Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:24 PM GMT

PDB ID	:	4RUF
Title	:	Human K2P4.1 (TRAAAK) potassium channel, W262S mutant
Authors	:	Lolicato, M.; Minor, D.L.Jr.
Deposited on	:	2014-11-19
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

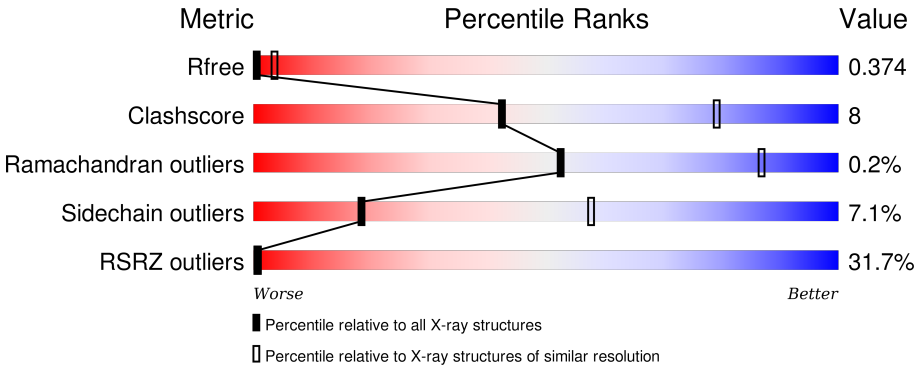
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 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}	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	309	33% 62% 19% • 17%
1	B	309	19% 65% 15% • 19%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	K	A	402	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3923 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 Potassium channel subfamily K member 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			1974	1302	321	344	7			
1	B	251	Total	C	N	O	S	0	0	0
			1943	1280	315	342	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	GLN	ASN	ENGINEERED MUTATION	UNP Q9NYG8
A	108	GLN	ASN	ENGINEERED MUTATION	UNP Q9NYG8
A	262	SER	TRP	ENGINEERED MUTATION	UNP Q9NYG8
A	301	SER	-	EXPRESSION TAG	UNP Q9NYG8
A	302	ASN	-	EXPRESSION TAG	UNP Q9NYG8
A	303	SER	-	EXPRESSION TAG	UNP Q9NYG8
A	304	LEU	-	EXPRESSION TAG	UNP Q9NYG8
A	305	GLU	-	EXPRESSION TAG	UNP Q9NYG8
A	306	VAL	-	EXPRESSION TAG	UNP Q9NYG8
A	307	LEU	-	EXPRESSION TAG	UNP Q9NYG8
A	308	PHE	-	EXPRESSION TAG	UNP Q9NYG8
A	309	GLN	-	EXPRESSION TAG	UNP Q9NYG8
B	104	GLN	ASN	ENGINEERED MUTATION	UNP Q9NYG8
B	108	GLN	ASN	ENGINEERED MUTATION	UNP Q9NYG8
B	262	SER	TRP	ENGINEERED MUTATION	UNP Q9NYG8
B	301	SER	-	EXPRESSION TAG	UNP Q9NYG8
B	302	ASN	-	EXPRESSION TAG	UNP Q9NYG8
B	303	SER	-	EXPRESSION TAG	UNP Q9NYG8
B	304	LEU	-	EXPRESSION TAG	UNP Q9NYG8
B	305	GLU	-	EXPRESSION TAG	UNP Q9NYG8
B	306	VAL	-	EXPRESSION TAG	UNP Q9NYG8
B	307	LEU	-	EXPRESSION TAG	UNP Q9NYG8
B	308	PHE	-	EXPRESSION TAG	UNP Q9NYG8
B	309	GLN	-	EXPRESSION TAG	UNP Q9NYG8

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

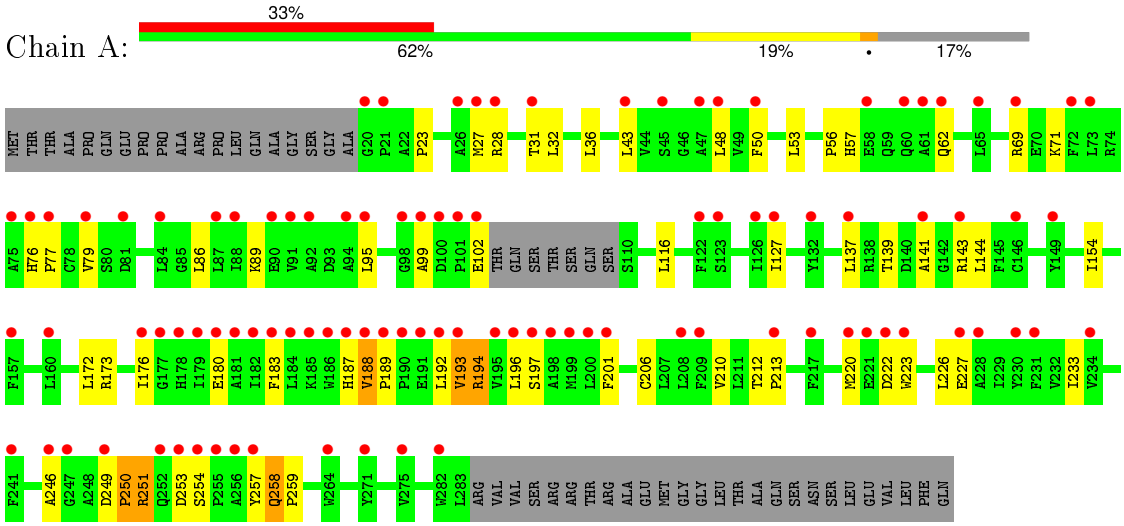
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total K 3 3	0	0
2	A	3	Total K 3 3	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

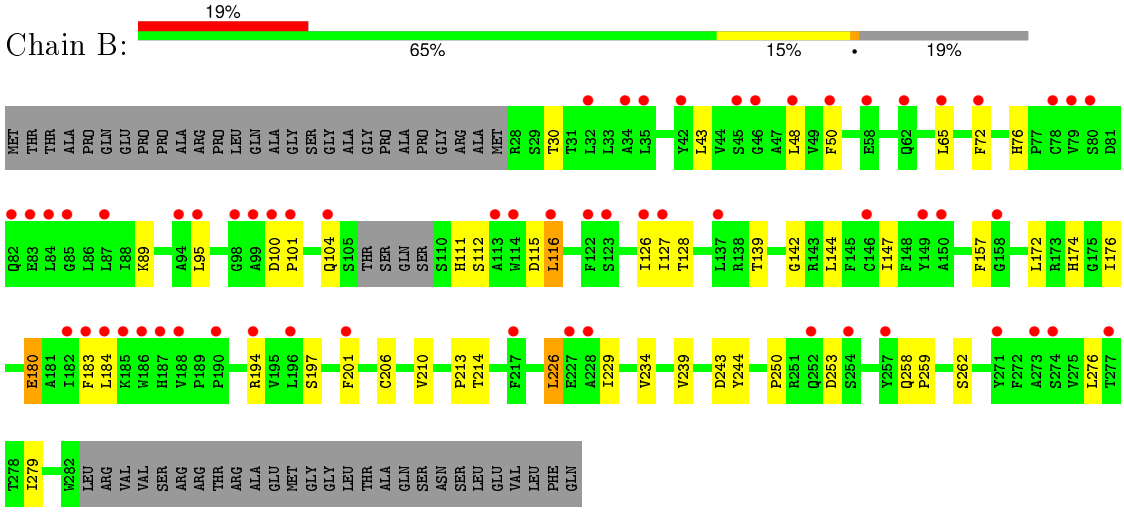
- Molecule 1: Potassium channel subfamily K member 4

Chain A:



- Molecule 1: Potassium channel subfamily K member 4

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.05Å 127.98Å 130.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.99 – 3.40 48.49 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (14.99-3.40) 99.9 (48.49-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.87 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.297 , 0.328 0.346 , 0.374	Depositor DCC
R_{free} test set	1031 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	129.7	Xtriage
Anisotropy	0.524	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.17 , 63.1	EDS
Estimated twinning fraction	0.026 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Outliers	5 of 20853 reflections (0.024%)	Xtriage
F_o,F_c correlation	0.80	EDS
Total number of atoms	3923	wwPDB-VP
Average B, all atoms (Å^2)	176.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: K

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	0.26	0/2024	0.48	0/2758
1	B	0.21	0/1992	0.38	0/2714
All	All	0.24	0/4016	0.43	0/5472

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	1974	0	1994	50	0
1	B	1943	0	1959	27	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
All	All	3923	0	3953	65	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 (65) 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:102:GLU:OE2	1:A:251:ARG:NH2	2.16	0.79
1:A:172:LEU:O	1:A:176:ILE:N	2.18	0.73
1:A:173:ARG:HA	1:A:176:ILE:HB	1.77	0.66
1:A:53:LEU:HD13	1:B:142:GLY:HA2	1.78	0.65
1:A:95:LEU:HD23	1:A:99:ALA:HB3	1.82	0.62
1:A:99:ALA:HB1	1:B:65:LEU:HD22	1.80	0.62
1:A:127:ILE:HA	1:A:154:ILE:HG12	1.86	0.58
1:A:220:MET:SD	1:A:257:TYR:OH	2.60	0.58
1:A:194:ARG:H	1:A:194:ARG:HD2	1.68	0.57
1:A:139:THR:HG22	1:A:141:ALA:H	1.71	0.56
1:A:192:LEU:O	1:A:196:LEU:N	2.35	0.56
1:A:226:LEU:HD11	1:B:144:LEU:HB2	1.88	0.55
1:A:188:VAL:HB	1:A:192:LEU:HD11	1.88	0.55
1:A:127:ILE:HD13	1:B:43:LEU:HD21	1.89	0.55
1:B:258:GLN:HB3	1:B:259:PRO:HD3	1.87	0.55
1:B:180:GLU:OE2	1:B:197:SER:OG	2.22	0.55
1:A:176:ILE:HD11	1:A:201:PHE:CD1	2.43	0.54
1:A:32:LEU:O	1:A:36:LEU:N	2.37	0.53
1:A:223:TRP:HZ2	1:A:246:ALA:HB3	1.74	0.53
1:A:223:TRP:CZ2	1:A:246:ALA:HB3	2.44	0.53
1:A:176:ILE:HG22	1:A:180:GLU:OE2	2.09	0.53
1:B:276:LEU:HD23	1:B:279:ILE:HD12	1.90	0.53
1:A:43:LEU:HD21	1:B:127:ILE:HD13	1.90	0.53
1:A:56:PRO:HB2	1:A:57:HIS:CE1	2.44	0.52
1:A:249:ASP:HB3	1:A:250:PRO:HD3	1.92	0.52
1:A:188:VAL:HB	1:A:192:LEU:HD21	1.93	0.51
1:B:176:ILE:HD13	1:B:201:PHE:CE1	2.46	0.51
1:A:23:PRO:O	1:A:27:MET:N	2.44	0.50
1:A:116:LEU:HD21	1:B:48:LEU:HD23	1.93	0.50
1:A:250:PRO:HB2	1:A:251:ARG:NE	2.27	0.50
1:A:28:ARG:O	1:A:31:THR:OG1	2.28	0.49
1:A:176:ILE:HD11	1:A:201:PHE:HD1	1.78	0.48
1:A:223:TRP:HB3	1:A:227:GLU:HB2	1.96	0.47
1:B:206:CYS:O	1:B:210:VAL:N	2.45	0.47
1:A:144:LEU:HB2	1:B:226:LEU:HD11	1.97	0.47
1:A:233:ILE:HD13	1:B:147:ILE:HG23	1.97	0.46
1:A:250:PRO:C	1:A:251:ARG:HE	2.19	0.46
1:A:194:ARG:CD	1:A:194:ARG:H	2.25	0.46
1:B:112:SER:HB3	1:B:115:ASP:HB3	1.98	0.46
1:A:183:PHE:O	1:A:188:VAL:HG23	2.16	0.45
1:B:259:PRO:O	1:B:262:SER:OG	2.27	0.45
1:B:116:LEU:HA	1:B:116:LEU:HD22	1.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:PRO:HB2	1:A:251:ARG:HE	1.82	0.45
1:A:192:LEU:HA	1:A:192:LEU:HD23	1.73	0.45
1:A:69:ARG:CZ	1:B:104:GLN:HB3	2.47	0.45
1:A:172:LEU:O	1:A:176:ILE:HG13	2.17	0.44
1:B:111:HIS:CG	1:B:250:PRO:HB3	2.51	0.44
1:A:48:LEU:HD23	1:B:116:LEU:HD21	1.99	0.44
1:A:212:THR:HB	1:A:213:PRO:HD3	2.00	0.44
1:A:79:VAL:HG22	1:B:76:HIS:CG	2.52	0.43
1:A:89:LYS:HE2	1:B:101:PRO:O	2.18	0.43
1:A:193:VAL:HA	1:A:194:ARG:HA	1.69	0.42
1:B:243:ASP:OD1	1:B:244:TYR:N	2.52	0.42
1:A:258:GLN:HB3	1:A:259:PRO:HD3	2.01	0.42
1:B:234:VAL:HG13	1:B:239:VAL:HB	2.00	0.41
1:A:76:HIS:HA	1:A:77:PRO:HD2	1.93	0.41
1:A:137:LEU:HD13	1:A:143:ARG:HA	2.02	0.41
1:B:214:THR:HG21	1:B:229:ILE:HG12	2.02	0.41
1:B:128:THR:HG22	1:B:157:PHE:CE2	2.56	0.41
1:A:71:LYS:HA	1:A:71:LYS:HD2	1.78	0.41
1:B:89:LYS:HE3	1:B:89:LYS:HB2	1.92	0.41
1:B:210:VAL:C	1:B:213:PRO:HD2	2.42	0.40
1:A:206:CYS:O	1:A:210:VAL:HB	2.21	0.40
1:A:188:VAL:HA	1:A:189:PRO:HD3	1.64	0.40
1:A:172:LEU:HA	1:A:172:LEU:HD23	1.96	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	253/309 (82%)	228 (90%)	24 (10%)	1 (0%)	39 79
1	B	247/309 (80%)	235 (95%)	12 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	500/618 (81%)	463 (93%)	36 (7%)	1 (0%)	52 87

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	250	PRO

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	204/248 (82%)	191 (94%)	13 (6%)	22 62
1	B	204/248 (82%)	188 (92%)	16 (8%)	16 52
All	All	408/496 (82%)	379 (93%)	29 (7%)	18 58

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	PHE
1	A	62	GLN
1	A	86	LEU
1	A	187	HIS
1	A	188	VAL
1	A	193	VAL
1	A	194	ARG
1	A	197	SER
1	A	222	ASP
1	A	251	ARG
1	A	253	ASP
1	A	254	SER
1	A	258	GLN
1	B	30	THR
1	B	50	PHE
1	B	72	PHE
1	B	95	LEU

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Mol	Chain	Res	Type
1	B	100	ASP
1	B	116	LEU
1	B	126	ILE
1	B	139	THR
1	B	172	LEU
1	B	174	HIS
1	B	180	GLU
1	B	183	PHE
1	B	184	LEU
1	B	194	ARG
1	B	226	LEU
1	B	253	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	257/309 (83%)	2.06	101 (39%) 0 1	100, 173, 304, 418	0
1	B	251/309 (81%)	1.41	60 (23%) 1 1	69, 158, 227, 311	0
All	All	508/618 (82%)	1.74	161 (31%) 1 1	69, 166, 273, 418	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	100	ASP	16.4
1	A	180	GLU	14.8
1	A	181	ALA	13.7
1	B	99	ALA	13.5
1	A	186	TRP	13.4
1	A	61	ALA	13.4
1	A	183	PHE	12.8
1	A	179	ILE	12.3
1	A	182	ILE	10.4
1	A	95	LEU	10.4
1	B	186	TRP	9.8
1	A	185	LYS	9.5
1	A	190	PRO	9.4
1	A	184	LEU	8.4
1	B	101	PRO	8.1
1	A	209	PHE	7.2
1	A	217	PHE	7.2
1	B	257	TYR	7.1
1	A	26	ALA	7.1
1	A	101	PRO	6.9
1	B	188	VAL	6.9
1	A	178	HIS	6.8
1	A	91	VAL	6.7
1	A	191	GLU	6.7

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Mol	Chain	Res	Type	RSRZ
1	B	50	PHE	6.3
1	B	62	GLN	6.2
1	A	177	GLY	6.1
1	A	246	ALA	6.0
1	A	81	ASP	6.0
1	A	73	LEU	6.0
1	B	104	GLN	5.8
1	A	50	PHE	5.6
1	A	254	SER	5.5
1	A	77	PRO	5.4
1	B	183	PHE	5.4
1	B	46	GLY	5.3
1	B	79	VAL	5.1
1	B	84	LEU	5.1
1	A	100	ASP	5.1
1	A	282	TRP	5.0
1	B	65	LEU	5.0
1	B	80	SER	5.0
1	B	48	LEU	5.0
1	A	176	ILE	4.9
1	A	193	VAL	4.9
1	A	195	VAL	4.9
1	A	187	HIS	4.8
1	A	88	ILE	4.7
1	A	197	SER	4.7
1	B	116	LEU	4.7
1	A	102	GLU	4.7
1	A	60	GLN	4.7
1	A	62	GLN	4.6
1	A	84	LEU	4.4
1	A	99	ALA	4.4
1	A	249	ASP	4.4
1	A	221	GLU	4.4
1	A	143	ARG	4.3
1	B	82	GLN	4.3
1	A	92	ALA	4.3
1	B	228	ALA	4.2
1	A	192	LEU	4.2
1	B	184	LEU	4.2
1	A	20	GLY	4.1
1	A	122	PHE	4.1
1	A	123	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	58	GLU	4.0
1	B	137	LEU	4.0
1	A	196	LEU	4.0
1	A	223	TRP	4.0
1	B	146	CYS	4.0
1	A	201	PHE	4.0
1	A	94	ALA	3.9
1	B	45	SER	3.8
1	B	254	SER	3.7
1	B	35	LEU	3.7
1	B	114	TRP	3.7
1	A	271	TYR	3.7
1	B	150	ALA	3.6
1	A	231	PHE	3.6
1	A	241	PHE	3.6
1	B	126	ILE	3.5
1	B	34	ALA	3.4
1	A	69	ARG	3.4
1	A	257	TYR	3.3
1	B	227	GLU	3.3
1	A	48	LEU	3.3
1	B	95	LEU	3.3
1	A	72	PHE	3.3
1	B	187	HIS	3.3
1	A	256	ALA	3.3
1	B	58	GLU	3.3
1	A	127	ILE	3.3
1	A	126	ILE	3.2
1	B	123	SER	3.2
1	B	190	PRO	3.2
1	A	79	VAL	3.2
1	A	45	SER	3.1
1	A	230	TYR	3.1
1	A	137	LEU	3.1
1	B	217	PHE	3.0
1	A	76	HIS	3.0
1	B	42	TYR	3.0
1	B	98	GLY	3.0
1	A	43	LEU	3.0
1	A	31	THR	3.0
1	A	252	GLN	2.9
1	A	220	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	78	CYS	2.9
1	A	149	TYR	2.9
1	B	201	PHE	2.9
1	B	127	ILE	2.8
1	A	65	LEU	2.8
1	A	227	GLU	2.8
1	A	247	GLY	2.8
1	B	277	THR	2.8
1	B	122	PHE	2.8
1	A	200	LEU	2.8
1	A	132	TYR	2.8
1	B	185	LYS	2.7
1	B	94	ALA	2.7
1	B	271	TYR	2.7
1	A	253	ASP	2.7
1	A	188	VAL	2.7
1	A	87	LEU	2.7
1	A	28	ARG	2.7
1	B	196	LEU	2.7
1	B	149	TYR	2.7
1	A	98	GLY	2.6
1	A	264	TRP	2.6
1	A	189	PRO	2.6
1	B	273	ALA	2.5
1	A	21	PRO	2.5
1	B	182	ILE	2.5
1	A	213	PRO	2.5
1	B	158	GLY	2.5
1	B	87	LEU	2.5
1	B	194	ARG	2.5
1	A	75	ALA	2.4
1	B	83	GLU	2.4
1	A	222	ASP	2.4
1	B	274	SER	2.4
1	A	234	VAL	2.4
1	B	72	PHE	2.4
1	B	85	GLY	2.3
1	A	199	MET	2.3
1	B	32	LEU	2.3
1	A	146	CYS	2.3
1	A	275	VAL	2.2
1	A	90	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	141	ALA	2.2
1	A	198	ALA	2.2
1	A	157	PHE	2.2
1	A	47	ALA	2.2
1	B	113	ALA	2.2
1	A	27	MET	2.1
1	B	252	GLN	2.1
1	A	255	PRO	2.1
1	A	208	LEU	2.1
1	A	160	LEU	2.1
1	A	228	ALA	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	K	A	402	1/1	0.75	0.44	3.30	191,191,191,191	0
2	K	A	403	1/1	0.94	0.28	-0.15	156,156,156,156	0
2	K	A	401	1/1	0.88	0.28	-0.17	169,169,169,169	0
2	K	B	401	1/1	0.78	0.22	-0.96	107,107,107,107	0
2	K	B	403	1/1	0.12	1.76	-	269,269,269,269	0
2	K	B	402	1/1	0.82	1.07	-	109,109,109,109	0

6.5 Other polymers (i)

There are no such residues in this entry.