



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:17 PM UTC

PDB ID : 6I1Z / pdb_00006i1z
Title : Outward facing structure of apo CST
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Deposited on : 2018-10-31
Resolution : 3.40 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

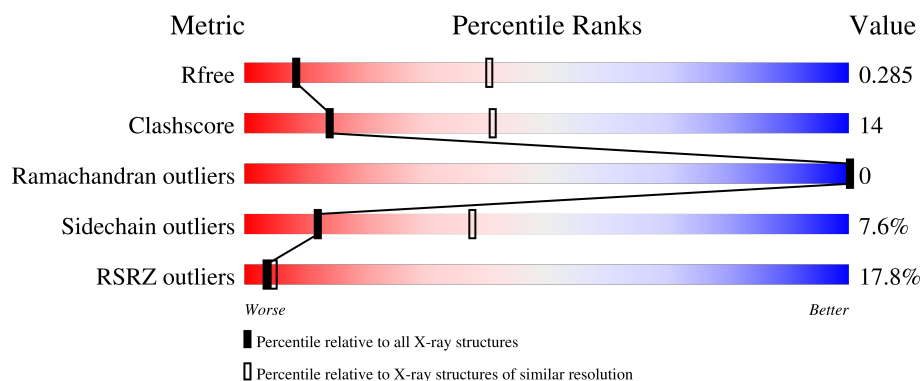
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	322	15% 66% 20% • 12%
1	B	322	17% 68% 20% • 10%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4290 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 CMP-sialic acid transporter 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2127	1410	323	378	16			
1	B	291	Total	C	N	O	S	0	0	0
			2163	1434	333	380	16			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	58	ARG	HIS	engineered mutation	UNP B4FZ94
A	59	THR	SER	engineered mutation	UNP B4FZ94
A	61	PRO	SER	engineered mutation	UNP B4FZ94
A	62	SER	PRO	engineered mutation	UNP B4FZ94
A	63	VAL	PRO	engineered mutation	UNP B4FZ94
B	58	ARG	HIS	engineered mutation	UNP B4FZ94
B	59	THR	SER	engineered mutation	UNP B4FZ94
B	61	PRO	SER	engineered mutation	UNP B4FZ94
B	62	SER	PRO	engineered mutation	UNP B4FZ94
B	63	VAL	PRO	engineered mutation	UNP B4FZ94

- Molecule 1: CMP-sialic acid transporter 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.58Å 69.46Å 102.03Å 82.83° 83.43° 68.22°	Depositor
Resolution (Å)	21.95 – 3.40 21.95 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.9 (21.95-3.40) 98.8 (21.95-3.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 3.37Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.268 , 0.286 0.273 , 0.285	Depositor DCC
R_{free} test set	816 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	145.8	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 101.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4290	wwPDB-VP
Average B, all atoms (Å ²)	174.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.12% 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	0.80	1/2170 (0.0%)	1.14	1/2966 (0.0%)
1	B	0.84	0/2210	1.17	7/3019 (0.2%)
All	All	0.82	1/4380 (0.0%)	1.16	8/5985 (0.1%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	168	LEU	C-O	-6.22	1.16	1.24

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	305	MET	CA-C-N	6.96	127.34	119.83
1	B	305	MET	C-N-CA	6.96	127.34	119.83
1	B	97	ASP	CA-C-N	6.75	128.28	119.84
1	B	97	ASP	C-N-CA	6.75	128.28	119.84
1	A	241	PHE	CA-CB-CG	6.68	120.48	113.80
1	B	19	ILE	CB-CA-C	-5.07	105.38	112.02
1	B	60	SER	CA-C-N	5.05	124.66	119.05
1	B	60	SER	C-N-CA	5.05	124.66	119.05

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	ARG	Sidechain

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	2127	0	2121	63	0
1	B	2163	0	2100	73	0
All	All	4290	0	4221	122	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 14.

All (122) 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:37:ILE:CG2	1:B:240:VAL:HG22	1.47	1.40
1:B:37:ILE:CG2	1:B:240:VAL:CG2	2.01	1.37
1:B:37:ILE:HG22	1:B:240:VAL:CG2	1.66	1.17
1:A:100:THR:HG23	1:A:155:LEU:HD13	1.24	1.16
1:A:295:ILE:HD11	1:B:137:VAL:HG11	1.18	1.13
1:A:295:ILE:HD11	1:B:137:VAL:CG1	1.85	1.05
1:B:253:LEU:O	1:B:257:SER:O	1.74	1.05
1:B:36:THR:C	1:B:38:PRO:HD2	1.80	1.05
1:B:37:ILE:HG21	1:B:240:VAL:CG2	1.85	1.00
1:A:295:ILE:CD1	1:B:137:VAL:HG11	1.93	0.98
1:B:36:THR:O	1:B:38:PRO:HD2	1.68	0.94
1:A:100:THR:CG2	1:A:155:LEU:HD13	1.96	0.94
1:A:291:LEU:O	1:A:295:ILE:HD13	1.66	0.93
1:A:134:LEU:HD11	1:B:134:LEU:HD11	1.53	0.90
1:B:37:ILE:HG21	1:B:240:VAL:HG23	1.53	0.88
1:A:253:LEU:O	1:A:257:SER:O	1.90	0.88
1:B:37:ILE:HG22	1:B:240:VAL:HG22	0.87	0.85
1:A:100:THR:HG23	1:A:155:LEU:CD1	2.08	0.83
1:B:36:THR:C	1:B:38:PRO:CD	2.52	0.83
1:A:76:VAL:HG22	1:A:201:PHE:CE1	2.16	0.81
1:B:37:ILE:CG2	1:B:240:VAL:HG23	2.08	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:HIS:CE1	1:A:89:GLN:OE1	2.35	0.79
1:B:253:LEU:O	1:B:257:SER:C	2.26	0.77
1:A:155:LEU:HD12	1:A:156:PHE:H	1.49	0.75
1:B:254:MET:HA	1:B:254:MET:HE2	1.68	0.75
1:B:260:ILE:HG21	1:B:303:TYR:CZ	2.23	0.73
1:A:260:ILE:HG21	1:A:303:TYR:CZ	2.24	0.73
1:B:221:LEU:H	1:B:221:LEU:HD23	1.54	0.72
1:B:20:LEU:HB3	1:B:239:VAL:HG12	1.72	0.72
1:A:85:HIS:HE1	1:A:89:GLN:OE1	1.73	0.71
1:B:37:ILE:HG21	1:B:240:VAL:HG22	1.55	0.71
1:B:301:GLN:HB3	1:B:305:MET:HE3	1.76	0.68
1:B:255:LYS:HD2	1:B:256:TYR:CE1	2.28	0.68
1:A:255:LYS:HD2	1:A:256:TYR:CE1	2.28	0.67
1:A:143:GLN:HG3	1:A:270:MET:HE1	1.77	0.67
1:B:37:ILE:HD12	1:B:38:PRO:HD3	1.77	0.66
1:B:37:ILE:N	1:B:38:PRO:CD	2.60	0.65
1:A:301:GLN:O	1:A:305:MET:HB2	1.98	0.64
1:B:301:GLN:O	1:B:305:MET:HB2	1.99	0.63
1:B:37:ILE:CG2	1:B:240:VAL:HG21	2.24	0.63
1:A:254:MET:HE2	1:A:254:MET:HA	1.82	0.61
1:B:181:GLU:OE2	1:B:185:LYS:HE3	2.00	0.61
1:B:36:THR:O	1:B:38:PRO:CD	2.44	0.60
1:B:35:ALA:O	1:B:38:PRO:CD	2.49	0.60
1:B:264:TYR:CD2	1:B:300:LEU:HD12	2.36	0.60
1:B:134:LEU:HB3	1:B:299:SER:HB2	1.83	0.59
1:A:181:GLU:OE2	1:A:185:LYS:HE3	2.02	0.59
1:B:255:LYS:CD	1:B:256:TYR:CE1	2.87	0.58
1:A:143:GLN:CG	1:A:270:MET:HE1	2.33	0.58
1:A:229:PHE:CB	1:A:232:TYR:CD1	2.87	0.58
1:A:255:LYS:CD	1:A:256:TYR:CE1	2.86	0.57
1:A:295:ILE:HD12	1:A:295:ILE:N	2.21	0.55
1:A:253:LEU:O	1:A:257:SER:C	2.50	0.54
1:B:255:LYS:HB3	1:B:256:TYR:CD1	2.43	0.54
1:A:155:LEU:CD1	1:A:156:PHE:H	2.20	0.54
1:B:250:VAL:O	1:B:254:MET:HG2	2.08	0.54
1:A:295:ILE:CD1	1:A:295:ILE:N	2.69	0.54
1:A:268:MET:HE1	1:A:296:CYS:HB3	1.90	0.53
1:B:271:LEU:HD22	1:B:293:ILE:HG13	1.91	0.53
1:B:37:ILE:O	1:B:38:PRO:C	2.51	0.52
1:A:255:LYS:HB3	1:A:256:TYR:CD1	2.44	0.52
1:A:143:GLN:CG	1:A:270:MET:CE	2.88	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:ILE:HG23	1:B:240:VAL:CG2	2.27	0.52
1:B:116:PHE:CE1	1:B:258:ASP:HB2	2.45	0.52
1:A:116:PHE:CE1	1:A:258:ASP:HB2	2.45	0.51
1:A:250:VAL:O	1:A:254:MET:HG2	2.10	0.51
1:B:264:TYR:CD2	1:B:300:LEU:CD1	2.94	0.51
1:A:291:LEU:HD11	1:B:140:THR:HG22	1.92	0.51
1:B:160:LEU:O	1:B:161:GLU:C	2.53	0.51
1:B:77:VAL:HB	1:B:78:PRO:HD3	1.94	0.50
1:A:229:PHE:CB	1:A:232:TYR:CE1	2.95	0.49
1:A:302:MET:HG3	1:B:130:MET:HE2	1.94	0.49
1:A:45:LYS:HD2	1:A:244:GLY:HA2	1.96	0.48
1:A:271:LEU:HD22	1:A:293:ILE:HG13	1.95	0.48
1:A:127:ILE:HD11	1:B:127:ILE:HD11	1.97	0.47
1:A:295:ILE:CD1	1:A:295:ILE:H	2.28	0.47
1:B:260:ILE:HG21	1:B:303:TYR:CE2	2.48	0.47
1:A:305:MET:HB3	1:A:310:LEU:HG	1.97	0.46
1:B:155:LEU:O	1:B:156:PHE:HB2	2.14	0.46
1:A:134:LEU:HB3	1:A:299:SER:HB2	1.98	0.46
1:A:147:CYS:HA	1:B:146:GLY:O	2.16	0.46
1:A:95:TYR:CE2	1:A:161:GLU:HB2	2.51	0.45
1:A:16:SER:HB2	1:A:242:ASN:HD21	1.82	0.45
1:B:35:ALA:O	1:B:38:PRO:HD3	2.15	0.45
1:B:117:ARG:O	1:B:121:LYS:HA	2.15	0.45
1:B:274:MET:HB3	1:B:289:LEU:HD13	1.98	0.45
1:A:302:MET:HG3	1:B:130:MET:CE	2.46	0.45
1:B:268:MET:CE	1:B:300:LEU:HD13	2.46	0.45
1:B:301:GLN:HB3	1:B:305:MET:CE	2.45	0.45
1:A:295:ILE:HD11	1:B:137:VAL:HG13	1.86	0.44
1:A:288:GLN:HG3	1:B:144:VAL:HG11	1.98	0.44
1:A:105:GLY:O	1:A:108:LYS:HG2	2.17	0.44
1:B:84:ILE:O	1:B:88:VAL:HG23	2.17	0.44
1:A:155:LEU:HD12	1:A:156:PHE:N	2.27	0.44
1:B:305:MET:HG2	1:B:306:PRO:HD2	2.00	0.43
1:B:312:GLU:C	1:B:313:LEU:HD23	2.43	0.43
1:A:255:LYS:HD2	1:A:256:TYR:HE1	1.82	0.43
1:B:221:LEU:H	1:B:221:LEU:CD2	2.27	0.43
1:B:179:TYR:HE1	1:B:183:LEU:HD21	1.83	0.43
1:B:134:LEU:HD23	1:B:134:LEU:HA	1.89	0.43
1:A:177:GLY:C	1:A:259:ASN:HD21	2.27	0.42
1:A:130:MET:HE2	1:B:302:MET:HG3	2.01	0.42
1:A:20:LEU:HB3	1:A:239:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:GLN:HG3	1:A:270:MET:CE	2.45	0.42
1:B:274:MET:HB3	1:B:289:LEU:CD1	2.50	0.42
1:B:96:VAL:HB	1:B:100:THR:HB	2.02	0.42
1:B:278:ILE:O	1:B:282:SER:HA	2.20	0.42
1:B:105:GLY:O	1:B:108:LYS:HG2	2.20	0.41
1:A:130:MET:HE3	1:B:301:GLN:HB2	2.02	0.41
1:A:229:PHE:HA	1:A:232:TYR:CD1	2.55	0.41
1:A:134:LEU:CD1	1:B:134:LEU:HD11	2.37	0.41
1:A:134:LEU:HA	1:A:134:LEU:HD23	1.85	0.41
1:A:16:SER:CB	1:A:242:ASN:HD21	2.34	0.41
1:A:107:LEU:HA	1:A:107:LEU:HD12	1.82	0.41
1:A:77:VAL:HB	1:A:78:PRO:HD3	2.02	0.41
1:A:116:PHE:HE1	1:A:258:ASP:HB2	1.85	0.41
1:B:254:MET:HA	1:B:254:MET:CE	2.47	0.41
1:B:305:MET:HA	1:B:306:PRO:HD3	1.87	0.41
1:A:141:THR:O	1:A:288:GLN:HB3	2.22	0.40
1:B:103:ILE:HD11	1:B:144:VAL:HG23	2.02	0.40
1:B:141:THR:O	1:B:288:GLN:HB3	2.21	0.40
1:A:122:ARG:HE	1:A:122:ARG:HB3	1.75	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	275/322 (85%)	269 (98%)	6 (2%)	0	100	100
1	B	281/322 (87%)	274 (98%)	7 (2%)	0	100	100
All	All	556/644 (86%)	543 (98%)	13 (2%)	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	225/288 (78%)	208 (92%)	17 (8%)	12	38
1	B	220/288 (76%)	203 (92%)	17 (8%)	12	37
All	All	445/576 (77%)	411 (92%)	34 (8%)	12	38

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	SER
1	A	68	GLU
1	A	90	PHE
1	A	98	PRO
1	A	103	ILE
1	A	107	LEU
1	A	132	ILE
1	A	144	VAL
1	A	178	VAL
1	A	200	THR
1	A	203	VAL
1	A	239	VAL
1	A	259	ASN
1	A	270	MET
1	A	273	THR
1	A	295	ILE
1	A	305	MET
1	B	37	ILE
1	B	40	LEU
1	B	62	SER
1	B	86	ASN
1	B	103	ILE
1	B	137	VAL
1	B	144	VAL
1	B	178	VAL
1	B	200	THR
1	B	203	VAL

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Mol	Chain	Res	Type
1	B	239	VAL
1	B	254	MET
1	B	257	SER
1	B	268	MET
1	B	273	THR
1	B	307	VAL
1	B	312	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	HIS
1	A	89	GLN
1	A	106	ASN
1	A	242	ASN
1	A	259	ASN
1	B	89	GLN
1	B	106	ASN
1	B	242	ASN
1	B	259	ASN

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	283/322 (87%)	0.70	47 (16%)  	76, 170, 242, 277	0
1	B	291/322 (90%)	0.90	55 (18%)  	94, 178, 263, 330	0
All	All	574/644 (89%)	0.80	102 (17%)  	76, 174, 251, 330	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	143	GLN	13.6
1	B	188	ASN	9.2
1	B	228	LEU	6.2
1	B	73	ARG	6.2
1	B	102	GLN	6.1
1	B	251	SER	5.6
1	A	186	LYS	5.1
1	B	100	THR	5.1
1	B	103	ILE	5.0
1	B	54	TRP	5.0
1	B	40	LEU	4.9
1	A	306	PRO	4.5
1	B	57	CYS	4.5
1	A	119	VAL	4.4
1	B	78	PRO	4.4
1	A	191	LEU	4.3
1	B	82	TYR	4.3
1	B	144	VAL	4.2
1	A	307	VAL	4.0
1	B	233	SER	4.0
1	B	206	ASN	3.9
1	A	164	LEU	3.9
1	B	285	ALA	3.9
1	A	75	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	273	THR	3.8
1	A	1	MET	3.8
1	A	40	LEU	3.8
1	A	168	LEU	3.8
1	B	119	VAL	3.7
1	A	162	GLY	3.7
1	A	163	TYR	3.6
1	A	184	MET	3.5
1	B	197	GLN	3.5
1	B	69	TRP	3.4
1	B	199	TYR	3.4
1	B	211	ILE	3.4
1	B	175	LEU	3.3
1	B	203	VAL	3.3
1	A	46	LEU	3.2
1	B	250	VAL	3.2
1	B	176	ALA	3.2
1	A	276	LEU	3.1
1	A	61	PRO	3.1
1	B	152	CYS	3.1
1	B	142	SER	3.0
1	B	140	THR	3.0
1	B	81	ILE	3.0
1	A	169	SER	2.9
1	A	267	SER	2.9
1	A	185	LYS	2.9
1	B	171	CYS	2.8
1	B	274	MET	2.8
1	B	301	GLN	2.8
1	A	90	PHE	2.8
1	A	280	LEU	2.8
1	A	231	GLY	2.8
1	B	121	LYS	2.8
1	B	191	LEU	2.7
1	B	201	PHE	2.7
1	A	88	VAL	2.7
1	A	57	CYS	2.7
1	B	270	MET	2.7
1	B	190	SER	2.7
1	A	80	VAL	2.7
1	B	187	ASN	2.7
1	B	170	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	103	ILE	2.6
1	A	282	SER	2.6
1	A	42	GLU	2.6
1	A	195	ASN	2.5
1	A	118	LEU	2.5
1	A	203	VAL	2.5
1	A	37	ILE	2.5
1	B	75	TYR	2.5
1	A	130	MET	2.5
1	B	310	LEU	2.5
1	A	206	ASN	2.5
1	B	214	ASP	2.4
1	B	307	VAL	2.4
1	A	160	LEU	2.4
1	B	221	LEU	2.4
1	B	305	MET	2.3
1	A	187	ASN	2.3
1	B	163	TYR	2.3
1	B	141	THR	2.3
1	A	284	LYS	2.3
1	A	271	LEU	2.2
1	B	210	LEU	2.2
1	B	99	SER	2.2
1	A	93	LEU	2.2
1	A	35	ALA	2.2
1	A	254	MET	2.2
1	B	172	LEU	2.2
1	B	189	ASP	2.2
1	A	192	TYR	2.2
1	A	17	GLN	2.2
1	A	71	SER	2.2
1	A	293	ILE	2.2
1	B	42	GLU	2.1
1	A	170	ALA	2.1
1	A	304	PHE	2.0
1	B	174	ALA	2.0

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 [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.