



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2023 – 01:10 PM EDT

PDB ID : 1OTT  
Title : Structure of the Escherichia coli ClC Chloride channel E148A mutant and Fab Complex  
Authors : Dutzler, R.; Campbell, E.B.; MacKinnon, R.  
Deposited on : 2003-03-23  
Resolution : 3.00 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](mailto: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>.

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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) : 1.13  
EDS : 2.35  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

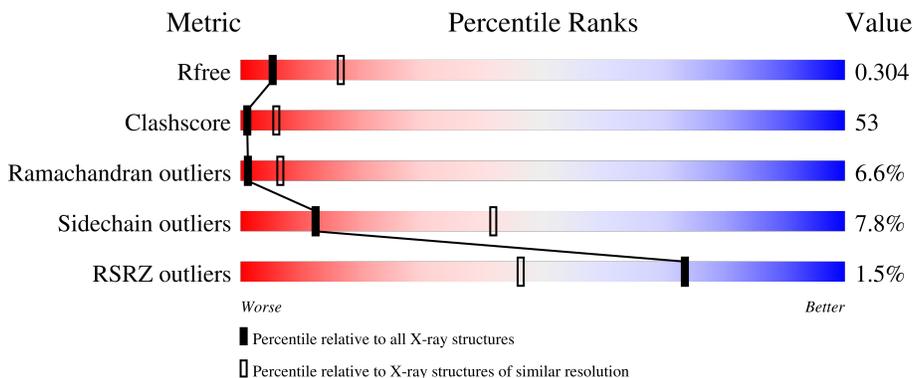
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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.



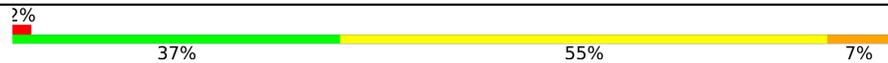
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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  $\geq 3$ , 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	465	
1	B	465	
2	C	222	
2	E	222	
3	D	211	

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Mol	Chain	Length	Quality of chain
3	F	211	 2% 37% 55% 7%

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
4	CL	A	466	-	-	X	-
4	CL	A	468	-	-	-	X
4	CL	B	466	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13221 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 Voltage-gated ClC-type chloride channel eriC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	444	3329	2188	560	561	20	0	0	0
1	B	441	3300	2172	553	555	20	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	148	ALA	GLU	engineered mutation	UNP P37019
B	148	ALA	GLU	engineered mutation	UNP P37019

- Molecule 2 is a protein called Fab fragment (Heavy chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	221	1672	1077	274	315	6	0	0	0
2	E	221	1672	1077	274	315	6	0	0	0

- Molecule 3 is a protein called Fab fragment (Light chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	211	1621	1008	271	334	8	0	0	0
3	F	211	1621	1008	271	334	8	0	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

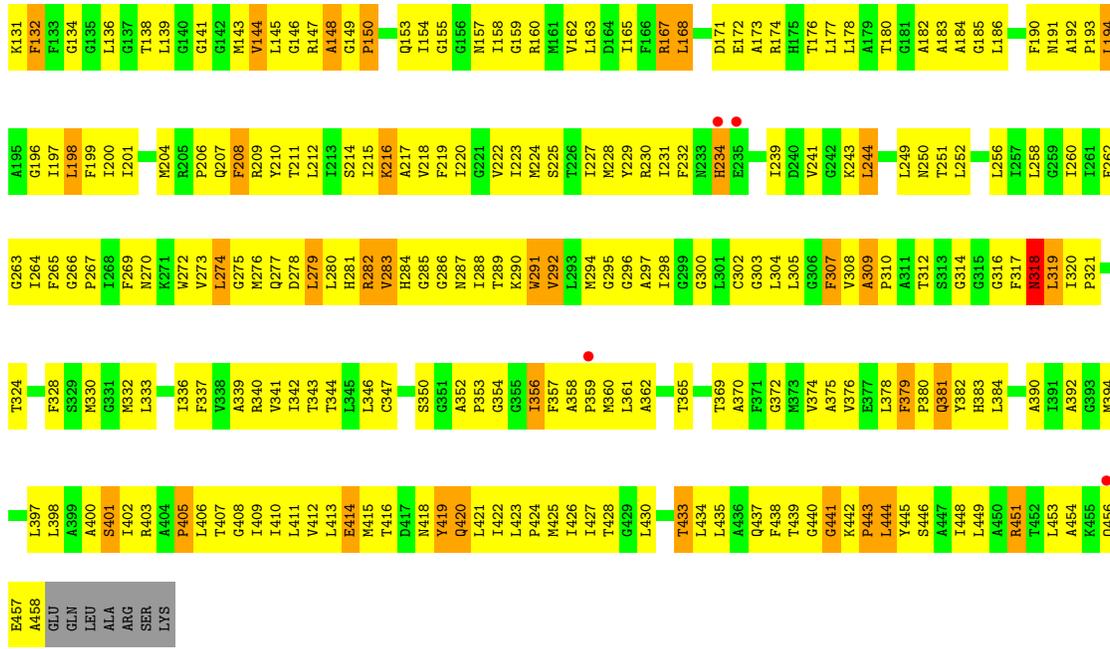
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Cl 3 3	0	0

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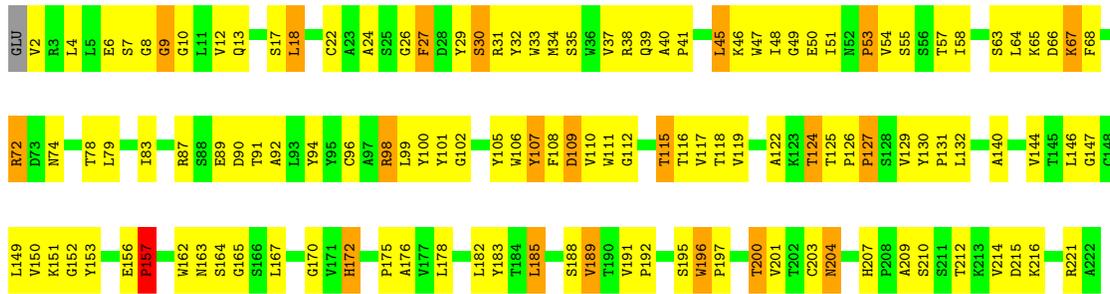
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	B	3	Total 3	Cl 3	0	0

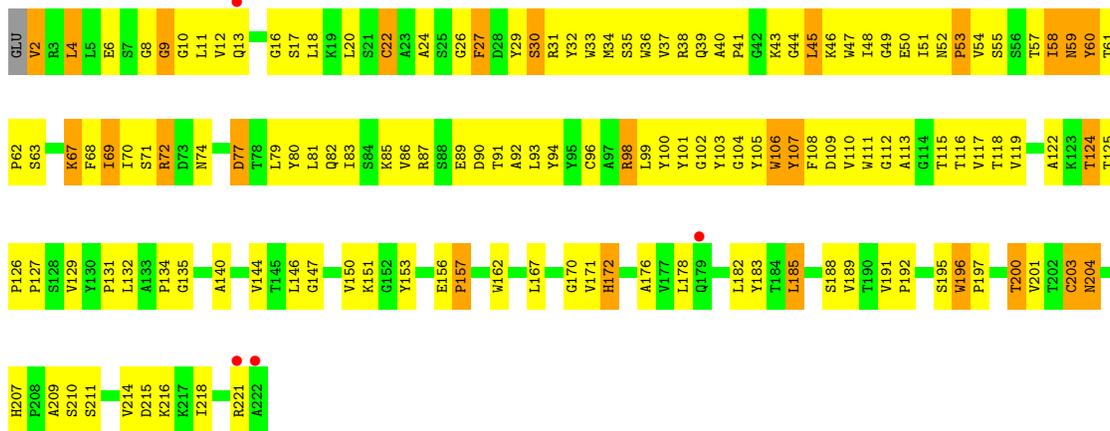




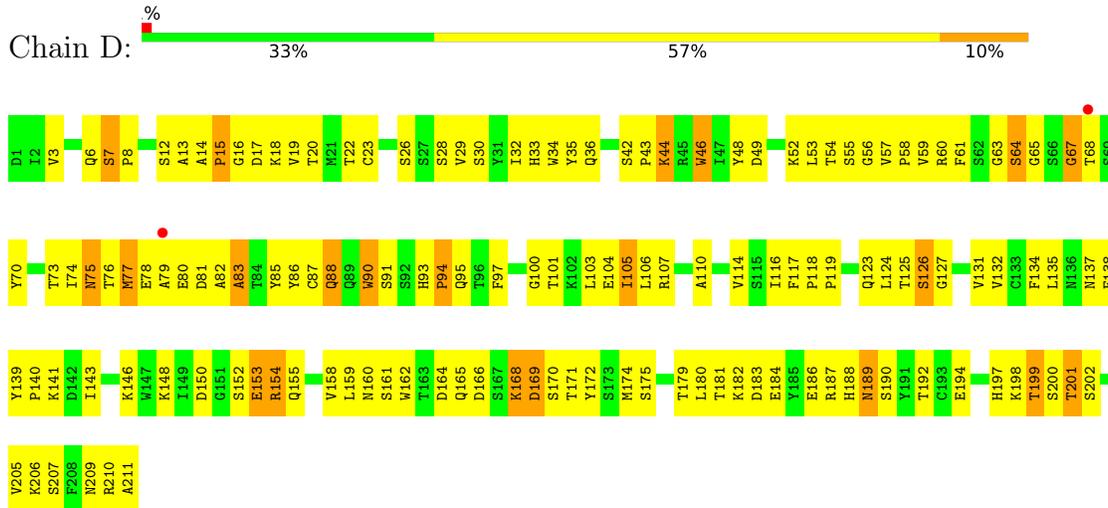
• Molecule 2: Fab fragment (Heavy chain)



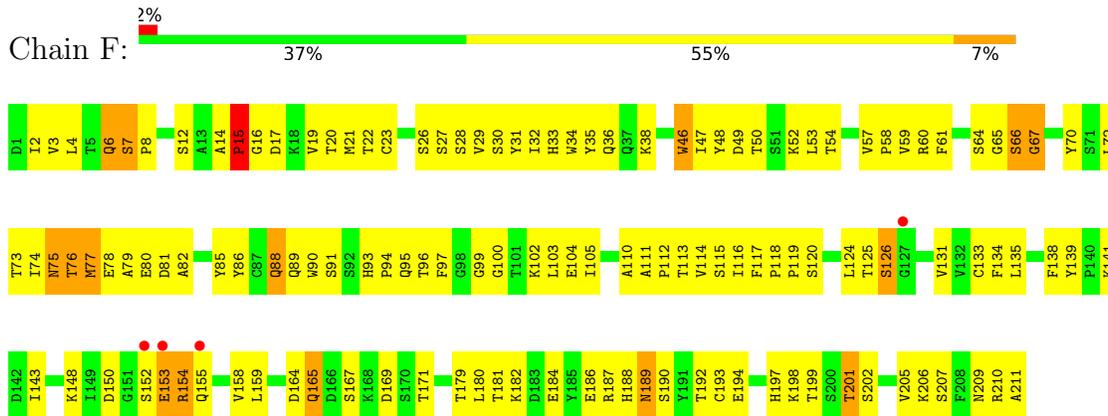
• Molecule 2: Fab fragment (Heavy chain)



- Molecule 3: Fab fragment (Light chain)



- Molecule 3: Fab fragment (Light chain)



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	231.61Å 95.72Å 169.82Å 90.00° 131.45° 90.00°	Depositor
Resolution (Å)	24.99 – 3.00 34.66 – 3.00	Depositor EDS
% Data completeness (in resolution range)	93.1 (24.99-3.00) 93.1 (34.66-3.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.62 (at 3.00Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.296 , 0.338 0.272 , 0.304	Depositor DCC
$R_{free}$ test set	2558 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	77.0	Xtrriage
Anisotropy	0.511	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 51.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.003 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	13221	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.43	0/3401	0.64	0/4616
1	B	0.47	0/3372	0.66	0/4578
2	C	0.48	0/1721	0.73	0/2355
2	E	0.50	0/1721	0.75	0/2355
3	D	0.43	0/1660	0.69	0/2257
3	F	0.50	0/1660	0.74	0/2257
All	All	0.47	0/13535	0.69	0/18418

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
3	F	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	F	139	TYR	Sidechain

### 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	3329	0	3483	442	0
1	B	3300	0	3456	446	0
2	C	1672	0	1654	141	0
2	E	1672	0	1654	170	0
3	D	1621	0	1546	154	0
3	F	1621	0	1546	166	0
4	A	3	0	0	4	0
4	B	3	0	0	4	0
All	All	13221	0	13339	1409	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 53.

The worst 5 of 1409 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)
3:D:16:GLY:HA2	3:D:76:THR:HG23	1.30	1.14
1:A:223:ILE:HD11	1:B:426:ILE:HG22	1.26	1.11
3:F:194:GLU:HG2	3:F:205:VAL:HG12	1.33	1.10
1:A:381:GLN:HE21	1:A:381:GLN:N	1.50	1.07
1:B:163:LEU:HD12	1:B:168:LEU:HD12	1.36	1.06

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	442/465 (95%)	307 (70%)	103 (23%)	32 (7%)	<b>1</b> <b>5</b>
1	B	439/465 (94%)	294 (67%)	117 (27%)	28 (6%)	<b>1</b> <b>7</b>
2	C	219/222 (99%)	176 (80%)	28 (13%)	15 (7%)	<b>1</b> <b>6</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	219/222 (99%)	171 (78%)	35 (16%)	13 (6%)	1	9
3	D	209/211 (99%)	169 (81%)	24 (12%)	16 (8%)	1	5
3	F	209/211 (99%)	164 (78%)	35 (17%)	10 (5%)	2	13
All	All	1737/1796 (97%)	1281 (74%)	342 (20%)	114 (7%)	1	6

5 of 114 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	ALA
1	A	171	ASP
1	A	283	VAL
1	A	309	ALA
1	A	438	PHE

### 5.3.2 Protein sidechains [i](#)

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	334/352 (95%)	309 (92%)	25 (8%)	13	43
1	B	331/352 (94%)	306 (92%)	25 (8%)	13	43
2	C	181/182 (100%)	162 (90%)	19 (10%)	7	27
2	E	181/182 (100%)	161 (89%)	20 (11%)	6	25
3	D	185/185 (100%)	174 (94%)	11 (6%)	19	54
3	F	185/185 (100%)	176 (95%)	9 (5%)	25	61
All	All	1397/1438 (97%)	1288 (92%)	109 (8%)	12	42

5 of 109 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	67	LYS
3	D	46	TRP
2	E	204	ASN
2	C	98	ARG

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Mol	Chain	Res	Type
2	C	200	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	93	HIS
3	F	137	ASN
3	D	136	ASN
3	D	189	ASN
3	F	189	ASN

### 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 monosaccharides 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 [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, 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	444/465 (95%)	-0.14	6 (1%) 75 49	52, 78, 101, 112	0
1	B	441/465 (94%)	-0.19	11 (2%) 57 29	47, 77, 104, 122	0
2	C	221/222 (99%)	-0.20	0 100 100	46, 77, 98, 128	0
2	E	221/222 (99%)	-0.25	4 (1%) 68 40	43, 79, 98, 119	0
3	D	211/211 (100%)	-0.07	2 (0%) 84 63	64, 91, 103, 110	0
3	F	211/211 (100%)	-0.16	4 (1%) 66 37	42, 73, 101, 112	0
All	All	1749/1796 (97%)	-0.17	27 (1%) 73 46	42, 79, 103, 128	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	235	GLU	5.1
1	A	72	ALA	4.5
1	A	168	LEU	4.1
1	B	70	HIS	3.7
1	B	72	ALA	3.5

### 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 monosaccharides 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
4	CL	A	468	1/1	0.60	0.71	117,117,117,117	0
4	CL	B	468	1/1	0.85	0.36	90,90,90,90	0
4	CL	B	466	1/1	0.86	0.19	66,66,66,66	0
4	CL	B	467	1/1	0.88	0.30	76,76,76,76	0
4	CL	A	466	1/1	0.90	0.50	76,76,76,76	0
4	CL	A	467	1/1	0.91	0.72	91,91,91,91	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.