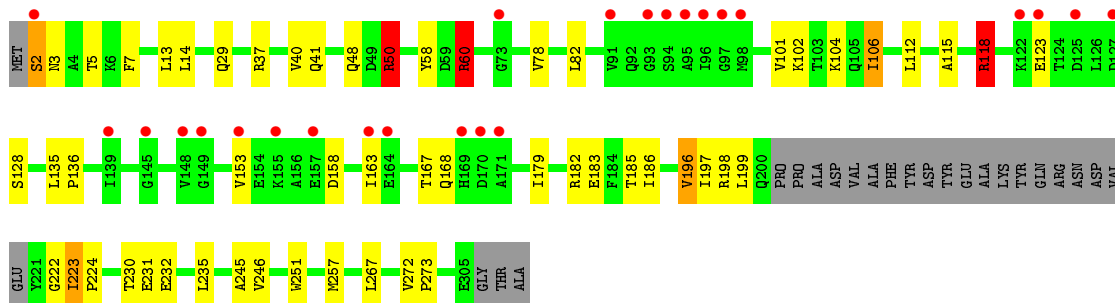
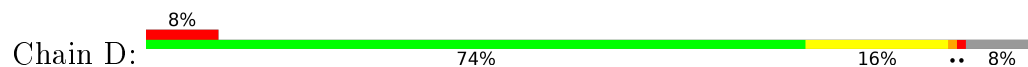


• Molecule 1: D-alanine-D-alanine ligase

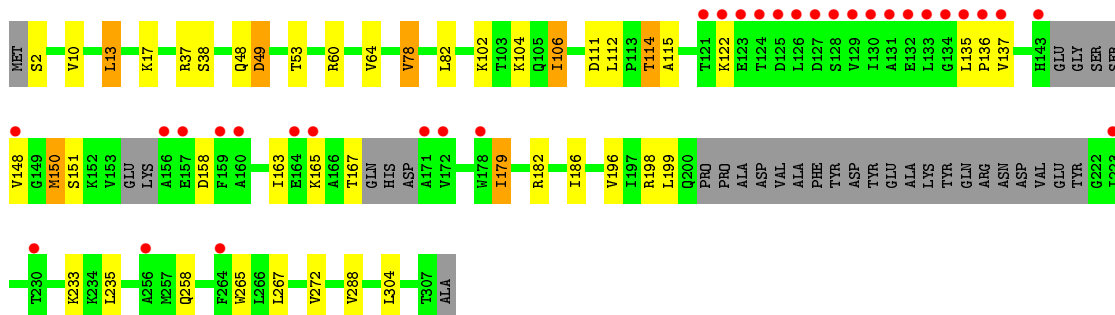
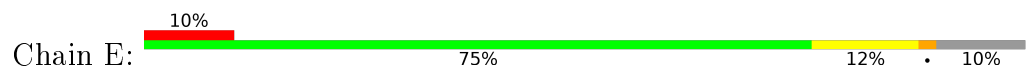




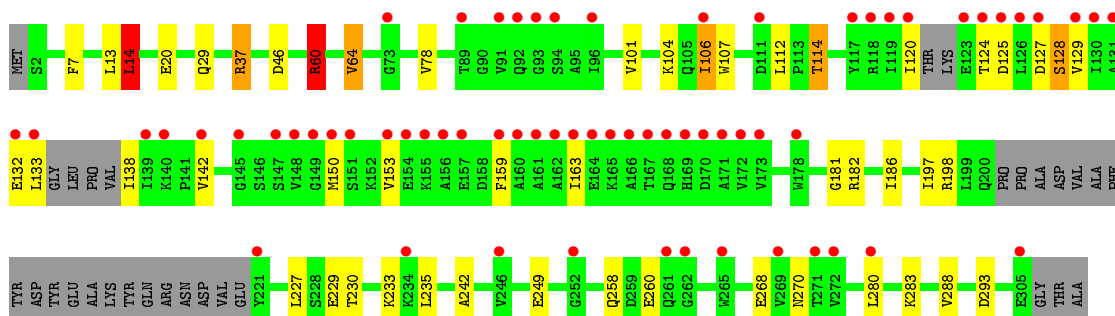
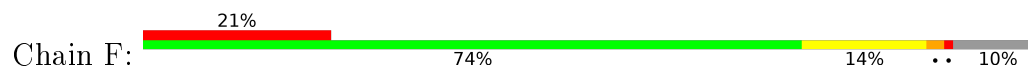
- Molecule 1: D-alanine–D-alanine ligase



- Molecule 1: D-alanine–D-alanine ligase



- Molecule 1: D-alanine–D-alanine ligase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	221.62Å 74.77Å 143.12Å 90.00° 103.27° 90.00°	Depositor
Resolution (Å)	36.05 – 2.19 36.05 – 2.19	Depositor EDS
% Data completeness (in resolution range)	98.4 (36.05-2.19) 98.5 (36.05-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.221 , 0.281 0.224 , 0.279	Depositor DCC
R_{free} test set	5778 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	45.2	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12910	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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	0.68	0/2175	0.86	4/2945 (0.1%)
1	B	0.70	0/2177	0.93	4/2948 (0.1%)
1	C	0.68	0/2117	0.86	5/2866 (0.2%)
1	D	0.68	0/2191	0.90	7/2968 (0.2%)
1	E	0.68	0/2115	0.87	4/2862 (0.1%)
1	F	0.68	0/2146	0.89	6/2903 (0.2%)
All	All	0.68	0/12921	0.89	30/17492 (0.2%)

There are no bond length outliers.

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	37	ARG	NE-CZ-NH2	-12.91	113.84	120.30
1	C	37	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	F	37	ARG	NE-CZ-NH1	8.55	124.57	120.30
1	D	60	ARG	NE-CZ-NH2	-8.47	116.06	120.30
1	D	37	ARG	NE-CZ-NH2	-7.89	116.35	120.30

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	2139	0	2144	21	0
1	B	2141	0	2146	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2082	0	2092	13	0
1	D	2154	0	2156	21	0
1	E	2083	0	2097	15	0
1	F	2112	0	2104	16	0
2	A	33	0	0	1	0
2	B	30	0	0	0	0
2	C	29	0	0	0	0
2	D	36	0	0	0	0
2	E	37	0	0	0	0
2	F	34	0	0	0	0
All	All	12910	0	12739	103	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 4.

The worst 5 of 103 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:E:179:ILE:HD11	1:E:265:TRP:CD1	2.20	0.76
1:A:122:LYS:HA	1:A:122:LYS:HE3	1.67	0.74
1:A:120:ILE:HA	1:A:124:THR:HG21	1.71	0.73
1:F:125:ASP:O	1:F:128:SER:OG	2.09	0.70
1:C:104:LYS:NZ	1:C:114:THR:OG1	2.25	0.69

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	276/308 (90%)	265 (96%)	11 (4%)	0	100	100
1	B	276/308 (90%)	264 (96%)	12 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	266/308 (86%)	252 (95%)	12 (4%)	2 (1%)	24	22
1	D	280/308 (91%)	266 (95%)	13 (5%)	1 (0%)	39	42
1	E	266/308 (86%)	255 (96%)	10 (4%)	1 (0%)	39	42
1	F	270/308 (88%)	253 (94%)	16 (6%)	1 (0%)	39	42
All	All	1634/1848 (88%)	1555 (95%)	74 (4%)	5 (0%)	46	50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	123	GLU
1	E	111	ASP
1	F	260	GLU
1	C	116	PRO
1	C	190	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	226/247 (92%)	195 (86%)	31 (14%)	4	3
1	B	227/247 (92%)	197 (87%)	30 (13%)	5	4
1	C	220/247 (89%)	193 (88%)	27 (12%)	6	5
1	D	228/247 (92%)	198 (87%)	30 (13%)	5	4
1	E	220/247 (89%)	191 (87%)	29 (13%)	5	4
1	F	223/247 (90%)	195 (87%)	28 (13%)	5	4
All	All	1344/1482 (91%)	1169 (87%)	175 (13%)	5	4

5 of 175 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	200	GLN
1	D	60	ARG

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Mol	Chain	Res	Type
1	F	163	ILE
1	C	230	THR
1	D	2	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	261	GLN
1	C	244	GLN
1	E	258	GLN
1	B	244	GLN
1	E	244	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	282/308 (91%)	0.36	21 (7%)	17 17	32, 49, 106, 133	0
1	B	282/308 (91%)	0.33	16 (5%)	27 27	31, 52, 98, 125	0
1	C	274/308 (88%)	0.91	49 (17%)	2 2	33, 57, 133, 163	0
1	D	284/308 (92%)	0.46	25 (8%)	12 11	32, 51, 106, 147	0
1	E	276/308 (89%)	0.56	32 (11%)	6 6	35, 57, 111, 131	0
1	F	278/308 (90%)	1.22	65 (23%)	1 1	34, 64, 143, 170	0
All	All	1676/1848 (90%)	0.64	208 (12%)	5 5	31, 54, 120, 170	0

The worst 5 of 208 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	159	PHE	12.0
1	F	126	LEU	9.6
1	D	148	VAL	9.3
1	F	148	VAL	8.3
1	F	172	VAL	8.1

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 [i](#)

There are no such residues in this entry.