



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:32 PM GMT

PDB ID : 1KPK
Title : Crystal Structure of the ClC Chloride Channel from E. coli
Authors : Dutzler, R.; Campbell, E.B.; Cadene, M.; Chait, B.T.; MacKinnon, R.
Deposited on : 2001-12-31
Resolution : 3.50 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

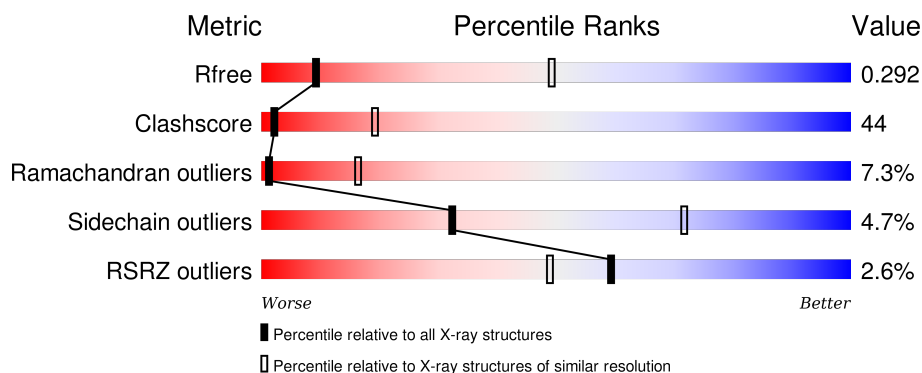
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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.



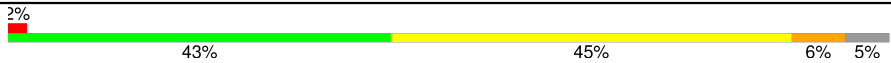
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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. 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>2%</div> <div>42%</div> <div>46%</div> <div>6%</div> <div>5%</div> </div>
1	B	473	<div> <div>2%</div> <div>41%</div> <div>47%</div> <div>7%</div> <div>5%</div> </div>
1	C	473	<div> <div>2%</div> <div>42%</div> <div>46%</div> <div>6%</div> <div>5%</div> </div>
1	D	473	<div> <div>4%</div> <div>42%</div> <div>46%</div> <div>6%</div> <div>5%</div> </div>
1	E	473	<div> <div>3%</div> <div>42%</div> <div>47%</div> <div>6%</div> <div>5%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	473	 A horizontal bar chart showing the quality of chain F. The bar is divided into five segments: a small red segment at the beginning labeled '2%', followed by a green segment labeled '43%', a yellow segment labeled '45%', an orange segment labeled '6%', and a small grey segment at the end labeled '5%'.

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 20274 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.

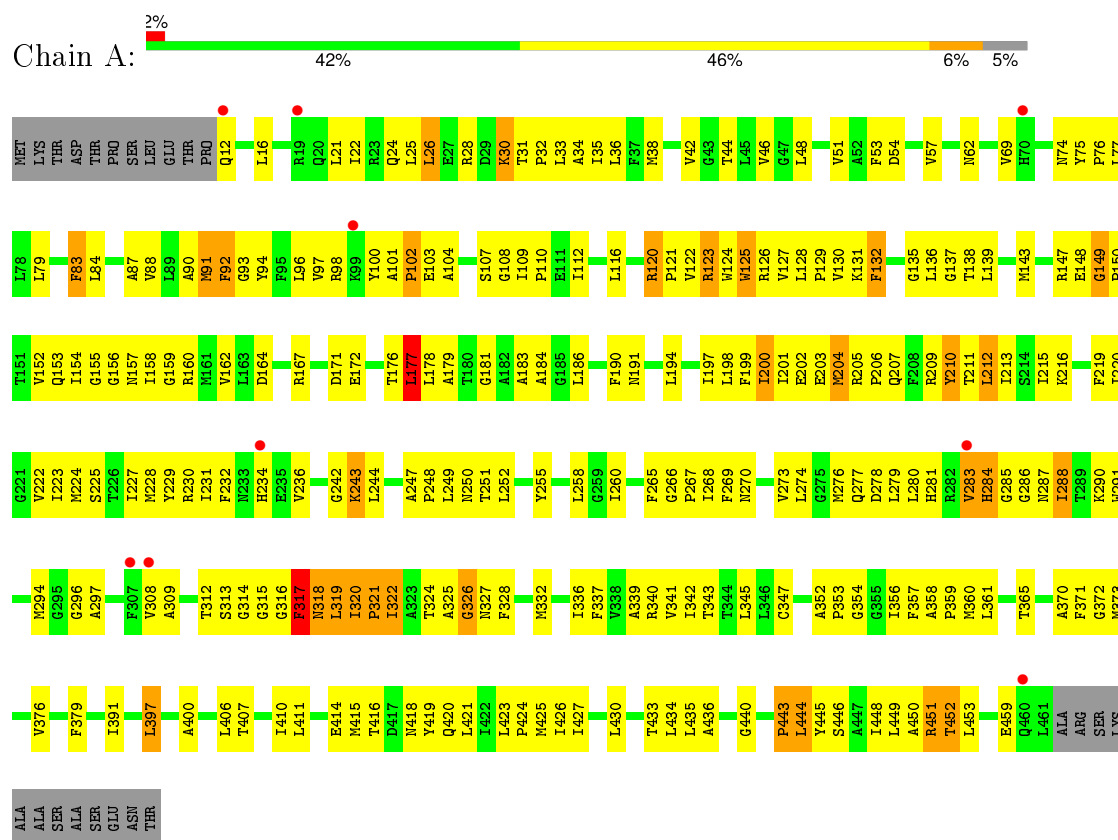
- Molecule 1 is a protein called putative channel transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	0	0
			3379	2219	570	570	20			
1	B	450	Total	C	N	O	S	0	0	0
			3379	2219	570	570	20			
1	C	450	Total	C	N	O	S	0	0	0
			3379	2219	570	570	20			
1	D	450	Total	C	N	O	S	0	0	0
			3379	2219	570	570	20			
1	E	450	Total	C	N	O	S	0	0	0
			3379	2219	570	570	20			
1	F	450	Total	C	N	O	S	0	0	0
			3379	2219	570	570	20			

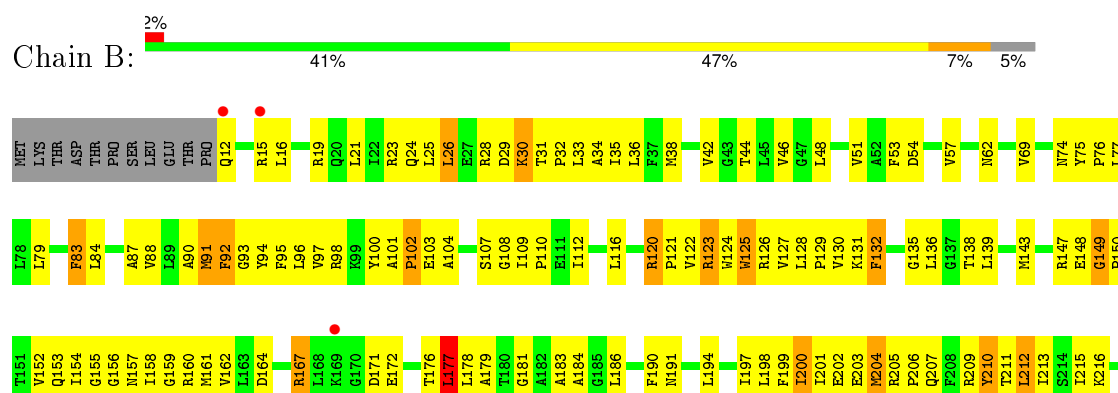
3 Residue-property plots

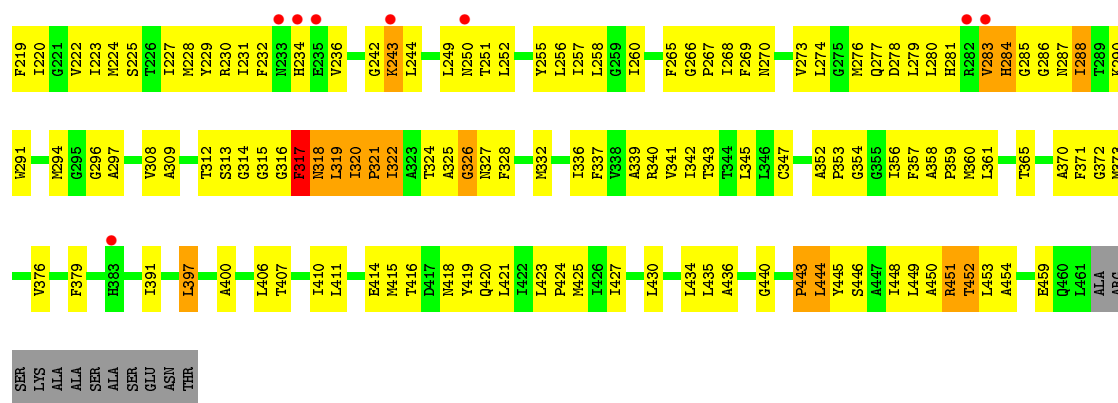
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: putative channel transporter

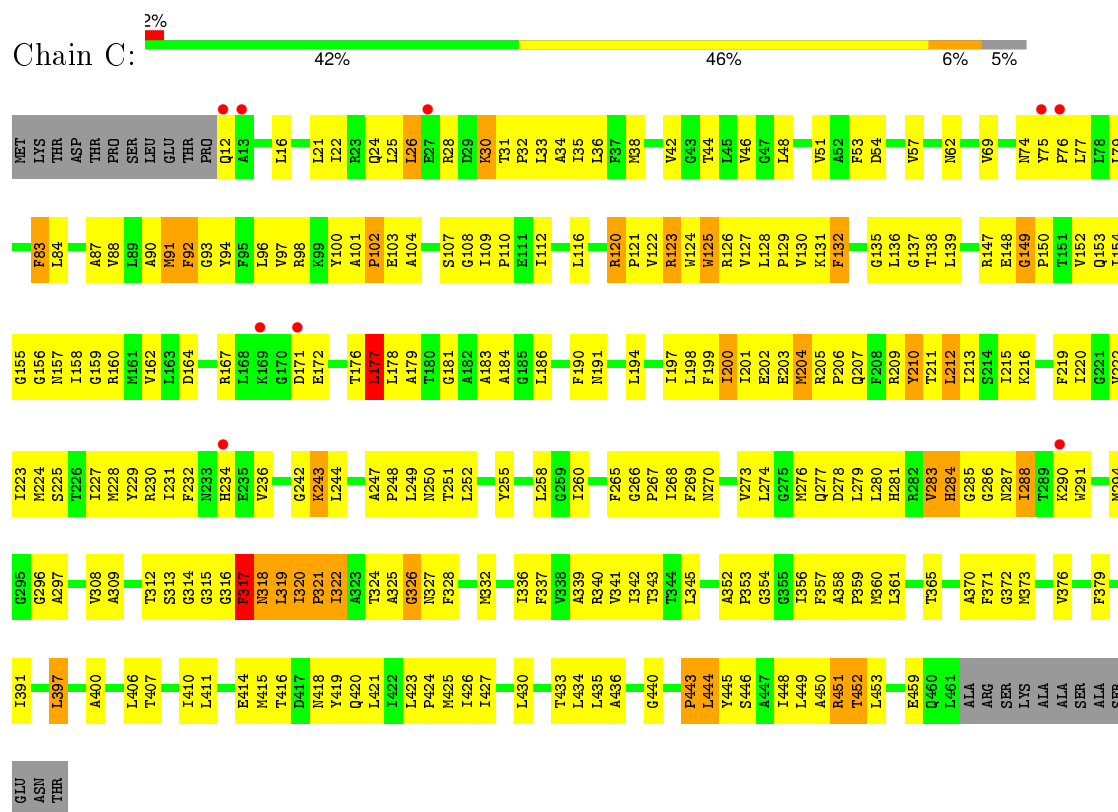


- Molecule 1: putative channel transporter

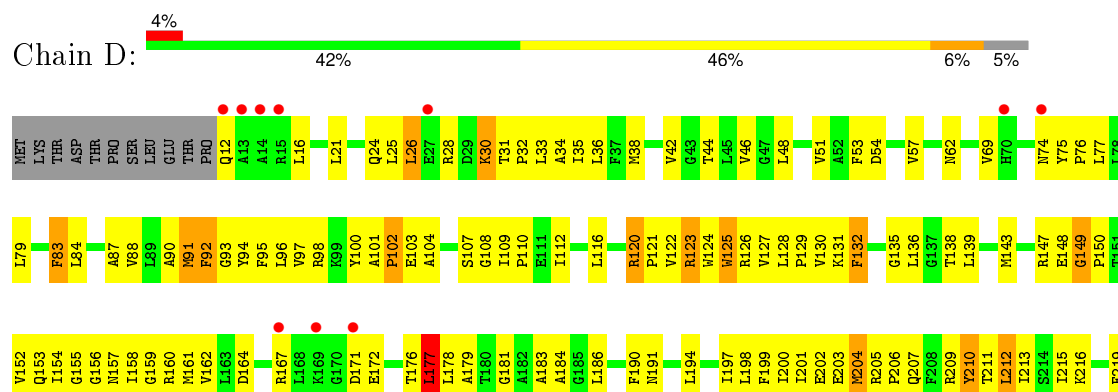


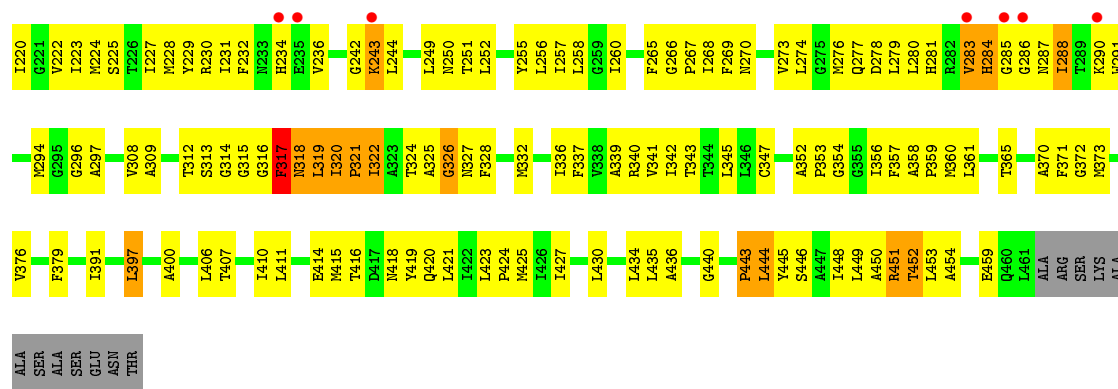


• Molecule 1: putative channel transporter

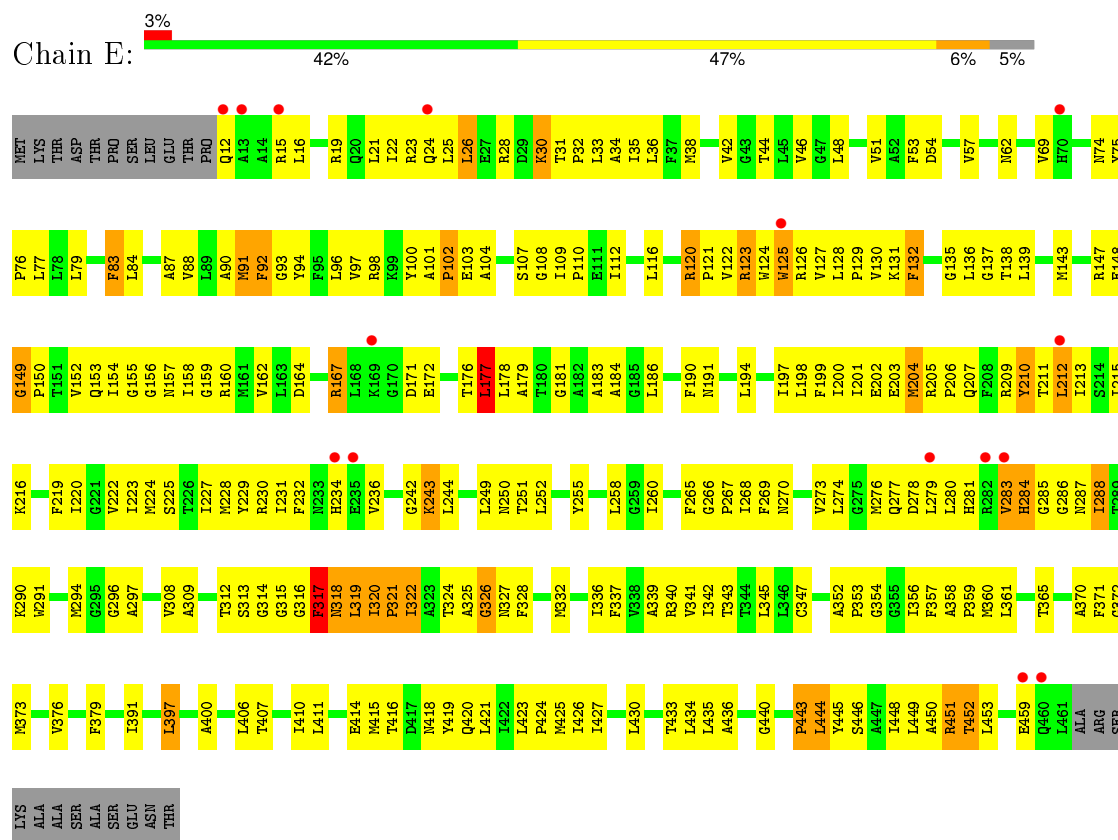


• Molecule 1: putative channel transporter

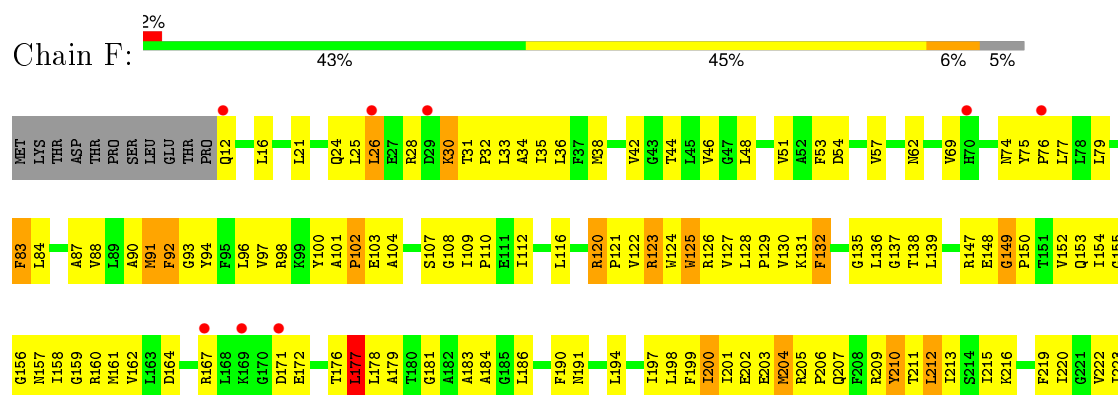




• Molecule 1: putative channel transporter



• Molecule 1: putative channel transporter



M224	V308	A400
S225	A309	L406
T226		T407
I227		
M228	T312	
Y229	S313	
P230	G314	T410
I231	G315	L411
F232	G316	
M233	F317	E414
N234	N318	M415
E235	I319	T416
Y236	I320	D417
	P321	M418
	I322	Y419
G242	A323	Q420
K243	T324	L421
L244	A325	T422
	G326	L423
I249	N327	P424
N250	F328	M425
T251		T426
L252	M332	I427
Y255		L430
	I336	
L258	F337	L434
	V338	L435
G259	A339	A436
I260	R340	
	V341	G440
F265	I342	
G266	T343	P443
P267	T344	L444
I268	I345	Y445
F269		S446
N270		A447
	A352	I448
	P353	L449
V273	G354	A450
L274	G355	R451
G275	I356	T452
M276	F357	L453
Q277	A358	A454
D278	P359	
L279	M360	
I280	L361	
H281		E459
R282		Q460
V283	T365	L461
H284		ALA
G285	A370	ARG
G286	F371	SER
N287	G372	LYS
I288	M373	ALA
T289		ALA
K290	V376	SER
H291		ALA
	F379	SER
		GLU
M294	I391	ASN
G295		THR
G296		
A297	I397	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.66Å 152.53Å 263.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50 19.97 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-3.50) 99.4 (19.97-3.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 3.52Å)	Xtriage
Refinement program	CNS 0.3	Depositor
R, R_{free}	0.290 , 0.301 0.285 , 0.292	Depositor DCC
R_{free} test set	5321 reflections (9.90%)	DCC
Wilson B-factor (Å ²)	125.9	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 55.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 53763 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	20274	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.49	0/3451	0.76	2/4683 (0.0%)
1	B	0.49	0/3451	0.76	2/4683 (0.0%)
1	C	0.49	0/3451	0.76	2/4683 (0.0%)
1	D	0.49	0/3451	0.76	2/4683 (0.0%)
1	E	0.49	0/3451	0.76	2/4683 (0.0%)
1	F	0.49	0/3451	0.76	2/4683 (0.0%)
All	All	0.49	0/20706	0.76	12/28098 (0.0%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	320	ILE	N-CA-C	5.97	127.11	111.00
1	F	320	ILE	N-CA-C	5.97	127.11	111.00
1	A	320	ILE	N-CA-C	5.96	127.10	111.00
1	C	320	ILE	N-CA-C	5.95	127.06	111.00
1	B	320	ILE	N-CA-C	5.95	127.06	111.00

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	3379	0	3537	338	0
1	B	3379	0	3537	336	52

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3379	0	3537	336	1
1	D	3379	0	3537	337	4
1	E	3379	0	3537	332	49
1	F	3379	0	3537	335	0
All	All	20274	0	21222	1844	53

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 44.

The worst 5 of 1844 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:D:200:ILE:HD13	1:D:204:MET:HG3	1.38	1.06
1:F:200:ILE:HD13	1:F:204:MET:HG3	1.38	1.05
1:B:200:ILE:HD13	1:B:204:MET:HG3	1.38	1.05
1:E:200:ILE:HD13	1:E:204:MET:HG3	1.38	1.05
1:F:322:ILE:HD12	1:F:322:ILE:N	1.74	1.03

The worst 5 of 53 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:ARG:CA	1:E:12:GLN:NE2[4_455]	0.70	1.50
1:B:16:LEU:CG	1:E:19:ARG:CZ[4_455]	0.73	1.47
1:B:19:ARG:NH1	1:E:16:LEU:CB[4_455]	0.88	1.32
1:B:12:GLN:CD	1:E:15:ARG:CB[4_455]	0.91	1.29
1:B:19:ARG:NH1	1:E:16:LEU:CG[4_455]	0.96	1.24

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	448/473 (95%)	340 (76%)	75 (17%)	33 (7%)	1	16
1	B	448/473 (95%)	340 (76%)	75 (17%)	33 (7%)	1	16
1	C	448/473 (95%)	340 (76%)	75 (17%)	33 (7%)	1	16
1	D	448/473 (95%)	340 (76%)	76 (17%)	32 (7%)	1	17
1	E	448/473 (95%)	340 (76%)	76 (17%)	32 (7%)	1	17
1	F	448/473 (95%)	340 (76%)	75 (17%)	33 (7%)	1	16
All	All	2688/2838 (95%)	2040 (76%)	452 (17%)	196 (7%)	1	16

5 of 196 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	LEU
1	B	319	LEU
1	C	319	LEU
1	D	319	LEU
1	E	319	LEU

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	339/358 (95%)	323 (95%)	16 (5%)	32	72
1	B	339/358 (95%)	323 (95%)	16 (5%)	32	72
1	C	339/358 (95%)	323 (95%)	16 (5%)	32	72
1	D	339/358 (95%)	323 (95%)	16 (5%)	32	72
1	E	339/358 (95%)	323 (95%)	16 (5%)	32	72
1	F	339/358 (95%)	323 (95%)	16 (5%)	32	72
All	All	2034/2148 (95%)	1938 (95%)	96 (5%)	32	72

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	317	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	132	PHE
1	F	212	LEU
1	C	322	ILE
1	D	30	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	327	ASN
1	D	207	GLN
1	F	277	GLN
1	C	418	ASN
1	D	62	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 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, 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	450/473 (95%)	-0.35	9 (2%) 68 59	51, 100, 147, 151	0
1	B	450/473 (95%)	-0.33	11 (2%) 62 52	51, 100, 147, 151	0
1	C	450/473 (95%)	-0.31	9 (2%) 68 59	51, 100, 147, 151	0
1	D	450/473 (95%)	-0.29	17 (3%) 44 36	51, 100, 147, 151	0
1	E	450/473 (95%)	-0.28	15 (3%) 50 41	51, 100, 147, 151	0
1	F	450/473 (95%)	-0.28	9 (2%) 68 59	51, 100, 147, 151	0
All	All	2700/2838 (95%)	-0.31	70 (2%) 59 49	51, 100, 147, 151	0

The worst 5 of 70 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	12	GLN	8.2
1	E	12	GLN	7.7
1	B	12	GLN	5.9
1	F	12	GLN	5.3
1	D	169	LYS	4.7

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.