



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:20 AM UTC

PDB ID : 5KF4 / pdb_00005kf4
Title : Crystal structure of FN3 domain (Residues P368-P466) of Human collagen XX
Authors : Xie, Y.; Cheng, Z.; Zhao, J.
Deposited on : 2016-06-12
Resolution : 2.50 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

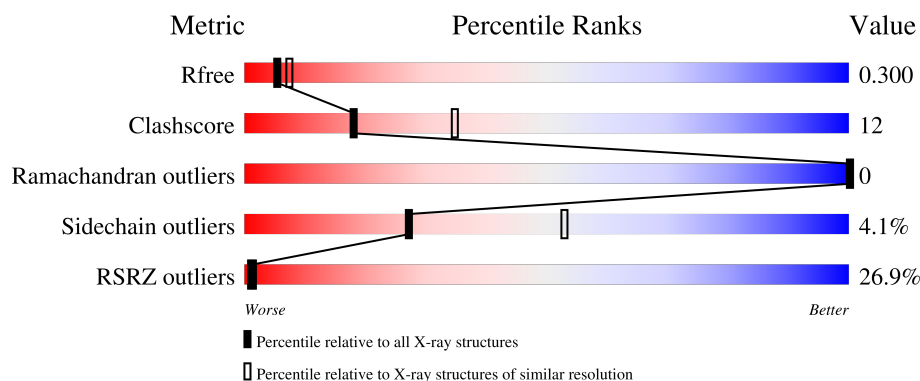
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	100	38% 59% 36% ..
1	B	100	6% 82% 17% .
1	C	100	22% 68% 27% ..
1	D	100	39% 65% 31% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2985 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 Collagen alpha-1(XX) chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	99	Total	C	N	O	0	0	0
			738	471	129	138			
1	B	99	Total	C	N	O	0	0	0
			738	471	129	138			
1	C	96	Total	C	N	O	0	0	0
			718	458	126	134			
1	D	97	Total	C	N	O	0	0	0
			723	461	127	135			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	367	GLY	-	expression tag	UNP Q9P218
B	367	GLY	-	expression tag	UNP Q9P218
C	367	GLY	-	expression tag	UNP Q9P218
D	367	GLY	-	expression tag	UNP Q9P218

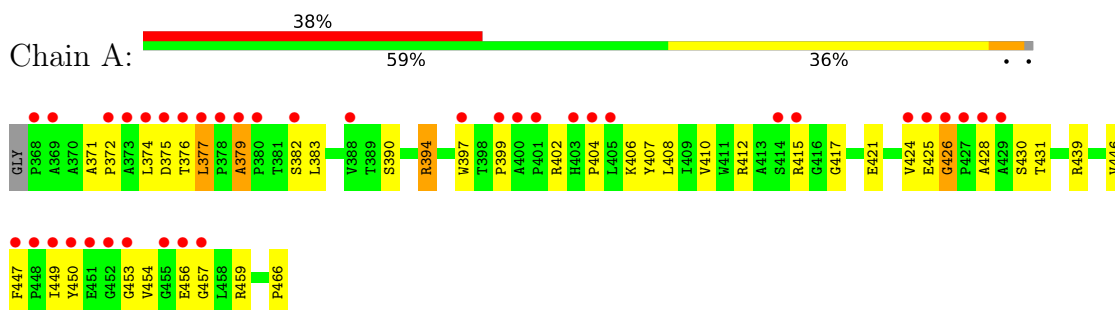
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	23	Total	O	0	0
			23	23		
2	B	18	Total	O	0	0
			18	18		
2	C	16	Total	O	0	0
			16	16		
2	D	11	Total	O	0	0
			11	11		

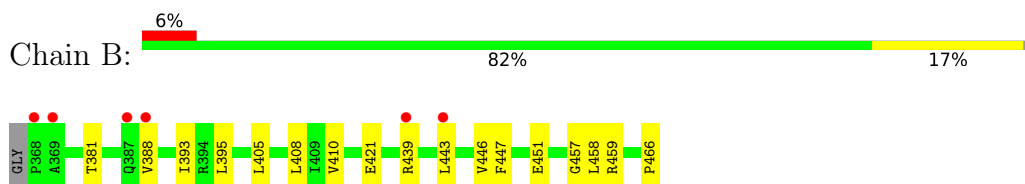
3 Residue-property plots [i](#)

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.

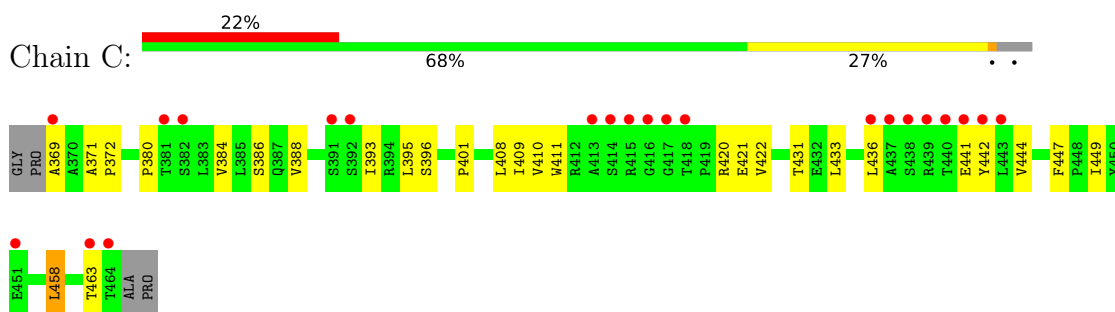
- Molecule 1: Collagen alpha-1(XX) chain



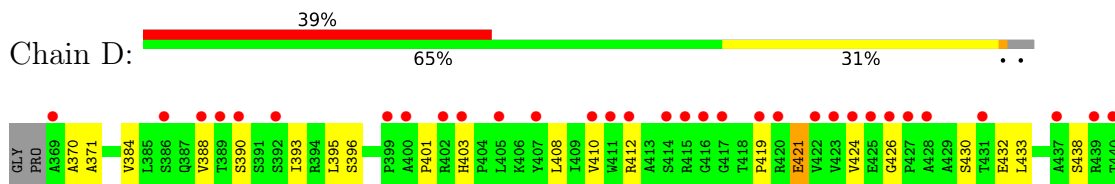
- Molecule 1: Collagen alpha-1(XX) chain



- Molecule 1: Collagen alpha-1(XX) chain



- Molecule 1: Collagen alpha-1(XX) chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.48Å 78.60Å 81.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.86 – 2.50 45.86 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.2 (45.86-2.50) 98.1 (45.86-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	11.90 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.258 , 0.284 0.281 , 0.300	Depositor DCC
R_{free} test set	640 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	1.232	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.002 for -h,l,k	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	2985	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.47 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.7868e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.37	0/758	0.94	6/1041 (0.6%)
1	B	0.34	0/758	0.78	0/1041
1	C	0.36	0/736	0.82	0/1011
1	D	0.41	0/741	0.93	4/1018 (0.4%)
All	All	0.37	0/2993	0.87	10/4111 (0.2%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	379	ALA	CA-C-N	-6.50	113.97	120.21
1	A	379	ALA	C-N-CA	-6.50	113.97	120.21
1	A	377	LEU	CA-C-N	-6.40	112.91	119.83
1	A	377	LEU	C-N-CA	-6.40	112.91	119.83
1	D	426	GLY	N-CA-C	5.77	124.10	112.34
1	D	421	GLU	N-CA-C	5.64	117.64	109.07
1	D	403	HIS	CA-C-N	5.36	126.71	120.98
1	D	403	HIS	C-N-CA	5.36	126.71	120.98
1	A	426	GLY	CA-C-N	-5.21	115.52	120.83
1	A	426	GLY	C-N-CA	-5.21	115.52	120.83

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	738	0	752	32	0
1	B	738	0	752	9	0
1	C	718	0	732	18	0
1	D	723	0	737	15	0
2	A	23	0	0	14	0
2	B	18	0	0	2	0
2	C	16	0	0	2	0
2	D	11	0	0	2	0
All	All	2985	0	2973	72	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 12.

All (72) 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:D:443:LEU:HD21	1:D:459:ARG:HD2	1.48	0.93
1:A:397:TRP:O	2:A:501:HOH:O	1.99	0.81
1:A:374:LEU:HG	2:A:507:HOH:O	1.85	0.76
1:D:410:VAL:HG22	1:D:421:GLU:HG2	1.68	0.75
1:B:451:GLU:OE2	2:B:501:HOH:O	2.03	0.75
1:A:459:ARG:NH1	2:A:506:HOH:O	2.20	0.75
1:B:439:ARG:HG2	1:B:466:PRO:HA	1.70	0.74
1:B:443:LEU:HD21	1:B:459:ARG:HD2	1.70	0.73
1:A:402:ARG:O	2:A:502:HOH:O	2.07	0.72
1:C:410:VAL:HG22	1:C:421:GLU:HG2	1.73	0.70
1:A:404:PRO:HG2	1:A:426:GLY:HA2	1.74	0.69
1:A:382:SER:HB2	1:C:458:LEU:HD12	1.75	0.69
1:B:410:VAL:HG22	1:B:421:GLU:HG2	1.75	0.67
1:A:453:GLY:O	2:A:503:HOH:O	2.14	0.66
1:C:409:ILE:HD13	1:C:431:THR:HG21	1.79	0.65
1:A:410:VAL:HG22	1:A:421:GLU:HG2	1.78	0.65
1:D:395:LEU:HD11	1:D:444:VAL:HG11	1.79	0.65
1:A:408:LEU:HB3	1:A:447:PHE:HB2	1.78	0.64
1:B:408:LEU:HB3	1:B:447:PHE:HB2	1.77	0.64
1:A:454:VAL:N	2:A:507:HOH:O	2.30	0.63
1:C:395:LEU:HD11	1:C:444:VAL:HG11	1.81	0.62
1:A:439:ARG:HG2	1:A:466:PRO:HA	1.82	0.62
1:D:370:ALA:C	2:D:503:HOH:O	2.42	0.62
1:D:412:ARG:HH21	1:D:419:PRO:HG3	1.66	0.61
1:C:401:PRO:HB3	1:D:401:PRO:HB3	1.82	0.60
1:C:441:GLU:HA	1:C:463:THR:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:PRO:O	1:A:426:GLY:HA3	2.02	0.59
1:C:388:VAL:HG13	1:C:393:ILE:HG22	1.87	0.57
1:A:428:ALA:O	2:A:504:HOH:O	2.18	0.56
1:C:393:ILE:HD11	1:C:433:LEU:HD12	1.88	0.56
1:A:404:PRO:HB3	1:A:450:TYR:CE1	2.41	0.56
1:A:399:PRO:HD3	2:A:501:HOH:O	2.07	0.55
1:D:446:VAL:O	1:D:457:GLY:HA3	2.07	0.55
1:D:371:ALA:N	2:D:503:HOH:O	2.40	0.53
1:C:386:SER:N	2:C:501:HOH:O	2.40	0.52
1:A:375:ASP:HA	1:A:456:GLU:HB2	1.91	0.52
1:D:408:LEU:HB3	1:D:447:PHE:HB2	1.91	0.52
1:A:446:VAL:O	1:A:457:GLY:HA3	2.10	0.51
1:C:380:PRO:HG2	1:C:458:LEU:HD22	1.92	0.51
1:D:441:GLU:HA	1:D:463:THR:HA	1.93	0.50
1:B:446:VAL:O	1:B:457:GLY:HA3	2.12	0.50
1:A:415:ARG:NH1	2:A:511:HOH:O	2.46	0.49
1:A:406:LYS:HD3	1:A:425:GLU:HA	1.95	0.48
1:C:369:ALA:N	2:C:503:HOH:O	2.46	0.48
1:D:388:VAL:HG13	1:D:393:ILE:HG22	1.96	0.47
1:A:406:LYS:HB2	1:A:449:ILE:HB	1.96	0.46
1:D:393:ILE:O	1:D:432:GLU:HG3	2.15	0.46
1:A:402:ARG:NH2	2:A:512:HOH:O	2.48	0.46
1:A:383:LEU:N	2:A:508:HOH:O	2.35	0.46
1:A:379:ALA:O	2:A:505:HOH:O	2.20	0.46
1:C:411:TRP:HZ3	1:C:422:VAL:HG12	1.80	0.46
1:A:412:ARG:NH2	1:A:417:GLY:O	2.50	0.45
1:A:425:GLU:N	1:A:425:GLU:OE1	2.51	0.44
1:D:393:ILE:HD13	1:D:462:VAL:HG11	1.99	0.43
1:C:408:LEU:HB2	1:C:449:ILE:HD11	2.00	0.43
1:A:375:ASP:OD1	1:A:376:THR:HG23	2.18	0.43
1:A:407:TYR:HB2	1:A:424:VAL:HG23	2.00	0.43
1:A:453:GLY:HA3	2:A:507:HOH:O	2.19	0.43
1:C:436:LEU:HD23	1:C:442:TYR:CD1	2.54	0.43
1:A:371:ALA:HA	1:A:372:PRO:HD3	1.88	0.43
1:C:371:ALA:HA	1:C:372:PRO:HD3	1.90	0.42
1:B:388:VAL:HG13	1:B:393:ILE:HG22	2.02	0.41
1:D:384:VAL:HB	1:D:396:SER:HB3	2.02	0.41
1:B:439:ARG:NH2	2:B:503:HOH:O	2.39	0.41
1:C:411:TRP:CZ3	1:C:422:VAL:HG12	2.56	0.41
1:A:394:ARG:NH2	1:A:430:SER:OG	2.54	0.41
1:A:402:ARG:HB3	2:A:502:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:384:VAL:HB	1:C:396:SER:OG	2.21	0.41
1:D:448:PRO:HB2	1:D:450:TYR:CE1	2.56	0.41
1:C:408:LEU:HB3	1:C:447:PHE:HB2	2.03	0.41
1:A:408:LEU:N	1:A:447:PHE:O	2.40	0.40
1:B:381:THR:C	1:B:458:LEU:HD11	2.46	0.40

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	97/100 (97%)	94 (97%)	3 (3%)	0	100	100
1	B	97/100 (97%)	94 (97%)	3 (3%)	0	100	100
1	C	94/100 (94%)	91 (97%)	3 (3%)	0	100	100
1	D	95/100 (95%)	91 (96%)	4 (4%)	0	100	100
All	All	383/400 (96%)	370 (97%)	13 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	80/80 (100%)	76 (95%)	4 (5%)	22	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	80/80 (100%)	78 (98%)	2 (2%)	42	69
1	C	78/80 (98%)	76 (97%)	2 (3%)	40	68
1	D	78/80 (98%)	73 (94%)	5 (6%)	16	33
All	All	316/320 (99%)	303 (96%)	13 (4%)	27	53

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	377	LEU
1	A	390	SER
1	A	394	ARG
1	A	431	THR
1	B	395	LEU
1	B	405	LEU
1	C	420	ARG
1	C	458	LEU
1	D	390	SER
1	D	424	VAL
1	D	430	SER
1	D	433	LEU
1	D	438	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	435	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides 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	99/100 (99%)	1.79	38 (38%) 1 0	13, 34, 70, 95	0
1	B	99/100 (99%)	0.62	6 (6%) 27 23	9, 18, 47, 58	0
1	C	96/100 (96%)	1.33	22 (22%) 2 1	8, 30, 74, 132	0
1	D	97/100 (97%)	1.88	39 (40%) 0 0	14, 35, 65, 129	0
All	All	391/400 (97%)	1.40	105 (26%) 1 1	8, 29, 69, 132	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	415	ARG	7.0
1	D	426	GLY	6.8
1	D	369	ALA	6.3
1	A	375	ASP	5.8
1	A	451	GLU	5.0
1	C	440	THR	4.9
1	C	464	THR	4.9
1	A	368	PRO	4.9
1	A	378	PRO	4.9
1	A	450	TYR	4.7
1	C	417	GLY	4.7
1	A	455	GLY	4.6
1	C	438	SER	4.6
1	D	412	ARG	4.5
1	D	442	TYR	4.5
1	D	388	VAL	4.5
1	A	427	PRO	4.5
1	A	369	ALA	4.5
1	B	369	ALA	4.3
1	C	414	SER	4.3
1	A	428	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	377	LEU	3.9
1	D	425	GLU	3.9
1	A	453	GLY	3.9
1	A	456	GLU	3.9
1	C	369	ALA	3.8
1	D	403	HIS	3.7
1	A	374	LEU	3.7
1	C	442	TYR	3.7
1	D	443	LEU	3.7
1	C	415	ARG	3.7
1	D	427	PRO	3.6
1	D	428	ALA	3.6
1	D	410	VAL	3.5
1	C	382	SER	3.5
1	C	437	ALA	3.5
1	A	372	PRO	3.5
1	A	429	ALA	3.5
1	D	464	THR	3.4
1	A	379	ALA	3.4
1	A	397	TRP	3.3
1	D	440	THR	3.3
1	A	425	GLU	3.3
1	A	382	SER	3.3
1	B	439	ARG	3.2
1	A	401	PRO	3.2
1	D	424	VAL	3.2
1	A	448	PRO	3.2
1	C	441	GLU	3.1
1	B	387	GLN	3.0
1	C	416	GLY	3.0
1	C	439	ARG	3.0
1	D	422	VAL	3.0
1	A	399	PRO	2.9
1	A	424	VAL	2.9
1	D	423	VAL	2.9
1	D	399	PRO	2.9
1	C	391	SER	2.9
1	D	414	SER	2.9
1	D	416	GLY	2.9
1	B	443	LEU	2.8
1	A	426	GLY	2.8
1	A	449	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	413	ALA	2.8
1	D	431	THR	2.8
1	D	456	GLU	2.8
1	A	405	LEU	2.7
1	C	392	SER	2.7
1	D	392	SER	2.7
1	D	419	PRO	2.7
1	D	417	GLY	2.6
1	D	402	ARG	2.6
1	B	388	VAL	2.6
1	A	452	GLY	2.6
1	C	463	THR	2.6
1	A	376	THR	2.6
1	A	447	PHE	2.5
1	D	462	VAL	2.5
1	D	386	SER	2.5
1	D	463	THR	2.5
1	D	405	LEU	2.4
1	D	390	SER	2.4
1	A	380	PRO	2.3
1	A	404	PRO	2.3
1	B	368	PRO	2.3
1	D	411	TRP	2.3
1	C	451	GLU	2.2
1	A	388	VAL	2.2
1	C	381	THR	2.2
1	A	403	HIS	2.2
1	A	457	GLY	2.2
1	D	450	TYR	2.2
1	A	415	ARG	2.2
1	A	414	SER	2.1
1	A	400	ALA	2.1
1	C	418	THR	2.1
1	D	420	ARG	2.1
1	A	373	ALA	2.1
1	D	439	ARG	2.1
1	C	436	LEU	2.1
1	D	389	THR	2.1
1	D	400	ALA	2.0
1	C	443	LEU	2.0
1	D	437	ALA	2.0
1	D	407	TYR	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.