



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 09:01 PM UTC

PDB ID : 3RFU / pdb_00003rfu
Title : Crystal structure of a copper-transporting PIB-type ATPase
Authors : Gourdon, P.; Liu, X.; Skjorringe, T.; Morth, J.P.; Birk Moller, L.; Panyella Pedersen, B.; Nissen, P.
Deposited on : 2011-04-07
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

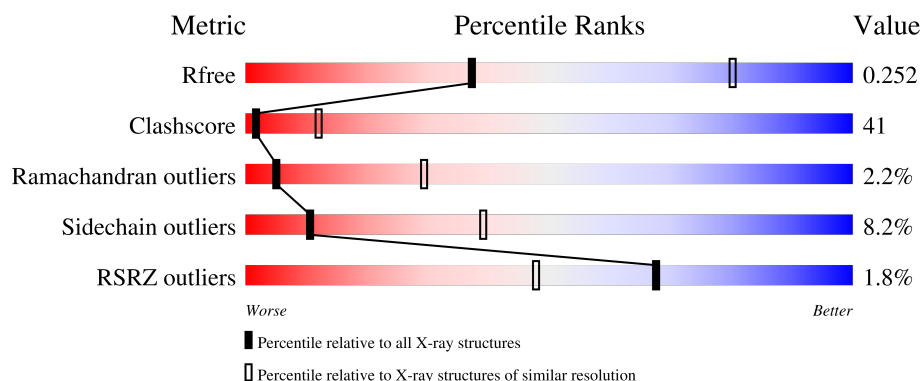
1 Overall quality at a glance

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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 ≥ 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	736	% 36% 47% 7% 10%
1	B	736	2% 37% 47% 7% 10%
1	C	736	2% 36% 47% 7% 10%
1	D	736	% 37% 47% 7% 10%

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
2	ALF	A	995	-	-	X	-

2 Entry composition [i](#)

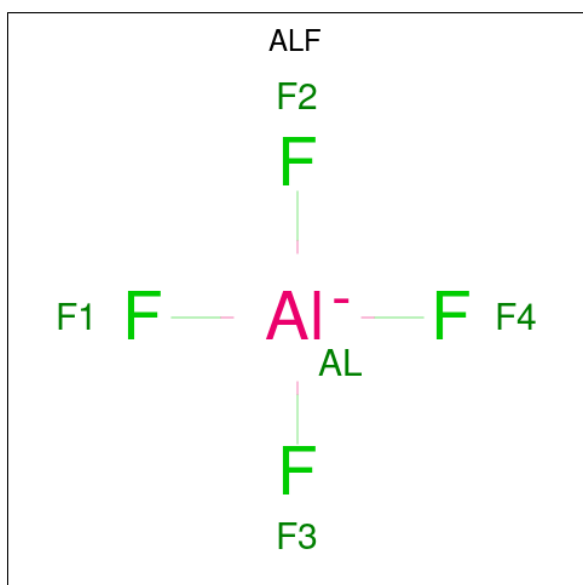
There are 4 unique types of molecules in this entry. The entry contains 19764 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Copper efflux ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	663	Total	C	N	O	S	0	0	0
			4934	3156	844	909	25			
1	B	663	Total	C	N	O	S	0	0	0
			4934	3156	844	909	25			
1	C	663	Total	C	N	O	S	0	0	0
			4934	3156	844	909	25			
1	D	663	Total	C	N	O	S	0	0	0
			4934	3156	844	909	25			

- Molecule 2 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Al	F	0	0
			5	1	4		
2	B	1	Total	Al	F	0	0
			5	1	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	Al	F	0	0
			5	1	4		
2	D	1	Total	Al	F	0	0
			5	1	4		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

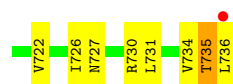
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	K	0	0
			1	1		
4	B	1	Total	K	0	0
			1	1		
4	C	1	Total	K	0	0
			1	1		
4	D	1	Total	K	0	0
			1	1		

- Molecule 1: Copper efflux ATPase





● Molecule 1: Copper efflux ATPase



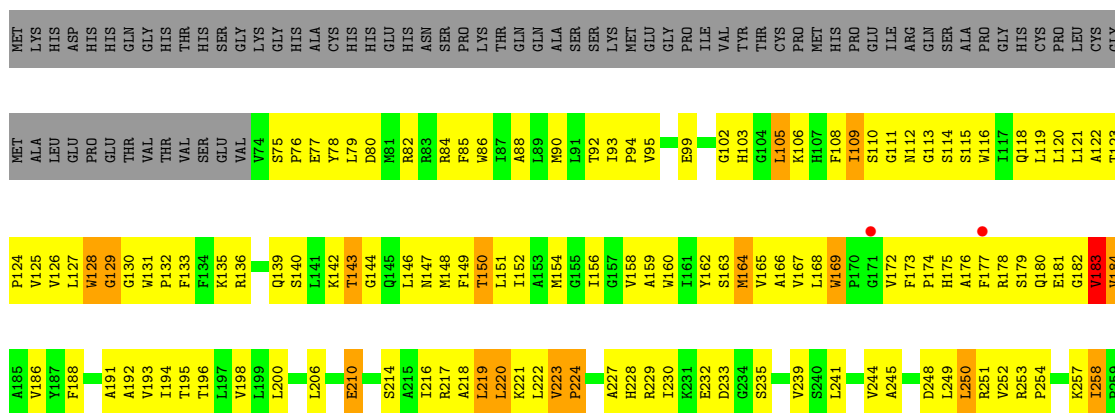
MET	LYS	HIS	ASP	HIS	HIS	GLN	GLY	HIS	THR	HIS	SER	GLY	LYS	GLY	HIS	P74	ALA	E77	Y78	L79	D80	M81	R82	R83	R84	F85	W86	I87	A88	L89	M90	I91	T92	I93	P94	V95	E99	G102	H103	G104	L105	K106	H107	F108	I109	S110	G111	N112	G113	S114	S115	W116	I117	Q118	L119	L120	L121	A122	CYS	GLY	T123
MET	ALA	LEU	GLU	PRO	GLU	THR	VAL	THR	VAL	SER	GLU	VAL	V74	S75	Q139	S140	L141	E77	Y78	L79	D80	M81	R82	R83	R84	F85	W86	I87	A88	L89	M90	I91	T92	I93	P94	V95	E99	G102	H103	G104	L105	K106	H107	F108	I109	S110	G111	N112	G113	S114	S115	W116	I117	Q118	L119	L120	L121	A122	CYS	GLY	T123
P124	V125	V126	L127	W128	G129	G130	W131	F132	F133	SER	SER	R136	Q139	S140	L141	E77	Y78	L79	D80	M81	R82	R83	R84	F85	W86	I87	A88	L89	M90	I91	T92	I93	P94	V95	E99	G102	H103	G104	L105	K106	H107	F108	I109	S110	G111	N112	G113	S114	S115	W116	I117	Q118	L119	L120	L121	A122	CYS	GLY	T123		
A185	V186	Y187	F188	A191	A192	V193	I194	T195	T196	L197	V198	L199	L200	L206	E210	S214	A215	L216	R217	A218	L219	L220	K221	L222	A223	G224	E225	G226	A227	H228	R229	W230	I231	E232	D233	G234	S235	V239	S240	L241	V244	A245	D248	L249	L250	R251	V252	R253	P254	E257	L258										
P259	V260	G261	G262	E263	V264	G265	E266	E267	E268	S269	F270	V271	D272	E273	S274	M275	V276	G277	G278	E279	P280	L281	P282	V283	A284	E285	A286	L287	L292	G293	A294	T295	L296	N297	Q298	T299	G300	S301	F302	V303	M304	K305	A306	L307	H308	V309	G310	S311	D312	T313	M314	L315	A316	R317	I318	V319	V322				
Q326	R329	L335	V339	S340	G341	W342	F343	V344	P345	A346	V347	F355	W358	A359	G362	P363	Q364	P365	A366	L367	S368	Y369	V375	S376	V377	L378	I379	I380	A381	C382	P383	C384	A385	L386	G387	L388	A389	T390	P391	M392	S393	I394	M395	V396	K400	Q403	V406	L407													
I408	A413	L414	E415	R416	M417	E418	K419	T422	L423	V424	V425	A426	K427	G429	T430	L431	T432	H435	L438	T439	R440	I441	V442	T443	F446	V447	N450	A451	L454	A455	L458	E459	H460	Q461	L466	A467	N468	V471	H472	A473	A474	K477	G478	L479	S480	L481	G482														
S483	V484	E488	A489	P490	T491	G492	G493	G494	V495	V496	G497	Q498	V499	D500	G501	H502	H503	V504	A505	I506	R510	L511	M512	Q513	E514	A520	P521	L522	F523	E524	D527	V536	M537	F538	M539	A540	V541	K544	T545	V546	A547	L548	I549	V550	V551	I555	K556	S557	S558	T559	P560	E561									
T562	I563	Q567	V574	M575	L576	T577	D578	D579	T583	V587	K595	V596	I600	M601	P602	E603	D604	K605	S606	R607	L612	K613	P614	K615	G616	L617	I618	V619	A620	M621	A622	G623	V626	D628	A629	P630	L632	D636	L637	G638	L639	A640	M641	G642	T645	D646															
V647	A648	I649	A652	G653	V654	T655	L656	L657	H658	G659	D660	L661	R662	G663	R668	R669	L670	S671	E672	S673	T674	Q680	F683	L687	V688	V690	L691	G692	V693	P694	L695	V699	L700	Y701	P702	L703	T704	G705	L706	L707	L708	S709	P710	M711	L712	A713	H717	A718	L719	V722											



● Molecule 1: Copper efflux ATPase



MET	LYS	ASP	HIS	HIS	GLN	GLY	THR	HIS	SER	GLY	LYS	GLY	HIS	ALA	CYS	HIS	HIS	GLU	HIS	ASN	SER	PRO	LYS	THR	GLN	GLN	ALA	SER	SER	LYS	MET	GLU	GLY	PRO	TLE	VAL	TYR	THR	CYS	PRO	MET	HIS	PRO	GLU	ILE	ARG	GLN	SER	ALA	PRO	GLY	HIS	CYS	PRO	LEU	CYS	GLY
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M717	A718	L719	V722	I726	N727	R730	L731	V734	I735	L736	G642	T645	V647	I649	A652	V654	T655	L656	L657	R658	G659	D660	L661	R662	G663	R668	R669	L670	S671	E672	S673	T674	M675	S676	Q680	F683	I687	Y688	N689	V690	L691	G692	V693	P694	L695	V699	L700	Y701	P702	L703	T704	G705	L706	L707	L708	S709	I712	A713	P560	E561	T562	I563	Q567	V574	M575	L576	T577	G578	D579	T583	G559	D660	L661	R662	G663	R668	L670	S671	E672	S673	T674	M675	S676	Q680	F683	I687	Y688	N689	V690	G692	V693	P694	L695	V699	L700	Y701	P702	L703	T704	G705	L706	L707	L708	S709	I712	A713	S480	L481	G482	S483	V484	E488	A489	P490	T491	G492	K493	G494	V495	V496	G497	Q498	V499	D500	G501	H502	H503	V504	A505	I506	R510	L511	M512	Q513	E514	A520	P521	L522	F523	E524	D527	V536	F538	M539	A540	V541	K544	T545	V546	A547	L548	V549	V551	T555	A556	T559	P560	E561	T562	I563	Q567	V574	M575	L576	T577	G578	D579	T583	G559	D660	L661	R662	G663	R668	L670	S671	E672	S673	T674	M675	S676	Q680	F683	I687	Y688	N689	V690	G692	V693	P694	L695	V699	L700	Y701	P702	L703	T704	G705	L706	L707	L708	S709	I712	A713	S480	L481	G482	S483	V484	E488	A489	P490	T491	G492	K493	G494	V495	V496	G497	Q498	V499	D500	G501	H502	H503	V504	A505	I506	R510	L511	M512	Q513	E514	A520	P521	L522	F523	E524	D527	V536	F538	M539	A540	V541	K544	T545	V546	A547	L548	V549	V551	T555	A556	T559	P560	E561	T562	I563	Q567	V574	M575	L576	T577	G578	D579	T583	G559	D660	L661	R662	G663	R668	L670	S671	E672	S673	T674	M675	S676	Q680	F683	I687	Y688	N689	V690	G692	V693	P694	L695	V699	L700	Y701	P702	L703	T704	G705	L706	L707	L708	S709	I712	A713	S480	L481	G482	S483	V484	E488	A489	P490	T491	G492	K493	G494	V495	V496	G497	Q498	V499	D500	G501	H502	H503	V504	A505	I506	R510	L511	M512	Q513	E514	A520	P521	L522	F523	E524	D527	V536	F538	M539	A540	V541	K544	T545	V546	A547	L548	V549	V551	T555	A556	T559	P560	E561	T562	I563	Q567	V574	M575	L576	T577	G578	D579	T583	G559	D660	L661	R662	G663	R668	L670	S671	E672	S673	T674	M675	S676	Q680	F683	I687	Y688	N689	V690	G692	V693	P694	L695	V699	L700	Y701	P702	L703	T704	G705	L706	L707	L708	S709	I712	A713	S480	L481	G482	S483	V484	E488	A489	P490	T491	G492	K493	G494	V495	V496	G497	Q498	V499	D500	G501	H502	H503	V504	A505	I506	R510	L511	M512	Q513	E514	A520	P521	L522	F523	E524	D527	V536	F538	M539	A540	V541	K544	T545	V546	A547	L548	V549	V551	T555	A556	T559	P560	E561	T562	I563	Q567	V574	M575	L576	T577	G578	D579	T583	G559	D660	L661	R662	G663	R668	L670	S671	E672	S673	T674	M675	S676	Q680	F683	I687	Y688	N689	V690	G692	V693	P694	L695	V699	L700	Y701	P702	L703	T704	G705	L706	L707	L708	S709	I712	A713	S480	L481	G482	S483	V484	E488	A489	P490	T491	G492	K493	G494	V495	V496	G497	Q498	V499	D500	G501	H502	H503	V504	A505	I506	R510	L511	M512	Q513	E514	A520	P521	L522	F523	E524	D527	V536	F538	M539	A540	V541	K544	T545	V546	A547	L548	V549	V551	T555	A556	T559	P560	E561	T562	I563	Q567	V574	M575	L576	T577	G578	D579	T583	G559	D660	L661	R662	G663	R668	L670	S671	E672	S673	T674	M675	S676	Q680	F683	I687	Y688	N689	V690	G692	V693	P694	L695	V699	L700	Y701	P702	L703	T704	G705	L706	L707	L708	S709	I712	A713	S480	L481	G482	S483	V484	E488	A489	P490	T491	G492	K493	G494	V495	V496	G497	Q498	V499	D500	G501	H502	H503	V504	A505	I506	R510	L511	M512	Q513	E514	A520	P521	L522	F523	E524	D527	V536	F538	M539	A540	V541	K544	T545	V546	A547	L548	V549	V551	T555	A556	T559	P560	E561	T562	I563	Q567	V574	M575	L576	T577	G578	D579	T583	G559	D660	L661	R662	G663	R668	L670	S671	E672	S673	T674	M675	S676	Q680	F683	I687	Y688	N689	V690	G692	V693	P694	L695	V699	L700	Y701	P702	L703	T704	G705	L706	L707	L708	S709	I712	A713	S480	L481	G482	S483	V484	E488	A489	P490	T491	G492	K493	G494	V495	V496	G497	Q498	V499	D500	G501	H502	H503	V504	A505	I506	R510	L511	M512	Q513	E514	A520	P521	L522	F523	E524	D527	V536	F538	M539	A540	V541	K544	T545	V546	A547	L548	V549	V551	T555	A556	T559	P560	E561	T562	I563	Q567	V574	M575	L576	T577	G578	D579	T583	G559	D660	L661	R662	G663	R668	L670	S671	E672	S673	T674	M675	S676	Q680	F683	I687	Y688	N689	V690	G692	V693	P694	L695	V699	L700	Y701	P702	L703	T704	G705	L706	L707	L708	S709	I712	A713	S480	L481	G482	S483	V484	E488	A489	P490	T491	G492	K493	G494	V495	V496	G497	Q498	V499	D500	G501	H502	H503	V504	A505	I506	R510	L511	M512	Q513	E514	A520	P521	L522	F523	E524	D527	V536	F538	M539	A540	V541	K544	T545	V546	A547	L548	V549	V551	T555	A556	T559	P560	E561	T562	I563	Q567	V574	M575	L576	T577	G578	D579	T583	G559	D660	L661	R662	G663	R668	L670	S671	E672	S673	T674	M675	S676	Q680	F683	I687	Y688	N689	V690	G692	V693	P694	L695	V699	L700	Y701	P702	L703	T704	G705	L706	L707	L708	S709	I712	A713	S480	L481	G482	S483	V484	E488	A489	P490	T491	G492	K493	G494	V495	V496	G497	Q498	V499	D500	G501	H502	H503	V504	A505	I506	R510	L511	M512	Q513	E514	A520	P521	L522	F523	E524	D527	V536	F538	M539	A540	V541	K544	T545	V546	A547	L548	V549	V551	T555	A556	T559	P560	E561	T562	I563	Q567	V574	M575	L576	T577	G578	D579	T583	G559	D660	L661	R662	G663	R668	L670	S671	E672	S673	T674	M675	S676	Q680	F683	I687	Y688	N689	V690	G692	V693	P694	L695	V699	L700	Y701	P702	L703	T704	G705	L706	L707	L708	S709	I712	A713	S480	L481	G482	S483	V484	E488	A489	P490	T491	G492	K493	G494	V495	V496	G497	Q498	V499	D500	G501	H502	H503	V504	A505	I506	R510	L511	M512	Q513	E514	A520	P521	L522	F523	E524	D527	V536	F538	M539	A540	V541	K544	T545	V546	A547	L548	V549	V551	T555	A556	T559	P560	E561	T562	I563	Q567	V574	M575	L576	T577	G578	D579	T583	G559	D660	L661	R662	G663	R668	L670	S671	E672	S673	T674	M675	S676	Q680	F683	I687	Y688	N689	V690	G692	V693	P694	L695	V699	L700	Y701	P702	L703	T704	G705	L706	L707	L708	S709	I712	A713	S480	L481	G482	S483	V484	E488	A489	P490	T491	G492	K493	G494	V495	V496	G497	Q498	V499	D500	G501	H502	H503	V504	A505	I506	R510	L511	M512	Q513	E514	A520	P521	L522	F523	E524	D527	V536	F538	M539	A540	V541	K544	T545	V546	A547	L548	V549	V551	T555	A556	T559	P560	E561	T562	I563	Q567	V574	M575	L576	T577	G578	D579	T583	G559	D660	L661	R662	G663	R668	L670	S671	E672	S673	T674	M675	S676	Q680	F683	I687	Y688	N689	V690	G692	V693	P694	L695	V699	L700	Y701	P702	L703	T704	G705	L706	L707	L708	S709	I712	A713	S480	L481	G482	S483	V484	E488	A489	P490	T491	G492	K493	G494	V495	V496	G497	Q498	V499	D500	G501	H502	H503	V504	A505	I506	R510	L511	M512	Q513	E514	A520	P521	L522	F523	E524	D527	V536	F538	M539	A540	V541	K544	T545	V546	A547	L548	V549	V551	T555	A556	T559	P560	E561	T562	I563	Q567	V574	M575	L576	T577	G578	D579	T583	G559	D660	L661	R662	G663	R668	L670	S671	E672	S673	T674	M675	S676	Q680	F683	I687	Y688	N689	V690	G692	V693	P694	L695	V699	L700	Y701	P702	L703	T704	G705	L706	L707	L708	S709	I712	A713	S480	L481	G482	S483	V484	E488	A489	P490	T491	G492	K493	G494	V495	V496	G497	Q498	V499	D500	G501	H502	H503	V504	A505	I506	R510	L511	M512	Q513	E514	A520	P521	L522	F523	E524	D527	V536	F538	M539	A540	V541	K544	T545	V546	A547	L548	V549	V551	T555	A556	T559	P560	E561	T562	I563	Q567	V574	M575	L576	T577	G578	D579	T583	G559	D660	L661	R662	G663	R668	L670	S671	E672	S673	T674	M675	S676	Q680	F683	I687	Y688	N689	V690	G692	V693	P694	L695	V699	L700	Y701	P702	L703	T704	G705	L706	L707	L708	S709	I712	A713	S480	L481	G482	S483	V484	E488	A489	P490	T491	G492	K493	G494	V495	V496	G497	Q498	V499	D500	G501	H502	H503	V504	A505	I506	R510	L511	M512	Q513	E514	A520	P521	L522	F523	E524	D527	V536	F538	M539	A540	V541	K544	T545	V546	A547	L548	V549	V551	T555	A556	T559	P560	E561	T562	I563	Q567	V574	M575	L576	T577	G578	D579	T583	G559	D660	L661	R662	G663	R668	L670	S671	E672	S673	T674	M675	S676	Q680	F683	I687	Y688	N689	V690	G692	V693	P694	L695	V699	L700	Y701	P702	L703	T704	G705	L706	L707	L708	S709	I712	A713	S480	L481	G482	S483	V484	E488	A489	P490	T491	G492	K493	G494	V495	V496	G497	Q498	V499	D500	G501	H502	H503	V504	A505	I506	R510	L511	M512	Q513	E514	A520	P521	L522	F523	E524	D527	V536	F538	M539	A540	V541	K544	T545	V546	A547	L548	V549	V551	T555	A556	T559	P560	E561	T562	I563	Q567	V574	M575</
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	44.15Å 72.98Å 329.95Å 89.96° 90.04° 90.22°	Depositor
Resolution (Å)	20.00 – 3.20 20.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.8 (20.00-3.20) 96.5 (20.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.235 , 0.261 (Not available) , 0.252	Depositor DCC
R_{free} test set	1945 reflections (2.44%)	wwPDB-VP
Wilson B-factor (Å ²)	89.5	Xtriage
Anisotropy	0.526	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 121.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.438 for h,-k,-l 0.428 for -h,k,-l 0.438 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19764	wwPDB-VP
Average B, all atoms (Å ²)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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, 0.333 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: K, MG, ALF

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	0.35	0/5017	0.90	19/6812 (0.3%)
1	B	0.35	0/5017	0.90	19/6812 (0.3%)
1	C	0.35	0/5017	0.90	19/6812 (0.3%)
1	D	0.35	0/5017	0.90	19/6812 (0.3%)
All	All	0.35	0/20068	0.90	76/27248 (0.3%)

There are no bond length outliers.

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	706	LEU	N-CA-C	8.80	118.61	108.49
1	D	706	LEU	N-CA-C	8.74	118.54	108.49
1	C	706	LEU	N-CA-C	8.73	118.53	108.49
1	A	706	LEU	N-CA-C	8.63	118.41	108.49
1	B	735	THR	N-CA-C	-7.54	103.15	111.36

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	4934	0	5125	408	0
1	B	4934	0	5125	416	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4934	0	5125	416	0
1	D	4934	0	5125	406	0
2	A	5	0	0	2	0
2	B	5	0	0	0	0
2	C	5	0	0	1	0
2	D	5	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	19764	0	20500	1634	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 41.

The worst 5 of 1634 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:B:123:THR:HG23	1:B:124:PRO:HD3	1.31	1.12
1:C:123:THR:HG23	1:C:124:PRO:HD3	1.31	1.12
1:A:123:THR:HG23	1:A:124:PRO:HD3	1.31	1.12
1:D:123:THR:HG23	1:D:124:PRO:HD3	1.31	1.12
1:A:662:ARG:HB2	1:A:663:GLY:HA3	1.34	1.09

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	661/736 (90%)	578 (87%)	69 (10%)	14 (2%)	5	31
1	B	661/736 (90%)	578 (87%)	68 (10%)	15 (2%)	5	29
1	C	661/736 (90%)	578 (87%)	69 (10%)	14 (2%)	5	31
1	D	661/736 (90%)	579 (88%)	68 (10%)	14 (2%)	5	31
All	All	2644/2944 (90%)	2313 (88%)	274 (10%)	57 (2%)	5	29

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	PRO
1	A	662	ARG
1	B	224	PRO
1	C	224	PRO
1	C	662	ARG

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	523/586 (89%)	481 (92%)	42 (8%)	11	40
1	B	523/586 (89%)	480 (92%)	43 (8%)	10	39
1	C	523/586 (89%)	480 (92%)	43 (8%)	10	39
1	D	523/586 (89%)	480 (92%)	43 (8%)	10	39
All	All	2092/2344 (89%)	1921 (92%)	171 (8%)	10	39

5 of 171 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	506	ILE
1	D	307	LEU
1	C	596	VAL
1	D	150	THR
1	D	424	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	513	GLN
1	D	513	GLN
1	B	567	GLN
1	D	567	GLN
1	D	112	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ALF	A	995	-	4,4,4	1.35	0	-		
2	ALF	B	995	-	4,4,4	1.37	0	-		
2	ALF	D	995	-	4,4,4	1.37	0	-		
2	ALF	C	995	-	4,4,4	1.35	0	-		

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.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	995	ALF	2	0
2	D	995	ALF	1	0
2	C	995	ALF	1	0

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	663/736 (90%)	-0.07	11 (1%) 69 49	56, 106, 243, 371	0
1	B	663/736 (90%)	-0.05	14 (2%) 63 43	55, 106, 244, 373	0
1	C	663/736 (90%)	-0.04	15 (2%) 61 41	55, 106, 244, 371	0
1	D	663/736 (90%)	-0.07	9 (1%) 73 54	56, 106, 244, 369	0
All	All	2652/2944 (90%)	-0.06	49 (1%) 67 48	55, 106, 244, 373	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	501	GLY	5.2
1	D	501	GLY	4.9
1	C	500	ASP	4.9
1	D	500	ASP	4.4
1	B	500	ASP	4.1

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 oligosaccharides 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, 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	K	B	997	1/1	0.79	0.17	154,154,154,154	0
4	K	C	997	1/1	0.81	0.12	144,144,144,144	0
4	K	A	997	1/1	0.83	0.14	141,141,141,141	0
4	K	D	997	1/1	0.84	0.14	160,160,160,160	0
2	ALF	D	995	5/5	0.95	0.10	57,62,80,127	0
2	ALF	B	995	5/5	0.96	0.08	48,60,80,130	0
3	MG	B	996	1/1	0.96	0.12	67,67,67,67	0
2	ALF	C	995	5/5	0.97	0.07	45,57,62,117	0
2	ALF	A	995	5/5	0.98	0.09	37,50,60,136	0
3	MG	C	996	1/1	0.98	0.12	58,58,58,58	0
3	MG	A	996	1/1	0.99	0.10	68,68,68,68	0
3	MG	D	996	1/1	0.99	0.15	77,77,77,77	0

6.5 Other polymers ⓘ

There are no such residues in this entry.