



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 04:24 am 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](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

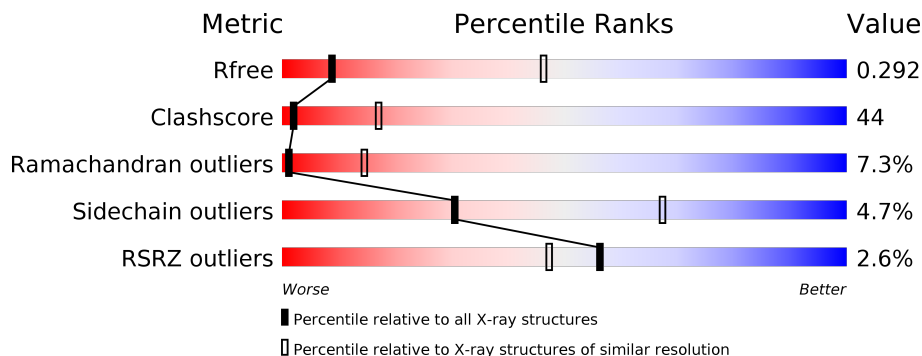
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	100719	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)
RSRZ outliers	101464	1226 (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  $\geq 3$ , 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	
1	B	473	
1	C	473	
1	D	473	
1	E	473	
1	F	473	

## 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.

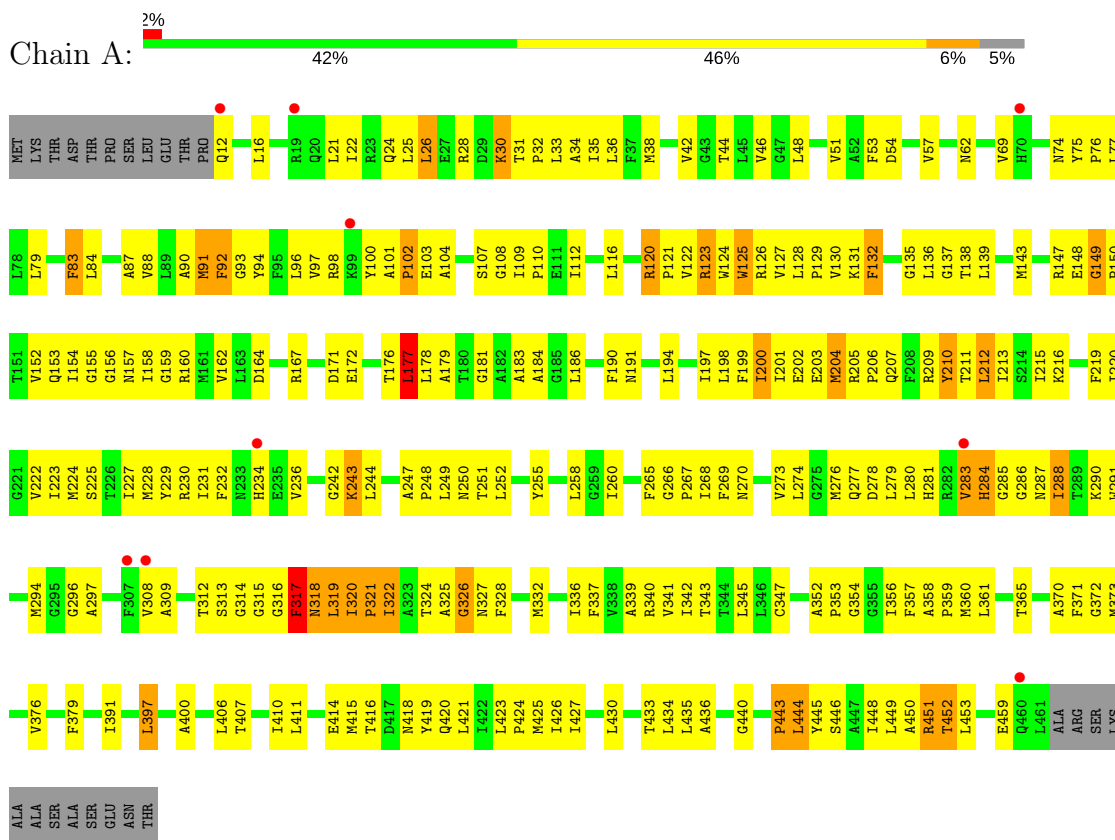
- Molecule 1 is a protein called putative channel transporter.

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			

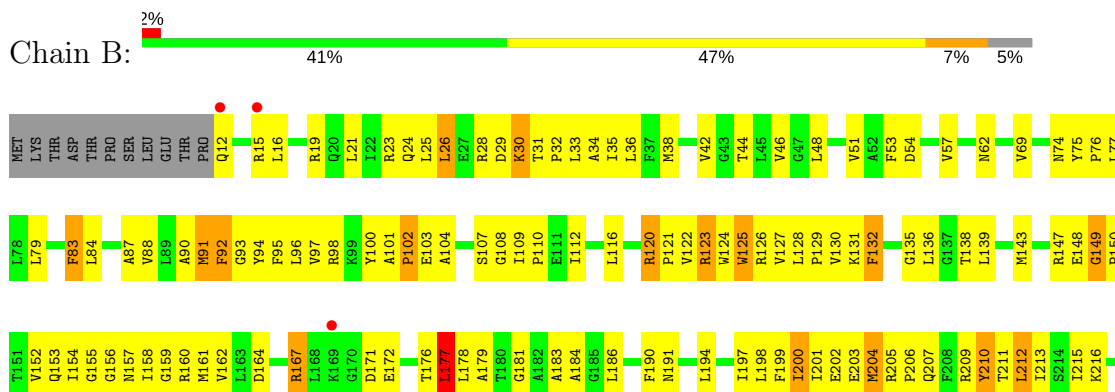
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

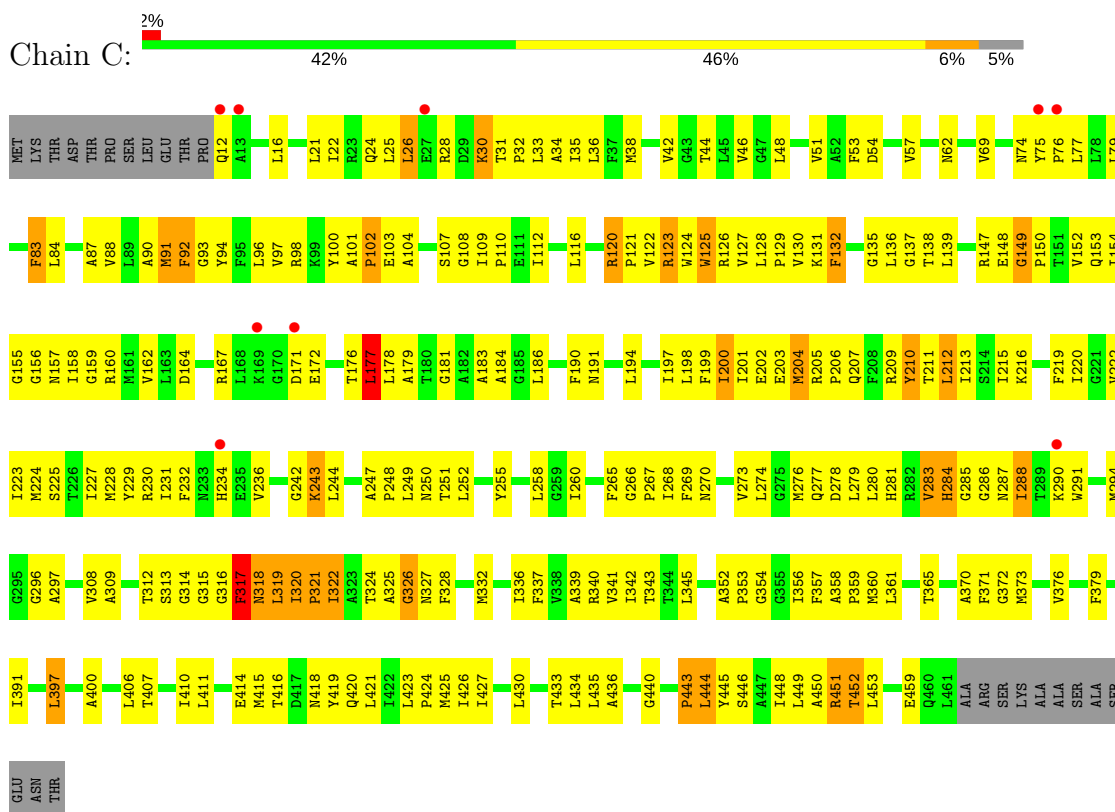
- Molecule 1: putative channel transporter



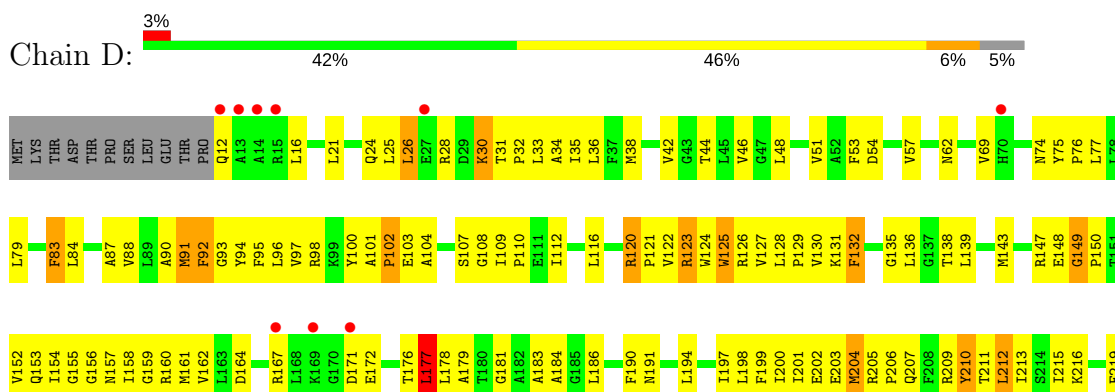
- Molecule 1: putative channel transporter

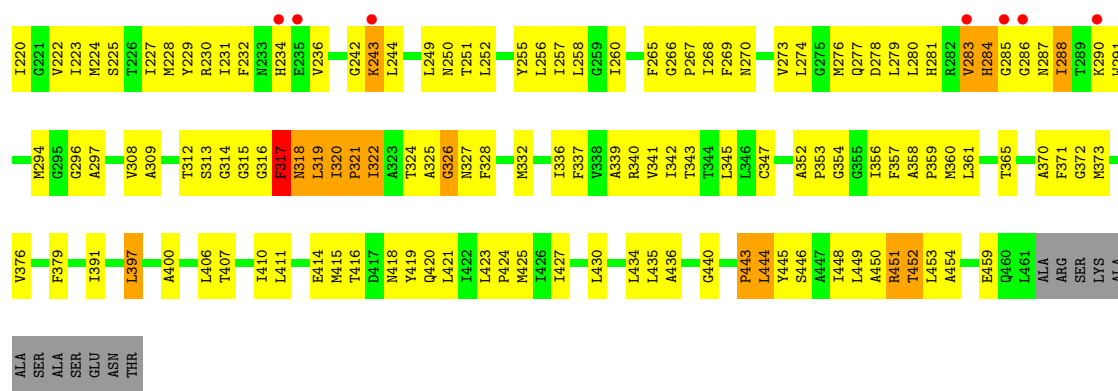


- Molecule 1: putative channel transporter

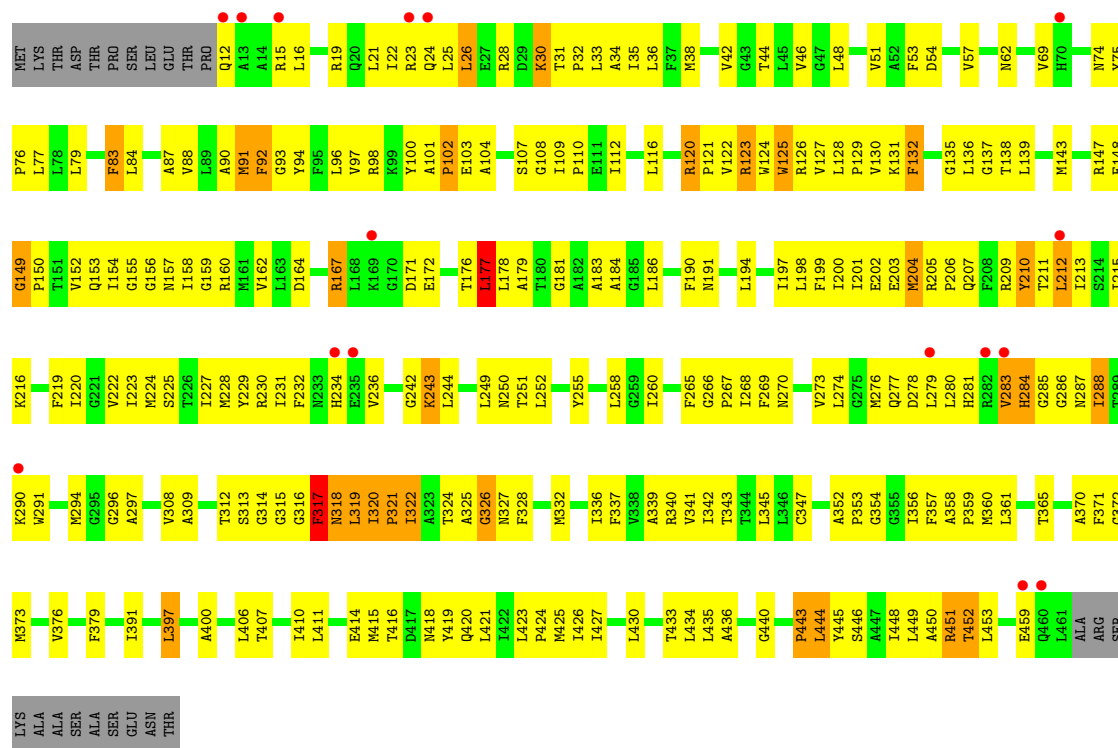
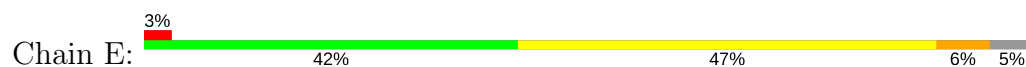


- Molecule 1: putative channel transporter

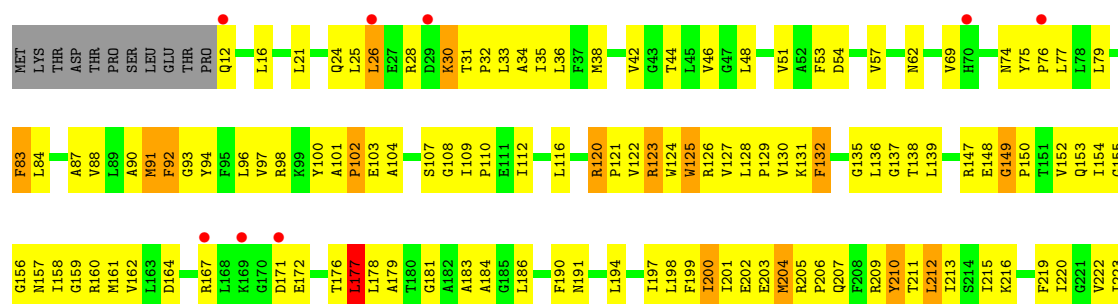
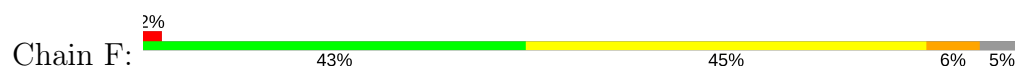




• Molecule 1: putative channel transporter



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M224	V308	A400	M225	A309	L406	M226	T407	M227	T410	M228	L411	M229	E414	M230	M415	M231	M416	M232	M417	M233	M418	M234	Y419	M235	Q420	M236	L421	M422	M237	L423	M238	P424	M239	L425	M240	L426	M241	L427	M242	L430	M243	L434	M244	L435	M245	L436	M246	L437	M247	L438	M248	L439	M249	L440	M250	P443	M251	L441	M252	L442	M253	L443	M254	L444	M255	L445	M256	L446	M257	L447	M258	L448	M259	L449	M260	L450	M261	L451	M262	L452	M263	L453	M264	L454	M265	E459	M266	Q460	M267	L461	M268	ALA	M269	ARG	M270	F337	M271	SER	M272	F338	LYS	M273	F339	ALA	M274	F340	SER	M275	F341	ALA	M276	F342	SER	M277	F343	ALA	M278	F344	SER	M279	F345	ALA	M280	F346	SER	M281	F347	ALA	M282	F348	SER	M283	F349	ALA	M284	F350	SER	M285	F351	ALA	M286	F352	SER	M287	F353	ALA	M288	F354	SER	M289	F355	ALA	M290	F356	SER	M291	F357	ALA	M292	F358	SER	M293	F359	ALA	M294	F360	SER	M295	F361	ALA	M296	F362	SER	M297	F363	ALA	M298	F364	SER	M299	F365	ALA	M300	F366	SER	M301	F367	ALA	M302	F368	SER	M303	F369	ALA	M304	F370	SER	M305	F371	ALA	M306	F372	SER	M307	F373	ALA	M308	F374	SER	M309	F375	ALA	M310	F376	SER	M311	F377	ALA	M312	F378	SER	M313	F379	ALA	M314	F380	SER	M315	F381	ALA	M316	F382	SER	M317	F383	ALA	M318	F384	SER	M319	F385	ALA	M320	F386	SER	M321	F387	ALA	M322	F388	SER	M323	F389	ALA	M324	F390	SER	M325	F391	ALA	M326	F392	SER	M327	F393	ALA	M328	F394	SER	M329	F395	ALA	M330	F396	SER	M331	F397	ALA	M332	F398	SER	M333	F399	ALA	M334	F400	SER	M335	F401	ALA	M336	F402	SER	M337	F403	ALA	M338	F404	SER	M339	F405	ALA	M340	F406	SER	M341	F407	ALA	M342	F408	SER	M343	F409	ALA	M344	F410	SER	M345	F411	ALA	M346	F412	SER	M347	F413	ALA	M348	F414	SER	M349	F415	ALA	M350	F416	SER	M351	F417	ALA	M352	F418	SER	M353	F419	ALA	M354	F420	SER	M355	F421	ALA	M356	F422	SER	M357	F423	ALA	M358	F424	SER	M359	F425	ALA	M360	F426	SER	M361	F427	ALA	M362	F428	SER	M363	F429	ALA	M364	F430	SER	M365	F431	ALA	M366	F432	SER	M367	F433	ALA	M368	F434	SER	M369	F435	ALA	M370	F436	SER	M371	F437	ALA	M372	F438	SER	M373	F439	ALA	M374	F440	SER	M375	F441	ALA	M376	F442	SER	M377	F443	ALA	M378	F444	SER	M379	F445	ALA	M380	F446	SER	M381	F447	ALA	M382	F448	SER	M383	F449	ALA	M384	F450	SER	M385	F451	ALA	M386	F452	SER	M387	F453	ALA	M388	F454	SER	M389	F455	ALA	M390	F456	SER	M391	F457	ALA	M392	F458	SER	M393	F459	ALA	M394	F460	SER	M395	F461	ALA	M396	F462	SER	M397	F463	ALA	M398	F464	SER	M399	F465	ALA	M400	F466	SER	M401	F467	ALA	M402	F468	SER	M403	F469	ALA	M404	F470	SER	M405	F471	ALA	M406	F472	SER	M407	F473	ALA	M408	F474	SER	M409	F475	ALA	M410	F476	SER	M411	F477	ALA	M412	F478	SER	M413	F479	ALA	M414	F480	SER	M415	F481	ALA	M416	F482	SER	M417	F483	ALA	M418	F484	SER	M419	F485	ALA	M420	F486	SER	M421	F487	ALA	M422	F488	SER	M423	F489	ALA	M424	F490	SER	M425	F491	ALA	M426	F492	SER	M427	F493	ALA	M428	F494	SER	M429	F495	ALA	M430	F496	SER	M431	F497	ALA	M432	F498	SER	M433	F499	ALA	M434	F500	SER	M435	F501	ALA	M436	F502	SER	M437	F503	ALA	M438	F504	SER	M439	F505	ALA	M440	F506	SER	M441	F507	ALA	M442	F508	SER	M443	F509	ALA	M444	F510	SER	M445	F511	ALA	M446	F512	SER	M447	F513	ALA	M448	F514	SER	M449	F515	ALA	M450	F516	SER	M451	F517	ALA	M452	F518	SER	M453	F519	ALA	M454	F520	SER	M455	F521	ALA	M456	F522	SER	M457	F523	ALA	M458	F524	SER	M459	F525	ALA	M460	F526	SER	M461	F527	ALA	M462	F528	SER	M463	F529	ALA	M464	F530	SER	M465	F531	ALA	M466	F532	SER	M467	F533	ALA	M468	F534	SER	M469	F535	ALA	M470	F536	SER	M471	F537	ALA	M472	F538	SER	M473	F539	ALA	M474	F540	SER	M475	F541	ALA	M476	F542	SER	M477	F543	ALA	M478	F544	SER	M479	F545	ALA	M480	F546	SER	M481	F547	ALA	M482	F548	SER	M483	F549	ALA	M484	F550	SER	M485	F551	ALA	M486	F552	SER	M487	F553	ALA	M488	F554	SER	M489	F555	ALA	M490	F556	SER	M491	F557	ALA	M492	F558	SER	M493	F559	ALA	M494	F560	SER	M495	F561	ALA	M496	F562	SER	M497	F563	ALA	M498	F564	SER	M499	F565	ALA	M500	F566	SER	M501	F567	ALA	M502	F568	SER	M503	F569	ALA	M504	F570	SER	M505	F571	ALA	M506	F572	SER	M507	F573	ALA	M508	F574	SER	M509	F575	ALA	M510	F576	SER	M511	F577	ALA	M512	F578	SER	M513	F579	ALA	M514	F580	SER	M515	F581	ALA	M516	F582	SER	M517	F583	ALA	M518	F584	SER	M519	F585	ALA	M520	F586	SER	M521	F587	ALA	M522	F588	SER	M523	F589	ALA	M524	F590	SER	M525	F591	ALA	M526	F592	SER	M527	F593	ALA	M528	F594	SER	M529	F595	ALA	M530	F596	SER	M531	F597	ALA	M532	F598	SER	M533	F599	ALA	M534	F600	SER	M535	F601	ALA	M536	F602	SER	M537	F603	ALA	M538	F604	SER	M539	F605	ALA	M540	F606	SER	M541	F607	ALA	M542	F608	SER	M543	F609	ALA	M544	F610	SER	M545	F611	ALA	M546	F612	SER	M547	F613	ALA	M548	F614	SER	M549	F615	ALA	M550	F616	SER	M551	F617	ALA	M552	F618	SER	M553	F619	ALA	M554	F620	SER	M555	F621	ALA	M556	F622	SER	M557	F623	ALA	M558	F624	SER	M559	F625	ALA	M560	F626	SER	M561	F627	ALA	M562	F628	SER	M563	F629	ALA	M564	F630	SER	M565	F631	ALA	M566	F632	SER	M567	F633	ALA	M568	F634	SER	M569	F635	ALA	M570	F636	SER	M571	F637	ALA	M572	F638	SER	M573	F639	ALA	M574	F640	SER	M575	F641	ALA	M576	F642	SER	M577	F643	ALA	M578	F644	SER	M579	F645	ALA	M580	F646	SER	M581	F647	ALA	M582	F648	SER	M583	F649	ALA	M584	F650	SER	M585	F651	ALA	M586	F652	SER	M587	F653	ALA	M588	F654	SER	M589	F655	ALA	M590	F656	SER	M591	F657	ALA	M592	F658	SER	M593	F659	ALA	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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	125.9	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 56.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	20274	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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](#)

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

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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:B:200:ILE:HD13	1:B:204:MET:HG3	1.38	1.05
1:F:200:ILE:HD13	1:F: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:N	1:F:322:ILE:HD12	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	14
1	B	448/473 (95%)	340 (76%)	75 (17%)	33 (7%)	1	14
1	C	448/473 (95%)	340 (76%)	75 (17%)	33 (7%)	1	14
1	D	448/473 (95%)	340 (76%)	76 (17%)	32 (7%)	1	15
1	E	448/473 (95%)	340 (76%)	76 (17%)	32 (7%)	1	15
1	F	448/473 (95%)	340 (76%)	75 (17%)	33 (7%)	1	14
All	All	2688/2838 (95%)	2040 (76%)	452 (17%)	196 (7%)	1	14

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%)	30	67
1	B	339/358 (95%)	323 (95%)	16 (5%)	30	67
1	C	339/358 (95%)	323 (95%)	16 (5%)	30	67
1	D	339/358 (95%)	323 (95%)	16 (5%)	30	67
1	E	339/358 (95%)	323 (95%)	16 (5%)	30	67
1	F	339/358 (95%)	323 (95%)	16 (5%)	30	67
All	All	2034/2148 (95%)	1938 (95%)	96 (5%)	30	67

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

Mol	Chain	Res	Type
1	C	317	PHE

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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, 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	450/473 (95%)	-0.37	9 (2%) 65 57	51, 100, 147, 151	0
1	B	450/473 (95%)	-0.35	11 (2%) 59 50	51, 100, 147, 151	0
1	C	450/473 (95%)	-0.34	9 (2%) 65 57	51, 100, 147, 151	0
1	D	450/473 (95%)	-0.32	16 (3%) 43 37	51, 100, 147, 151	0
1	E	450/473 (95%)	-0.31	16 (3%) 43 37	51, 100, 147, 151	0
1	F	450/473 (95%)	-0.30	9 (2%) 65 57	51, 100, 147, 151	0
All	All	2700/2838 (95%)	-0.33	70 (2%) 56 47	51, 100, 147, 151	0

The worst 5 of 70 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	12	GLN	8.1
1	E	12	GLN	7.7
1	B	12	GLN	5.9
1	F	12	GLN	5.3
1	D	169	LYS	4.9

### 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.