



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:20 PM UTC

PDB ID : 2YKH / pdb_00002ykh
Title : Sensor region of a sensor histidine kinase
Authors : Preu, J.; Panjikar, S.; Morth, P.; Jaiswal, R.; Karunakar, P.; Tucker, P.A.
Deposited on : 2011-05-27
Resolution : 2.78 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

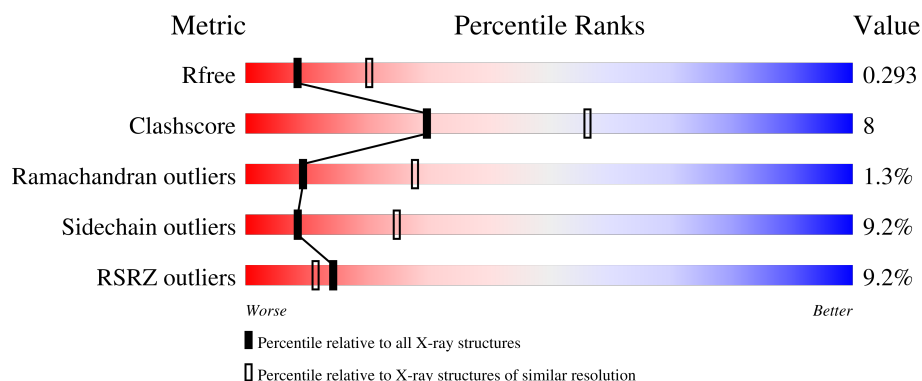
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

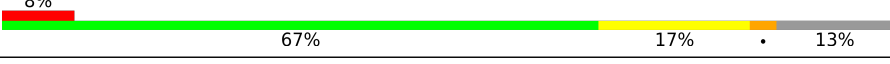
The reported resolution of this entry is 2.78 Å.

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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	305	 8% 67% 16% •• 13%
1	B	305	 8% 67% 17% • 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4033 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 PROBABLE SENSOR HISTIDINE KINASE PDTAS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			1985	1238	359	378	10			
1	B	265	Total	C	N	O	S	0	1	0
			1991	1241	360	380	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP O05846
A	0	ALA	-	expression tag	UNP O05846
B	-1	GLY	-	expression tag	UNP O05846
B	0	ALA	-	expression tag	UNP O05846

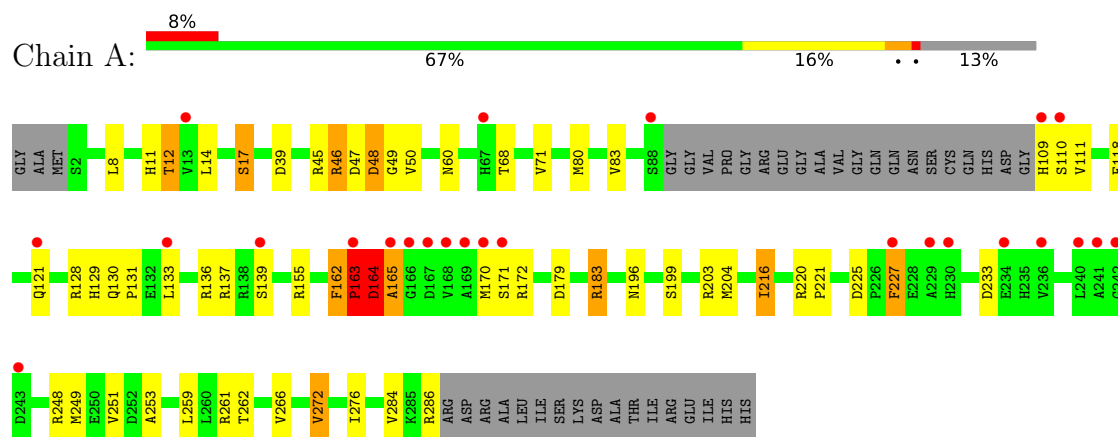
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	29	Total	O	0	0
			29	29		
2	B	28	Total	O	0	0
			28	28		

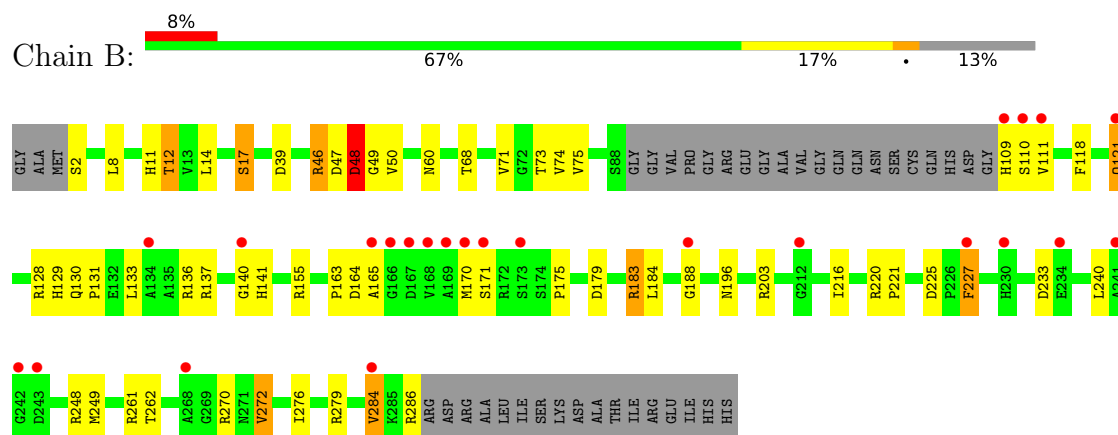
3 Residue-property plots

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: PROBABLE SENSOR HISTIDINE KINASE PDTAS



• Molecule 1: PROBABLE SENSOR HISTIDINE KINASE PDTAS



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.92Å 79.53Å 102.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.88 – 2.78 19.88 – 2.78	Depositor EDS
% Data completeness (in resolution range)	97.6 (19.88-2.78) 97.2 (19.88-2.78)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.248 , 0.299 0.242 , 0.293	Depositor DCC
R_{free} test set	957 reflections (6.18%)	wwPDB-VP
Wilson B-factor (Å ²)	42.9	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 26.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	4033	wwPDB-VP
Average B, all atoms (Å ²)	43.0	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 23.73 % 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 4.3974e-03.*

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	0.74	0/2019	1.02	7/2752 (0.3%)
1	B	0.72	0/2028	0.95	4/2764 (0.1%)
All	All	0.73	0/4047	0.98	11/5516 (0.2%)

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	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	162	PHE	CA-C-N	9.92	132.24	119.84
1	A	162	PHE	C-N-CA	9.92	132.24	119.84
1	A	163	PRO	CA-C-N	7.21	135.31	121.54
1	A	163	PRO	C-N-CA	7.21	135.31	121.54
1	A	171	SER	N-CA-C	6.40	118.13	108.46
1	B	171	SER	N-CA-C	6.30	117.98	108.46
1	B	270	ARG	N-CA-C	5.87	119.04	109.59
1	B	121	GLN	N-CA-C	5.75	118.58	109.50
1	B	140	GLY	N-CA-C	-5.45	103.00	111.12
1	A	164	ASP	N-CA-CB	5.40	119.62	110.49
1	A	121	GLN	N-CA-C	5.38	118.00	109.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	PHE	Peptide
1	A	163	PRO	Peptide
1	B	163	PRO	Peptide

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	1985	0	1972	34	0
1	B	1991	0	1981	36	0
2	A	29	0	0	5	0
2	B	28	0	0	5	0
All	All	4033	0	3953	67	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 8.

All (67) 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:60:ASN:HB3	2:B:2010:HOH:O	1.32	1.21
1:A:12:THR:HG23	1:A:14:LEU:H	1.40	0.87
1:B:12:THR:HG23	1:B:14:LEU:H	1.39	0.86
1:B:121:GLN:HB3	2:B:2015:HOH:O	1.76	0.84
1:A:8:LEU:O	1:A:12:THR:HG22	1.83	0.78
1:A:17:SER:HB3	1:A:118:PHE:CE2	2.23	0.74
1:A:17:SER:HB3	1:A:118:PHE:HE2	1.51	0.73
1:B:284:VAL:HG23	2:B:2027:HOH:O	1.89	0.72
1:A:225:ASP:OD2	1:A:227:PHE:HB2	1.95	0.67
1:B:8:LEU:O	1:B:12:THR:HG22	1.95	0.66
1:A:60:ASN:OD1	2:A:2004:HOH:O	2.13	0.66
1:B:46:ARG:CD	1:B:48:ASP:HB2	2.25	0.65
1:B:225:ASP:OD2	1:B:227:PHE:HB2	1.97	0.65
1:B:17:SER:HB3	1:B:118:PHE:HE2	1.61	0.64
1:B:46:ARG:HD2	1:B:48:ASP:HB2	1.80	0.64
1:A:39:ASP:HB2	1:A:129:HIS:HB2	1.80	0.63
1:A:46:ARG:HD2	1:A:50:VAL:HB	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ARG:HG3	2:A:2016:HOH:O	2.00	0.61
1:B:17:SER:HB3	1:B:118:PHE:CE2	2.35	0.60
1:A:179:ASP:O	1:A:196:ASN:HB3	2.05	0.57
1:A:131:PRO:HB2	1:A:136:ARG:HG2	1.87	0.55
1:B:183:ARG:NH2	1:B:272:VAL:O	2.40	0.55
1:A:183:ARG:NH2	1:A:272:VAL:O	2.39	0.55
1:A:71:VAL:HB	1:B:203:ARG:NH2	2.22	0.54
1:B:220:ARG:NH1	1:B:233:ASP:OD2	2.41	0.54
1:B:220:ARG:HD2	2:B:2023:HOH:O	2.08	0.53
1:B:39:ASP:HB2	1:B:129:HIS:HB2	1.90	0.52
1:B:141:HIS:HB2	2:B:2019:HOH:O	2.10	0.52
1:B:109:HIS:HB2	1:B:130:GLN:O	2.10	0.51
1:A:109:HIS:HB2	1:A:130:GLN:O	2.11	0.51
1:A:170:MET:HB2	1:A:248:ARG:HH21	1.75	0.50
1:B:46:ARG:HD3	1:B:48:ASP:HB2	1.92	0.50
1:B:262:THR:HG22	1:B:276:ILE:HG13	1.93	0.50
1:A:266:VAL:CG2	2:A:2025:HOH:O	2.60	0.50
1:B:11:HIS:O	1:B:46:ARG:HB3	2.12	0.49
1:A:80:MET:HE2	1:A:83:VAL:HG21	1.96	0.48
1:B:131:PRO:HB2	1:B:136:ARG:HG2	1.96	0.48
1:A:47:ASP:C	1:A:49:GLY:N	2.72	0.47
1:A:47:ASP:C	1:A:49:GLY:H	2.21	0.47
1:A:262:THR:HG22	1:A:276:ILE:HG13	1.95	0.47
1:B:46:ARG:HD2	1:B:50:VAL:HB	1.97	0.47
1:A:203:ARG:NH2	1:B:71:VAL:HB	2.28	0.47
1:A:220:ARG:NH1	1:A:233:ASP:OD2	2.47	0.47
1:A:216:ILE:HD13	1:A:216:ILE:HA	1.71	0.46
1:A:45:ARG:HB3	2:A:2008:HOH:O	2.16	0.45
1:B:220:ARG:HB3	1:B:221:PRO:HD3	1.97	0.45
1:B:184:LEU:HD23	1:B:184:LEU:HA	1.79	0.44
1:B:111:VAL:HA	1:B:128:ARG:O	2.18	0.44
1:B:48:ASP:HB3	1:B:50:VAL:HG23	2.00	0.44
1:A:11:HIS:O	1:A:46:ARG:HB3	2.18	0.43
1:B:170:MET:HB2	1:B:248:ARG:HH21	1.83	0.42
1:B:50:VAL:HG11	1:B:74:VAL:HG13	2.01	0.42
1:A:45:ARG:NE	2:A:2008:HOH:O	2.50	0.42
1:B:47:ASP:C	1:B:49:GLY:N	2.77	0.42
1:B:47:ASP:C	1:B:49:GLY:H	2.28	0.42
1:A:111:VAL:HA	1:A:128:ARG:O	2.20	0.42
1:A:164:ASP:O	1:A:165:ALA:C	2.63	0.41
1:B:188:GLY:HA3	1:B:240:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ARG:HD3	1:A:48:ASP:HB2	2.02	0.41
1:A:203:ARG:NH1	1:B:2:SER:OG	2.53	0.41
1:A:220:ARG:HB3	1:A:221:PRO:HD3	2.02	0.41
1:A:204:MET:HG2	1:A:253:ALA:HB3	2.02	0.41
1:B:175:PRO:HB3	1:B:279:ARG:HB2	2.02	0.41
1:B:73:THR:HG22	1:B:75:VAL:HG23	2.03	0.41
1:A:46:ARG:CD	1:A:48:ASP:HB2	2.51	0.40
1:B:179:ASP:O	1:B:196:ASN:HB3	2.20	0.40
1:A:216:ILE:CD1	1:A:233:ASP:HA	2.52	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	261/305 (86%)	240 (92%)	17 (6%)	4 (2%)	8	25
1	B	262/305 (86%)	241 (92%)	18 (7%)	3 (1%)	11	32
All	All	523/610 (86%)	481 (92%)	35 (7%)	7 (1%)	9	28

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	PRO
1	A	164	ASP
1	A	48	ASP
1	B	48	ASP
1	A	165	ALA
1	B	165	ALA
1	B	164	ASP

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	211/241 (88%)	189 (90%)	22 (10%)	7	20
1	B	213/241 (88%)	196 (92%)	17 (8%)	11	31
All	All	424/482 (88%)	385 (91%)	39 (9%)	8	25

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	THR
1	A	17	SER
1	A	46	ARG
1	A	68	THR
1	A	110	SER
1	A	133	LEU
1	A	137	ARG
1	A	139	SER
1	A	155	ARG
1	A	164	ASP
1	A	172	ARG
1	A	183	ARG
1	A	199	SER
1	A	216	ILE
1	A	227	PHE
1	A	249	MET
1	A	251	VAL
1	A	259	LEU
1	A	261	ARG
1	A	272	VAL
1	A	284	VAL
1	A	286	ARG
1	B	12	THR
1	B	17	SER
1	B	46	ARG
1	B	48	ASP
1	B	68	THR

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Mol	Chain	Res	Type
1	B	110	SER
1	B	133	LEU
1	B	137	ARG
1	B	155	ARG
1	B	183	ARG
1	B	216	ILE
1	B	227	PHE
1	B	249	MET
1	B	261	ARG
1	B	272	VAL
1	B	284	VAL
1	B	286	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	109	HIS
1	B	21	HIS
1	B	60	ASN
1	B	67	HIS
1	B	109	HIS

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 [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	265/305 (86%)	0.54	25 (9%)	14 11	24, 42, 65, 79	0
1	B	265/305 (86%)	0.49	24 (9%)	15 12	24, 42, 65, 79	1 (0%)
All	All	530/610 (86%)	0.52	49 (9%)	14 11	24, 42, 66, 79	1 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	169	ALA	5.7
1	A	166	GLY	4.8
1	A	227	PHE	4.8
1	B	165	ALA	4.5
1	B	167	ASP	4.5
1	B	168	VAL	4.4
1	A	168	VAL	4.2
1	B	140	GLY	4.1
1	B	169	ALA	4.0
1	A	165	ALA	4.0
1	A	171	SER	3.9
1	B	171	SER	3.6
1	B	110	SER	3.5
1	B	166	GLY	3.4
1	A	109	HIS	3.2
1	A	88	SER	3.2
1	A	167	ASP	3.1
1	B	284	VAL	3.1
1	B	230	HIS	3.1
1	A	234	GLU	3.1
1	A	121	GLN	3.0
1	A	110	SER	2.9
1	B	242	GLY	2.9
1	B	111	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	67	HIS	2.9
1	B	170	MET	2.8
1	A	133	LEU	2.8
1	B	121	GLN	2.7
1	B	109	HIS	2.7
1	A	163	PRO	2.7
1	A	230	HIS	2.6
1	B	188	GLY	2.6
1	B	134	ALA	2.6
1	A	242	GLY	2.5
1	A	243	ASP	2.5
1	A	13	VAL	2.5
1	B	268	ALA	2.5
1	B	173	SER	2.4
1	A	240	LEU	2.4
1	A	139	SER	2.4
1	B	234	GLU	2.4
1	A	236	VAL	2.4
1	B	241	ALA	2.3
1	B	227	PHE	2.3
1	A	229	ALA	2.3
1	B	243	ASP	2.2
1	B	212	GLY	2.1
1	A	241	ALA	2.1
1	A	170	MET	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 ⓘ

There are no such residues in this entry.