



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:02 PM GMT

PDB ID : 4GX5
Title : GsuK Channel
Authors : Kong, C.; Zeng, W.; Ye, S.; Chen, L.; Sauer, D.B.; Lam, Y.; Derebe, M.G.; Jiang, Y.
Deposited on : 2012-09-03
Resolution : 3.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

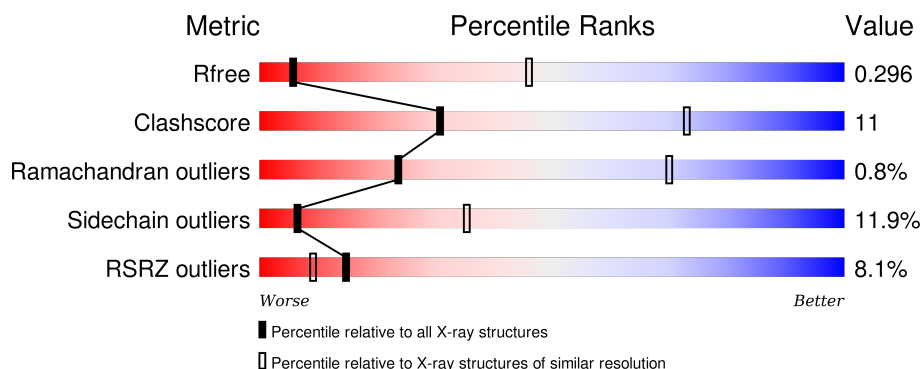
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)

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 $\leq 5\%$. 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	565	<div> <div>4%</div> <div>48%</div> <div>15%</div> <div>•</div> <div>34%</div> </div>
1	B	565	<div> <div>11%</div> <div>66%</div> <div>26%</div> <div>5%</div> <div>•</div> </div>
1	C	565	<div> <div>10%</div> <div>65%</div> <div>28%</div> <div>•</div> <div>•</div> </div>
1	D	565	<div> <div>2%</div> <div>47%</div> <div>15%</div> <div>•</div> <div>33%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CA	C	607	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14266 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 TrkA domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	0	0
			2922	1882	506	523	11			
1	B	548	Total	C	N	O	S	0	0	0
			4208	2695	729	769	15			
1	C	546	Total	C	N	O	S	0	0	0
			4188	2684	723	766	15			
1	D	376	Total	C	N	O	S	0	0	0
			2928	1885	507	525	11			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	EXPRESSION TAG	UNP Q74FS9
A	5	GLN	-	EXPRESSION TAG	UNP Q74FS9
A	6	ARG	-	EXPRESSION TAG	UNP Q74FS9
A	7	GLY	-	EXPRESSION TAG	UNP Q74FS9
A	8	SER	-	EXPRESSION TAG	UNP Q74FS9
A	52	ALA	GLU	ENGINEERED MUTATION	UNP Q74FS9
A	77	GLU	GLN	ENGINEERED MUTATION	UNP Q74FS9
A	565	LEU	-	EXPRESSION TAG	UNP Q74FS9
A	566	VAL	-	EXPRESSION TAG	UNP Q74FS9
A	567	PRO	-	EXPRESSION TAG	UNP Q74FS9
A	568	ARG	-	EXPRESSION TAG	UNP Q74FS9
B	4	MET	-	EXPRESSION TAG	UNP Q74FS9
B	5	GLN	-	EXPRESSION TAG	UNP Q74FS9
B	6	ARG	-	EXPRESSION TAG	UNP Q74FS9
B	7	GLY	-	EXPRESSION TAG	UNP Q74FS9
B	8	SER	-	EXPRESSION TAG	UNP Q74FS9
B	52	ALA	GLU	ENGINEERED MUTATION	UNP Q74FS9
B	77	GLU	GLN	ENGINEERED MUTATION	UNP Q74FS9
B	565	LEU	-	EXPRESSION TAG	UNP Q74FS9
B	566	VAL	-	EXPRESSION TAG	UNP Q74FS9
B	567	PRO	-	EXPRESSION TAG	UNP Q74FS9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	568	ARG	-	EXPRESSION TAG	UNP Q74FS9
C	4	MET	-	EXPRESSION TAG	UNP Q74FS9
C	5	GLN	-	EXPRESSION TAG	UNP Q74FS9
C	6	ARG	-	EXPRESSION TAG	UNP Q74FS9
C	7	GLY	-	EXPRESSION TAG	UNP Q74FS9
C	8	SER	-	EXPRESSION TAG	UNP Q74FS9
C	52	ALA	GLU	ENGINEERED MUTATION	UNP Q74FS9
C	77	GLU	GLN	ENGINEERED MUTATION	UNP Q74FS9
C	565	LEU	-	EXPRESSION TAG	UNP Q74FS9
C	566	VAL	-	EXPRESSION TAG	UNP Q74FS9
C	567	PRO	-	EXPRESSION TAG	UNP Q74FS9
C	568	ARG	-	EXPRESSION TAG	UNP Q74FS9
D	4	MET	-	EXPRESSION TAG	UNP Q74FS9
D	5	GLN	-	EXPRESSION TAG	UNP Q74FS9
D	6	ARG	-	EXPRESSION TAG	UNP Q74FS9
D	7	GLY	-	EXPRESSION TAG	UNP Q74FS9
D	8	SER	-	EXPRESSION TAG	UNP Q74FS9
D	52	ALA	GLU	ENGINEERED MUTATION	UNP Q74FS9
D	77	GLU	GLN	ENGINEERED MUTATION	UNP Q74FS9
D	565	LEU	-	EXPRESSION TAG	UNP Q74FS9
D	566	VAL	-	EXPRESSION TAG	UNP Q74FS9
D	567	PRO	-	EXPRESSION TAG	UNP Q74FS9
D	568	ARG	-	EXPRESSION TAG	UNP Q74FS9

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	6	Total K 6 6	0	0
2	C	6	Total K 6 6	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Zn 1 1	0	0
3	A	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0

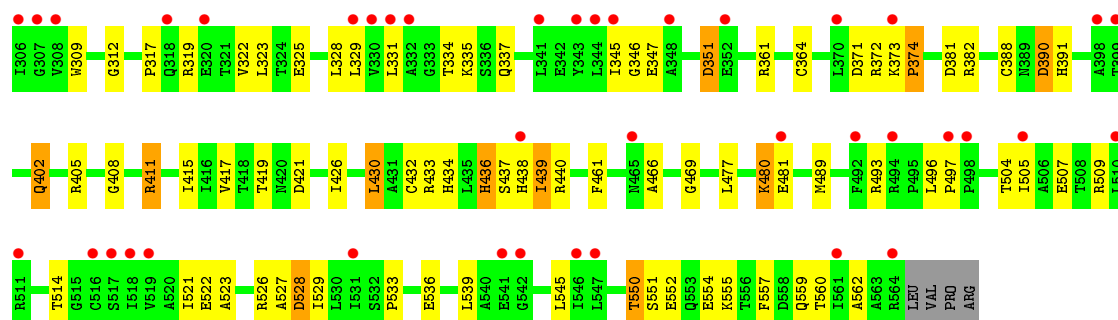
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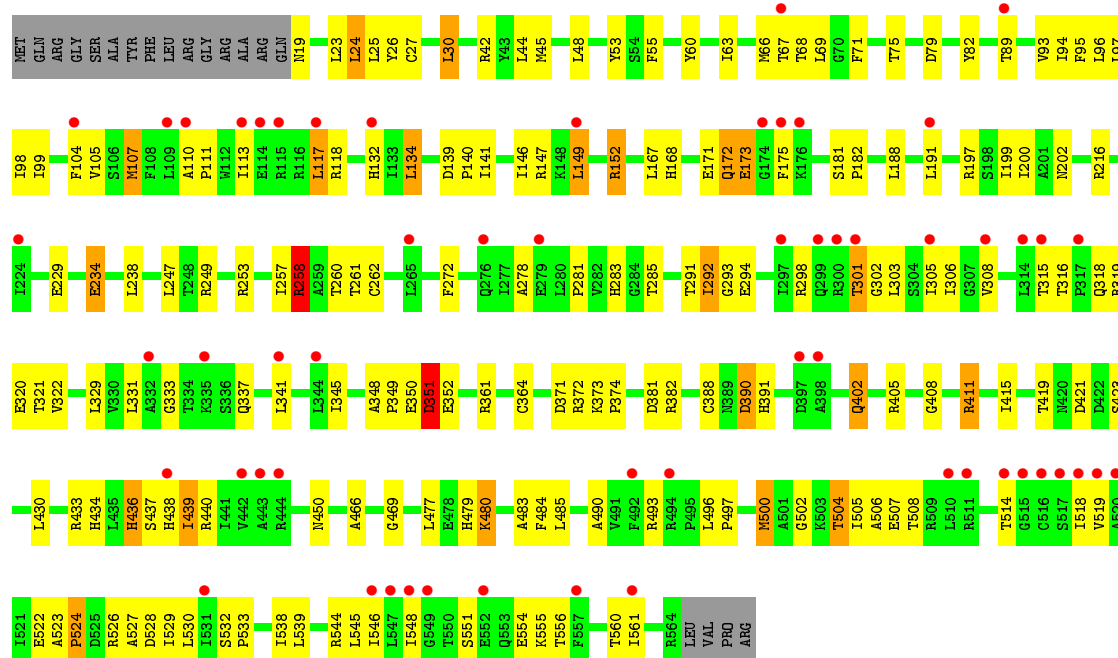
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Zn	0	0
			1	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

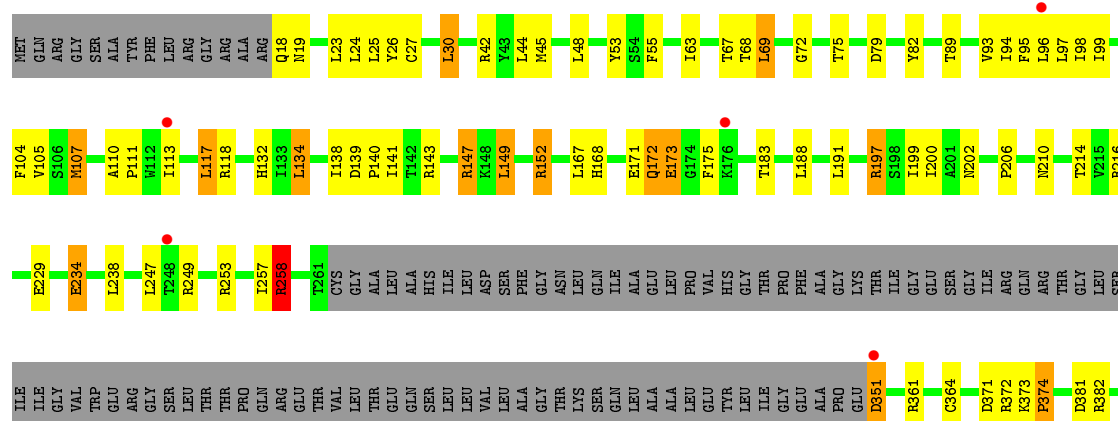
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		
4	C	2	Total	Ca	0	0
			2	2		



• Molecule 1: TrkA domain protein



• Molecule 1: TrkA domain protein





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	234.98Å 108.36Å 165.79Å 90.00° 134.96° 90.00°	Depositor
Resolution (Å)	45.39 – 3.70 49.34 – 3.70	Depositor EDS
% Data completeness (in resolution range)	86.8 (45.39-3.70) 86.5 (49.34-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 3.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.261 , 0.293 0.261 , 0.296	Depositor DCC
R_{free} test set	1383 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	153.1	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 187.4	EDS
Estimated twinning fraction	0.287 for -h-2*l,k,h+l 0.045 for -h,-k,h+l 0.044 for -h-2*l,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 27492 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14266	wwPDB-VP
Average B, all atoms (Å ²)	229.0	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 38.05 % 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 3.9078e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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, ZN, CA

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	0.33	0/2982	0.86	18/4060 (0.4%)
1	B	0.30	0/4291	0.76	17/5843 (0.3%)
1	C	0.31	0/4271	0.76	17/5817 (0.3%)
1	D	0.33	0/2988	0.86	17/4068 (0.4%)
All	All	0.32	0/14532	0.80	69/19788 (0.3%)

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	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	382	ARG	NE-CZ-NH2	13.17	126.88	120.30
1	B	258	ARG	NE-CZ-NH1	-12.93	113.83	120.30
1	A	249	ARG	NE-CZ-NH2	12.84	126.72	120.30
1	C	249	ARG	NE-CZ-NH2	12.81	126.71	120.30
1	A	382	ARG	NE-CZ-NH1	-12.74	113.93	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	173	GLU	Peptide
1	B	173	GLU	Peptide
1	C	173	GLU	Peptide
1	D	173	GLU	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	2922	0	2964	63	0
1	B	4208	0	4288	108	0
1	C	4188	0	4268	99	0
1	D	2928	0	2969	62	0
2	A	6	0	0	0	0
2	C	6	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
All	All	14266	0	14489	312	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 11.

The worst 5 of 312 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:C:117:LEU:HB2	1:D:117:LEU:HD11	1.43	1.00
1:A:117:LEU:HB2	1:B:117:LEU:HD11	1.49	0.95
1:C:523:ALA:HB3	1:C:526:ARG:HD3	1.64	0.78
1:D:19:ASN:HB3	1:D:107:MET:HG3	1.66	0.77
1:B:19:ASN:HB3	1:B:107:MET:HG3	1.67	0.76

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	371/565 (66%)	346 (93%)	23 (6%)	2 (0%)	34	77
1	B	546/565 (97%)	509 (93%)	33 (6%)	4 (1%)	26	72
1	C	544/565 (96%)	498 (92%)	40 (7%)	6 (1%)	17	65
1	D	372/565 (66%)	345 (93%)	25 (7%)	2 (0%)	34	77
All	All	1833/2260 (81%)	1698 (93%)	121 (7%)	14 (1%)	24	70

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	351	ASP
1	A	374	PRO
1	B	374	PRO
1	C	374	PRO
1	D	374	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	313/463 (68%)	275 (88%)	38 (12%)	6	34
1	B	449/463 (97%)	398 (89%)	51 (11%)	7	38
1	C	447/463 (96%)	393 (88%)	54 (12%)	6	34
1	D	314/463 (68%)	276 (88%)	38 (12%)	6	34
All	All	1523/1852 (82%)	1342 (88%)	181 (12%)	6	35

5 of 181 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	481	GLU
1	C	134	LEU
1	D	258	ARG
1	B	536	GLU
1	C	25	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	267	HIS
1	B	276	GLN
1	B	337	GLN

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 20 ligands modelled in this entry, 20 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 [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, 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	375/565 (66%)	0.22	20 (5%) 30 20	126, 189, 324, 425	0
1	B	548/565 (96%)	0.54	61 (11%) 7 5	135, 230, 370, 487	0
1	C	546/565 (96%)	0.54	57 (10%) 8 6	124, 223, 381, 519	0
1	D	376/565 (66%)	0.27	12 (3%) 51 35	124, 187, 332, 475	0
All	All	1845/2260 (81%)	0.42	150 (8%) 15 9	124, 205, 368, 519	0

The worst 5 of 150 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	516	CYS	17.2
1	B	307	GLY	12.1
1	D	398	ALA	10.3
1	C	114	GLU	8.6
1	C	519	VAL	8.6

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
4	CA	C	607	1/1	0.93	0.27	2.33	138,138,138,138	0
4	CA	B	602	1/1	0.90	0.20	0.30	175,175,175,175	0
4	CA	A	606	1/1	0.93	0.17	-1.17	173,173,173,173	0
2	K	A	603	1/1	0.82	0.21	-1.27	169,169,169,169	1
2	K	C	602	1/1	0.54	0.16	-1.32	153,153,153,153	1
2	K	A	601	1/1	0.99	0.12	-1.37	166,166,166,166	1
2	K	A	602	1/1	0.93	0.19	-1.84	154,154,154,154	1
2	K	C	604	1/1	0.99	0.07	-1.97	143,143,143,143	1
2	K	C	603	1/1	0.67	0.14	-2.34	160,160,160,160	1
4	CA	C	606	1/1	0.85	0.10	-4.42	185,185,185,185	0
3	ZN	B	601	1/1	0.98	0.28	-	134,134,134,134	0
2	K	C	601	1/1	0.99	0.12	-	207,207,207,207	1
2	K	A	608	1/1	0.74	0.19	-	225,225,225,225	1
3	ZN	C	605	1/1	0.98	0.28	-	152,152,152,152	0
2	K	C	608	1/1	0.72	0.50	-	241,241,241,241	1
3	ZN	D	601	1/1	0.99	0.24	-	149,149,149,149	0
2	K	C	609	1/1	0.83	0.78	-	200,200,200,200	1
2	K	A	604	1/1	0.99	0.12	-	186,186,186,186	1
3	ZN	A	605	1/1	0.98	0.25	-	160,160,160,160	0
2	K	A	607	1/1	0.90	0.81	-	199,199,199,199	1

6.5 Other polymers [i](#)

There are no such residues in this entry.