



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:18 am GMT

PDB ID : 2XEX  
Title : CRYSTAL STRUCTURE OF STAPHYLOCOCCUS AUREUS ELONGATION FACTOR G  
Authors : Chen, Y.; Koripella, R.K.; Sanyal, S.; Selmer, M.  
Deposited on : 2010-05-19  
Resolution : 1.90 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

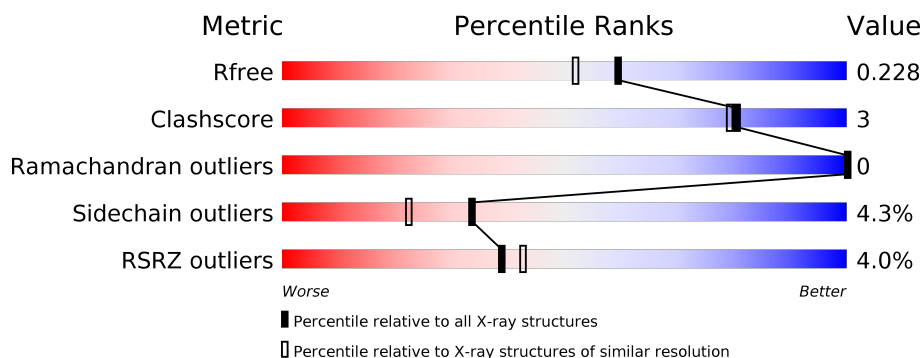
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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  $\geq 3$ , 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	693	<div> <div>4%</div> <div> <div></div> <div>88%</div> <div>8%</div> <div>•</div> </div> </div>
1	B	693	<div> <div>4%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div>••</div> </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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	K	A	1694	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10865 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 ELONGATION FACTOR G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	664	Total	C	N	O	S	0	0	1
			5130	3218	865	1019	28			
1	B	675	Total	C	N	O	S	0	0	1
			5222	3275	880	1037	30			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	K	0	0
			1	1		
2	A	1	Total	K	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

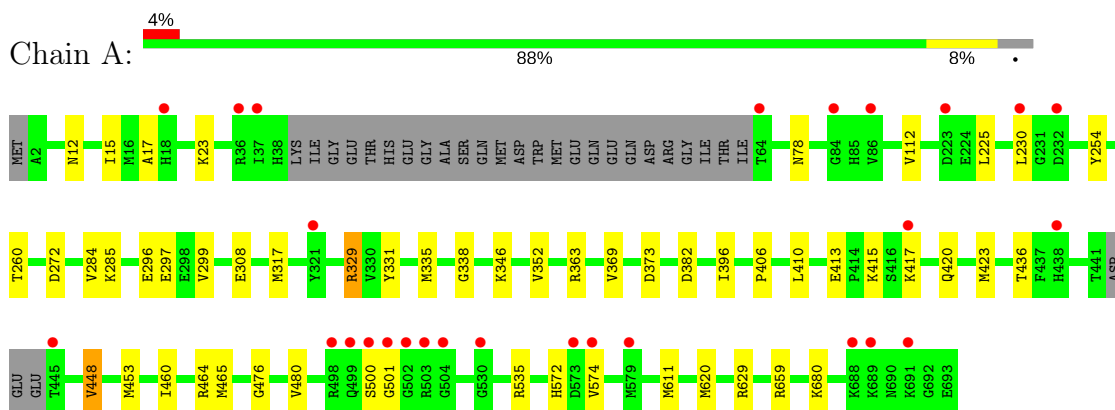
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	245	Total	O	0	0
			245	245		
4	B	264	Total	O	0	0
			264	264		

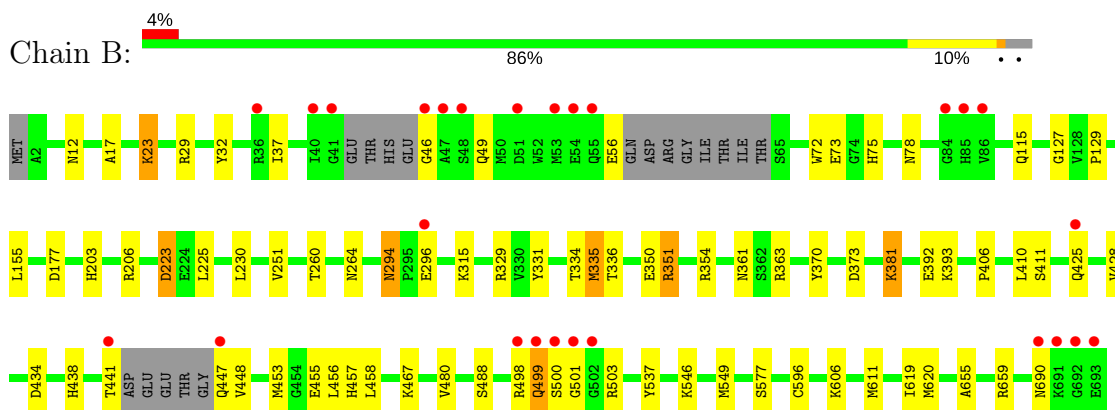
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: ELONGATION FACTOR G



#### • Molecule 1: ELONGATION FACTOR G



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.16Å 137.34Å 125.36Å 90.00° 94.93° 90.00°	Depositor
Resolution (Å)	46.20 – 1.90 46.20 – 1.90	Depositor EDS
% Data completeness (in resolution range)	92.7 (46.20-1.90) 92.8 (46.20-1.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.187 , 0.224 0.192 , 0.228	Depositor DCC
$R_{free}$ test set	4777 reflections (4.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.9	Xtriage
Anisotropy	0.674	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 54.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10865	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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 ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.91	2/5220 (0.0%)	0.77	4/7058 (0.1%)
1	B	0.91	2/5313 (0.0%)	0.75	3/7179 (0.0%)
All	All	0.91	4/10533 (0.0%)	0.76	7/14237 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	254	TYR	CD2-CE2	6.30	1.48	1.39
1	A	308	GLU	CB-CG	5.66	1.62	1.52
1	B	72	TRP	CB-CG	5.50	1.60	1.50
1	B	655	ALA	CA-CB	5.07	1.63	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	659	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	A	629	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	272	ASP	CB-CG-OD2	6.16	123.84	118.30
1	B	659	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	B	354	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	B	177	ASP	CB-CG-OD2	5.68	123.41	118.30
1	A	272	ASP	CB-CG-OD1	-5.07	113.74	118.30

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	5130	0	5039	21	0
1	B	5222	0	5121	43	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	245	0	0	0	0
4	B	264	0	0	1	0
All	All	10865	0	10160	64	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 (64) 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:294:ASN:HD21	1:B:296:GLU:HG2	1.24	1.01
1:B:351:ARG:HH11	1:B:351:ARG:HG3	1.33	0.93
1:B:351:ARG:HH11	1:B:351:ARG:CG	1.85	0.89
1:B:350:GLU:OE1	1:B:381:LYS:HE3	1.72	0.88
1:B:29:ARG:HH11	1:B:264:ASN:HD21	1.18	0.87
1:B:37:ILE:HG12	1:B:361:ASN:ND2	1.90	0.86
1:B:32:TYR:HA	1:B:37:ILE:HD12	1.61	0.82
1:B:203:HIS:HD2	1:B:206:ARG:HH11	1.29	0.79
1:B:453:MET:H	1:B:457:HIS:HD2	1.29	0.76
1:A:423:MET:HG3	1:A:465:MET:CE	2.18	0.74
1:B:294:ASN:ND2	1:B:296:GLU:HG2	2.01	0.73
1:A:406:PRO:HA	1:A:453:MET:HE1	1.71	0.72
1:A:423:MET:HG3	1:A:465:MET:HE3	1.72	0.71
1:B:37:ILE:HG12	1:B:361:ASN:HD22	1.55	0.71
1:B:49:GLN:NE2	1:B:264:ASN:OD1	2.25	0.70
1:B:498:ARG:HG2	1:B:499:GLN:H	1.59	0.67
1:B:203:HIS:CD2	1:B:206:ARG:HH11	2.13	0.66
1:A:299:VAL:HG11	1:A:396:ILE:HD12	1.79	0.64
1:B:12:ASN:HD22	1:B:78:ASN:HB2	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:ILE:O	1:A:464:ARG:HG3	2.01	0.60
1:B:546:LYS:HA	1:B:549:MET:HE2	1.85	0.59
1:B:406:PRO:HD3	1:B:438:HIS:CD2	2.39	0.57
1:A:572:HIS:CE1	1:A:574:VAL:HG22	2.39	0.57
1:A:423:MET:SD	1:A:448:VAL:HG11	2.45	0.57
1:B:46:GLY:O	1:B:49:GLN:HG3	2.05	0.55
1:B:434:ASP:OD2	1:B:457:HIS:HE1	1.88	0.55
1:A:572:HIS:HE1	1:A:574:VAL:HG22	1.72	0.55
1:A:410:LEU:HD11	1:A:476:GLY:O	2.07	0.55
1:B:335:MET:HG2	1:B:336:THR:N	2.21	0.54
1:A:17:ALA:HB3	1:A:23:LYS:HB2	1.88	0.54
1:B:441:THR:HG22	1:B:448:VAL:HG22	1.90	0.53
1:B:127:GLY:O	1:B:129:PRO:HD3	2.09	0.53
1:A:284:VAL:HG22	1:A:285:LYS:H	1.75	0.52
1:B:351:ARG:NH1	1:B:351:ARG:CG	2.54	0.51
1:B:498:ARG:HH11	1:B:498:ARG:HB2	1.76	0.51
1:B:453:MET:H	1:B:457:HIS:CD2	2.18	0.50
1:B:203:HIS:HD2	1:B:206:ARG:HD3	1.76	0.50
1:B:411:SER:OG	1:B:447:GLN:OE1	2.29	0.49
1:A:299:VAL:CG1	1:A:396:ILE:HD12	2.41	0.49
1:B:498:ARG:NH1	1:B:498:ARG:HB2	2.27	0.49
1:B:410:LEU:HB2	1:B:458:LEU:HD13	1.94	0.48
1:B:606:LYS:HE2	4:B:2259:HOH:O	2.14	0.47
1:A:284:VAL:HG22	1:A:285:LYS:N	2.29	0.47
1:A:12:ASN:HD22	1:A:78:ASN:HB2	1.79	0.47
1:B:203:HIS:CD2	1:B:206:ARG:HD3	2.49	0.47
1:A:329:ARG:HG2	1:A:331:TYR:CZ	2.50	0.47
1:B:17:ALA:O	1:B:23:LYS:HE2	2.15	0.47
1:B:223:ASP:OD1	1:B:223:ASP:N	2.46	0.47
1:A:500:SER:HA	1:A:501:GLY:HA2	1.64	0.46
1:B:329:ARG:HG2	1:B:331:TYR:CZ	2.50	0.45
1:A:436:THR:O	1:A:453:MET:HE2	2.18	0.44
1:A:15:ILE:O	1:A:23:LYS:HE3	2.18	0.43
1:B:455:GLU:HG3	1:B:456:LEU:N	2.34	0.43
1:A:338:GLY:N	1:A:352:VAL:O	2.43	0.43
1:B:498:ARG:CG	1:B:499:GLN:H	2.30	0.43
1:B:115:GLN:CD	1:B:115:GLN:H	2.22	0.42
1:B:37:ILE:HG12	1:B:361:ASN:HD21	1.78	0.42
1:B:500:SER:HA	1:B:501:GLY:HA2	1.71	0.42
1:B:488:SER:HB2	1:B:596:CYS:HA	2.01	0.42
1:B:537:TYR:OH	1:B:577:SER:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:ARG:HB2	1:A:535:ARG:HE	1.56	0.41
1:B:370:TYR:O	1:B:373:ASP:HB2	2.20	0.41
1:A:369:VAL:HG12	1:A:373:ASP:HB2	2.03	0.41
1:B:73:GLU:O	1:B:75:HIS:HD2	2.04	0.40

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	658/693 (95%)	644 (98%)	14 (2%)	0	100	100
1	B	667/693 (96%)	651 (98%)	16 (2%)	0	100	100
All	All	1325/1386 (96%)	1295 (98%)	30 (2%)	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	553/579 (96%)	532 (96%)	21 (4%)	38	27
1	B	562/579 (97%)	535 (95%)	27 (5%)	30	18
All	All	1115/1158 (96%)	1067 (96%)	48 (4%)	33	22

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	VAL
1	A	225	LEU
1	A	230	LEU
1	A	260	THR
1	A	296	GLU
1	A	297	GLU
1	A	317	MET
1	A	329	ARG
1	A	335	MET
1	A	346	LYS
1	A	363	ARG
1	A	382	ASP
1	A	413	GLU
1	A	415	LYS
1	A	417	LYS
1	A	420	GLN
1	A	448	VAL
1	A	480	VAL
1	A	611	MET
1	A	620	MET
1	A	680	LYS
1	B	23	LYS
1	B	56	GLU
1	B	155	LEU
1	B	223	ASP
1	B	225	LEU
1	B	230	LEU
1	B	251	VAL
1	B	260	THR
1	B	294	ASN
1	B	315	LYS
1	B	334	THR
1	B	335	MET
1	B	351	ARG
1	B	363	ARG
1	B	381	LYS
1	B	392	GLU
1	B	393	LYS
1	B	425	GLN
1	B	428	VAL
1	B	467	LYS
1	B	480	VAL

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Mol	Chain	Res	Type
1	B	499	GLN
1	B	503	ARG
1	B	611	MET
1	B	619	ILE
1	B	620	MET
1	B	690	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	78	ASN
1	A	158	ASN
1	A	290	HIS
1	A	409	HIS
1	A	505	GLN
1	B	12	ASN
1	B	49	GLN
1	B	75	HIS
1	B	78	ASN
1	B	158	ASN
1	B	203	HIS
1	B	250	ASN
1	B	264	ASN
1	B	294	ASN
1	B	359	HIS
1	B	361	ASN
1	B	425	GLN
1	B	457	HIS
1	B	505	GLN
1	B	690	ASN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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

### 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<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	664/693 (95%)	0.13	27 (4%) 38 42	7, 20, 37, 62	0
1	B	675/693 (97%)	0.07	26 (3%) 40 44	10, 20, 39, 70	0
All	All	1339/1386 (96%)	0.10	53 (3%) 39 43	7, 20, 38, 70	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	501	GLY	8.7
1	A	500	SER	8.2
1	B	47	ALA	6.0
1	B	692	GLY	5.3
1	B	500	SER	5.1
1	A	499	GLN	4.8
1	A	503	ARG	4.5
1	A	445	THR	4.5
1	B	55	GLN	4.4
1	B	86	VAL	3.9
1	A	504	GLY	3.6
1	A	84	GLY	3.6
1	A	37	ILE	3.6
1	A	498	ARG	3.5
1	B	693	GLU	3.3
1	B	441	THR	3.2
1	A	574	VAL	3.1
1	A	688	LYS	3.1
1	A	230	LEU	3.0
1	A	689	LYS	3.0
1	A	64	THR	2.9
1	B	46	GLY	2.9
1	B	691	LYS	2.8
1	A	691	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	86	VAL	2.7
1	A	573	ASP	2.7
1	A	530	GLY	2.6
1	B	425	GLN	2.5
1	A	36	ARG	2.5
1	B	51	ASP	2.5
1	B	499	GLN	2.4
1	B	84	GLY	2.4
1	B	501	GLY	2.4
1	B	54	GLU	2.4
1	B	36	ARG	2.4
1	B	53	MET	2.4
1	A	438	HIS	2.4
1	B	296	GLU	2.4
1	B	40	ILE	2.3
1	A	223	ASP	2.3
1	B	48	SER	2.3
1	A	579	MET	2.2
1	B	690	ASN	2.2
1	A	502	GLY	2.2
1	A	417	LYS	2.2
1	B	85	HIS	2.2
1	B	502	GLY	2.2
1	A	232	ASP	2.1
1	B	447	GLN	2.1
1	A	321	TYR	2.1
1	B	41	GLY	2.0
1	B	498	ARG	2.0
1	A	18	HIS	2.0

## 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 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	K	A	1694	1/1	0.96	0.17	5.30	46,46,46,46	0
2	K	B	1694	1/1	0.95	0.14	0.28	51,51,51,51	0
3	CL	B	1693	1/1	0.98	0.10	0.24	24,24,24,24	0
3	CL	A	1693	1/1	0.95	0.09	-0.10	33,33,33,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.