Full wwPDB X-ray Structure Validation Report (i)

Sep 7, 2026 – 09:21 PM JST

PDB ID	:	21AZ / pdb_000021az
Title	:	Ectodomain of Arabidopsis cell-surface hydrogen peroxide sensor HPCA1/CARD1
Authors	:	Wang, J.; Yang, Q.; Zhao, D.; Li, J.
Deposited on	:	2025-12-05
Resolution	:	2.00 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 (i) 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 (i)) were used in the production of this report:

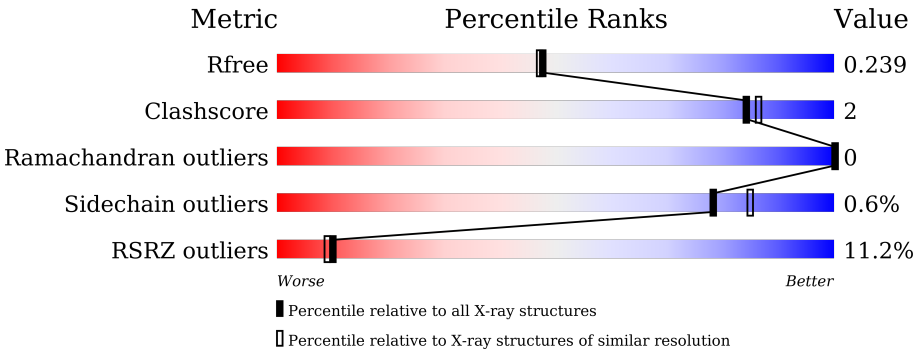
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 <=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	552	4% 88% 6% 6%
1	B	552	17% 86% 6% 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8566 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.

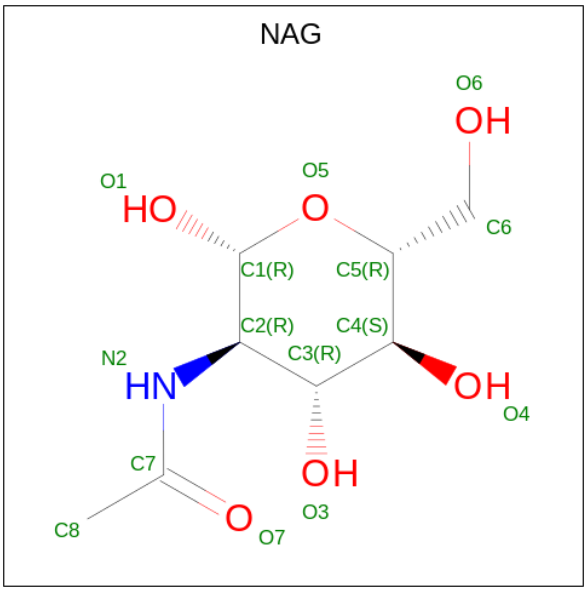
- Molecule 1 is a protein called Leucine-rich repeat receptor protein kinase HPCA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	0	0
			4025	2586	653	771	15			
1	B	510	Total	C	N	O	S	0	0	0
			3967	2551	643	758	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	547	HIS	-	expression tag	UNP Q8GZ99
A	548	HIS	-	expression tag	UNP Q8GZ99
A	549	HIS	-	expression tag	UNP Q8GZ99
A	550	HIS	-	expression tag	UNP Q8GZ99
A	551	HIS	-	expression tag	UNP Q8GZ99
A	552	HIS	-	expression tag	UNP Q8GZ99
B	547	HIS	-	expression tag	UNP Q8GZ99
B	548	HIS	-	expression tag	UNP Q8GZ99
B	549	HIS	-	expression tag	UNP Q8GZ99
B	550	HIS	-	expression tag	UNP Q8GZ99
B	551	HIS	-	expression tag	UNP Q8GZ99
B	552	HIS	-	expression tag	UNP Q8GZ99

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0

- Molecule 3 is water.

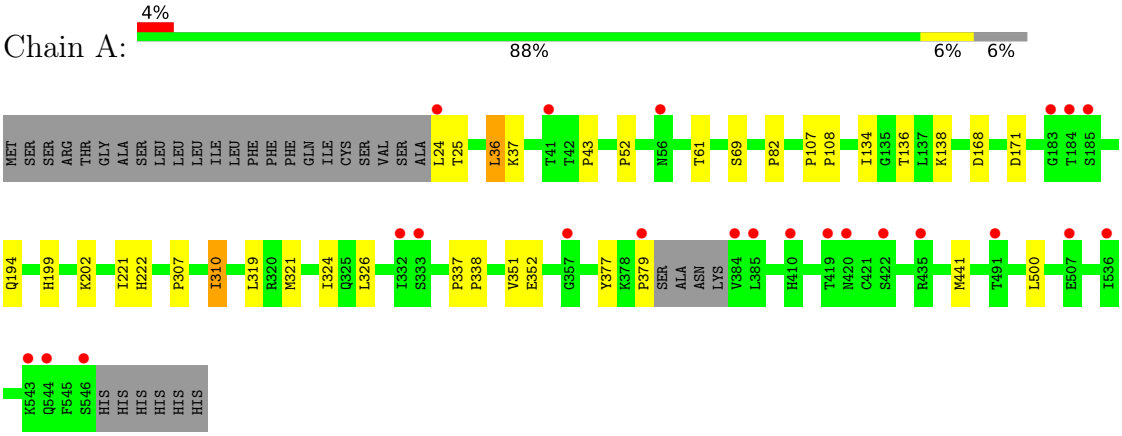
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	308	Total O 308 308	0	0
3	B	168	Total O 168 168	0	0

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.

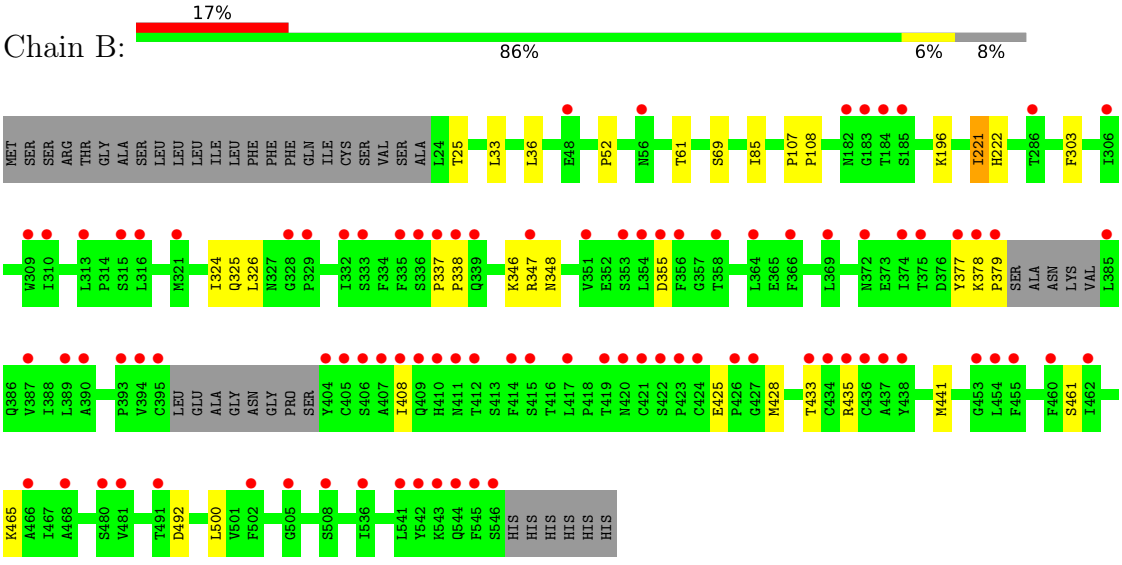
• Molecule 1: Leucine-rich repeat receptor protein kinase HPCA1

Chain A:



• Molecule 1: Leucine-rich repeat receptor protein kinase HPCA1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	118.85Å 41.89Å 129.79Å 90.00° 110.83° 90.00°	Depositor
Resolution (Å)	32.36 – 2.00 32.36 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (32.36-2.00) 99.8 (32.36-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.214 , 0.239 0.214 , 0.239	Depositor DCC
R_{free} test set	2000 reflections (2.44%)	wwPDB-VP
Wilson B-factor (Å^2)	27.7	Xtriage
Anisotropy	0.696	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 35.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8566	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.13	0/4124	0.34	0/5622
1	B	0.12	0/4064	0.33	0/5538
All	All	0.12	0/8188	0.33	0/11160

There are no bond length outliers.

There are no bond angle outliers.

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	4025	0	3990	17	0
1	B	3967	0	3935	20	0
2	A	56	0	52	0	0
2	B	42	0	39	0	0
3	A	308	0	0	0	0
3	B	168	0	0	1	0
All	All	8566	0	8016	37	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 2.

All (37) 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:326:LEU:H	1:B:348:ASN:HD22	1.28	0.80
1:A:25:THR:HG21	1:A:52:PRO:HD2	1.73	0.70
1:B:196:LYS:HG3	1:B:221:ILE:HD13	1.77	0.66
1:B:346:LYS:HG2	1:B:347:ARG:HG3	1.81	0.62
1:B:221:ILE:HG22	1:B:222:HIS:CD2	2.42	0.55
1:A:37:LYS:HG3	1:A:43:PRO:HB3	1.90	0.54
1:B:441:MET:HG2	1:B:500:LEU:HG	1.90	0.54
1:A:61:THR:HB	1:A:69:SER:HB3	1.88	0.54
1:B:355:ASP:HB2	1:B:378:LYS:HD3	1.90	0.52
1:A:351:VAL:HG23	1:A:352:GLU:HG3	1.92	0.51
1:A:221:ILE:HG22	1:A:222:HIS:CD2	2.46	0.50
1:B:326:LEU:H	1:B:348:ASN:ND2	2.05	0.49
1:A:168:ASP:HA	1:A:199:HIS:HB2	1.93	0.49
1:A:136:THR:HA	1:A:138:LYS:HE2	1.95	0.48
1:B:492:ASP:HB2	3:B:773:HOH:O	2.14	0.47
1:B:461:SER:O	1:B:465:LYS:HG3	2.16	0.46
1:B:61:THR:HB	1:B:69:SER:HB3	1.97	0.46
1:A:36:LEU:HD23	1:A:82:PRO:HD2	1.99	0.45
1:B:324:ILE:HG13	1:B:326:LEU:HG	1.99	0.44
1:A:307:PRO:HB2	1:A:310:ILE:HD13	1.99	0.44
1:B:433:THR:OG1	1:B:435:ARG:HD2	2.17	0.44
1:A:324:ILE:HG13	1:A:326:LEU:HG	2.00	0.44
1:A:441:MET:HG2	1:A:500:LEU:HG	2.00	0.44
1:B:33:LEU:HD12	1:B:52:PRO:HG2	1.99	0.44
1:B:377:TYR:O	1:B:379:PRO:HD3	2.17	0.43
1:A:319:LEU:HD21	1:A:321:MET:HE2	2.00	0.43
1:B:337:PRO:HA	1:B:338:PRO:HD3	1.85	0.42
1:B:25:THR:HG21	1:B:52:PRO:HD2	2.02	0.42
1:A:107:PRO:HA	1:A:108:PRO:HD3	1.93	0.41
1:B:36:LEU:HD11	1:B:85:ILE:HD13	2.03	0.41
1:A:377:TYR:O	1:A:379:PRO:HD3	2.21	0.41
1:A:194:GLN:H	1:A:194:GLN:CD	2.28	0.40
1:A:171:ASP:OD1	1:A:202:LYS:HD2	2.21	0.40
1:B:303:PHE:HA	1:B:325:GLN:O	2.21	0.40
1:B:425:GLU:HB2	1:B:428:MET:HE3	2.03	0.40
1:A:337:PRO:HA	1:A:338:PRO:HD3	1.86	0.40
1:B:107:PRO:HA	1:B:108:PRO:HD3	1.95	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	515/552 (93%)	490 (95%)	25 (5%)	0	100	100
1	B	504/552 (91%)	476 (94%)	28 (6%)	0	100	100
All	All	1019/1104 (92%)	966 (95%)	53 (5%)	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	466/495 (94%)	462 (99%)	4 (1%)	70	78
1	B	460/495 (93%)	458 (100%)	2 (0%)	84	89
All	All	926/990 (94%)	920 (99%)	6 (1%)	78	85

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	36	LEU
1	A	134	ILE
1	A	310	ILE
1	B	221	ILE
1	B	408	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	HIS
1	A	325	GLN
1	A	370	GLN
1	A	386	GLN
1	A	391	ASN
1	A	409	GLN
1	A	493	HIS
1	B	34	ASN
1	B	208	ASN
1	B	222	HIS
1	B	269	ASN
1	B	325	GLN
1	B	348	ASN
1	B	370	GLN
1	B	391	ASN
1	B	493	HIS

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)

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	A	603	1	14,14,15	0.79	0	17,19,21	0.97	0
2	NAG	B	602	1	14,14,15	0.78	0	17,19,21	1.04	0
2	NAG	A	604	1	14,14,15	0.80	0	17,19,21	1.12	1 (5%)
2	NAG	B	603	1	14,14,15	0.81	0	17,19,21	1.25	2 (11%)
2	NAG	B	601	1	14,14,15	0.79	0	17,19,21	1.03	1 (5%)
2	NAG	A	602	1	14,14,15	0.68	0	17,19,21	1.07	1 (5%)
2	NAG	A	601	1	14,14,15	0.77	0	17,19,21	1.10	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	603	1	-	0/6/23/26	0/1/1/1
2	NAG	B	602	1	-	0/6/23/26	0/1/1/1
2	NAG	A	604	1	-	0/6/23/26	0/1/1/1
2	NAG	B	603	1	-	0/6/23/26	0/1/1/1
2	NAG	B	601	1	-	0/6/23/26	0/1/1/1
2	NAG	A	602	1	-	0/6/23/26	0/1/1/1
2	NAG	A	601	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	604	NAG	C1-O5-C5	3.16	116.47	112.19
2	A	602	NAG	C1-O5-C5	3.12	116.42	112.19
2	A	601	NAG	C1-O5-C5	2.97	116.22	112.19
2	B	603	NAG	C1-O5-C5	2.68	115.83	112.19
2	B	603	NAG	O5-C1-C2	-2.36	107.56	111.29
2	B	601	NAG	C1-O5-C5	2.34	115.36	112.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	519/552 (94%)	0.27	23 (4%) 39 38	17, 27, 44, 68	0
1	B	510/552 (92%)	0.97	92 (18%) 3 3	20, 35, 61, 78	0
All	All	1029/1104 (93%)	0.61	115 (11%) 10 9	17, 30, 54, 78	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	184	THR	5.9
1	B	395	CYS	5.7
1	B	332	ILE	5.4
1	A	184	THR	4.6
1	B	377	TYR	4.6
1	A	24	LEU	4.5
1	B	394	VAL	4.3
1	B	379	PRO	4.3
1	B	544	GLN	4.2
1	A	420	ASN	4.2
1	B	408	ILE	4.1
1	B	404	TYR	4.1
1	A	544	GLN	4.0
1	A	332	ILE	4.0
1	B	385	LEU	3.9
1	B	183	GLY	3.8
1	A	379	PRO	3.7
1	A	384	VAL	3.7
1	A	543	LYS	3.6
1	B	436	CYS	3.6
1	B	410	HIS	3.6
1	B	411	ASN	3.5
1	B	405	CYS	3.4
1	B	541	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	393	PRO	3.3
1	B	389	LEU	3.2
1	B	354	LEU	3.2
1	B	536	ILE	3.2
1	B	419	THR	3.1
1	B	543	LYS	3.1
1	B	329	PRO	3.0
1	B	423	PRO	3.0
1	B	390	ALA	3.0
1	B	434	CYS	3.0
1	A	422	SER	3.0
1	B	56	ASN	3.0
1	B	309	TRP	3.0
1	B	358	THR	3.0
1	B	433	THR	2.9
1	B	491	THR	2.9
1	A	333	SER	2.9
1	B	375	THR	2.9
1	B	185	SER	2.8
1	A	419	THR	2.8
1	B	337	PRO	2.8
1	B	409	GLN	2.7
1	A	410	HIS	2.7
1	B	366	PHE	2.7
1	B	426	PRO	2.7
1	B	372	ASN	2.7
1	B	422	SER	2.7
1	B	424	CYS	2.7
1	B	502	PHE	2.6
1	B	313	LEU	2.6
1	A	185	SER	2.6
1	B	351	VAL	2.6
1	B	374	ILE	2.6
1	B	427	GLY	2.6
1	B	437	ALA	2.6
1	A	385	LEU	2.6
1	B	505	GLY	2.6
1	B	335	PHE	2.5
1	B	328	GLY	2.5
1	A	56	ASN	2.5
1	B	468	ALA	2.5
1	B	310	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	481	VAL	2.5
1	B	435	ARG	2.5
1	B	545	PHE	2.4
1	B	306	ILE	2.4
1	B	347	ARG	2.4
1	B	48	GLU	2.4
1	B	356	PHE	2.4
1	B	460	PHE	2.4
1	B	421	CYS	2.4
1	B	369	LEU	2.3
1	A	357	GLY	2.3
1	B	378	LYS	2.3
1	B	438	TYR	2.3
1	B	420	ASN	2.3
1	A	435	ARG	2.3
1	B	546	SER	2.3
1	B	387	VAL	2.3
1	B	414	PHE	2.3
1	B	455	PHE	2.3
1	B	339	GLN	2.3
1	A	41	THR	2.2
1	A	507	GLU	2.2
1	B	406	SER	2.2
1	B	508	SER	2.2
1	B	454	LEU	2.2
1	A	546	SER	2.2
1	A	536	ILE	2.2
1	B	364	LEU	2.2
1	B	338	PRO	2.1
1	B	462	ILE	2.1
1	B	353	SER	2.1
1	A	491	THR	2.1
1	B	407	ALA	2.1
1	B	466	ALA	2.1
1	B	315	SER	2.1
1	B	316	LEU	2.1
1	B	417	LEU	2.1
1	B	321	MET	2.1
1	B	412	THR	2.1
1	B	480	SER	2.1
1	B	542	TYR	2.1
1	B	333	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	415	SER	2.1
1	B	355	ASP	2.0
1	B	286	THR	2.0
1	A	183	GLY	2.0
1	B	453	GLY	2.0
1	B	336	SER	2.0
1	B	182	ASN	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	A	602	14/15	0.74	0.14	34,44,49,54	0
2	NAG	B	603	14/15	0.80	0.12	37,42,53,54	0
2	NAG	A	604	14/15	0.85	0.11	30,37,44,46	0
2	NAG	B	601	14/15	0.86	0.12	30,33,43,48	0
2	NAG	B	602	14/15	0.86	0.11	32,38,43,46	0
2	NAG	A	603	14/15	0.86	0.10	26,34,44,47	0
2	NAG	A	601	14/15	0.93	0.07	18,23,32,37	0

6.5 Other polymers (i)

There are no such residues in this entry.