



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 02:42 AM GMT

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 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/ValidationPDFNotes.html>

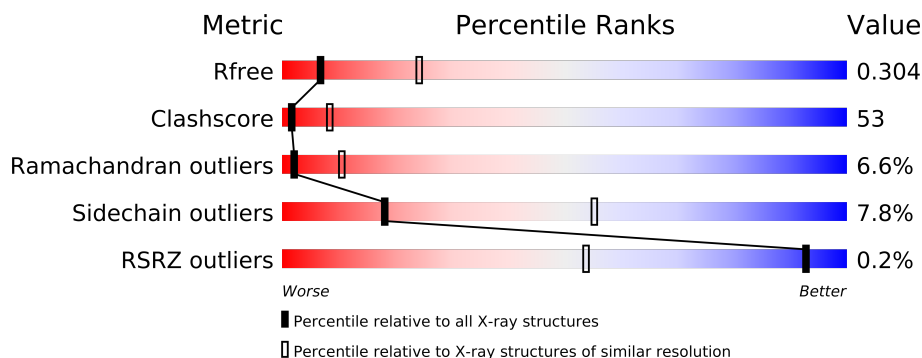
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	465	
1	B	465	
2	C	222	
2	E	222	
3	D	211	
3	F	211	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	CL	A	467	-	X
4	CL	A	468	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13221 atoms, of which 0 are hydrogen and 0 are deuterium.

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
1	A	444	Total	C	N	O	S	0	0	0
			3329	2188	560	561	20			
1	B	441	Total	C	N	O	S	0	0	0
			3300	2172	553	555	20			

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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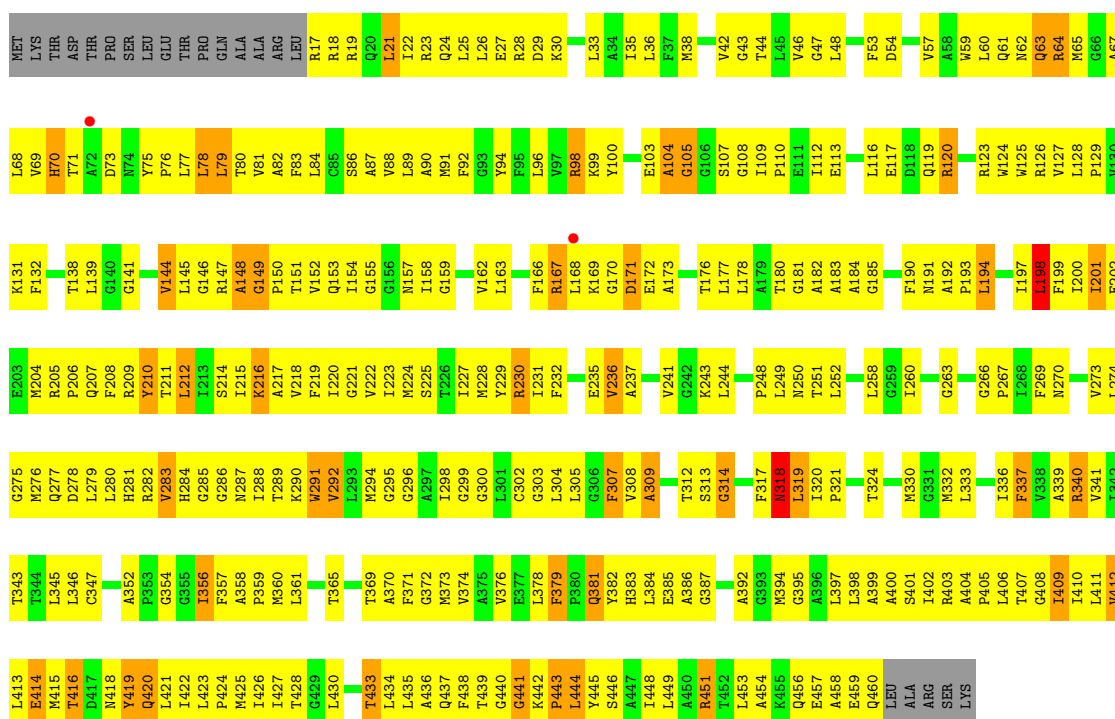
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Cl	0	0
			3	3		

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 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.

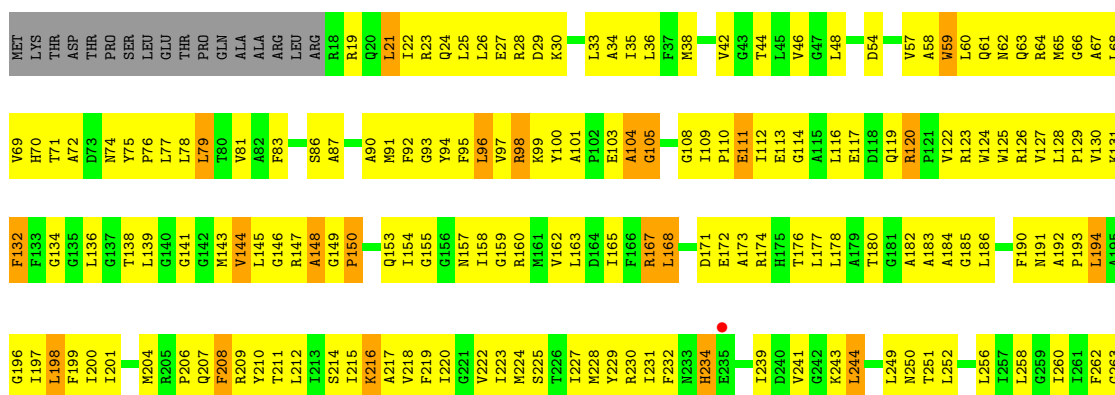
- Molecule 1: Voltage-gated ClC-type chloride channel eriC

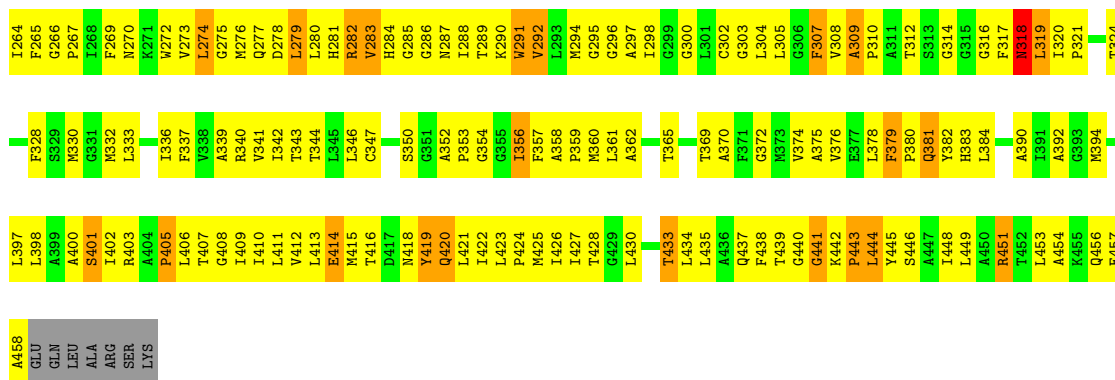
Chain A:



- Molecule 1: Voltage-gated ClC-type chloride channel eriC

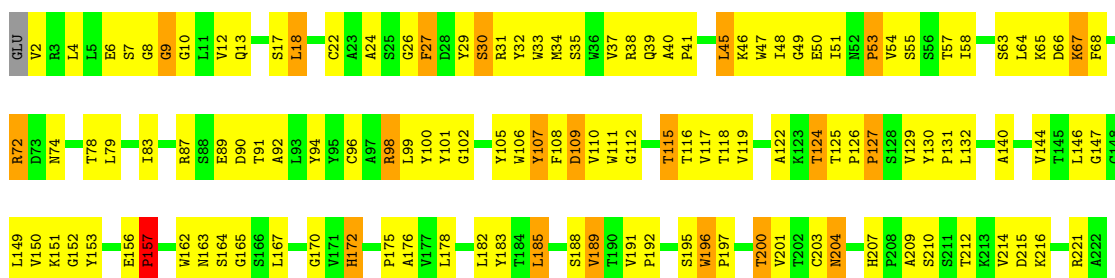
Chain B:





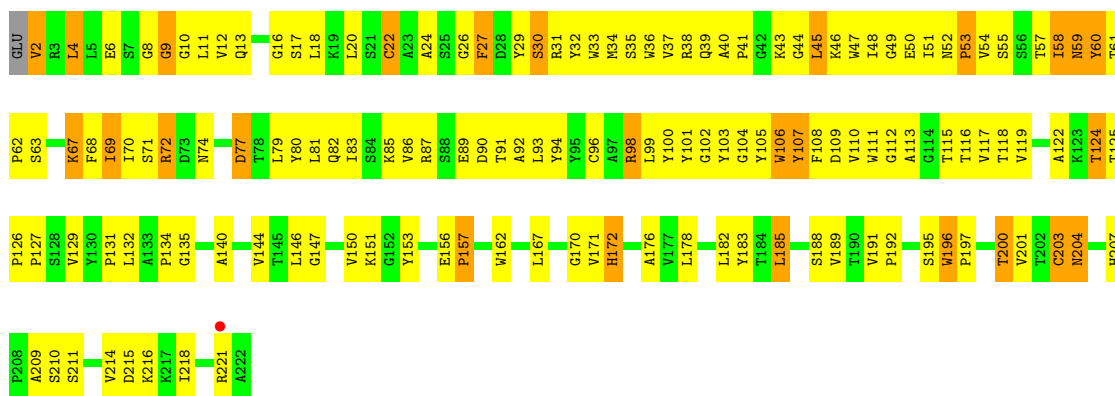
• Molecule 2: Fab fragment (Heavy chain)

Chain C:



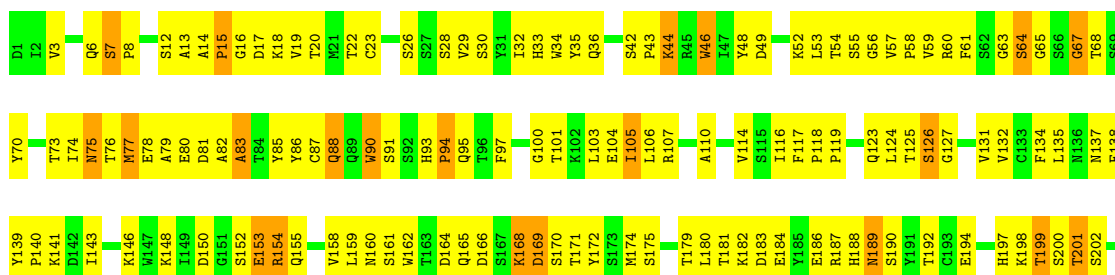
• Molecule 2: Fab fragment (Heavy chain)

Chain E:



• Molecule 3: Fab fragment (Light chain)

Chain D:



V205
K206
S207
F208
N209
R210
A211

● Molecule 3: Fab fragment (Light chain)

Chain F:

D1	I2	V3	L4	T5	Q6	S7	P8		S12	A13	A14	P15	G16	D17	K18	V19	T20	M21	T22	C23		S26	S27	S28	V29	S30	S31	I32	H33	W34	Y35	Q36	Q37	K38		W46	I47	Y48	D49	T50	S51	K52	L53	T54		V57	P58	V59	R60	F61		S64	G65	S66	G67		Y70	S71	L72
T73	I74	N75	T76	M77	E78	A79	E80	D81	A82		Y85	Y86	G87	Q88	Q89	W90	S91	S92	H93	P94	Q95	T96	F97	G98	G99	G100	T101	K102	L103	E104	I105		A110	A111	P112	T113	V114	S115	T116	F117	P118	P119	S120		L124	T125	S126		V131	V132	C133	F134	L135		F138	Y139	P140	K141	D142
I143		K148	I149	D150	G151	S152	E153	R154	Q155		V158	L159		D164	Q165	D166	S167	K168	D169	S170	T171		T179	L180	T181	K182	D183	E184	Y185	E186	R187	H188	M189	S190	Y191	T192	C193	E194		H197	K198	T199	S200	T201	S202		V205	K206	S207	F208	N209	R210	A211						

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 3.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.296 , 0.338 0.272 , 0.304	Depositor DCC
R_{free} test set	2556 reflections (4.91%)	DCC
Wilson B-factor (Å ²)	77.0	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 56.4	EDS
Estimated twinning fraction	0.003 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 52146 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	13221	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 53.

The worst 5 of 1409 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:N	1:A:381:GLN:HE21	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

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	442/465 (95%)	307 (70%)	103 (23%)	32 (7%)	2	8
1	B	439/465 (94%)	294 (67%)	117 (27%)	28 (6%)	2	11
2	C	219/222 (99%)	176 (80%)	28 (13%)	15 (7%)	2	10
2	E	219/222 (99%)	171 (78%)	35 (16%)	13 (6%)	2	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	209/211 (99%)	169 (81%)	24 (12%)	16 (8%)	1	7
3	F	209/211 (99%)	164 (78%)	35 (17%)	10 (5%)	4	20
All	All	1737/1796 (97%)	1281 (74%)	342 (20%)	114 (7%)	2	10

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 ⓘ

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%)	19	57
1	B	331/352 (94%)	306 (92%)	25 (8%)	19	57
2	C	181/182 (100%)	162 (90%)	19 (10%)	10	37
2	E	181/182 (100%)	161 (89%)	20 (11%)	9	34
3	D	185/185 (100%)	174 (94%)	11 (6%)	28	70
3	F	185/185 (100%)	176 (95%)	9 (5%)	35	78
All	All	1397/1438 (97%)	1288 (92%)	109 (8%)	18	55

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

Mol	Chain	Res	Type
1	B	451	ARG
2	C	115	THR
3	F	6	GLN
2	C	4	LEU
2	C	63	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such

sidechains are listed below:

Mol	Chain	Res	Type
1	B	207	GLN
1	B	287	ASN
3	F	137	ASN
1	B	270	ASN
1	B	318	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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.

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(Å ²)	Q<0.9
1	A	444/465 (95%)	-0.15	2 (0%) 88 36	52, 78, 101, 112	0
1	B	441/465 (94%)	-0.21	1 (0%) 93 54	47, 77, 104, 122	0
2	C	221/222 (99%)	-0.17	0 100 100	46, 77, 98, 128	0
2	E	221/222 (99%)	-0.19	1 (0%) 88 36	43, 79, 98, 119	0
3	D	211/211 (100%)	-0.11	0 100 100	64, 91, 103, 110	0
3	F	211/211 (100%)	-0.14	0 100 100	42, 73, 101, 112	0
All	All	1749/1796 (97%)	-0.17	4 (0%) 93 54	42, 79, 103, 128	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	168	LEU	2.8
1	B	235	GLU	2.7
1	A	72	ALA	2.4
2	E	221	ARG	2.3

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 ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	CL	A	467	1/1	0.55	4.60	91,91,91,91	0
4	CL	A	468	1/1	0.46	2.85	117,117,117,117	0
4	CL	A	466	1/1	0.40	1.20	76,76,76,76	0
4	CL	B	468	1/1	0.34	0.74	90,90,90,90	0
4	CL	B	467	1/1	0.26	-0.04	76,76,76,76	0
4	CL	B	466	1/1	0.15	-2.07	66,66,66,66	0

6.5 Other polymers ⓘ

There are no such residues in this entry.