



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:38 AM UTC

PDB ID : 5DE2 / pdb\_00005de2  
Title : Structural mechanism of Nek7 activation by Nek9-induced dimerisation  
Authors : Haq, T.; Bayliss, R.  
Deposited on : 2015-08-25  
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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (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

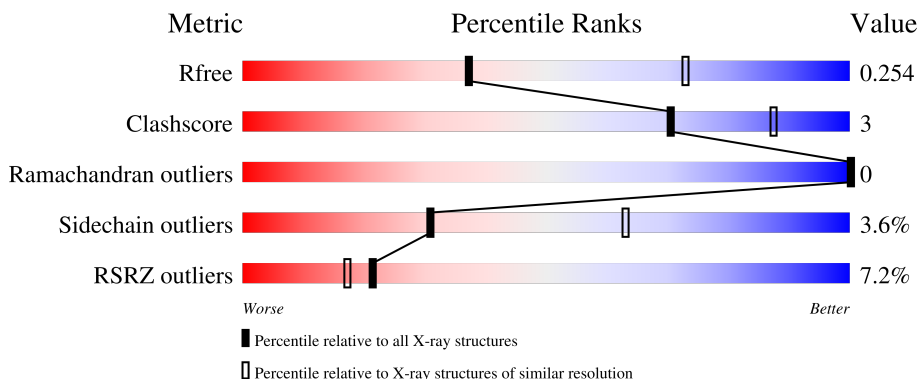
# 1 Overall quality at a glance

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  $\geq 3$ , 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	310	 3% (poor fit), 76% (0-1 outliers), 10% (2 outliers), 14% (3+ outliers)
1	B	310	 2% (poor fit), 72% (0-1 outliers), 12% (2 outliers), 15% (3+ outliers)
2	C	19	 79% (poor fit), 74% (0-1 outliers), 11% (2 outliers), 16% (3+ outliers)
2	D	19	 47% (poor fit), 37% (0-1 outliers), 11% (2 outliers), 53% (3+ outliers)

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4452 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 Serine/threonine-protein kinase Nek7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	267	Total	C	N	O	S	0	0	0
			2126	1360	366	382	18			
1	B	262	Total	C	N	O	S	0	2	0
			2105	1350	363	374	18			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	97	PHE	TYR	engineered mutation	UNP Q8TDX7
A	303	LEU	-	expression tag	UNP Q8TDX7
A	304	GLU	-	expression tag	UNP Q8TDX7
A	305	HIS	-	expression tag	UNP Q8TDX7
A	306	HIS	-	expression tag	UNP Q8TDX7
A	307	HIS	-	expression tag	UNP Q8TDX7
A	308	HIS	-	expression tag	UNP Q8TDX7
A	309	HIS	-	expression tag	UNP Q8TDX7
A	310	HIS	-	expression tag	UNP Q8TDX7
B	97	PHE	TYR	engineered mutation	UNP Q8TDX7
B	303	LEU	-	expression tag	UNP Q8TDX7
B	304	GLU	-	expression tag	UNP Q8TDX7
B	305	HIS	-	expression tag	UNP Q8TDX7
B	306	HIS	-	expression tag	UNP Q8TDX7
B	307	HIS	-	expression tag	UNP Q8TDX7
B	308	HIS	-	expression tag	UNP Q8TDX7
B	309	HIS	-	expression tag	UNP Q8TDX7
B	310	HIS	-	expression tag	UNP Q8TDX7

- Molecule 2 is a protein called Serine/threonine-protein kinase Nek9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	16	Total	C	N	O	S	0	0	0
			135	89	22	23	1			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	D	9	76	49	15	12	0	0	0

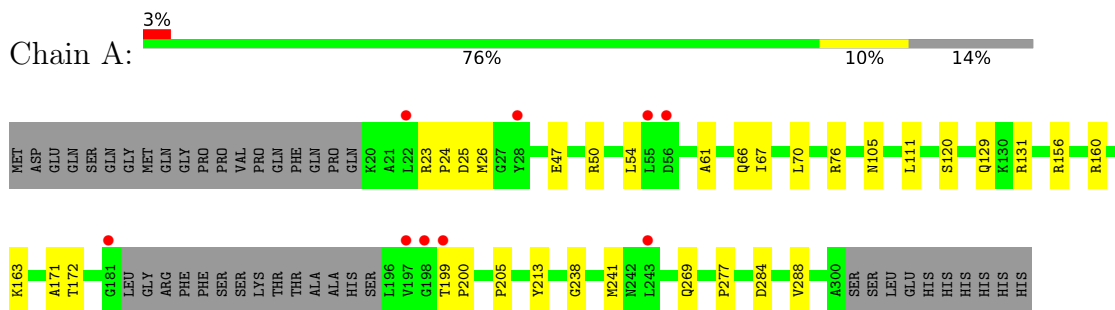
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	O	0	0
			4	4		
3	B	6	Total	O	0	0
			6	6		

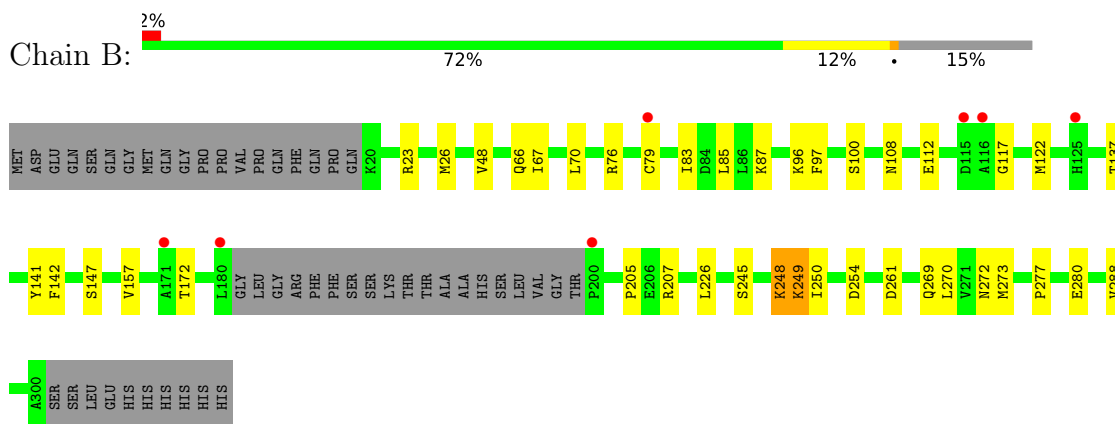
### 3 Residue-property plots [i](#)

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.

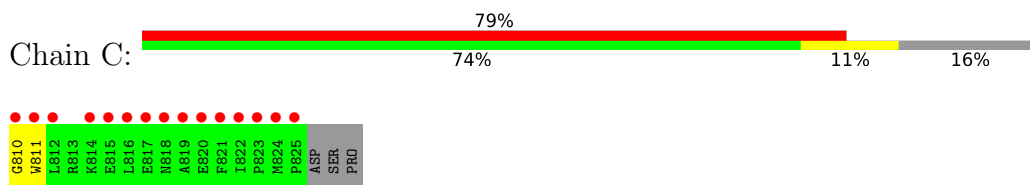
- Molecule 1: Serine/threonine-protein kinase Nek7



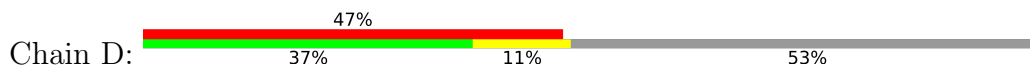
- Molecule 1: Serine/threonine-protein kinase Nek7



- Molecule 2: Serine/threonine-protein kinase Nek9



- Molecule 2: Serine/threonine-protein kinase Nek9



•	G810
•	W811
•	L812
•	R813
•	R814
•	E815
•	L816
•	E817
•	R818
	ALA
	GLU
	PHE
	ILE
	PRO
	MET
	PRO
	ASP
	SER
	PRO

## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.12Å 88.12Å 155.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	54.48 – 2.78 54.48 – 2.78	Depositor EDS
% Data completeness (in resolution range)	99.9 (54.48-2.78) 99.9 (54.48-2.78)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.58 (at 2.77Å)	Xtrriage
Refinement program	BUSTER 2.10.1	Depositor
R, $R_{free}$	0.206 , 0.254 0.204 , 0.254	Depositor DCC
$R_{free}$ test set	930 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.4	Xtrriage
Anisotropy	0.083	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 36.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.044 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4452	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.82	0/2174	1.31	8/2939 (0.3%)
1	B	0.78	0/2160	1.26	6/2919 (0.2%)
2	C	0.76	0/139	1.20	2/187 (1.1%)
2	D	0.63	0/77	1.06	0/102
All	All	0.80	0/4550	1.28	16/6147 (0.3%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	284	ASP	CA-CB-CG	5.79	118.39	112.60
1	B	250	ILE	CA-C-N	5.30	128.16	120.79
1	B	250	ILE	C-N-CA	5.30	128.16	120.79
1	B	207	ARG	CA-C-N	5.25	127.66	120.46
1	B	207	ARG	C-N-CA	5.25	127.66	120.46
1	A	288	VAL	CA-C-N	5.25	127.31	120.28
1	A	288	VAL	C-N-CA	5.25	127.31	120.28
1	A	120	SER	CA-C-N	5.19	127.18	120.44
1	A	120	SER	C-N-CA	5.19	127.18	120.44
1	A	24	PRO	CA-C-N	5.17	127.21	120.28
1	A	24	PRO	C-N-CA	5.17	127.21	120.28
2	C	810	GLY	CA-C-N	5.04	127.29	120.38
2	C	810	GLY	C-N-CA	5.04	127.29	120.38
1	B	147	SER	CA-C-N	5.02	126.97	120.44
1	B	147	SER	C-N-CA	5.02	126.97	120.44
1	A	50	ARG	N-CA-C	-5.02	101.06	109.24

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	2126	0	2106	10	0
1	B	2105	0	2090	20	0
2	C	135	0	132	1	0
2	D	76	0	74	2	0
3	A	4	0	0	0	0
3	B	6	0	0	0	0
All	All	4452	0	4402	30	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 3.

All (30) 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:137:THR:O	1:B:141:TYR:HD2	1.71	0.74
1:A:199:THR:HB	1:A:200:PRO:HD2	1.72	0.71
1:B:269:GLN:HG3	1:B:273:MET:HE2	1.77	0.66
1:A:67:ILE:HB	1:A:76:ARG:HG3	1.84	0.60
1:B:122:MET:HE1	1:B:141:TYR:CZ	2.38	0.59
1:B:205:PRO:HG2	1:B:277:PRO:HA	1.86	0.56
1:B:141:TYR:OH	2:D:815:GLU:OE1	2.24	0.54
1:A:66:GLN:HB2	1:A:70:LEU:HD12	1.90	0.53
1:B:117:GLY:HA3	2:D:811:TRP:HZ2	1.74	0.52
1:B:100:SER:HA	1:B:108:ASN:O	2.10	0.52
1:B:137:THR:O	1:B:141:TYR:CD2	2.58	0.52
1:B:245:SER:HA	1:B:248:LYS:HD3	1.93	0.50
1:A:160:ARG:HA	1:A:213:TYR:CE1	2.46	0.50
1:B:249:LYS:HB2	1:B:254:ASP:HB3	1.93	0.49
1:B:23:ARG:HH21	1:B:26:MET:HE2	1.76	0.49
1:B:96:LYS:HB2	1:B:112:GLU:HB2	1.95	0.48
1:A:129:GLN:HB3	1:A:131:ARG:HD3	1.96	0.48
1:A:171:ALA:HA	2:C:811:TRP:HD1	1.80	0.46
1:B:87:LYS:HG2	1:B:97:PHE:CE2	2.51	0.45
1:A:160:ARG:HA	1:A:213:TYR:CZ	2.51	0.45
1:B:79:CYS:O	1:B:83:ILE:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:GLY:HA3	1:A:241:MET:HE2	1.99	0.44
1:A:205:PRO:HG2	1:A:277:PRO:HA	2.00	0.44
1:B:142:PHE:CE1	1:B:226:LEU:HB2	2.53	0.42
1:B:67:ILE:HB	1:B:76:ARG:HG3	2.00	0.42
1:B:66:GLN:HB2	1:B:70:LEU:HB2	2.02	0.42
1:B:85:LEU:HB3	1:B:157:VAL:HG22	2.01	0.41
1:A:61:ALA:HB3	1:A:111:LEU:HB2	2.03	0.41
1:B:270:LEU:HD21	1:B:288:VAL:HG13	2.02	0.41
1:B:87:LYS:HG2	1:B:97:PHE:HE2	1.86	0.41

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	263/310 (85%)	252 (96%)	11 (4%)	0	100	100
1	B	260/310 (84%)	245 (94%)	15 (6%)	0	100	100
2	C	14/19 (74%)	13 (93%)	1 (7%)	0	100	100
2	D	7/19 (37%)	7 (100%)	0	0	100	100
All	All	544/658 (83%)	517 (95%)	27 (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	228/274 (83%)	218 (96%)	10 (4%)	25	56
1	B	226/274 (82%)	219 (97%)	7 (3%)	35	68
2	C	14/17 (82%)	14 (100%)	0	100	100
2	D	7/17 (41%)	7 (100%)	0	100	100
All	All	475/582 (82%)	458 (96%)	17 (4%)	31	63

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
1	A	25	ASP
1	A	26	MET
1	A	47	GLU
1	A	54	LEU
1	A	105	ASN
1	A	156	ARG
1	A	163	LYS
1	A	172	THR
1	A	269	GLN
1	B	48	VAL
1	B	172	THR
1	B	248	LYS
1	B	249	LYS
1	B	261	ASP
1	B	272	ASN
1	B	280	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	ASN
1	B	29	ASN
1	B	153	HIS
2	D	818	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	267/310 (86%)	0.20	9 (3%) 48 41	43, 61, 98, 110	1 (0%)
1	B	262/310 (84%)	0.23	7 (2%) 56 48	39, 61, 90, 95	2 (0%)
2	C	16/19 (84%)	3.34	15 (93%) 0 0	68, 80, 84, 84	16 (100%)
2	D	9/19 (47%)	3.34	9 (100%) 0 0	79, 82, 88, 96	9 (100%)
All	All	554/658 (84%)	0.36	40 (7%) 21 17	39, 62, 91, 110	28 (5%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	822	ILE	5.2
1	B	115	ASP	5.2
1	A	181	GLY	4.8
2	C	820	GLU	4.7
2	C	825	PRO	4.6
2	C	810	GLY	4.6
2	D	812	LEU	4.6
2	D	811	TRP	4.1
2	D	816	LEU	4.0
2	D	810	GLY	4.0
2	C	816	LEU	4.0
2	C	812	LEU	3.7
2	C	819	ALA	3.4
1	B	180	LEU	3.3
1	A	197	VAL	3.3
2	C	814	LYS	3.2
2	D	815	GLU	3.2
2	C	821	PHE	3.2
2	D	817	GLU	3.1
2	C	811	TRP	3.1
1	A	55	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	C	823	PRO	2.8
1	B	116	ALA	2.6
1	A	22	LEU	2.6
2	D	818	ASN	2.6
1	B	79	CYS	2.5
1	A	243	LEU	2.5
2	C	817	GLU	2.4
1	A	56	ASP	2.4
1	A	199	THR	2.4
1	A	28	TYR	2.3
2	C	815	GLU	2.3
2	D	814	LYS	2.3
1	B	200	PRO	2.3
1	B	171	ALA	2.3
1	A	198	GLY	2.3
2	D	813	ARG	2.2
2	C	824	MET	2.2
2	C	818	ASN	2.2
1	B	125[A]	HIS	2.1

## 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.