



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2018 – 10:34 pm GMT

PDB ID : 2EXW  
Title : Crystal structure of a EcCIC-Fab complex in the absence of bound ions  
Authors : Lobet, S.; Dutzler, R.  
Deposited on : 2005-11-09  
Resolution : 3.20 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.

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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 : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

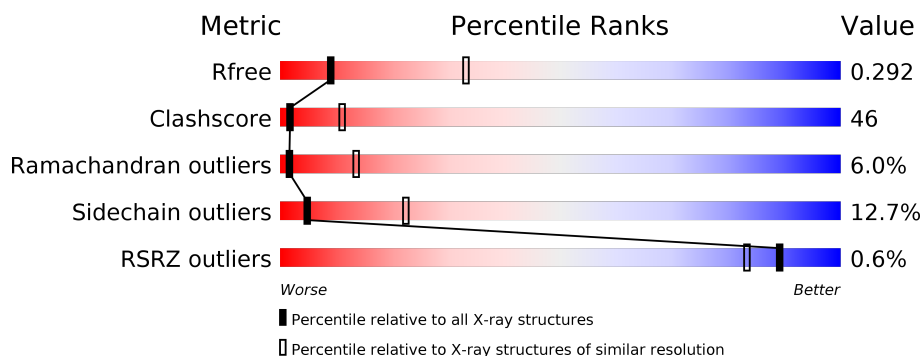
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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))
$R_{free}$	111664	1121 (3.22-3.18)
Clashscore	122126	1091 (3.20-3.20)
Ramachandran outliers	120053	1074 (3.20-3.20)
Sidechain outliers	120020	1073 (3.20-3.20)
RSRZ outliers	108989	1083 (3.22-3.18)

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	473	<div> <div>42%</div> <div>46%</div> <div>5%</div> <div>6%</div> </div>
1	B	473	<div> <div>42%</div> <div>45%</div> <div>6%</div> <div>7%</div> </div>
2	C	222	<div> <div>%</div> <div>36%</div> <div>47%</div> <div>14%</div> <div>.</div> </div>
2	E	222	<div> <div>%</div> <div>31%</div> <div>50%</div> <div>17%</div> <div>.</div> </div>
3	D	211	<div> <div>29%</div> <div>54%</div> <div>16%</div> <div>.</div> </div>
3	F	211	<div> <div>%</div> <div>28%</div> <div>55%</div> <div>15%</div> <div>.</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13223 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 H(+)/Cl(-) exchange transporter clcA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3333	2190	560	563	20			
1	B	441	Total	C	N	O	S	0	0	0
			3304	2174	553	557	20			

- 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			

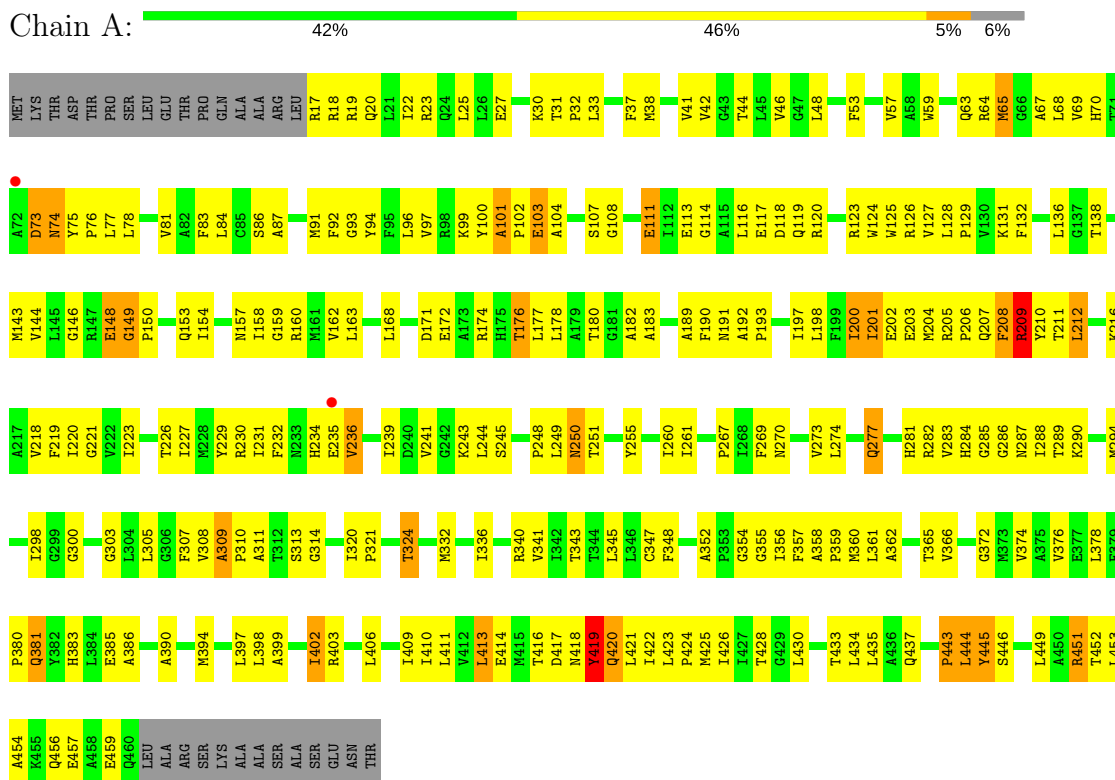
- Molecule 3 is a protein called Fab Fragment (Light Chain).

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			

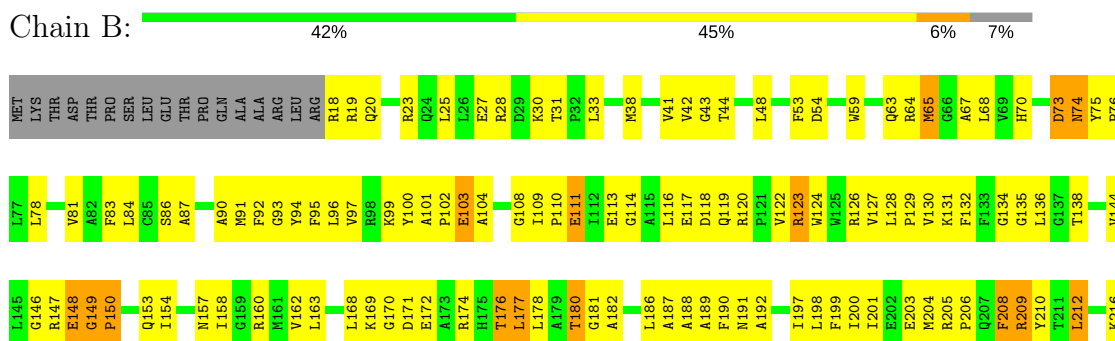
### 3 Residue-property plots

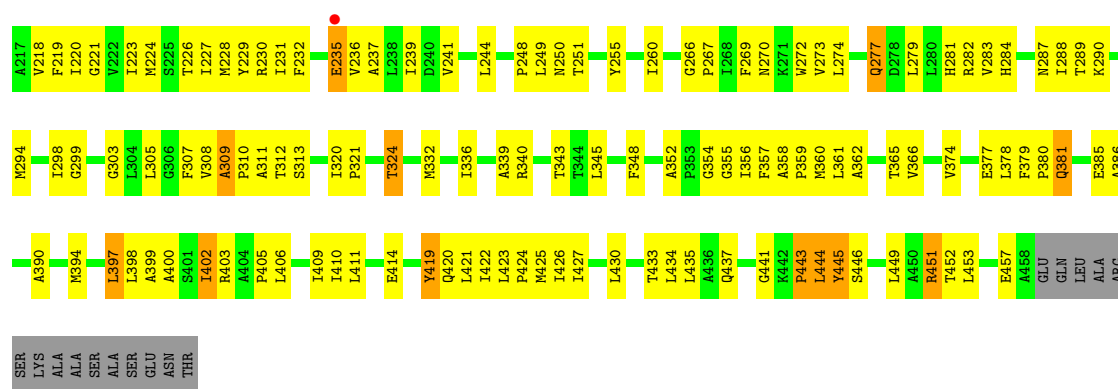
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: H(+)/Cl(-) exchange transporter clcA

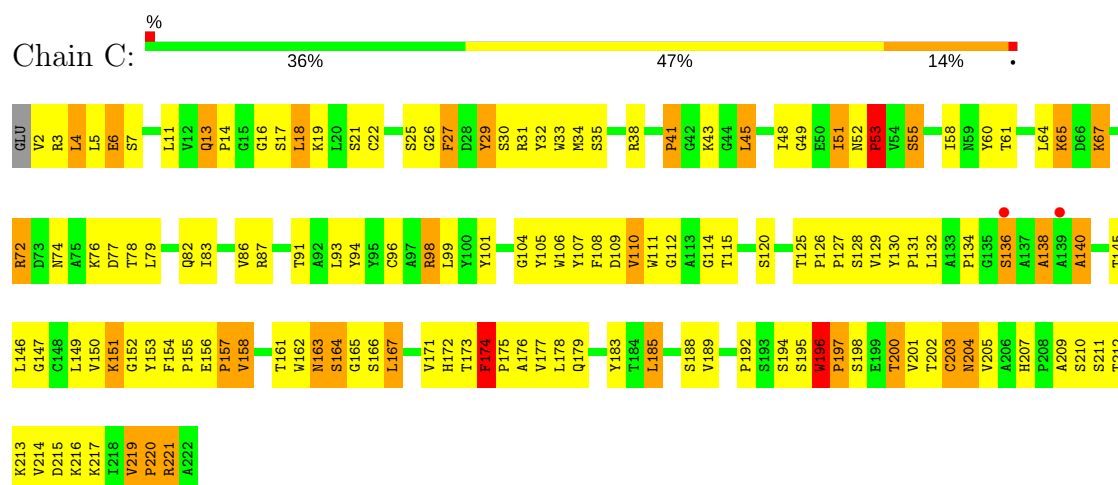


- Molecule 1: H(+)/Cl(-) exchange transporter clcA

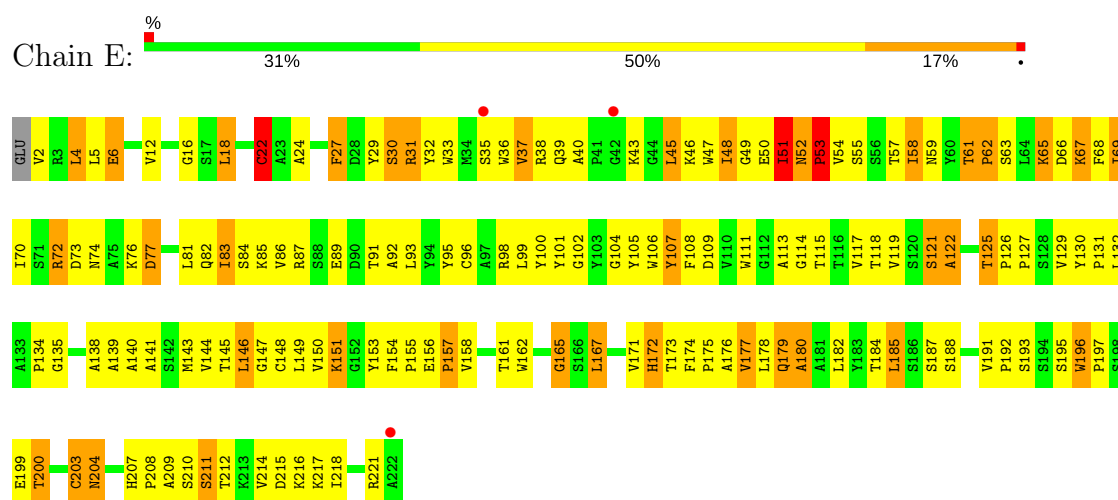




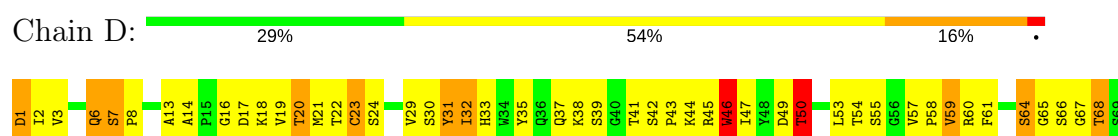
• Molecule 2: Fab Fragment (Heavy Chain)

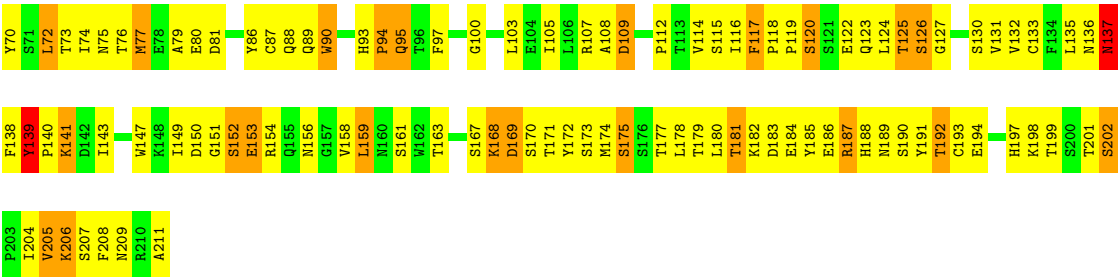


• Molecule 2: Fab Fragment (Heavy Chain)

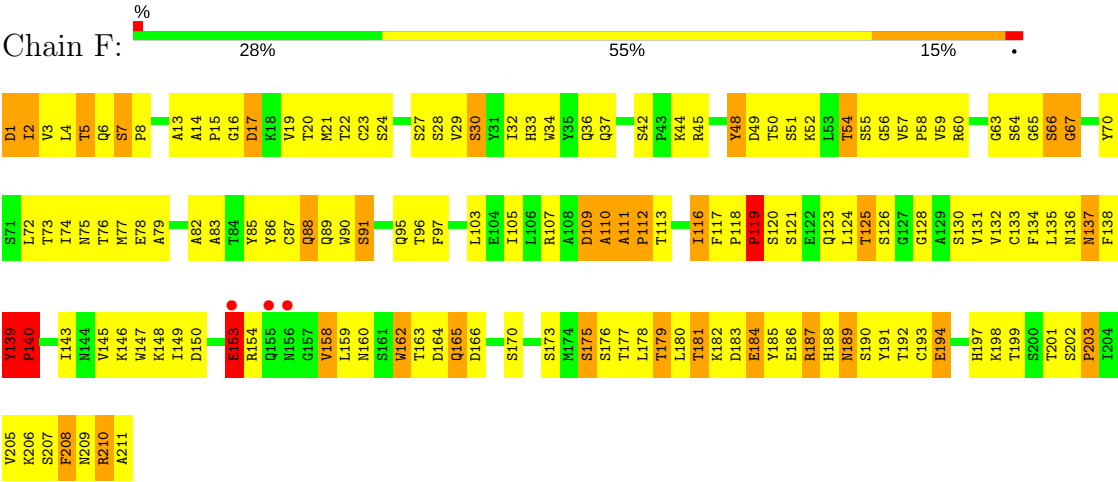


• Molecule 3: Fab Fragment (Light Chain)





● 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, $\alpha$ , $\beta$ , $\gamma$	219.83Å 122.44Å 151.34Å 90.00° 128.16° 90.00°	Depositor
Resolution (Å)	19.98 – 3.20 19.98 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.0 (19.98-3.20) 98.1 (19.98-3.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.93 (at 3.22Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.268 , 0.314 0.261 , 0.292	Depositor DCC
$R_{free}$ test set	2524 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	86.6	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 61.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	13223	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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

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	0/3405	0.65	0/4621
1	B	0.48	0/3376	0.68	0/4583
2	C	0.56	0/1721	0.94	4/2355 (0.2%)
2	E	0.56	0/1721	0.94	4/2355 (0.2%)
3	D	0.44	0/1660	0.85	1/2257 (0.0%)
3	F	0.72	6/1660 (0.4%)	1.04	8/2257 (0.4%)
All	All	0.52	6/13543 (0.0%)	0.82	17/18428 (0.1%)

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
2	C	0	1
2	E	0	1
3	D	0	1
3	F	0	1
All	All	0	6

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	139	TYR	C-O	-8.93	1.06	1.23
3	F	140	PRO	CA-C	7.08	1.67	1.52
3	F	140	PRO	C-O	5.35	1.33	1.23
3	F	139	TYR	CD2-CE2	5.27	1.47	1.39
3	F	140	PRO	N-CA	5.16	1.56	1.47

The worst 5 of 17 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	139	TYR	C-N-CA	-8.08	88.07	122.00
3	F	110	ALA	N-CA-C	7.11	130.20	111.00
3	F	140	PRO	CA-N-CD	-6.57	102.30	111.50
3	F	140	PRO	CA-C-O	6.33	135.38	120.20
2	E	22	CYS	CA-CB-SG	6.07	124.92	114.00

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	419	TYR	Sidechain
1	B	419	TYR	Sidechain
2	C	29	TYR	Sidechain
3	D	139	TYR	Sidechain
2	E	101	TYR	Sidechain

## 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	3333	0	3484	289	0
1	B	3304	0	3457	269	0
2	C	1672	0	1654	183	0
2	E	1672	0	1654	165	0
3	D	1621	0	1546	194	0
3	F	1621	0	1546	234	0
All	All	13223	0	13341	1220	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 46.

The worst 5 of 1220 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)
2:E:207:HIS:ND1	2:E:210:SER:HB2	1.52	1.23
1:A:235:GLU:O	1:A:236:VAL:HG23	1.47	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ILE:HD11	1:B:426:ILE:HG22	1.33	1.10
3:F:7:SER:HB2	3:F:22:THR:HB	1.34	1.08
3:D:16:GLY:HA2	3:D:76:THR:HG23	1.35	1.07

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	442/473 (93%)	361 (82%)	62 (14%)	19 (4%)	3	22
1	B	439/473 (93%)	342 (78%)	81 (18%)	16 (4%)	4	26
2	C	219/222 (99%)	166 (76%)	39 (18%)	14 (6%)	1	11
2	E	219/222 (99%)	173 (79%)	30 (14%)	16 (7%)	1	8
3	D	209/211 (99%)	159 (76%)	28 (13%)	22 (10%)	0	3
3	F	209/211 (99%)	158 (76%)	33 (16%)	18 (9%)	1	5
All	All	1737/1812 (96%)	1359 (78%)	273 (16%)	105 (6%)	2	13

5 of 105 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	ASP
1	A	209	ARG
1	A	236	VAL
1	A	309	ALA
1	B	73	ASP

### 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	335/358 (94%)	312 (93%)	23 (7%)	17	53
1	B	332/358 (93%)	310 (93%)	22 (7%)	18	55
2	C	181/182 (100%)	149 (82%)	32 (18%)	2	10
2	E	181/182 (100%)	141 (78%)	40 (22%)	1	5
3	D	185/185 (100%)	153 (83%)	32 (17%)	2	11
3	F	185/185 (100%)	156 (84%)	29 (16%)	3	13
All	All	1399/1450 (96%)	1221 (87%)	178 (13%)	5	22

5 of 178 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	24	SER
3	D	156	ASN
3	F	143	ILE
3	D	41	THR
3	D	77	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	270	ASN
1	B	327	ASN
3	F	89	GLN
1	B	284	HIS
1	B	381	GLN

### 5.3.3 RNA ⓘ

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](#)

There are no ligands in this entry.

## 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	444/473 (93%)	-0.37	2 (0%) 90 86	48, 77, 111, 138	0
1	B	441/473 (93%)	-0.44	1 (0%) 94 94	41, 71, 115, 151	0
2	C	221/222 (99%)	-0.25	2 (0%) 84 76	43, 71, 106, 160	0
2	E	221/222 (99%)	-0.07	3 (1%) 75 63	37, 78, 121, 145	0
3	D	211/211 (100%)	-0.03	0 100 100	52, 91, 118, 128	0
3	F	211/211 (100%)	-0.12	3 (1%) 75 63	26, 70, 123, 140	0
All	All	1749/1812 (96%)	-0.26	11 (0%) 89 83	26, 76, 117, 160	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	222	ALA	3.6
1	B	235	GLU	3.4
1	A	235	GLU	2.8
1	A	72	ALA	2.7
2	C	136	SER	2.3

### 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.