



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 27, 2023 – 02:01 AM EDT

PDB ID : 3FH6  
Title : Crystal structure of the resting state maltose transporter from *E. coli*  
Authors : Khare, D.; Oldham, M.L.; Orelle, C.; Davidson, A.L.; Chen, J.  
Deposited on : 2008-12-08  
Resolution : 4.50 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

<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>.

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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 : 2.35  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

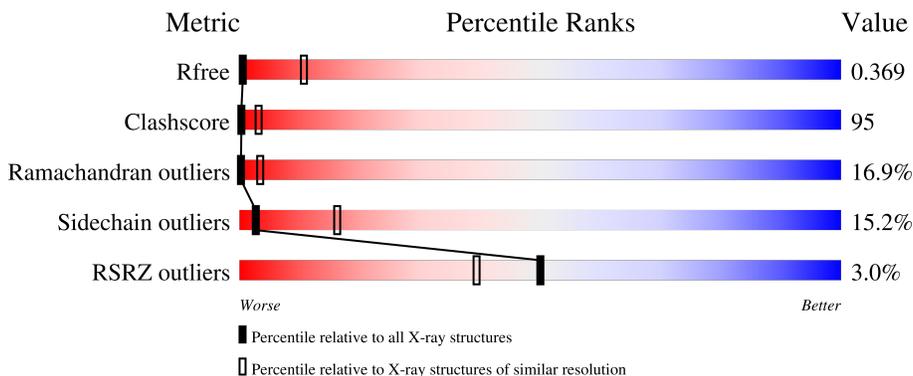
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.50 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.



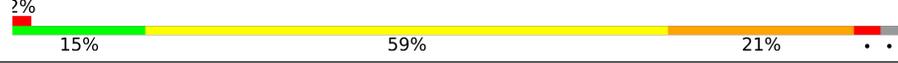
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1055 (5.20-3.80)
Clashscore	141614	1123 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)
RSRZ outliers	127900	1101 (5.30-3.70)

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  $\geq 3$ , 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	F	480	 9% 41% 14% 34%
1	H	480	 4% 9% 42% 14%
2	G	296	 2% 17% 52% 14%
2	I	296	 2% 17% 52% 14%
3	A	381	 2% 12% 60% 22%

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Mol	Chain	Length	Quality of chain
3	B	381	
3	C	381	
3	D	381	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 20236 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 Maltose transport system permease protein malF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	F	316	2418	1607	378	418	15	0	0	0
1	H	316	2418	1607	378	418	15	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	35	MET	-	expression tag	UNP P02916
H	35	MET	-	expression tag	UNP P02916

- Molecule 2 is a protein called Maltose transport system permease protein malG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	G	254	1942	1308	306	319	9	0	0	0
2	I	254	1942	1308	306	319	9	0	0	0

- Molecule 3 is a protein called Maltose/maltodextrin import ATP-binding protein malK.

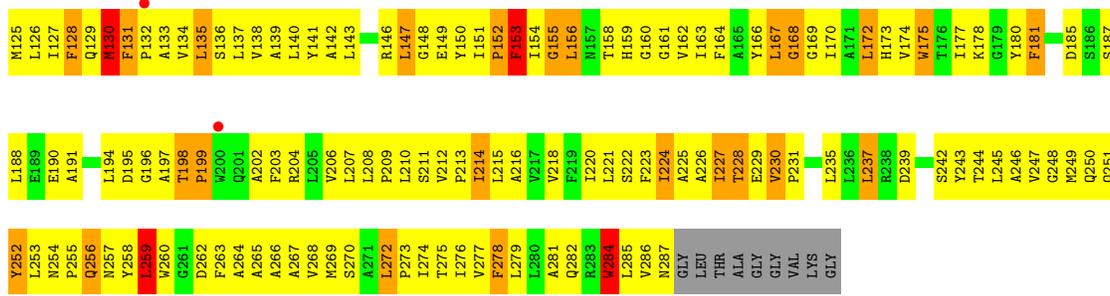
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	371	2876	1819	515	529	13	0	0	0
3	B	372	2882	1822	516	531	13	0	0	0
3	C	371	2876	1819	515	529	13	0	0	0
3	D	372	2882	1822	516	531	13	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

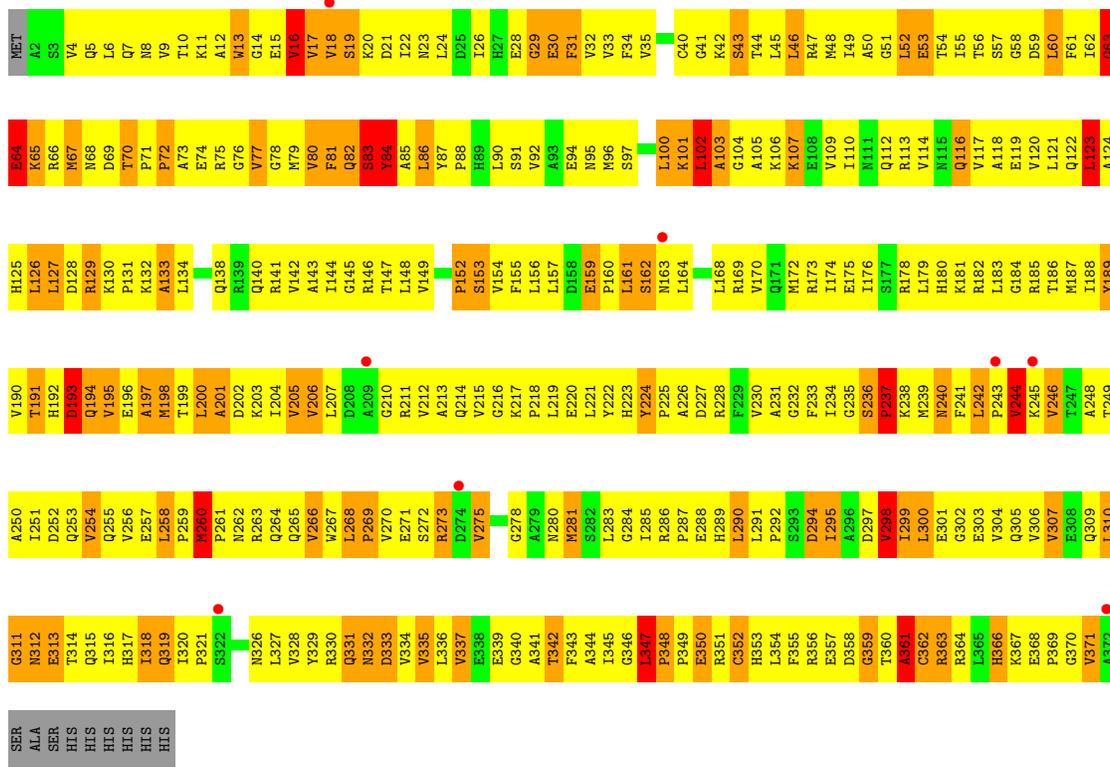
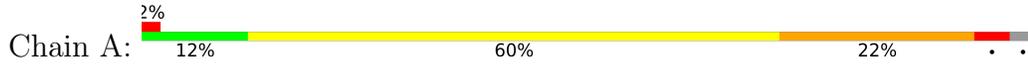
Chain	Residue	Modelled	Actual	Comment	Reference
A	372	ALA	-	expression tag	UNP P68187
A	373	SER	-	expression tag	UNP P68187
A	374	ALA	-	expression tag	UNP P68187
A	375	SER	-	expression tag	UNP P68187
A	376	HIS	-	expression tag	UNP P68187
A	377	HIS	-	expression tag	UNP P68187
A	378	HIS	-	expression tag	UNP P68187
A	379	HIS	-	expression tag	UNP P68187
A	380	HIS	-	expression tag	UNP P68187
A	381	HIS	-	expression tag	UNP P68187
B	372	ALA	-	expression tag	UNP P68187
B	373	SER	-	expression tag	UNP P68187
B	374	ALA	-	expression tag	UNP P68187
B	375	SER	-	expression tag	UNP P68187
B	376	HIS	-	expression tag	UNP P68187
B	377	HIS	-	expression tag	UNP P68187
B	378	HIS	-	expression tag	UNP P68187
B	379	HIS	-	expression tag	UNP P68187
B	380	HIS	-	expression tag	UNP P68187
B	381	HIS	-	expression tag	UNP P68187
C	372	ALA	-	expression tag	UNP P68187
C	373	SER	-	expression tag	UNP P68187
C	374	ALA	-	expression tag	UNP P68187
C	375	SER	-	expression tag	UNP P68187
C	376	HIS	-	expression tag	UNP P68187
C	377	HIS	-	expression tag	UNP P68187
C	378	HIS	-	expression tag	UNP P68187
C	379	HIS	-	expression tag	UNP P68187
C	380	HIS	-	expression tag	UNP P68187
C	381	HIS	-	expression tag	UNP P68187
D	372	ALA	-	expression tag	UNP P68187
D	373	SER	-	expression tag	UNP P68187
D	374	ALA	-	expression tag	UNP P68187
D	375	SER	-	expression tag	UNP P68187
D	376	HIS	-	expression tag	UNP P68187
D	377	HIS	-	expression tag	UNP P68187
D	378	HIS	-	expression tag	UNP P68187
D	379	HIS	-	expression tag	UNP P68187
D	380	HIS	-	expression tag	UNP P68187
D	381	HIS	-	expression tag	UNP P68187



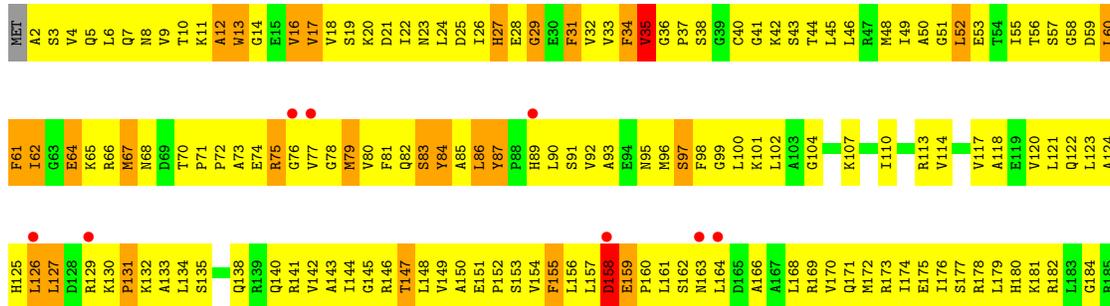
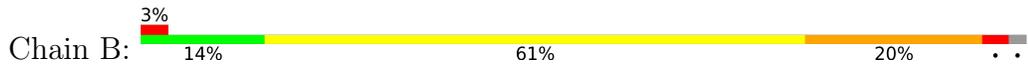


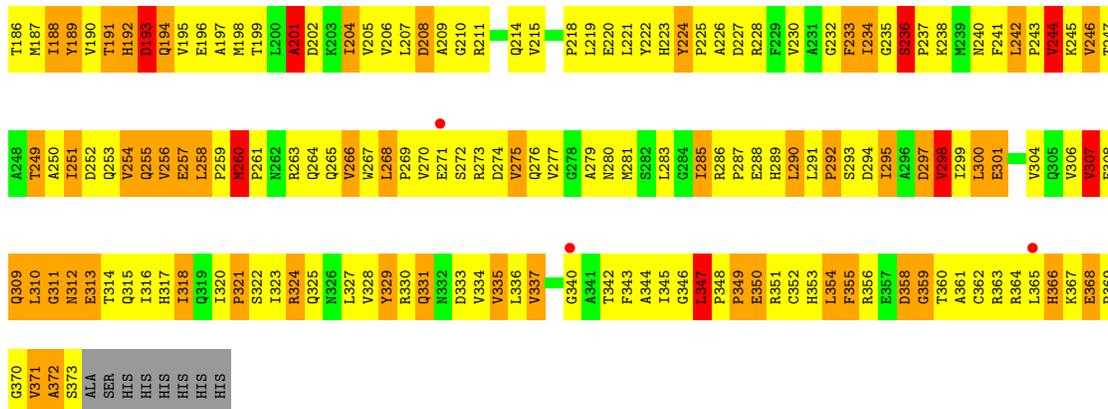


• Molecule 3: Maltose/maltodextrin import ATP-binding protein malK

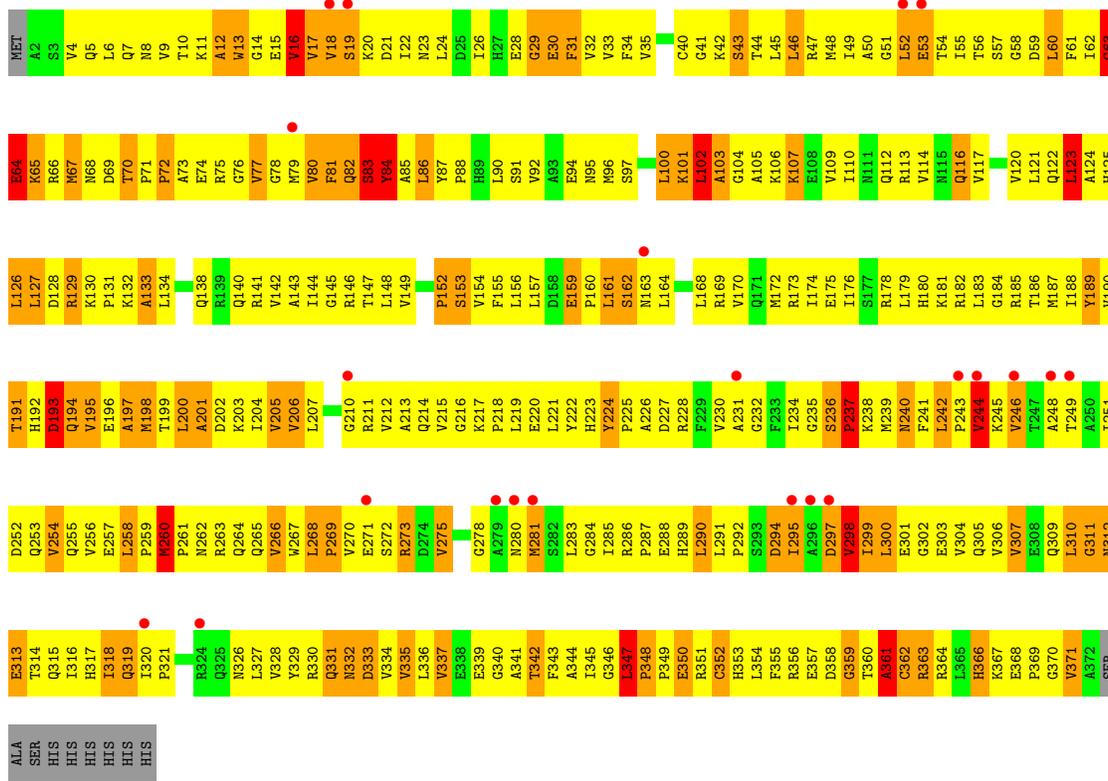
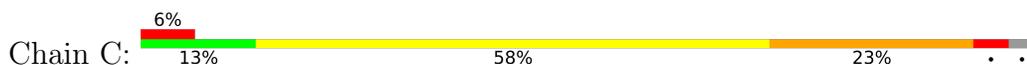


• Molecule 3: Maltose/maltodextrin import ATP-binding protein malK

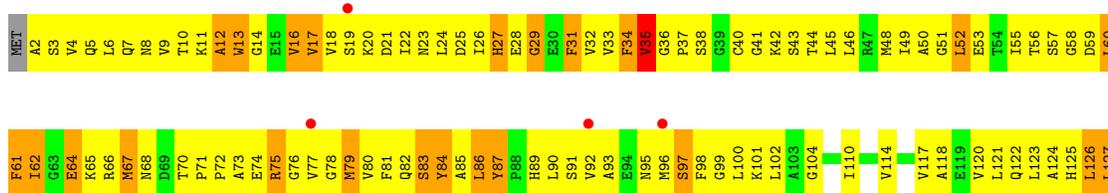
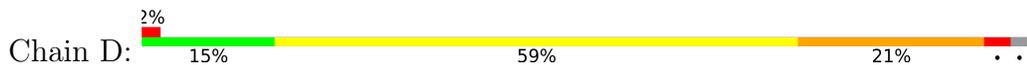




• Molecule 3: Maltose/maltodextrin import ATP-binding protein malK



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HIS	T314	Q253	E128	T191	Q254	T192	R129	Q255	H193	Q256	R130	Q257	K131	Q258	R132	Q259	K133	Q260	R134	Q261	K135	Q262	R136	Q263	K137	Q264	R138	Q265	K138	Q266	R139	Q267	K139	Q268	R140	Q269	K140	Q270	R141	Q271	K141	Q272	R142	Q273	K142	Q274	R143	Q275	K143	Q276	R144	Q277	K144	Q278	R145	Q279	K145	Q280	R146	Q281	K146	Q282	R147	Q283	K147	Q284	R148	Q285	K148	Q286	R149	Q287	K149	Q288	R150	Q289	K150	Q290	R151	Q291	K151	Q292	R152	Q293	K152	Q294	R153	Q295	K153	Q296	R154	Q297	K154	Q298	R155	Q299	K155	Q300	R156	Q301	K156	Q302	R157	Q303	K157	Q304	R158	Q305	K158	Q306	R159	Q307	K159	Q308	R160	Q309	K160	Q310	R161	Q311	K161	Q312	R162	Q313	K162	Q314	R163	Q315	K163	Q316	R164	Q317	K164	Q318	R165	Q319	K165	Q320	R166	Q321	K166	Q322	R167	Q323	K167	Q324	R168	Q325	K168	Q326	R169	Q327	K169	Q328	R170	Q329	K170	Q330	R171	Q331	K171	Q332	R172	Q333	K172	Q334	R173	Q335	K173	Q336	R174	Q337	K174	Q338	R175	Q339	K175	Q340	R176	Q341	K176	Q342	R177	Q343	K177	Q344	R178	Q345	K178	Q346	R179	Q347	K179	Q348	R180	Q349	K180	Q350	R181	Q351	K181	Q352	R182	Q353	K182	Q354	R183	Q355	K183	Q356	R184	Q357	K184	Q358	R185	Q359	K185	Q360	R186	Q361	K186	Q362	R187	Q363	K187	Q364	R188	Q365	K188	Q366	R189	Q367	K189	Q368	R190	Q369	K190	Q370	R191	Q371	K191	Q372	R192	Q373	K192	Q374	R193	Q375	K193	Q376	R194	Q377	K194	Q378	R195	Q379	K195	Q380	R196	Q381	K196	Q382	R197	Q383	K197	Q384	R198	Q385	K198	Q386	R199	Q387	K199	Q388	R200	Q389	K200	Q390	R201	Q391	K201	Q392	R202	Q393	K202	Q394	R203	Q395	K203	Q396	R204	Q397	K204	Q398	R205	Q399	K205	Q400	R206	Q401	K206	Q402	R207	Q403	K207	Q404	R208	Q405	K208	Q406	R209	Q407	K209	Q408	R210	Q409	K210	Q410	R211	Q411	K211	Q412	R212	Q413	K212	Q414	R213	Q415	K213	Q416	R214	Q417	K214	Q418	R215	Q419	K215	Q420	R216	Q421	K216	Q422	R217	Q423	K217	Q424	R218	Q425	K218	Q426	R219	Q427	K219	Q428	R220	Q429	K220	Q430	R221	Q431	K221	Q432	R222	Q433	K222	Q434	R223	Q435	K223	Q436	R224	Q437	K224	Q438	R225	Q439	K225	Q440	R226	Q441	K226	Q442	R227	Q443	K227	Q444	R228	Q445	K228	Q446	R229	Q447	K229	Q448	R230	Q449	K230	Q450	R231	Q451	K231	Q452	R232	Q453	K232	Q454	R233	Q455	K233	Q456	R234	Q457	K234	Q458	R235	Q459	K235	Q460	R236	Q461	K236	Q462	R237	Q463	K237	Q464	R238	Q465	K238	Q466	R239	Q467	K239	Q468	R240	Q469	K240	Q470	R241	Q471	K241	Q472	R242	Q473	K242	Q474	R243	Q475	K243	Q476	R244	Q477	K244	Q478	R245	Q479	K245	Q480	R246	Q481	K246	Q482	R247	Q483	K247	Q484	R248	Q485	K248	Q486	R249	Q487	K249	Q488	R250	Q489	K250	Q490	R251	Q491	K251	Q492	R252	Q493	K252	Q494	R253	Q495	K253	Q496	R254	Q497	K254	Q498	R255	Q499	K255	Q500	R256	Q501	K256	Q502	R257	Q503	K257	Q504	R258	Q505	K258	Q506	R259	Q507	K259	Q508	R260	Q509	K260	Q510	R261	Q511	K261	Q512	R262	Q513	K262	Q514	R263	Q515	K263	Q516	R264	Q517	K264	Q518	R265	Q519	K265	Q520	R266	Q521	K266	Q522	R267	Q523	K267	Q524	R268	Q525	K268	Q526	R269	Q527	K269	Q528	R270	Q529	K270	Q530	R271	Q531	K271	Q532	R272	Q533	K272	Q534	R273	Q535	K273	Q536	R274	Q537	K274	Q538	R275	Q539	K275	Q540	R276	Q541	K276	Q542	R277	Q543	K277	Q544	R278	Q545	K278	Q546	R279	Q547	K279	Q548	R280	Q549	K280	Q550	R281	Q551	K281	Q552	R282	Q553	K282	Q554	R283	Q555	K283	Q556	R284	Q557	K284	Q558	R285	Q559	K285	Q560	R286	Q561	K286	Q562	R287	Q563	K287	Q564	R288	Q565	K288	Q566	R289	Q567	K289	Q568	R290	Q569	K290	Q570	R291	Q571	K291	Q572	R292	Q573	K292	Q574	R293	Q575	K293	Q576	R294	Q577	K294	Q578	R295	Q579	K295	Q580	R296	Q581	K296	Q582	R297	Q583	K297	Q584	R298	Q585	K298	Q586	R299	Q587	K299	Q588	R300	Q589	K300	Q590	R301	Q591	K301	Q592	R302	Q593	K302	Q594	R303	Q595	K303	Q596	R304	Q597	K304	Q598	R305	Q599	K305	Q600	R306	Q601	K306	Q602	R307	Q603	K307	Q604	R308	Q605	K308	Q606	R309	Q607	K309	Q608	R310	Q609	K310	Q610	R311	Q611	K311	Q612	R312	Q613	K312	Q614	R313	Q615	K313	Q616	R314	Q617	K314	Q618	R315	Q619	K315	Q620	R316	Q621	K316	Q622	R317	Q623	K317	Q624	R318	Q625	K318	Q626	R319	Q627	K319	Q628	R320	Q629	K320	Q630	R321	Q631	K321	Q632	R322	Q633	K322	Q634	R323	Q635	K323	Q636	R324	Q637	K324	Q638	R325	Q639	K325	Q640	R326	Q641	K326	Q642	R327	Q643	K327	Q644	R328	Q645	K328	Q646	R329	Q647	K329	Q648	R330	Q649	K330	Q650	R331	Q651	K331	Q652	R332	Q653	K332	Q654	R333	Q655	K333	Q656	R334	Q657	K334	Q658	R335	Q659	K335	Q660	R336	Q661	K336	Q662	R337	Q663	K337	Q664	R338	Q665	K338	Q666	R339	Q667	K339	Q668	R340	Q669	K340	Q670	R341	Q671	K341	Q672	R342	Q673	K342	Q674	R343	Q675	K343	Q676	R344	Q677	K344	Q678	R345	Q679	K345	Q680	R346	Q681	K346	Q682	R347	Q683	K347	Q684	R348	Q685	K348	Q686	R349	Q687	K349	Q688	R350	Q689	K350	Q690	R351	Q691	K351	Q692	R352	Q693	K352	Q694	R353	Q695	K353	Q696	R354	Q697	K354	Q698	R355	Q699	K355	Q700	R356	Q701	K356	Q702	R357	Q703	K357	Q704	R358	Q705	K358	Q706	R359	Q707	K359	Q708	R360	Q709	K360	Q710	R361	Q711	K361	Q712	R362	Q713	K362	Q714	R363	Q715	K363	Q716	R364	Q717	K364	Q718	R365	Q719	K365	Q720	R366	Q721	K366	Q722	R367	Q723	K367	Q724	R368	Q725	K368	Q726	R369	Q727	K369	Q728	R370	Q729	K370	Q730	R371	Q731	K371	Q732	R372	Q733	K372	Q734	R373	Q735	K373	Q736	R374	Q737	K374	Q738	R375	Q739	K375	Q740	R376	Q741	K376	Q742	R377	Q743	K377	Q744	R378	Q745	K378	Q746	R379	Q747	K379	Q748	R380	Q749	K380	Q750	R381	Q751	K381	Q752	R382	Q753	K382	Q754	R383	Q755	K383	Q756	R384	Q757	K384	Q758	R385	Q759	K385	Q760	R386	Q761	K386	Q762	R387	Q763	K387	Q764	R388	Q765	K388	Q766	R389	Q767	K389	Q768	R390	Q769	K390	Q770	R391	Q771	K391	Q772	R392	Q773	K392	Q774	R393	Q775	K393	Q776	R394	Q777	K394	Q778	R395	Q779	K395	Q780	R396	Q781	K396	Q782	R397	Q783	K397	Q784	R398	Q785	K398	Q786	R399	Q787	K399	Q788	R400	Q789	K400	Q790	R401	Q791	K401	Q792	R402	Q793	K402	Q794	R403	Q795	K403	Q796	R404	Q797	K404	Q798	R405	Q799	K405	Q800	R406	Q801	K406	Q802	R407	Q803	K407	Q804	R408	Q805	K408	Q806	R409	Q807	K409	Q808	R410	Q809	K410	Q810	R411	Q811	K411	Q812	R412	Q813	K412	Q814	R413	Q815	K413	Q816	R414	Q817	K414	Q818	R415	Q819	K415	Q820	R416	Q821	K416	Q822	R417	Q823	K417	Q824	R418	Q825	K418	Q826	R419	Q827	K419	Q828	R420	Q829	K420	Q830	R421	Q831	K421	Q832	R422	Q833	K422	Q834	R423	Q835	K423	Q836	R424	Q837	K424	Q838	R425	Q839	K425	Q840	R426	Q841	K426	Q842	R427	Q843	K427	Q844	R428	Q845	K428	Q846	R429	Q847	K429	Q848	R430	Q849	K430	Q850	R431	Q851	K431	Q852	R432	Q853	K432	Q854	R433	Q855	K433	Q856	R434	Q857	K434	Q858	R435	Q859	K435	Q860	R436	Q861	K436	Q862	R437	Q863	K437	Q864	R438	Q865	K438	Q866	R439	Q867	K439	Q868	R440	Q869	K440	Q870	R441	Q871	K441	Q872	R442	Q873	K442	Q874	R443	Q875	K443	Q876	R444	Q877	K444	Q878	R445	Q879	K445	Q880	R446	Q881	K446	Q882	R447	Q883	K447	Q884	R448	Q885	K448	Q886	R449	Q887	K449	Q888	R450	Q889	K450	Q890	R451	Q891	K451	Q892	R452	Q893	K452	Q894	R453	Q895	K453	Q896	R454	Q897	K454	Q898	R455	Q899	K455	Q900	R456	Q901	K456	Q902	R457	Q903	K457	Q904	R458	Q905	K458	Q906	R459	Q907	K459	Q908	R460	Q909	K460	Q910	R461	Q911	K461	Q912	R462	Q913	K462	Q914	R463	Q915	K463	Q916	R464	Q917	K464	Q918	R465	Q919	K465	Q920	R466	Q921	K466	Q922	R467	Q923	K467	Q924	R468	Q925	K468	Q926	R469	Q927	K469	Q928	R470	Q929	K470	Q930	R471	Q931	K471	Q932	R472	Q933	K472	Q934	R473	Q935	K473	Q936	R474	Q937	K474	Q938	R475	Q939	K475	Q940	R476	Q941	K476	Q942	R477	Q943	K477	Q944	R478	Q945	K478	Q946	R479	Q947	K479	Q948	R480	Q949	K480	Q950	R481	Q951	K481	Q952	R482	Q953	K482	Q954	R483	Q955	K483	Q956	R484	Q957	K484	Q958	R485	Q959	K485	Q960	R486	Q961	K486	Q962	R487	Q963	K487	Q964	R488	Q965	K488	Q966	R489	Q967	K489	Q968	R490	Q969	K490	Q970	R491	Q
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## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	171.10Å 209.48Å 438.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 4.50 49.19 – 4.50	Depositor EDS
% Data completeness (in resolution range)	85.2 (50.00-4.50) 85.2 (49.19-4.50)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 4.45Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.340 , 0.363 0.354 , 0.369	Depositor DCC
$R_{free}$ test set	2038 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	216.6	Xtrriage
Anisotropy	0.633	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.18 , 150.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	20236	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	300.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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	F	0.51	0/2473	0.85	3/3365 (0.1%)
1	H	0.51	0/2473	0.85	2/3365 (0.1%)
2	G	0.49	0/1992	0.87	5/2724 (0.2%)
2	I	0.50	0/1992	0.87	5/2724 (0.2%)
3	A	0.46	1/2926 (0.0%)	0.90	6/3968 (0.2%)
3	B	0.49	1/2932 (0.0%)	0.92	2/3976 (0.1%)
3	C	0.46	1/2926 (0.0%)	0.90	6/3968 (0.2%)
3	D	0.49	1/2932 (0.0%)	0.92	2/3976 (0.1%)
All	All	0.49	4/20646 (0.0%)	0.89	31/28066 (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
3	A	0	1
3	C	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	159	GLU	CD-OE2	6.81	1.33	1.25
3	A	159	GLU	CD-OE2	6.79	1.33	1.25
3	D	159	GLU	CD-OE2	6.50	1.32	1.25
3	B	159	GLU	CD-OE2	6.49	1.32	1.25

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	259	LEU	N-CA-C	-7.22	91.50	111.00
2	I	259	LEU	N-CA-C	-7.22	91.51	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	196	GLY	N-CA-C	6.62	129.66	113.10
2	I	196	GLY	N-CA-C	6.62	129.66	113.10
1	H	380	GLY	N-CA-C	6.46	129.24	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	84	TYR	Sidechain
3	C	84	TYR	Sidechain

## 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	F	2418	0	2476	555	0
1	H	2418	0	2476	557	0
2	G	1942	0	2008	362	0
2	I	1942	0	2008	365	0
3	A	2876	0	2942	582	15
3	B	2882	0	2947	557	12
3	C	2876	0	2942	571	9
3	D	2882	0	2947	549	5
All	All	20236	0	20746	3892	31

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 95.

The worst 5 of 3892 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:F:347:ILE:HG23	1:F:348:ASN:H	1.03	1.15
3:D:157:LEU:HD23	3:D:160:PRO:HG3	1.30	1.13
1:F:275:LYS:H	1:F:276:PRO:HD2	1.07	1.13
1:F:387:LEU:HD21	1:F:429:LEU:HD13	1.29	1.12
3:C:79:MET:HG2	3:C:80:VAL:H	1.14	1.12

The worst 5 of 31 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)
3:A:182:ARG:O	3:B:324:ARG:NH1[2_565]	0.90	1.30
3:C:267:TRP:NE1	3:C:267:TRP:NE1[3_555]	1.15	1.05
3:B:340:GLY:O	3:B:340:GLY:O[2_565]	1.19	1.01
3:B:276:GLN:OE1	3:D:274:ASP:N[2_565]	1.26	0.94
3:A:119:GLU:CG	3:A:119:GLU:CD[2_565]	1.27	0.93

## 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	F	310/480 (65%)	209 (67%)	61 (20%)	40 (13%)	0	5
1	H	310/480 (65%)	209 (67%)	61 (20%)	40 (13%)	0	5
2	G	250/296 (84%)	179 (72%)	38 (15%)	33 (13%)	0	4
2	I	250/296 (84%)	179 (72%)	38 (15%)	33 (13%)	0	4
3	A	369/381 (97%)	198 (54%)	97 (26%)	74 (20%)	0	2
3	B	370/381 (97%)	203 (55%)	95 (26%)	72 (20%)	0	2
3	C	369/381 (97%)	198 (54%)	96 (26%)	75 (20%)	0	2
3	D	370/381 (97%)	203 (55%)	95 (26%)	72 (20%)	0	2
All	All	2598/3076 (84%)	1578 (61%)	581 (22%)	439 (17%)	0	3

5 of 439 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	90	ALA
1	F	92	THR
1	F	94	TYR
1	F	96	SER
1	F	98	ASN

### 5.3.2 Protein sidechains [i](#)

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	F	253/394 (64%)	201 (79%)	52 (21%)	1	7
1	H	253/394 (64%)	201 (79%)	52 (21%)	1	7
2	G	198/237 (84%)	166 (84%)	32 (16%)	2	15
2	I	198/237 (84%)	166 (84%)	32 (16%)	2	15
3	A	314/323 (97%)	273 (87%)	41 (13%)	4	20
3	B	315/323 (98%)	276 (88%)	39 (12%)	4	22
3	C	314/323 (97%)	273 (87%)	41 (13%)	4	20
3	D	315/323 (98%)	276 (88%)	39 (12%)	4	22
All	All	2160/2554 (85%)	1832 (85%)	328 (15%)	3	16

5 of 328 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	130	MET
3	C	342	THR
2	I	181	PHE
3	C	83	SER
3	D	127	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	309	GLN
3	D	276	GLN
1	H	376	ASN
3	D	264	GLN
3	D	82	GLN

### 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 monosaccharides 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	F	316/480 (65%)	-0.31	3 (0%) 84 77	187, 310, 422, 493	0
1	H	316/480 (65%)	0.04	19 (6%) 21 18	187, 310, 422, 493	0
2	G	254/296 (85%)	-0.19	5 (1%) 65 56	204, 296, 401, 510	0
2	I	254/296 (85%)	-0.29	5 (1%) 65 56	204, 296, 401, 510	0
3	A	371/381 (97%)	-0.08	8 (2%) 62 52	195, 296, 384, 474	0
3	B	372/381 (97%)	-0.06	11 (2%) 50 39	150, 281, 361, 454	0
3	C	371/381 (97%)	0.15	22 (5%) 22 19	195, 296, 384, 474	0
3	D	372/381 (97%)	-0.15	7 (1%) 66 58	150, 281, 361, 454	0
All	All	2626/3076 (85%)	-0.10	80 (3%) 50 39	150, 294, 398, 510	0

The worst 5 of 80 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	280	ASN	6.5
1	H	56	ILE	6.2
1	H	483	ASP	5.7
3	C	281	MET	5.5
3	C	244	VAL	5.4

### 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 monosaccharides in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.