



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:14 AM UTC

PDB ID : 6FIB / pdb_00006fib
Title : Structure of human 4-1BB ligand
Authors : Joseph, C.; Claus, C.; Ferrara, C.; von Hirschheydt, T.; Prince, C.; Funk, D.; Klein, C.; Benz, J.
Deposited on : 2018-01-17
Resolution : 2.70 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 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

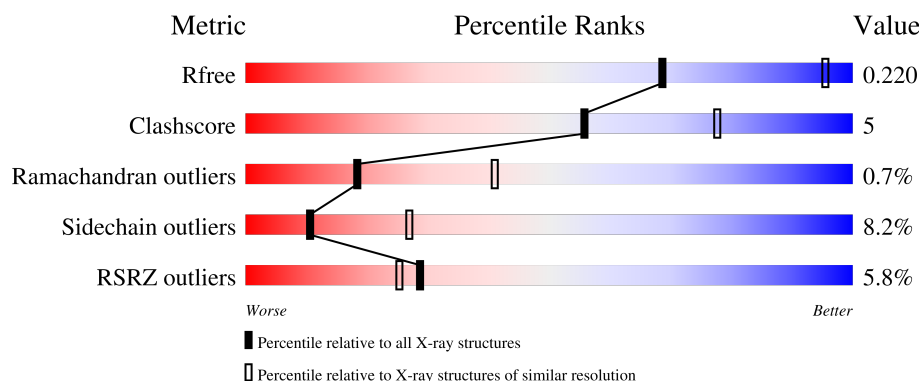
1 Overall quality at a glance

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)

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	188	2% 60% 15% .. 22%
2	B	311	3% 38% 6% . 55%
3	C	292	4% 40% 9% . 50%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3347 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 Tumor necrosis factor ligand superfamily member 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	0	0	0
			1100	706	195	198	1			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	249	GLY	-	expression tag	UNP P41273
A	250	GLY	-	expression tag	UNP P41273
A	251	GLY	-	expression tag	UNP P41273
A	252	GLY	-	expression tag	UNP P41273
A	253	SER	-	expression tag	UNP P41273
A	254	GLY	-	expression tag	UNP P41273
A	255	GLY	-	expression tag	UNP P41273
A	256	GLY	-	expression tag	UNP P41273
A	257	GLY	-	expression tag	UNP P41273
A	258	SER	-	expression tag	UNP P41273

- Molecule 2 is a protein called Tumor necrosis factor ligand superfamily member 9,4-1BBL-CH/CL fusion.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	140	Total	C	N	O	S	0	0	0
			1063	683	189	190	1			

- Molecule 3 is a protein called Tumor necrosis factor ligand superfamily member 9, Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	146	Total	C	N	O	S	0	0	0
			1102	706	198	197	1			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	70	ARG	-	expression tag	UNP P41273
C	249	GLY	-	linker	UNP P41273
C	250	GLY	-	linker	UNP P41273
C	251	GLY	-	linker	UNP P41273
C	252	GLY	-	linker	UNP P41273
C	253	SER	-	linker	UNP P41273
C	254	GLY	-	linker	UNP P41273
C	255	GLY	-	linker	UNP P41273
C	256	GLY	-	linker	UNP P41273
C	257	GLY	-	linker	UNP P41273
C	288	GLU	LYS	conflict	UNP A8K008
C	354	GLU	LYS	conflict	UNP A8K008

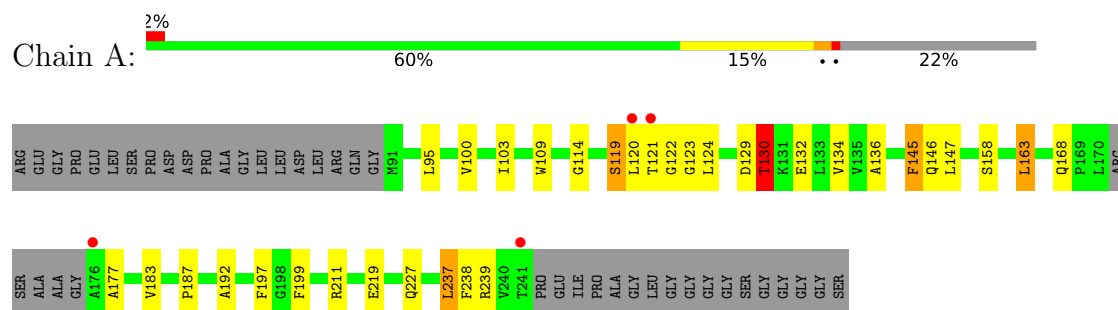
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	22	Total 22	O 22	0	0
4	B	29	Total 29	O 29	0	0
4	C	31	Total 31	O 31	0	0

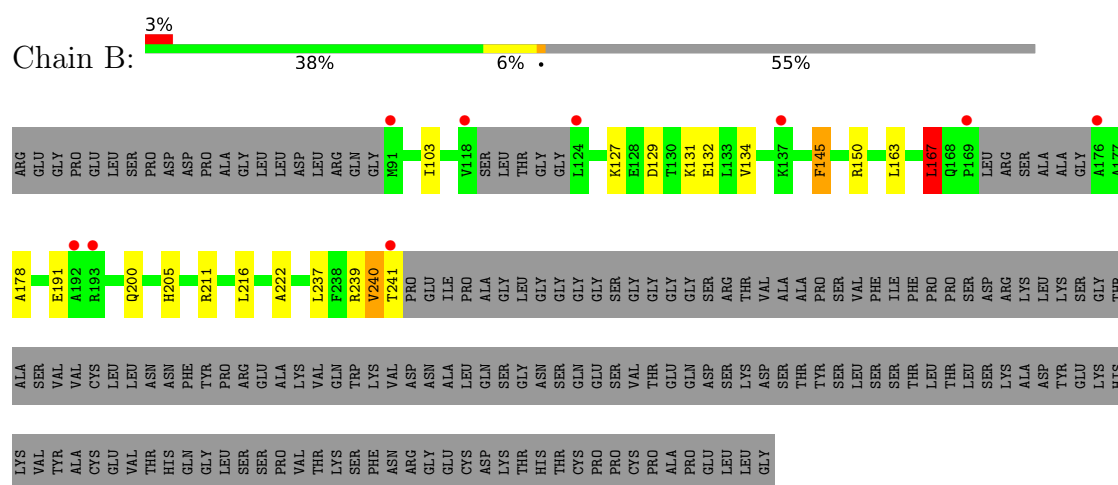
3 Residue-property plots [i](#)

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.

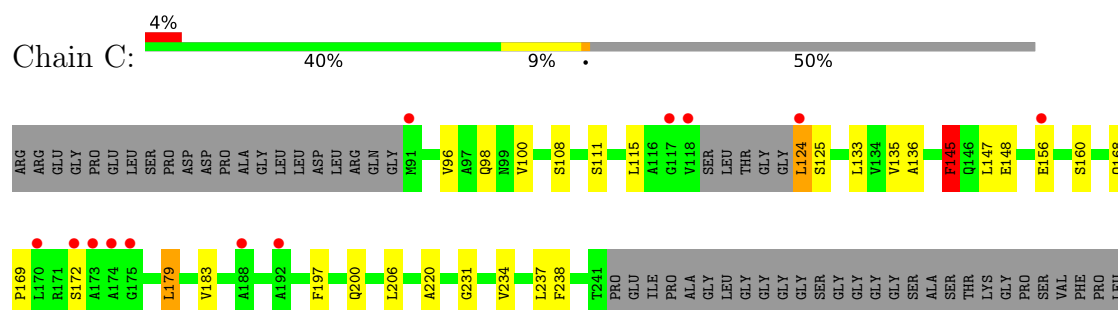
- Molecule 1: Tumor necrosis factor ligand superfamily member 9



- Molecule 2: Tumor necrosis factor ligand superfamily member 9,4-1BBL -CH/CL fusion



- Molecule 3: Tumor necrosis factor ligand superfamily member 9, Uncharacterized protein



[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	119.59Å 119.59Å 104.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	103.57 – 2.70 103.57 – 2.70	Depositor EDS
% Data completeness (in resolution range)	61.9 (103.57-2.70) 62.0 (103.57-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.69Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.166 , 0.221 0.174 , 0.220	Depositor DCC
R_{free} test set	696 reflections (2.97%)	wwPDB-VP
Wilson B-factor (Å ²)	84.7	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 84.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.037 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3347	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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	0.86	1/1122 (0.1%)	1.41	11/1524 (0.7%)
2	B	0.84	0/1084	1.28	8/1471 (0.5%)
3	C	0.86	0/1124	1.36	6/1526 (0.4%)
All	All	0.85	1/3330 (0.0%)	1.35	25/4521 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	103	ILE	CG1-CD1	5.25	1.72	1.51

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	PHE	CA-CB-CG	10.35	124.14	113.80
2	B	145	PHE	CA-CB-CG	9.30	123.10	113.80
3	C	145	PHE	CA-CB-CG	7.40	121.20	113.80
3	C	100	VAL	N-CA-CB	7.13	117.49	111.64
1	A	177	ALA	CA-C-N	6.92	129.86	120.38
1	A	177	ALA	C-N-CA	6.92	129.86	120.38
3	C	98	GLN	CB-CG-CD	-6.77	101.09	112.60
2	B	127	LYS	CA-C-N	6.65	129.49	120.38
2	B	127	LYS	C-N-CA	6.65	129.49	120.38
1	A	130	THR	N-CA-C	-6.40	99.21	109.96
2	B	167	LEU	CA-C-N	6.35	128.96	120.58
2	B	167	LEU	C-N-CA	6.35	128.96	120.58
2	B	129	ASP	CA-CB-CG	6.34	118.94	112.60
1	A	238	PHE	CA-CB-CG	6.28	120.08	113.80
3	C	125	SER	N-CA-C	6.21	118.54	110.53
1	A	121	THR	CA-C-N	5.46	129.94	121.32
1	A	121	THR	C-N-CA	5.46	129.94	121.32
3	C	220	ALA	CA-C-N	5.34	130.61	122.65
3	C	220	ALA	C-N-CA	5.34	130.61	122.65
1	A	114	GLY	CA-C-N	5.32	129.12	120.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	GLY	C-N-CA	5.32	129.12	120.23
2	B	222	ALA	CA-C-N	5.09	127.36	120.38
2	B	222	ALA	C-N-CA	5.09	127.36	120.38
1	A	120	LEU	CA-C-N	5.01	126.99	120.28
1	A	120	LEU	C-N-CA	5.01	126.99	120.28

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	1100	0	1114	13	0
2	B	1063	0	1073	10	0
3	C	1102	0	1116	15	0
4	A	22	0	0	0	0
4	B	29	0	0	0	0
4	C	31	0	0	0	0
All	All	3347	0	3303	31	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 5.

All (31) 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:B:167:LEU:HD11	2:B:178:ALA:HB2	1.73	0.70
1:A:197:PHE:CZ	3:C:200:GLN:HG3	2.31	0.66
3:C:96:VAL:HG11	3:C:231:GLY:HA2	1.83	0.60
2:B:205:HIS:HB2	3:C:115:LEU:HD23	1.85	0.59
3:C:133:LEU:HD21	3:C:237:LEU:HD21	1.85	0.58
2:B:103:ILE:O	2:B:216:LEU:HD23	2.05	0.56
1:A:147:LEU:HD22	1:A:163:LEU:HG	1.88	0.55
1:A:123:GLY:C	1:A:136:ALA:HB2	2.34	0.52
3:C:96:VAL:CG1	3:C:231:GLY:HA2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:LEU:HB3	1:A:109:TRP:HB3	1.93	0.51
2:B:200:GLN:HG3	3:C:197:PHE:CZ	2.47	0.50
2:B:240:VAL:HG11	3:C:238:PHE:HB2	1.93	0.50
1:A:100:VAL:HG12	1:A:227:GLN:HG2	1.94	0.48
3:C:124:LEU:N	3:C:136:ALA:HB2	2.29	0.47
1:A:124:LEU:HD12	1:A:136:ALA:H	1.79	0.47
2:B:134:VAL:HG12	2:B:211:ARG:HG2	1.96	0.47
1:A:197:PHE:HZ	3:C:200:GLN:HG3	1.80	0.45
3:C:96:VAL:HG22	3:C:234:VAL:HG22	1.98	0.45
2:B:239:ARG:HG2	2:B:241:THR:H	1.82	0.44
2:B:200:GLN:HG3	3:C:197:PHE:HZ	1.83	0.43
1:A:134:VAL:HG12	1:A:211:ARG:HG2	2.00	0.43
1:A:197:PHE:CE2	1:A:199:PHE:HB2	2.53	0.43
1:A:124:LEU:HD23	1:A:237:LEU:HD13	1.99	0.43
2:B:163:LEU:HD23	2:B:163:LEU:HA	1.78	0.42
1:A:122:GLY:C	1:A:124:LEU:H	2.28	0.42
3:C:168:GLN:HA	3:C:169:PRO:C	2.45	0.42
1:A:187:PRO:HG3	2:B:191:GLU:HG2	2.02	0.42
1:A:130:THR:HB	1:A:132:GLU:HG3	2.02	0.41
3:C:135:VAL:HG21	3:C:206:LEU:HD13	2.01	0.41
3:C:145:PHE:CZ	3:C:179:LEU:HB3	2.56	0.41
3:C:147:LEU:HD23	3:C:183:VAL:CG2	2.51	0.41

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	142/188 (76%)	131 (92%)	9 (6%)	2 (1%)	9	23
2	B	134/311 (43%)	125 (93%)	9 (7%)	0	100	100
3	C	142/292 (49%)	137 (96%)	4 (3%)	1 (1%)	18	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	418/791 (53%)	393 (94%)	22 (5%)	3 (1%)	18	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	ALA
3	C	172	SER
1	A	119	SER

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	112/137 (82%)	100 (89%)	12 (11%)	6	16
2	B	108/247 (44%)	101 (94%)	7 (6%)	15	37
3	C	111/227 (49%)	103 (93%)	8 (7%)	13	32
All	All	331/611 (54%)	304 (92%)	27 (8%)	10	27

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	SER
1	A	129	ASP
1	A	130	THR
1	A	145	PHE
1	A	146	GLN
1	A	158	SER
1	A	163	LEU
1	A	168	GLN
1	A	183	VAL
1	A	219	GLU
1	A	237	LEU
1	A	239	ARG
2	B	131	LYS

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Mol	Chain	Res	Type
2	B	132	GLU
2	B	145	PHE
2	B	150	ARG
2	B	167	LEU
2	B	237	LEU
2	B	240	VAL
3	C	108	SER
3	C	111	SER
3	C	124	LEU
3	C	145	PHE
3	C	148	GLU
3	C	156	GLU
3	C	160	SER
3	C	179	LEU

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	215	HIS
2	B	168	GLN
3	C	166	HIS
3	C	168	GLN
3	C	210	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

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	146/188 (77%)	0.22	4 (2%) 56 53	56, 84, 135, 164	0
2	B	140/311 (45%)	0.26	9 (6%) 25 22	57, 84, 134, 146	0
3	C	146/292 (50%)	0.22	12 (8%) 17 15	55, 78, 127, 159	0
All	All	432/791 (54%)	0.23	25 (5%) 29 25	55, 82, 134, 164	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	118	VAL	5.9
1	A	120	LEU	4.1
2	B	118	VAL	3.9
3	C	117	GLY	3.7
3	C	174	ALA	3.6
3	C	170	LEU	3.4
3	C	192	ALA	3.1
2	B	91	MET	3.1
3	C	188	ALA	3.1
2	B	241	THR	3.0
3	C	91	MET	2.9
3	C	175	GLY	2.8
3	C	124	LEU	2.8
3	C	172	SER	2.7
2	B	169	PRO	2.7
1	A	176	ALA	2.4
3	C	173	ALA	2.4
2	B	176	ALA	2.4
2	B	192	ALA	2.4
2	B	137	LYS	2.3
3	C	156	GLU	2.1
2	B	193	ARG	2.1
2	B	124	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	121	THR	2.0
1	A	241	THR	2.0

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.