



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 05:19 AM UTC

PDB ID : 6KXG / pdb_00006kxg
Title : Crystal structure of caspase-11-CARD
Authors : Liu, M.Z.Y.; Jin, T.C.
Deposited on : 2019-09-11
Resolution : 2.81 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

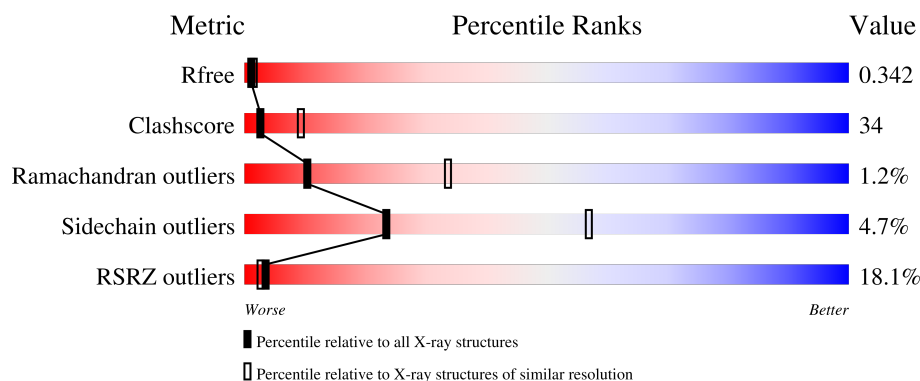
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	462	13% 55% 35% 8%
1	B	462	19% 46% 36% 14%
1	C	462	17% 50% 39% 9%
1	D	462	16% 48% 37% 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12882 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 caspase-11-CARD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3319	2140	541	630	8			
1	B	399	Total	C	N	O	S	0	0	0
			3079	1987	495	590	7			
1	C	419	Total	C	N	O	S	0	0	0
			3258	2096	534	620	8			
1	D	415	Total	C	N	O	S	0	0	0
			3223	2074	525	616	8			

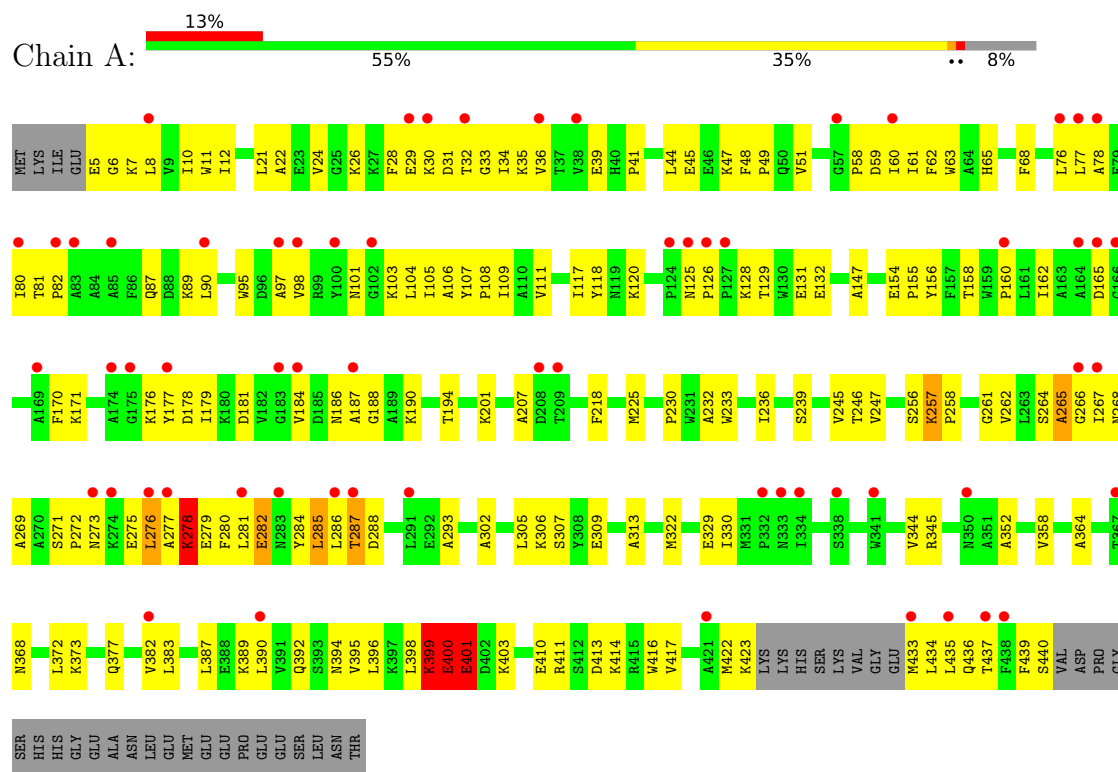
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	O	0	0
			3	3		

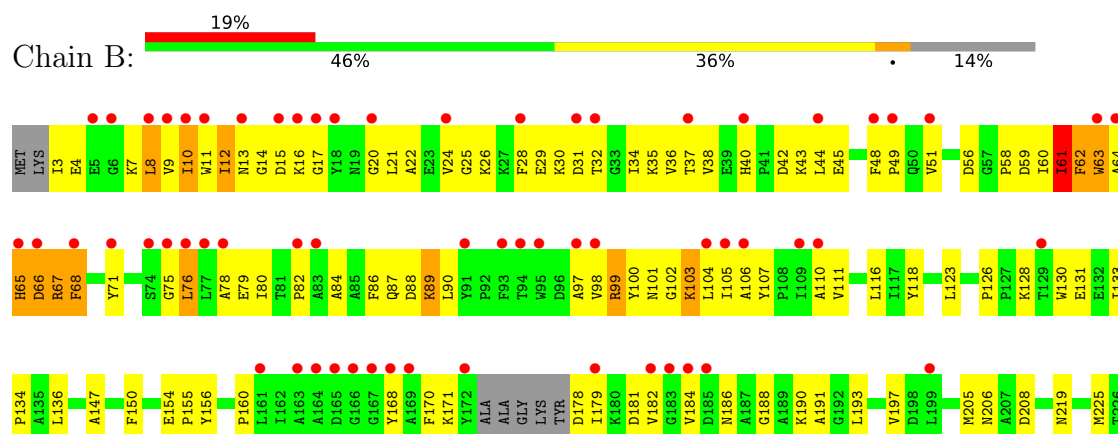
3 Residue-property plots

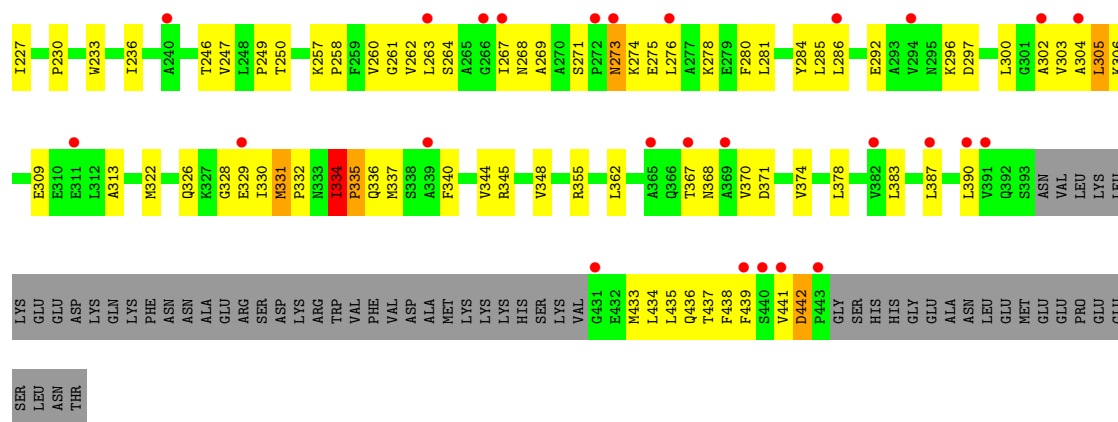
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: caspase-11-CARD

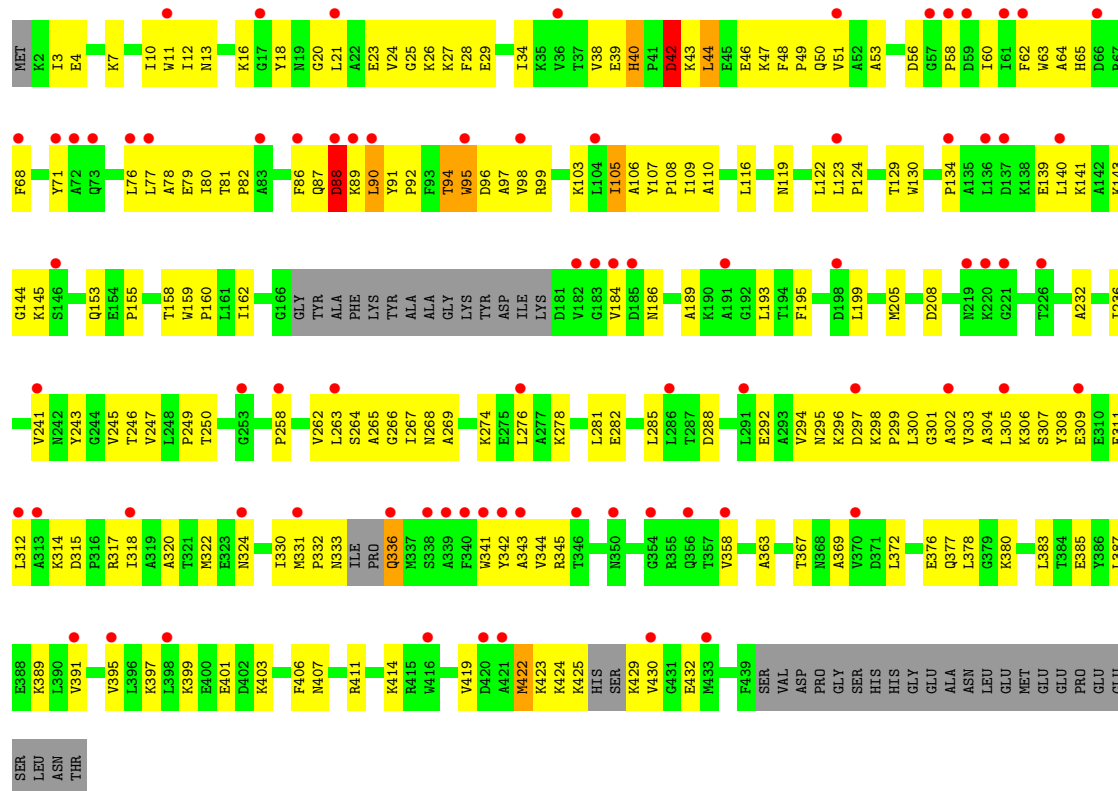


• Molecule 1: caspase-11-CARD

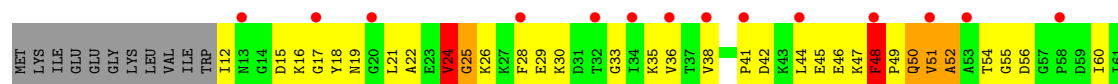




• Molecule 1: caspase-11-CARD



• Molecule 1: caspase-11-CARD



F62	K143	S234	L312	A313	N235	K314	T238	S239	A240	V241	N242	Y243	G244	V245	Q254	K257	P258	G261	V262	L263	S264	G266	I267	N268	A269	A270	S271	P272	N273	K274	E275	L276	A277	K278	N283	Y284	L285	G290	L291	E292	A293	V294	M295	K298	P299	L300	G301	A302	V303	K306	S307	Y308	E309	E310	E311	W233	A409
F63	G144	K145	K145	S146	A147	L148	F150	N151	L152	Q153	E154	P155	P160	L161	I162	A163	A164	D165	K171	Y172	ALA	ALA	GLY	LYS	TYR	D178	I179	K190	L196	V197	D198	L199	I200	M205	N206	A207	D208	T209	D210	N219	K220	G221	E222	T223	A224	N225	T226	I227	N228	G229	P230	L140	K141	A142			
F64	H65	D66	R67	F68	G69	G70	Y71	A72	Q73	S74	G75	L76	T80	T81	P82	A83	A84	D88	T94	Y95	D96	A97	V98	R99	Y100	N101	G102	K103	L104	I105	V111	E112	I117	Y118	N119	L122	T129	W130	E131	E132	I133	P134	A135	L136	D137	K138	E139	L140	K141	A142							
E410	R411	S412	D413	K414	R415	W416	W417	F418	V419	D420	A421	M422	LYS	LYS	LYS	HIS	SER	LYS	VAL	G431	E432	M433	L434	L435	Q436	T437	F438	F439	SER	VAL	ASP	PRO	GLY	SER	HIS	HIS	GLY	GLU	ALA	ASN	LEU	GLU	MET	GLU	GLU	PRO	GLU	SER	LEU	ASN	THR						

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.31Å 145.16Å 187.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.67 – 2.81 38.67 – 2.81	Depositor EDS
% Data completeness (in resolution range)	97.4 (38.67-2.81) 97.3 (38.67-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.305 , 0.340 0.307 , 0.342	Depositor DCC
R_{free} test set	2573 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	84.1	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 92.9	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	0.89	EDS
Total number of atoms	12882	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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	0.36	0/3394	0.59	5/4603 (0.1%)
1	B	0.35	1/3149 (0.0%)	0.65	8/4278 (0.2%)
1	C	0.32	0/3326	0.57	4/4504 (0.1%)
1	D	0.36	0/3294	0.66	6/4467 (0.1%)
All	All	0.35	1/13163 (0.0%)	0.62	23/17852 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	61	ILE	CA-CB	-5.64	1.51	1.55

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	52	ALA	N-CA-C	-9.35	102.00	113.97
1	B	331	MET	CA-C-N	7.67	127.72	119.89
1	B	331	MET	C-N-CA	7.67	127.72	119.89
1	C	18	TYR	N-CA-C	-7.45	104.34	113.50
1	D	312	LEU	N-CA-C	-6.85	104.74	113.23

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	3319	0	3306	178	0
1	B	3079	0	3055	260	0
1	C	3258	0	3257	228	0
1	D	3223	0	3198	222	0
2	A	3	0	0	0	0
All	All	12882	0	12816	871	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 34.

The worst 5 of 871 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:12:ILE:HD11	1:B:62:PHE:CD2	1.41	1.51
1:B:66:ASP:HB3	1:B:331:MET:SD	1.66	1.34
1:C:63:TRP:CD1	1:C:64:ALA:H	1.44	1.33
1:B:80:ILE:HD12	1:B:107:TYR:CZ	1.67	1.28
1:C:63:TRP:CD1	1:C:64:ALA:N	2.01	1.26

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	423/462 (92%)	393 (93%)	26 (6%)	4 (1%)	14	41
1	B	393/462 (85%)	357 (91%)	32 (8%)	4 (1%)	12	38
1	C	411/462 (89%)	389 (95%)	19 (5%)	3 (1%)	18	47
1	D	409/462 (88%)	365 (89%)	36 (9%)	8 (2%)	6	21
All	All	1636/1848 (88%)	1504 (92%)	113 (7%)	19 (1%)	10	34

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	LYS
1	A	399	LYS
1	A	400	GLU
1	B	335	PRO
1	C	241	VAL

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	342/373 (92%)	329 (96%)	13 (4%)	29	64
1	B	318/373 (85%)	299 (94%)	19 (6%)	17	47
1	C	338/373 (91%)	328 (97%)	10 (3%)	36	72
1	D	333/373 (89%)	312 (94%)	21 (6%)	16	45
All	All	1331/1492 (89%)	1268 (95%)	63 (5%)	23	57

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	305	LEU
1	D	334	ILE
1	C	88	ASP
1	D	333	ASN
1	D	422	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	283	ASN
1	D	408	ASN
1	C	65	HIS
1	C	73	GLN
1	C	356	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 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	427/462 (92%)	1.06	62 (14%) 6 4	54, 108, 184, 260	0
1	B	399/462 (86%)	1.24	88 (22%) 2 2	58, 114, 222, 270	0
1	C	419/462 (90%)	1.22	78 (18%) 3 2	58, 116, 221, 264	0
1	D	415/462 (89%)	1.25	73 (17%) 4 3	60, 115, 222, 331	0
All	All	1660/1848 (89%)	1.19	301 (18%) 3 3	54, 114, 220, 331	0

The worst 5 of 301 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	17	GLY	5.8
1	D	119	ASN	5.7
1	B	183	GLY	5.6
1	C	66	ASP	5.6
1	C	17	GLY	5.3

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.