wwPDB X-ray Structure Validation Summary Report (i)

Sep 12, 2023 – 12:50 AM EDT

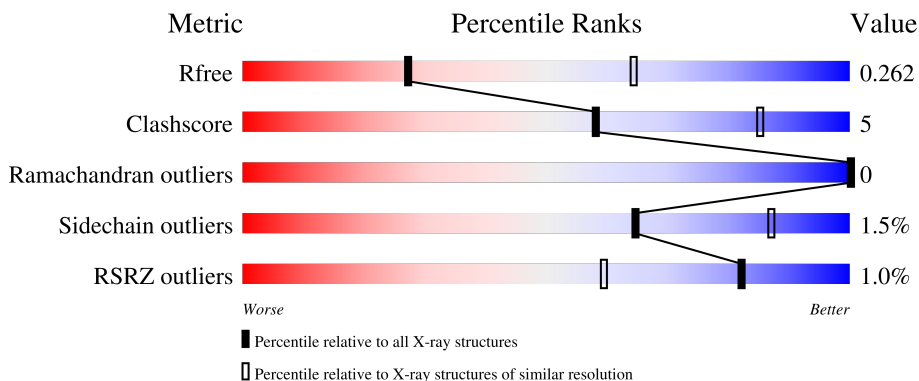|		
PDB ID	:	4L76
Title	:	Ca2+-bound E212Q mutant MthK RCK domain
Authors	:	Smith, F.J.; Rothberg, B.S.
Deposited on	:	2013-06-13
Resolution	:	2.99 Å(reported)

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 2.99 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.
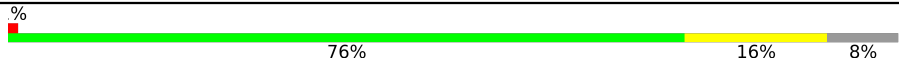
Metric	Percentile Ranks	Value
Rfree		0.262
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		1.5%
RSRZ outliers		1.0%

Worse   *Better*

▉ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 <=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	242	2% 82% 12% 6%
1	B	242	83% 9% 7%
1	C	242	% 79% 12% · 9%
1	D	242	75% 17% 8%
1	E	242	% 83% 9% 8%

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Mol	Chain	Length	Quality of chain
1	F	242	

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	CA	D	404	-	-	-	X

2   Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10218 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 Calcium-gated potassium channel MthK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1712	1072	299	334	7			
1	B	224	Total	C	N	O	S	0	0	0
			1715	1068	308	332	7			
1	C	221	Total	C	N	O	S	0	0	0
			1693	1057	297	332	7			
1	D	222	Total	C	N	O	S	0	0	0
			1684	1051	305	321	7			
1	E	223	Total	C	N	O	S	0	0	0
			1705	1064	302	332	7			
1	F	223	Total	C	N	O	S	0	0	0
			1693	1056	300	330	7			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	212	GLN	GLU	engineered mutation	UNP O27564
A	337	LEU	-	expression tag	UNP O27564
A	338	VAL	-	expression tag	UNP O27564
A	339	PRO	-	expression tag	UNP O27564
A	340	ARG	-	expression tag	UNP O27564
A	341	GLY	-	expression tag	UNP O27564
A	342	SER	-	expression tag	UNP O27564
A	343	HIS	-	expression tag	UNP O27564
A	344	HIS	-	expression tag	UNP O27564
A	345	HIS	-	expression tag	UNP O27564
A	346	HIS	-	expression tag	UNP O27564
A	347	HIS	-	expression tag	UNP O27564
A	348	HIS	-	expression tag	UNP O27564
B	212	GLN	GLU	engineered mutation	UNP O27564
B	337	LEU	-	expression tag	UNP O27564
B	338	VAL	-	expression tag	UNP O27564
B	339	PRO	-	expression tag	UNP O27564

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Chain	Residue	Modelled	Actual	Comment	Reference
B	340	ARG	-	expression tag	UNP O27564
B	341	GLY	-	expression tag	UNP O27564
B	342	SER	-	expression tag	UNP O27564
B	343	HIS	-	expression tag	UNP O27564
B	344	HIS	-	expression tag	UNP O27564
B	345	HIS	-	expression tag	UNP O27564
B	346	HIS	-	expression tag	UNP O27564
B	347	HIS	-	expression tag	UNP O27564
B	348	HIS	-	expression tag	UNP O27564
C	212	GLN	GLU	engineered mutation	UNP O27564
C	337	LEU	-	expression tag	UNP O27564
C	338	VAL	-	expression tag	UNP O27564
C	339	PRO	-	expression tag	UNP O27564
C	340	ARG	-	expression tag	UNP O27564
C	341	GLY	-	expression tag	UNP O27564
C	342	SER	-	expression tag	UNP O27564
C	343	HIS	-	expression tag	UNP O27564
C	344	HIS	-	expression tag	UNP O27564
C	345	HIS	-	expression tag	UNP O27564
C	346	HIS	-	expression tag	UNP O27564
C	347	HIS	-	expression tag	UNP O27564
C	348	HIS	-	expression tag	UNP O27564
D	212	GLN	GLU	engineered mutation	UNP O27564
D	337	LEU	-	expression tag	UNP O27564
D	338	VAL	-	expression tag	UNP O27564
D	339	PRO	-	expression tag	UNP O27564
D	340	ARG	-	expression tag	UNP O27564
D	341	GLY	-	expression tag	UNP O27564
D	342	SER	-	expression tag	UNP O27564
D	343	HIS	-	expression tag	UNP O27564
D	344	HIS	-	expression tag	UNP O27564
D	345	HIS	-	expression tag	UNP O27564
D	346	HIS	-	expression tag	UNP O27564
D	347	HIS	-	expression tag	UNP O27564
D	348	HIS	-	expression tag	UNP O27564
E	212	GLN	GLU	engineered mutation	UNP O27564
E	337	LEU	-	expression tag	UNP O27564
E	338	VAL	-	expression tag	UNP O27564
E	339	PRO	-	expression tag	UNP O27564
E	340	ARG	-	expression tag	UNP O27564
E	341	GLY	-	expression tag	UNP O27564
E	342	SER	-	expression tag	UNP O27564

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Chain	Residue	Modelled	Actual	Comment	Reference
E	343	HIS	-	expression tag	UNP O27564
E	344	HIS	-	expression tag	UNP O27564
E	345	HIS	-	expression tag	UNP O27564
E	346	HIS	-	expression tag	UNP O27564
E	347	HIS	-	expression tag	UNP O27564
E	348	HIS	-	expression tag	UNP O27564
F	212	GLN	GLU	engineered mutation	UNP O27564
F	337	LEU	-	expression tag	UNP O27564
F	338	VAL	-	expression tag	UNP O27564
F	339	PRO	-	expression tag	UNP O27564
F	340	ARG	-	expression tag	UNP O27564
F	341	GLY	-	expression tag	UNP O27564
F	342	SER	-	expression tag	UNP O27564
F	343	HIS	-	expression tag	UNP O27564
F	344	HIS	-	expression tag	UNP O27564
F	345	HIS	-	expression tag	UNP O27564
F	346	HIS	-	expression tag	UNP O27564
F	347	HIS	-	expression tag	UNP O27564
F	348	HIS	-	expression tag	UNP O27564

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Ca 2	0	0
2	B	2	Total 2	Ca 2	0	0
2	C	2	Total 2	Ca 2	0	0
2	D	3	Total 3	Ca 3	0	0
2	E	3	Total 3	Ca 3	0	0
2	F	1	Total 1	Ca 1	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Na 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total Na 1 1		0	0

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total O 1 1		0	0

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.
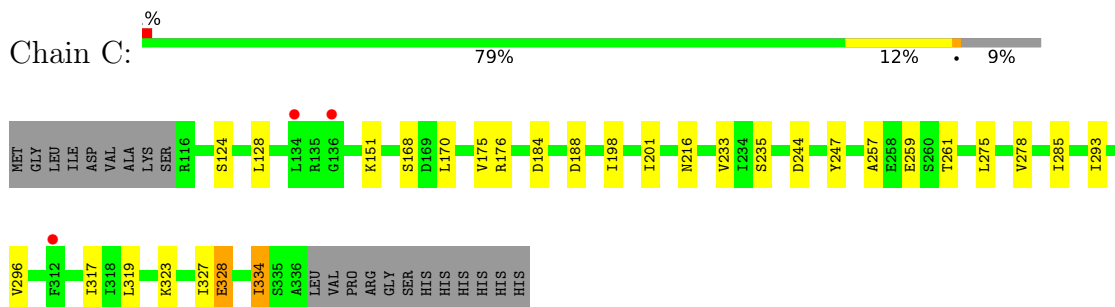
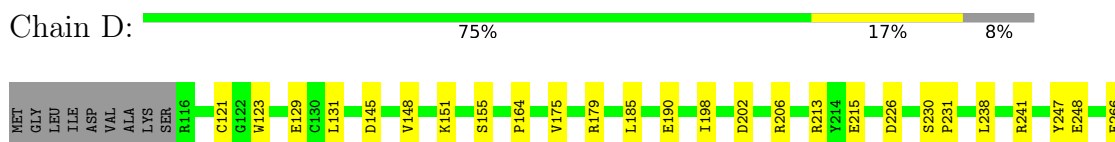• Molecule 1: Calcium-gated potassium channel MthK
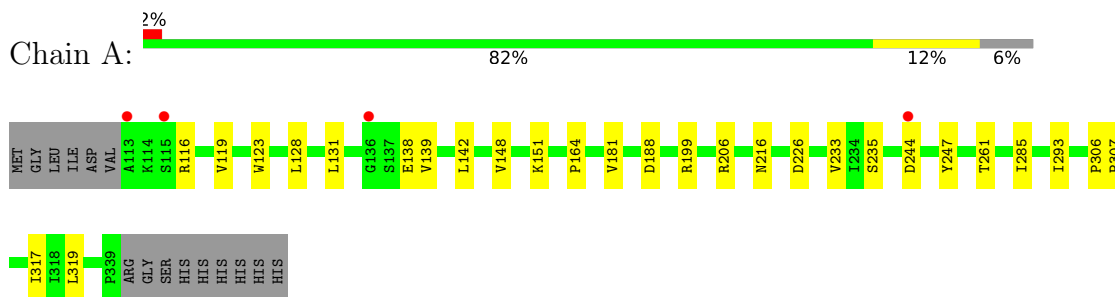
• Molecule 1: Calcium-gated potassium channel MthK

• Molecule 1: Calcium-gated potassium channel MthK

• Molecule 1: Calcium-gated potassium channel MthK

• Molecule 1: Calcium-gated potassium channel MthK

Chain E:

• Molecule 1: Calcium-gated potassium channel MthK

Chain F:
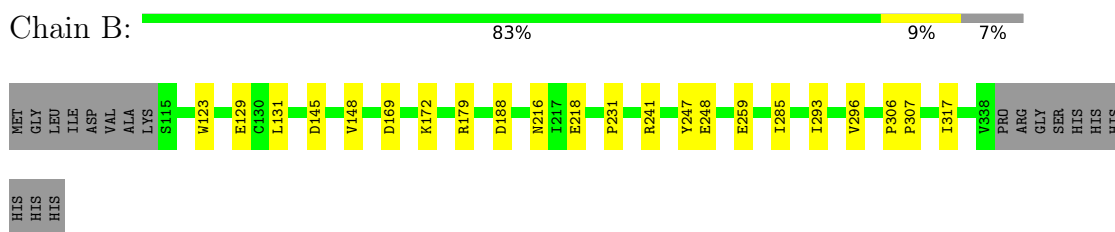
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	118.88Å 118.88Å 356.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.56 – 2.99 44.56 – 2.99	Depositor EDS
% Data completeness (in resolution range)	98.8 (44.56-2.99) 90.3 (44.56-2.99)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.217 , 0.263 0.217 , 0.262	Depositor DCC
R_{free} test set	2000 reflections (6.49%)	wwPDB-VP
Wilson B-factor (Å^2)	77.4	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 55.7	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10218	wwPDB-VP
Average B, all atoms (Å^2)	104.0	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 55.83 % 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 2.9873e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NA

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	0.36	0/1734	0.55	0/2350
1	B	0.39	0/1736	0.53	0/2346
1	C	0.32	0/1714	0.49	0/2317
1	D	0.34	0/1705	0.50	0/2307
1	E	0.33	0/1726	0.51	0/2333
1	F	0.37	0/1714	0.55	0/2320
All	All	0.35	0/10329	0.52	0/13973

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 (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	1712	0	1695	18	0
1	B	1715	0	1712	17	0
1	C	1693	0	1689	21	0
1	D	1684	0	1678	28	0
1	E	1705	0	1700	14	0
1	F	1693	0	1674	24	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	D	1	0	0	1	0
All	All	10218	0	10148	97	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 5.

The worst 5 of 97 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:E:116:ARG:HG3	1:E:179:ARG:HD2	1.70	0.73
1:F:281:LEU:HB2	1:F:308:ARG:HB2	1.76	0.67
1:D:213:ARG:NH2	1:D:215:GLU:OE1	2.28	0.67
1:F:285:ILE:HG21	1:F:293:ILE:HD11	1.77	0.66
1:A:285:ILE:HG21	1:A:293:ILE:HD11	1.79	0.64

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	225/242 (93%)	221 (98%)	4 (2%)	0	100	100
1	B	222/242 (92%)	219 (99%)	3 (1%)	0	100	100
1	C	219/242 (90%)	216 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	220/242 (91%)	217 (99%)	3 (1%)	0	100	100
1	E	221/242 (91%)	217 (98%)	4 (2%)	0	100	100
1	F	221/242 (91%)	219 (99%)	2 (1%)	0	100	100
All	All	1328/1452 (92%)	1309 (99%)	19 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	183/207 (88%)	182 (100%)	1 (0%)	88	96
1	B	185/207 (89%)	184 (100%)	1 (0%)	88	96
1	C	184/207 (89%)	179 (97%)	5 (3%)	44	77
1	D	179/207 (86%)	177 (99%)	2 (1%)	73	90
1	E	184/207 (89%)	181 (98%)	3 (2%)	62	86
1	F	181/207 (87%)	177 (98%)	4 (2%)	52	81
All	All	1096/1242 (88%)	1080 (98%)	16 (2%)	65	87

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	296	VAL
1	F	261	THR
1	D	328	GLU
1	F	146	GLU
1	D	296	VAL

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

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 15 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, 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(Å²)	Q<0.9
1	A	227/242 (93%)	0.02	4 (1%)	68	40	70, 95, 125, 150	0
1	B	224/242 (92%)	-0.01	0	100	100	69, 92, 118, 164	0
1	C	221/242 (91%)	0.15	3 (1%)	75	49	81, 112, 154, 184	0
1	D	222/242 (91%)	0.02	1 (0%)	91	75	78, 101, 134, 160	0
1	E	223/242 (92%)	0.14	3 (1%)	77	51	81, 112, 151, 162	0
1	F	223/242 (92%)	0.02	3 (1%)	77	51	72, 97, 125, 148	0
All	All	1340/1452 (92%)	0.06	14 (1%)	82	59	69, 101, 140, 184	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	115	SER	3.8
1	C	136	GLY	3.5
1	E	136	GLY	3.1
1	C	312	PHE	2.9
1	A	113	ALA	2.8

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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. 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	B-factors(Å^2)	Q<0.9
2	CA	A	401	1/1	0.34	0.20	135,135,135,135	0
2	CA	F	401	1/1	0.47	0.17	124,124,124,124	0
2	CA	C	401	1/1	0.56	0.23	152,152,152,152	0
2	CA	B	401	1/1	0.57	0.25	140,140,140,140	0
3	NA	D	403	1/1	0.65	0.17	88,88,88,88	0
3	NA	B	403	1/1	0.66	0.22	71,71,71,71	0
2	CA	D	404	1/1	0.74	0.42	171,171,171,171	0
2	CA	D	401	1/1	0.80	0.14	126,126,126,126	0
2	CA	B	402	1/1	0.86	0.09	97,97,97,97	0
2	CA	E	403	1/1	0.89	0.20	175,175,175,175	0
2	CA	E	401	1/1	0.90	0.05	136,136,136,136	0
2	CA	D	402	1/1	0.91	0.12	113,113,113,113	0
2	CA	C	402	1/1	0.92	0.06	138,138,138,138	0
2	CA	A	402	1/1	0.94	0.09	84,84,84,84	0
2	CA	E	402	1/1	0.96	0.15	112,112,112,112	0

6.5 Other polymers ⓘ

There are no such residues in this entry.