



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 06:43 AM UTC

PDB ID : 4N5Q / pdb_00004n5q
Title : Crystal structure of the N-terminal ankyrin repeat domain of TRPV3
Authors : Shi, D.J.; Ye, S.; Cao, X.; Wang, K.W.; Zhang, R.
Deposited on : 2013-10-10
Resolution : 1.95 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

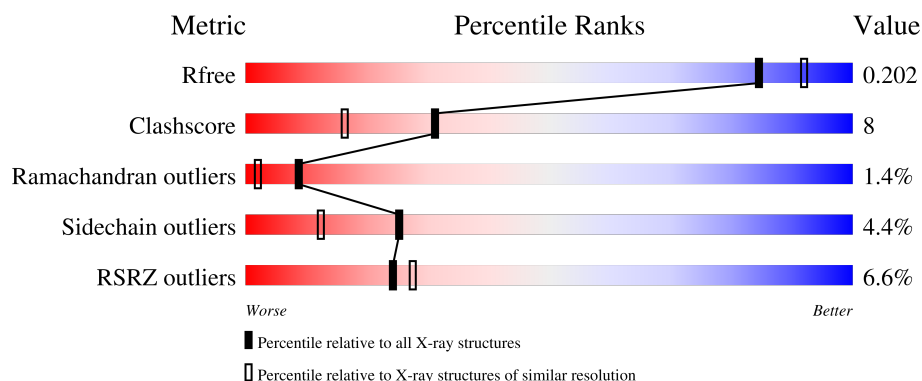
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	257	5% 81% 13% • •
1	B	257	8% 82% 12% • ••

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4545 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 Transient receptor potential cation channel subfamily V member 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			1978	1243	346	377	12			
1	B	254	Total	C	N	O	S	0	1	0
			2029	1274	358	384	13			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	117	MET	-	expression tag	UNP Q8K424
A	368	HIS	-	expression tag	UNP Q8K424
A	369	HIS	-	expression tag	UNP Q8K424
A	370	HIS	-	expression tag	UNP Q8K424
A	371	HIS	-	expression tag	UNP Q8K424
A	372	HIS	-	expression tag	UNP Q8K424
A	373	HIS	-	expression tag	UNP Q8K424
B	117	MET	-	expression tag	UNP Q8K424
B	368	HIS	-	expression tag	UNP Q8K424
B	369	HIS	-	expression tag	UNP Q8K424
B	370	HIS	-	expression tag	UNP Q8K424
B	371	HIS	-	expression tag	UNP Q8K424
B	372	HIS	-	expression tag	UNP Q8K424
B	373	HIS	-	expression tag	UNP Q8K424

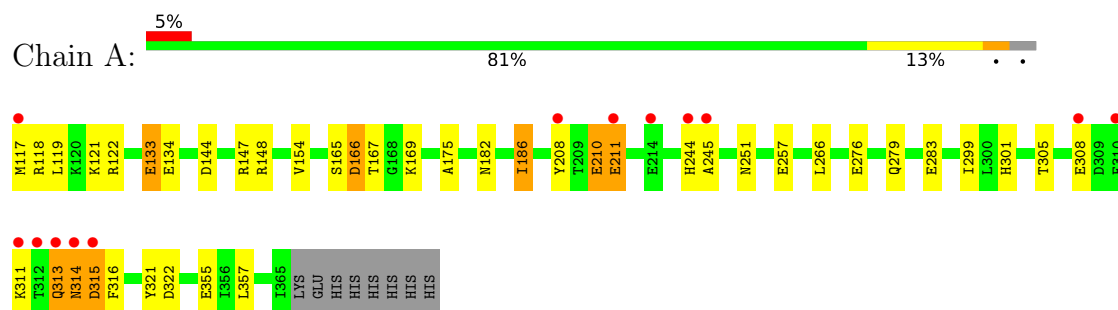
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	275	Total	O	0	0
			275	275		
2	B	263	Total	O	0	0
			263	263		

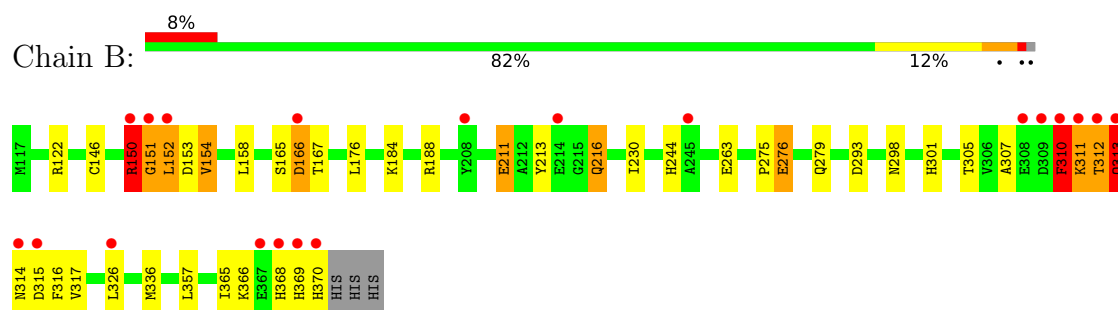
3 Residue-property plots [i](#)

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: Transient receptor potential cation channel subfamily V member 3



- Molecule 1: Transient receptor potential cation channel subfamily V member 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.52Å 78.56Å 82.97Å 90.00° 93.30° 90.00°	Depositor
Resolution (Å)	41.40 – 1.95 41.40 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.3 (41.40-1.95) 92.9 (41.40-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 1.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.169 , 0.201 0.170 , 0.202	Depositor DCC
R_{free} test set	2913 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4545	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% 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	0.88	1/2005 (0.0%)	1.01	3/2705 (0.1%)
1	B	0.86	0/2062	1.02	8/2781 (0.3%)
All	All	0.87	1/4067 (0.0%)	1.02	11/5486 (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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	154	VAL	CA-CB	7.51	1.58	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	312	THR	N-CA-C	-7.08	103.50	111.14
1	B	369	HIS	N-CA-C	6.74	119.88	108.90
1	B	166	ASP	N-CA-CB	-6.48	100.45	109.91
1	B	165	SER	CA-C-N	6.30	128.97	120.65
1	B	165	SER	C-N-CA	6.30	128.97	120.65
1	B	150	ARG	N-CA-C	6.06	123.70	110.80
1	B	154	VAL	N-CA-CB	5.54	114.77	110.45
1	B	151	GLY	N-CA-C	5.29	125.72	113.18
1	A	165	SER	CA-C-N	5.14	127.93	120.79
1	A	165	SER	C-N-CA	5.14	127.93	120.79
1	A	166	ASP	N-CA-CB	-5.14	102.01	109.82

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	310	PHE	Peptide

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	1978	0	1989	29	0
1	B	2029	0	2034	38	0
2	A	275	0	0	11	0
2	B	263	0	0	9	0
All	All	4545	0	4023	66	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 (66) 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:A:321:TYR:OH	2:A:554:HOH:O	1.87	0.92
1:B:279:GLN:OE1	2:B:504:HOH:O	1.96	0.84
1:A:210:GLU:OE1	2:A:644:HOH:O	1.95	0.83
1:B:370:HIS:ND1	2:B:557:HOH:O	2.10	0.82
1:B:153:ASP:OD2	2:B:645:HOH:O	2.00	0.79
1:A:257:GLU:OE2	2:A:514:HOH:O	2.01	0.78
1:A:313:GLN:O	1:A:315:ASP:N	2.20	0.72
1:B:314:ASN:C	1:B:316:PHE:H	1.96	0.72
1:B:314:ASN:O	1:B:316:PHE:N	2.22	0.72
1:B:370:HIS:CG	2:B:557:HOH:O	2.45	0.70
1:B:313:GLN:CD	1:B:314:ASN:H	2.01	0.69
1:B:311:LYS:HG2	1:B:313:GLN:HG3	1.76	0.68
1:A:322:ASP:OD2	2:A:565:HOH:O	2.12	0.68
1:A:134:GLU:OE1	2:A:557:HOH:O	2.12	0.67
1:B:150:ARG:HA	1:B:154:VAL:HG23	1.78	0.66
1:B:151:GLY:O	1:B:152:LEU:HB2	1.96	0.65
1:B:211:GLU:H	1:B:211:GLU:CD	2.04	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ASP:OD1	2:A:588:HOH:O	2.13	0.64
1:B:298:ASN:HD22	1:B:336:MET:HE2	1.62	0.64
1:B:310:PHE:HD2	1:B:311:LYS:N	1.98	0.61
1:A:314:ASN:ND2	1:A:355:GLU:OE1	2.36	0.59
1:B:276:GLU:H	1:B:276:GLU:CD	2.09	0.59
1:B:370:HIS:HB3	2:B:557:HOH:O	2.05	0.56
1:A:313:GLN:O	1:A:313:GLN:NE2	2.40	0.55
1:A:121:LYS:NZ	2:A:581:HOH:O	2.41	0.54
1:A:118:ARG:HH21	1:B:122:ARG:NH1	2.06	0.53
1:A:133:GLU:CD	1:A:133:GLU:H	2.17	0.53
1:A:279:GLN:O	1:A:283:GLU:HG3	2.10	0.51
1:A:175:ALA:HB2	1:A:186:ILE:HD11	1.92	0.51
1:B:122:ARG:HD2	2:B:533:HOH:O	2.10	0.51
1:B:365:ILE:O	1:B:368:HIS:HB3	2.10	0.51
1:A:313:GLN:C	1:A:315:ASP:H	2.16	0.51
1:B:275:PRO:O	1:B:279:GLN:HG3	2.12	0.49
1:B:301:HIS:O	1:B:305:THR:HG23	2.12	0.49
1:B:314:ASN:C	1:B:316:PHE:N	2.63	0.48
1:B:326:LEU:HD11	1:B:366:LYS:HZ3	1.79	0.47
1:B:244:HIS:HD2	2:B:549:HOH:O	1.96	0.47
1:B:311:LYS:HB3	1:B:313:GLN:O	2.15	0.47
1:B:216:GLN:HG3	2:B:426:HOH:O	2.14	0.46
1:A:244:HIS:CD2	2:A:529:HOH:O	2.69	0.46
1:B:176:LEU:HD21	1:B:230:ILE:HG21	1.96	0.46
1:A:251:ASN:ND2	2:A:560:HOH:O	2.38	0.45
1:B:166:ASP:HB3	1:B:167:THR:HG23	1.97	0.45
1:A:313:GLN:C	1:A:315:ASP:N	2.74	0.45
1:A:166:ASP:HB3	1:A:167:THR:HG23	1.99	0.45
1:B:146:CYS:SG	1:B:158:LEU:HD21	2.58	0.44
1:A:169:LYS:HE2	1:A:208:TYR:OH	2.17	0.44
1:A:117:MET:HG3	1:A:119:LEU:H	1.81	0.44
1:A:301:HIS:O	1:A:305:THR:HG23	2.17	0.44
1:B:263:GLU:OE1	1:B:293:ASP:HB2	2.17	0.44
1:B:326:LEU:HD11	1:B:366:LYS:NZ	2.33	0.44
1:B:312:THR:OG1	1:B:313:GLN:N	2.50	0.44
1:A:211:GLU:H	1:A:211:GLU:CD	2.24	0.43
1:A:266:LEU:HG	1:A:299:ILE:HD12	2.01	0.43
1:B:307:ALA:HB2	1:B:317:VAL:HG11	2.00	0.43
1:B:184:LYS:O	1:B:188:ARG:HG3	2.19	0.43
1:B:310:PHE:HD2	1:B:311:LYS:H	1.66	0.42
1:B:310:PHE:CD2	1:B:311:LYS:N	2.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ARG:HD2	2:A:557:HOH:O	2.18	0.42
1:A:245:ALA:HB3	2:A:550:HOH:O	2.19	0.41
1:A:182:ASN:O	1:A:186:ILE:HG23	2.21	0.41
1:B:150:ARG:HA	1:B:154:VAL:CG2	2.48	0.41
1:A:313:GLN:C	1:A:313:GLN:HE21	2.27	0.41
1:B:213:TYR:HE1	2:B:558:HOH:O	2.03	0.41
1:B:275:PRO:HD2	1:B:276:GLU:OE1	2.21	0.41
1:A:117:MET:HE3	1:A:117:MET:HB2	1.86	0.41

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	247/257 (96%)	239 (97%)	6 (2%)	2 (1%)	16	7
1	B	253/257 (98%)	238 (94%)	10 (4%)	5 (2%)	6	1
All	All	500/514 (97%)	477 (95%)	16 (3%)	7 (1%)	9	2

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	311	LYS
1	A	314	ASN
1	B	150	ARG
1	B	152	LEU
1	B	310	PHE
1	B	315	ASP
1	B	313	GLN

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	212/220 (96%)	200 (94%)	12 (6%)	18	6
1	B	218/220 (99%)	211 (97%)	7 (3%)	34	20
All	All	430/440 (98%)	411 (96%)	19 (4%)	25	12

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	GLU
1	A	147	ARG
1	A	148	ARG
1	A	186	ILE
1	A	210	GLU
1	A	211	GLU
1	A	276	GLU
1	A	308	GLU
1	A	313	GLN
1	A	315	ASP
1	A	316	PHE
1	A	357	LEU
1	B	211	GLU
1	B	216	GLN
1	B	276	GLU
1	B	310	PHE
1	B	311	LYS
1	B	313	GLN
1	B	357	LEU

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	140	GLN
1	A	143	GLN
1	A	197	ASN

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Mol	Chain	Res	Type
1	A	273	ASN
1	B	140	GLN
1	B	251	ASN
1	B	279	GLN
1	B	369	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](#)

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	249/257 (96%)	-0.07	13 (5%) 33 37	17, 29, 63, 124	0
1	B	254/257 (98%)	0.07	20 (7%) 18 21	17, 28, 76, 122	1 (0%)
All	All	503/514 (97%)	0.00	33 (6%) 24 27	17, 29, 69, 124	1 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	152	LEU	8.3
1	A	310	PHE	6.5
1	B	312	THR	5.7
1	A	312	THR	5.7
1	B	370	HIS	5.6
1	B	368	HIS	5.4
1	B	310	PHE	5.2
1	B	151	GLY	4.8
1	B	314	ASN	4.4
1	A	313	GLN	4.2
1	B	309	ASP	3.9
1	A	315	ASP	3.9
1	A	314	ASN	3.6
1	B	150	ARG	3.6
1	B	367	GLU	3.5
1	A	308	GLU	3.4
1	B	313	GLN	3.4
1	A	311	LYS	3.3
1	B	308	GLU	3.2
1	A	117	MET	3.1
1	B	326	LEU	2.6
1	B	166	ASP	2.6
1	B	245	ALA	2.6
1	B	214	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	245	ALA	2.5
1	A	214	GLU	2.4
1	B	315	ASP	2.3
1	B	369	HIS	2.3
1	A	211	GLU	2.2
1	B	311	LYS	2.2
1	A	208	TYR	2.2
1	B	208	TYR	2.1
1	A	244	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.