



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:37 AM UTC

PDB ID : 8H4O / pdb_00008h4o
Title : Crystal Structure of nucleotide-free Irgb6_T95D mutant
Authors : Saijo-Hamano, Y.; Okuma, H.; Sakai, N.; Kato, T.; Imasaki, T.; Nitta, R.
Deposited on : 2022-10-11
Resolution : 2.05 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

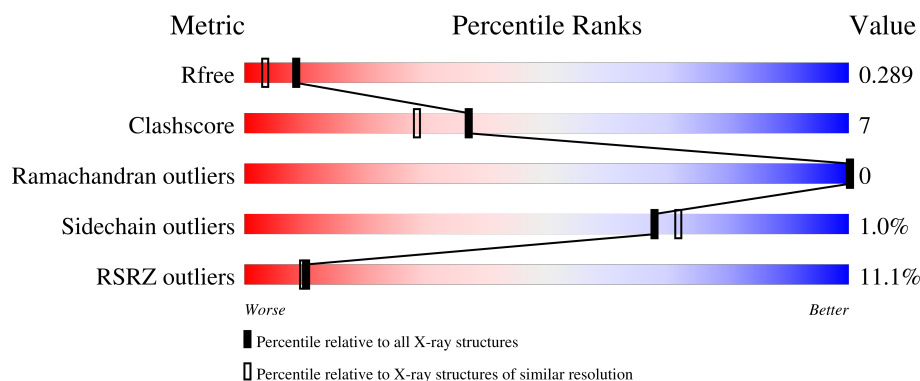
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	417	4% 82% 13% 5%
1	B	417	17% 76% 19% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6489 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 T-cell-specific guanine nucleotide triphosphate-binding protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	0	0
			3197	2068	515	603	11			
1	B	396	Total	C	N	O	S	0	0	0
			3195	2066	517	601	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q3T9E4
A	0	PRO	-	expression tag	UNP Q3T9E4
A	95	ASP	THR	engineered mutation	UNP Q3T9E4
B	-1	GLY	-	expression tag	UNP Q3T9E4
B	0	PRO	-	expression tag	UNP Q3T9E4
B	95	ASP	THR	engineered mutation	UNP Q3T9E4

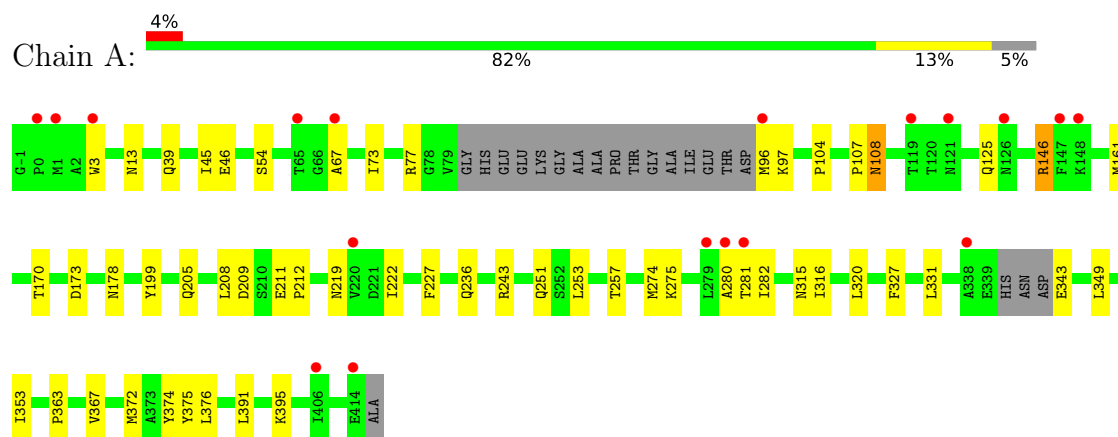
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	71	Total	O	0	0
			71	71		
2	B	26	Total	O	0	0
			26	26		

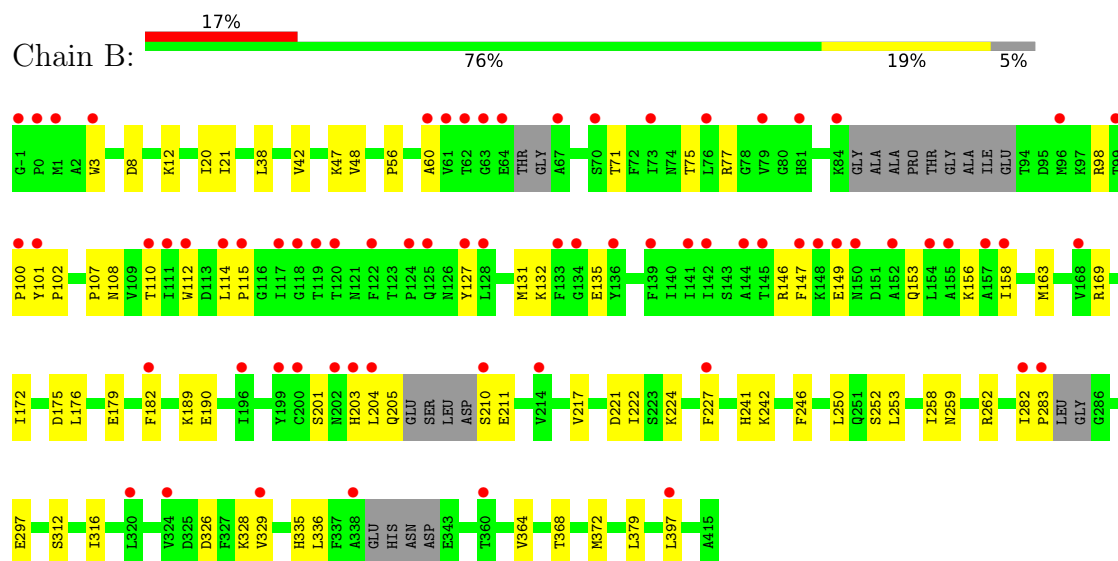
3 Residue-property plots [i](#)

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: T-cell-specific guanine nucleotide triphosphate-binding protein 2



- Molecule 1: T-cell-specific guanine nucleotide triphosphate-binding protein 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.53Å 80.61Å 147.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.55 – 2.05 40.55 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.3 (40.55-2.05) 99.6 (40.55-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.20_4459: ???	Depositor
R, R_{free}	0.226 , 0.283 (Not available) , 0.289	Depositor DCC
R_{free} test set	2000 reflections (3.65%)	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6489	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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	0.39	0/3271	0.54	0/4423
1	B	0.33	0/3267	0.50	0/4412
All	All	0.36	0/6538	0.52	0/8835

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	ARG	Sidechain

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	3197	0	3183	42	0
1	B	3195	0	3175	53	0
2	A	71	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	26	0	0	0	0
All	All	6489	0	6358	90	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.

All (90) 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:169:ARG:NH2	1:B:175:ASP:OD2	2.05	0.90
1:B:368:THR:HG22	1:B:372:MET:HE2	1.63	0.81
1:A:280:ALA:HB3	1:A:367:VAL:HG21	1.64	0.78
1:B:252:SER:HB3	1:B:258:ILE:HD11	1.65	0.78
1:A:236:GLN:O	2:A:501:HOH:O	2.08	0.72
1:A:349:LEU:HD11	1:A:376:LEU:HD21	1.72	0.72
1:B:397:LEU:HD23	1:B:397:LEU:O	1.93	0.69
1:A:243:ARG:NH2	2:A:501:HOH:O	2.24	0.69
1:B:282:ILE:HG13	1:B:283:PRO:HD2	1.75	0.67
1:A:96:MET:N	2:A:503:HOH:O	2.27	0.66
1:A:363:PRO:HG3	1:A:374:TYR:CD2	2.30	0.66
1:A:54:SER:HB3	1:B:107:PRO:HG3	1.78	0.66
1:B:210:SER:OG	1:B:211:GLU:N	2.26	0.65
1:B:190:GLU:OE1	1:B:190:GLU:N	2.31	0.63
1:B:328:LYS:O	1:B:335:HIS:NE2	2.33	0.62
1:B:201:SER:HA	1:B:204:LEU:HD12	1.82	0.60
1:A:349:LEU:HD13	1:A:372:MET:SD	2.42	0.60
1:B:149:GLU:HG2	1:B:203:HIS:NE2	2.18	0.59
1:B:3:TRP:CZ3	1:B:38:LEU:HD21	2.38	0.58
1:A:107:PRO:HB3	1:B:100:PRO:HB2	1.87	0.57
1:B:21:ILE:HG22	1:B:48:VAL:HG11	1.87	0.56
1:A:45:ILE:HD13	1:A:274:MET:HE2	1.87	0.56
1:B:336:LEU:HD21	1:B:379:LEU:HG	1.90	0.54
1:B:259:ASN:OD1	1:B:262:ARG:NH1	2.41	0.53
1:A:161:MET:HA	1:A:161:MET:HE2	1.89	0.53
1:A:251:GLN:O	1:A:257:THR:HG21	2.08	0.53
1:B:149:GLU:O	1:B:153:GLN:HG2	2.09	0.53
1:A:39:GLN:CD	1:B:282:ILE:HD11	2.34	0.52
1:B:98:ARG:NH1	1:B:132:LYS:HD2	2.24	0.52
1:A:73:ILE:O	1:A:77:ARG:HG3	2.08	0.52
1:B:326:ASP:O	1:B:329:VAL:HG12	2.10	0.52
1:A:320:LEU:HD21	1:A:395:LYS:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:GLN:CB	1:A:253:LEU:HD23	2.40	0.52
1:A:67:ALA:O	1:A:170:THR:HG21	2.11	0.51
1:B:115:PRO:O	1:B:127:TYR:OH	2.17	0.51
1:B:222:ILE:HB	1:B:227:PHE:CD1	2.46	0.51
1:B:77:ARG:NH2	1:B:101:TYR:HD2	2.09	0.50
1:A:282:ILE:CG2	1:B:42:VAL:HG11	2.42	0.50
1:A:222:ILE:HG22	1:A:227:PHE:CE2	2.46	0.50
1:B:222:ILE:HD11	1:B:253:LEU:HB2	1.94	0.50
1:A:77:ARG:HB3	1:A:104:PRO:HD3	1.94	0.49
1:B:368:THR:CG2	1:B:372:MET:HE2	2.39	0.49
1:B:115:PRO:HD2	1:B:131:MET:CE	2.42	0.49
1:A:170:THR:OG1	1:A:219:ASN:OD1	2.24	0.48
1:A:327:PHE:CE2	1:A:331:LEU:HD11	2.49	0.48
1:B:246:PHE:O	1:B:250:LEU:HD22	2.13	0.47
1:A:349:LEU:HD11	1:A:376:LEU:CD2	2.43	0.47
1:A:205:GLN:HG2	1:A:211:GLU:HA	1.95	0.47
1:B:169:ARG:HG3	1:B:172:ILE:HD11	1.97	0.47
1:A:280:ALA:O	1:A:367:VAL:HG22	2.16	0.46
1:A:316:ILE:CD1	1:A:391:LEU:HD13	2.45	0.46
1:A:178:ASN:ND2	2:A:502:HOH:O	2.15	0.46
1:A:251:GLN:HB2	1:A:253:LEU:HD23	1.97	0.46
1:B:221:ASP:HB3	1:B:224:LYS:CD	2.45	0.46
1:B:176:LEU:HD21	1:B:189:LYS:HG3	1.98	0.45
1:B:60:ALA:HB1	1:B:114:LEU:HD22	1.97	0.45
1:B:146:ARG:HG3	1:B:147:PHE:N	2.30	0.45
1:B:71:THR:O	1:B:75:THR:OG1	2.25	0.45
1:B:312:SER:O	1:B:316:ILE:HD12	2.17	0.45
1:A:208:LEU:HD12	1:A:212:PRO:HG3	1.98	0.45
1:B:179:GLU:HA	1:B:182:PHE:HD2	1.80	0.45
1:B:8:ASP:OD2	1:B:12:LYS:NZ	2.40	0.44
1:B:56:PRO:O	1:B:242:LYS:NZ	2.49	0.44
1:B:158:ILE:HG23	1:B:163:MET:HB2	1.99	0.44
1:B:156:LYS:HD2	1:B:156:LYS:HA	1.80	0.44
1:A:46:GLU:HG2	1:A:275:LYS:HG3	2.00	0.44
1:B:20:ILE:O	1:B:241:HIS:HD2	2.01	0.44
1:B:169:ARG:HG3	1:B:172:ILE:CD1	2.48	0.44
1:A:282:ILE:HG21	1:B:42:VAL:HG11	2.00	0.43
1:B:175:ASP:OD1	1:B:175:ASP:C	2.61	0.43
1:A:353:ILE:HG12	1:A:375:TYR:CD2	2.54	0.43
1:A:173:ASP:OD1	1:A:173:ASP:N	2.47	0.43
1:A:108:ASN:OD1	1:A:108:ASN:N	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:GLU:HA	1:B:297:GLU:OE1	2.18	0.42
1:B:56:PRO:HA	1:B:108:ASN:HB3	2.02	0.42
1:B:205:GLN:OE1	1:B:211:GLU:HG2	2.20	0.42
1:B:3:TRP:NE1	1:B:364:VAL:HB	2.34	0.42
1:A:343:GLU:O	1:A:343:GLU:HG2	2.20	0.42
1:B:189:LYS:HB3	1:B:190:GLU:OE1	2.20	0.42
1:A:125:GLN:H	1:A:125:GLN:CD	2.28	0.41
1:A:320:LEU:HD23	1:A:320:LEU:HA	1.87	0.41
1:A:349:LEU:HD23	1:A:349:LEU:HA	1.84	0.41
1:B:132:LYS:HB3	1:B:135:GLU:HG3	2.01	0.41
1:A:146:ARG:HD3	1:A:199:TYR:CE1	2.56	0.41
1:B:102:PRO:HA	1:B:110:THR:HA	2.02	0.41
1:A:327:PHE:HE2	1:A:331:LEU:HD11	1.86	0.41
1:A:316:ILE:H	1:A:316:ILE:HG13	1.59	0.40
1:A:3:TRP:CD1	1:A:3:TRP:N	2.87	0.40
1:B:47:LYS:HD3	1:B:47:LYS:HA	1.88	0.40
1:B:100:PRO:HB3	1:B:112:TRP:CH2	2.56	0.40

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	391/417 (94%)	381 (97%)	10 (3%)	0	100	100
1	B	384/417 (92%)	371 (97%)	13 (3%)	0	100	100
All	All	775/834 (93%)	752 (97%)	23 (3%)	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	352/365 (96%)	346 (98%)	6 (2%)	53	53
1	B	351/365 (96%)	350 (100%)	1 (0%)	86	90
All	All	703/730 (96%)	696 (99%)	7 (1%)	68	72

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	97	LYS
1	A	108	ASN
1	A	209	ASP
1	A	281	THR
1	A	315	ASN
1	B	217	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	203	HIS
1	A	205	GLN
1	A	251	GLN
1	B	36	ASN
1	B	39	GLN
1	B	108	ASN
1	B	315	ASN

5.3.3 RNA ⓘ

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	397/417 (95%)	0.47	18 (4%) 38 38	32, 49, 73, 88	0
1	B	396/417 (94%)	1.08	70 (17%) 4 3	36, 61, 98, 117	0
All	All	793/834 (95%)	0.78	88 (11%) 10 10	32, 54, 91, 117	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	338	ALA	4.7
1	B	67	ALA	4.5
1	B	182	PHE	4.3
1	B	199	TYR	4.2
1	B	154	LEU	3.8
1	B	76	LEU	3.8
1	B	-1	GLY	3.4
1	A	280	ALA	3.4
1	B	147	PHE	3.4
1	A	147	PHE	3.3
1	B	0	PRO	3.2
1	B	200	CYS	3.2
1	A	96	MET	3.2
1	B	62	THR	3.1
1	A	3	TRP	3.1
1	B	397	LEU	3.1
1	B	157	ALA	3.1
1	B	61	VAL	3.1
1	B	111	ILE	3.1
1	B	142	ILE	3.0
1	B	282	ILE	3.0
1	B	203	HIS	3.0
1	B	227	PHE	3.0
1	B	114	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	127	TYR	2.9
1	B	117	ILE	2.9
1	B	60	ALA	2.8
1	B	112	TRP	2.8
1	B	128	LEU	2.7
1	B	210	SER	2.7
1	B	133	PHE	2.7
1	B	110	THR	2.7
1	B	96	MET	2.7
1	B	100	PRO	2.7
1	B	136	TYR	2.7
1	B	145	THR	2.6
1	B	141	ILE	2.6
1	B	63	GLY	2.6
1	B	149	GLU	2.6
1	A	338	ALA	2.6
1	B	79	VAL	2.6
1	B	283	PRO	2.6
1	B	3	TRP	2.6
1	B	152	ALA	2.5
1	B	155	ALA	2.5
1	A	67	ALA	2.5
1	B	64	GLU	2.5
1	B	204	LEU	2.5
1	A	148	LYS	2.5
1	A	0	PRO	2.4
1	B	360	THR	2.4
1	B	84	LYS	2.4
1	B	158	ILE	2.4
1	B	214	VAL	2.4
1	A	119	THR	2.4
1	A	406	ILE	2.4
1	A	1	MET	2.4
1	B	1	MET	2.3
1	A	281	THR	2.3
1	B	101	TYR	2.3
1	B	150	ASN	2.3
1	A	279	LEU	2.3
1	A	121	ASN	2.3
1	B	134	GLY	2.3
1	B	320	LEU	2.3
1	B	324	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	124	PRO	2.3
1	B	202	ASN	2.3
1	B	119	THR	2.2
1	A	414	GLU	2.2
1	B	122	PHE	2.2
1	A	65	THR	2.2
1	B	115	PRO	2.2
1	B	148	LYS	2.2
1	B	81	HIS	2.2
1	B	73	ILE	2.2
1	B	168	VAL	2.2
1	B	144	ALA	2.2
1	B	139	PHE	2.1
1	B	196	ILE	2.1
1	B	99	THR	2.1
1	B	70	SER	2.1
1	A	126	ASN	2.1
1	B	118	GLY	2.1
1	A	220	VAL	2.1
1	B	329	VAL	2.0
1	B	125	GLN	2.0
1	B	120	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.