



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:46 AM GMT

PDB ID : 2TAA
Title : STRUCTURE AND POSSIBLE CATALYTIC RESIDUES OF TAKA-AMYLASE A
Authors : Kusunoki, M.; Matsuura, Y.; Tanaka, N.; Kakudo, M.
Deposited on : 1982-10-18
Resolution : 3.00 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

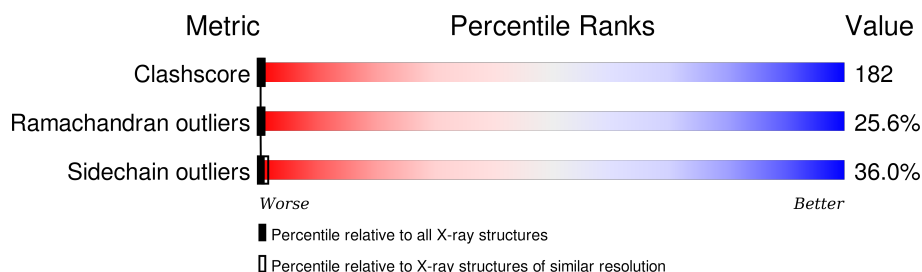
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	478	
1	B	478	
1	C	478	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11073 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 TAKA-AMYLASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	0	0	0
			3690	2332	593	746	19			
1	B	478	Total	C	N	O	S	0	0	0
			3690	2332	593	746	19			
1	C	478	Total	C	N	O	S	0	0	0
			3690	2332	593	746	19			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

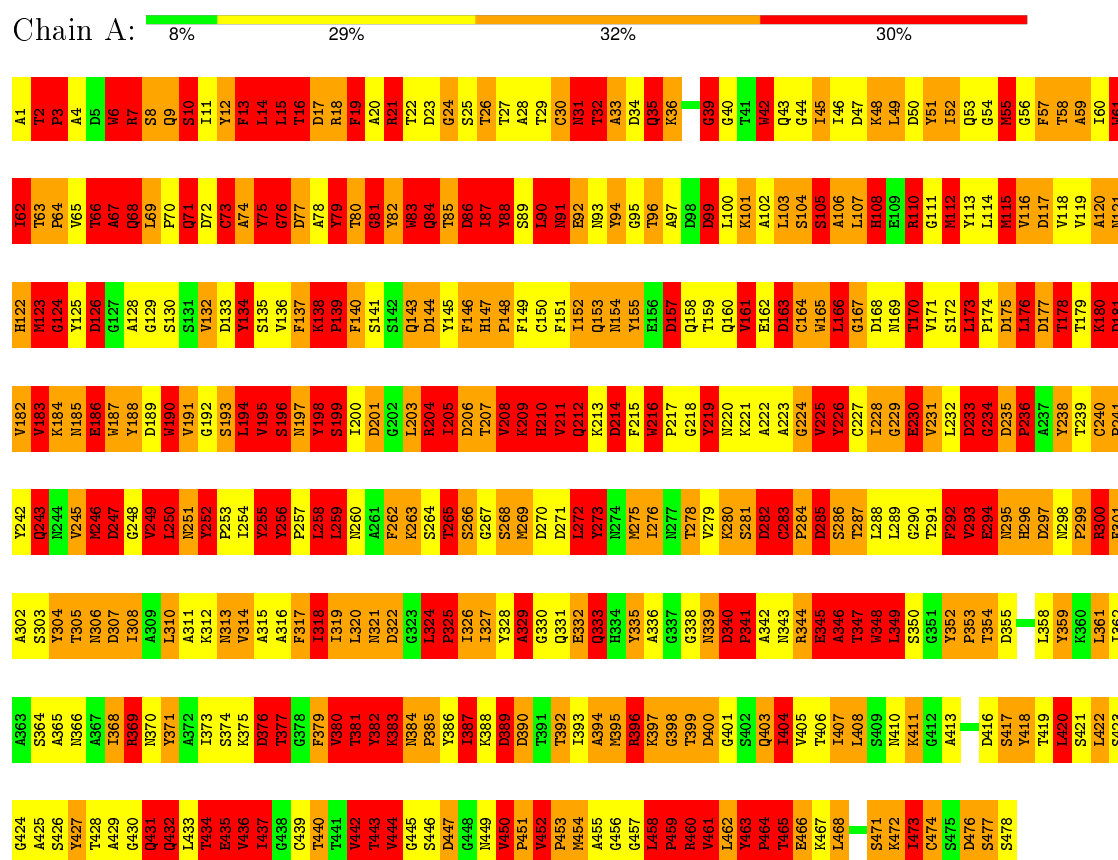
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

3 Residue-property plots

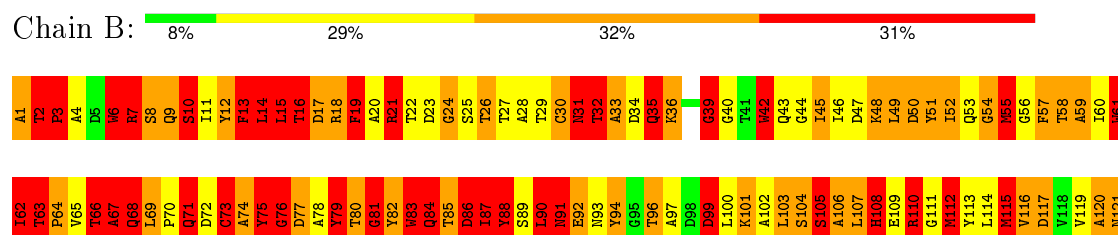
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

• Molecule 1: TAKA-AMYLASE A



• Molecule 1: TAKA-AMYLASE A



N428	N429	N430	N431	N432	N433	N434	N435	N436	N437	N438	N439	N440	N441	N442	N443	N444	N445	N446	N447	N448	N449	N450	N451	N452	N453	N454	N455	N456	N457	N458	N459	N460	N461	N462	N463	N464	N465	N466	N467	N468	N469	N470	N471	N472	N473	N474	N475	N476	N477	N478	N479	N480	N481	N482	N483	N484	N485	N486	N487	N488	N489	N490	N491	N492	N493	N494	N495	N496	N497	N498	N499	N500																																																																																																																																																																																																																																																				
K367	K368	K369	K370	K371	K372	K373	K374	K375	K376	K377	K378	K379	K380	K381	K382	K383	K384	K385	K386	K387	K388	K389	K390	K391	K392	K393	K394	K395	K396	K397	K398	K399	K400	K401	K402	K403	K404	K405	K406	K407	K408	K409	K410	K411	K412	K413	K414	K415	K416	K417	K418	K419	K420	K421	K422	K423	K424	K425	K426	K427	K428	K429	K430	K431	K432	K433	K434	K435	K436	K437	K438	K439	K440	K441	K442	K443	K444	K445	K446	K447	K448	K449	K450	K451	K452	K453	K454	K455	K456	K457	K458	K459	K460	K461	K462	K463	K464	K465	K466	K467	K468	K469	K470	K471	K472	K473	K474	K475	K476	K477	K478	K479	K480	K481	K482	K483	K484	K485	K486	K487	K488	K489	K490	K491	K492	K493	K494	K495	K496	K497	K498	K499	K500																																																																																																																																																																																							
N306	N307	N308	N309	N310	N311	N312	N313	N314	N315	N316	N317	N318	N319	N320	N321	N322	N323	N324	N325	N326	N327	N328	N329	N330	N331	N332	N333	N334	N335	N336	N337	N338	N339	N340	N341	N342	N343	N344	N345	N346	N347	N348	N349	N350	N351	N352	N353	N354	N355	N356	N357	N358	N359	N360	N361	N362	N363	N364	N365	N366	N367	N368	N369	N370	N371	N372	N373	N374	N375	N376	N377	N378	N379	N380	N381	N382	N383	N384	N385	N386	N387	N388	N389	N390	N391	N392	N393	N394	N395	N396	N397	N398	N399	N400	N401	N402	N403	N404	N405	N406	N407	N408	N409	N410	N411	N412	N413	N414	N415	N416	N417	N418	N419	N420	N421	N422	N423	N424	N425	N426	N427	N428	N429	N430	N431	N432	N433	N434	N435	N436	N437	N438	N439	N440	N441	N442	N443	N444	N445	N446	N447	N448	N449	N450	N451	N452	N453	N454	N455	N456	N457	N458	N459	N460	N461	N462	N463	N464	N465	N466	N467	N468	N469	N470	N471	N472	N473	N474	N475	N476	N477	N478	N479	N480	N481	N482	N483	N484	N485	N486	N487	N488	N489	N490	N491	N492	N493	N494	N495	N496	N497	N498	N499	N500																																																																																																																										
K246	K247	K248	K249	K250	K251	K252	K253	K254	K255	K256	K257	K258	K259	K260	K261	K262	K263	K264	K265	K266	K267	K268	K269	K270	K271	K272	K273	K274	K275	K276	K277	K278	K279	K280	K281	K282	K283	K284	K285	K286	K287	K288	K289	K290	K291	K292	K293	K294	K295	K296	K297	K298	K299	K300	K301	K302	K303	K304	K305	K306	K307	K308	K309	K310	K311	K312	K313	K314	K315	K316	K317	K318	K319	K320	K321	K322	K323	K324	K325	K326	K327	K328	K329	K330	K331	K332	K333	K334	K335	K336	K337	K338	K339	K340	K341	K342	K343	K344	K345	K346	K347	K348	K349	K350	K351	K352	K353	K354	K355	K356	K357	K358	K359	K360	K361	K362	K363	K364	K365	K366	K367	K368	K369	K370	K371	K372	K373	K374	K375	K376	K377	K378	K379	K380	K381	K382	K383	K384	K385	K386	K387	K388	K389	K390	K391	K392	K393	K394	K395	K396	K397	K398	K399	K400	K401	K402	K403	K404	K405	K406	K407	K408	K409	K410	K411	K412	K413	K414	K415	K416	K417	K418	K419	K420	K421	K422	K423	K424	K425	K426	K427	K428	K429	K430	K431	K432	K433	K434	K435	K436	K437	K438	K439	K440	K441	K442	K443	K444	K445	K446	K447	K448	K449	K450	K451	K452	K453	K454	K455	K456	K457	K458	K459	K460	K461	K462	K463	K464	K465	K466	K467	K468	K469	K470	K471	K472	K473	K474	K475	K476	K477	K478	K479	K480	K481	K482	K483	K484	K485	K486	K487	K488	K489	K490	K491	K492	K493	K494	K495	K496	K497	K498	K499	K500																																																														
K184	K185	K186	K187	K188	K189	K190	K191	K192	K193	K194	K195	K196	K197	K198	K199	K200	K201	K202	K203	K204	K205	K206	K207	K208	K209	K210	K211	K212	K213	K214	K215	K216	K217	K218	K219	K220	K221	K222	K223	K224	K225	K226	K227	K228	K229	K230	K231	K232	K233	K234	K235	K236	K237	K238	K239	K240	K241	K242	K243	K244	K245	K246	K247	K248	K249	K250	K251	K252	K253	K254	K255	K256	K257	K258	K259	K260	K261	K262	K263	K264	K265	K266	K267	K268	K269	K270	K271	K272	K273	K274	K275	K276	K277	K278	K279	K280	K281	K282	K283	K284	K285	K286	K287	K288	K289	K290	K291	K292	K293	K294	K295	K296	K297	K298	K299	K300	K301	K302	K303	K304	K305	K306	K307	K308	K309	K310	K311	K312	K313	K314	K315	K316	K317	K318	K319	K320	K321	K322	K323	K324	K325	K326	K327	K328	K329	K330	K331	K332	K333	K334	K335	K336	K337	K338	K339	K340	K341	K342	K343	K344	K345	K346	K347	K348	K349	K350	K351	K352	K353	K354	K355	K356	K357	K358	K359	K360	K361	K362	K363	K364	K365	K366	K367	K368	K369	K370	K371	K372	K373	K374	K375	K376	K377	K378	K379	K380	K381	K382	K383	K384	K385	K386	K387	K388	K389	K390	K391	K392	K393	K394	K395	K396	K397	K398	K399	K400	K401	K402	K403	K404	K405	K406	K407	K408	K409	K410	K411	K412	K413	K414	K415	K416	K417	K418	K419	K420	K421	K422	K423	K424	K425	K426	K427	K428	K429	K430	K431	K432	K433	K434	K435	K436	K437	K438	K439	K440	K441	K442	K443	K444	K445	K446	K447	K448	K449	K450	K451	K452	K453	K454	K455	K456	K457	K458	K459	K460	K461	K462	K463	K464	K465	K466	K467	K468	K469	K470	K471	K472	K473	K474	K475	K476	K477	K478	K479	K480	K481	K482	K483	K484	K485	K486	K487	K488	K489	K490	K491	K492	K493	K494	K495	K496	K497	K498	K499	K500
K184	K185	K186	K187	K188	K189	K190	K191	K192	K193	K194	K195	K196	K197	K198	K199	K200	K201	K202	K203	K204	K205	K206	K207	K208	K209	K210	K211	K212	K213	K214	K215	K216	K217	K218	K219	K220	K221	K222	K223	K224	K225	K226	K227	K228	K229	K230	K231	K232	K233	K234	K235	K236	K237	K238	K239	K240	K241	K242	K243	K244	K245	K246	K247	K248	K249	K250	K251	K252	K253	K254	K255	K256	K257	K258	K259	K260	K261	K262	K263	K264	K265	K266	K267	K268	K269	K270	K271	K272	K273	K274	K275	K276	K277	K278	K279	K280	K281	K282	K283	K284	K285	K286	K287	K288	K289	K290	K291	K292	K293	K294	K295	K296	K297	K298	K299	K300	K301	K302	K303	K304	K305	K306	K307	K308	K309	K310	K311	K312	K313	K314	K315	K316	K317	K318	K319	K320	K321	K322	K323	K324	K325	K326	K327	K328	K329	K330	K331	K332	K333	K334	K335	K336	K337	K338	K339	K340	K341	K342	K343	K344	K345	K346	K347	K348	K349	K350	K351	K352	K353	K354	K355	K356	K357	K358	K359	K360	K361	K362	K363	K364	K365	K366	K367	K368	K369	K370	K371	K372	K373	K374	K375	K376	K377	K378	K379	K380	K381	K382	K383	K384	K385	K386	K387	K388	K389	K390	K391	K392	K393	K394	K395	K396	K397	K398	K399	K400	K401	K402	K403	K404	K405	K406	K407	K408	K409	K410	K411	K412	K413	K414	K415	K416	K417	K418	K419	K420	K421	K422	K423	K424	K425	K426	K427	K428	K429	K430	K431	K432	K433	K434	K435	K436	K437	K438	K439	K440	K441	K442	K443	K444	K445	K446	K447	K448	K449	K450	K451	K452	K453	K454	K455	K456	K457	K458	K459	K460	K461	K462	K463	K464	K465	K466	K467	K468	K469	K470	K471	K472	K473	K474	K475	K476	K477	K478	K479	K480	K481	K482	K483	K484	K485	K486	K487	K488	K489	K490	K491	K492	K493	K494	K495	K496	K497	K498	K499	K500
K184	K185	K186	K187	K188	K189	K190	K191	K192	K193	K194	K195	K196	K197	K198	K199	K200	K201	K202	K203	K204	K205	K206	K207	K208	K209	K210	K211	K212	K213	K214	K215	K216	K217	K218	K219	K220	K221	K222	K223	K224	K225	K226	K227	K228	K229	K230	K231	K232	K233	K234	K235	K236	K237	K238	K239	K240	K241	K242	K243	K244	K245	K246	K247	K248	K249	K250	K251	K252	K253	K254	K255	K256	K257	K258	K259	K260	K261	K262	K263	K264	K265	K266	K267	K268	K269	K270	K271	K272	K273	K274	K275	K276	K277	K278	K279	K280	K281	K282	K283	K284	K285	K286	K287	K288	K289	K290	K291	K292	K293	K294	K295	K296	K297	K298	K299	K300	K301	K302	K303	K304	K305	K306	K307	K308	K309	K310	K311	K312	K313	K314	K315	K316	K317	K318	K319	K320	K321	K322	K323	K324	K325	K326	K327	K328	K329	K330	K331	K332	K333	K334	K335	K336	K337	K338	K339	K340	K341	K342	K343	K344	K345	K346	K347	K348	K349	K350	K351	K352	K353	K354	K355	K356	K357	K358	K359	K360	K361	K362	K363	K364	K365	K366	K367	K368	K369	K370	K371	K372	K373	K374	K375	K376	K377	K378	K379	K380	K381	K382	K383	K384	K385	K386	K387	K388	K389	K390	K391	K392	K393	K394	K395	K396	K397	K398	K399	K400	K401	K402	K403	K404	K405	K406	K407	K408	K409	K410	K411	K412	K413	K414	K415	K416	K417	K418	K419	K420	K421	K422	K423	K424	K425	K426	K427	K428	K429	K430	K431	K432	K433	K434	K435	K436	K43																																																															

• Molecule 1: TAKA-AMYLASE A

Chain C: 9% 28% 33% 30%

S426	S427	T428	A429	C430	Q431	O432	L433	B434	E435	V436	I437	G438	C439	T440	T441	V442	T443	V444	G445	S446	P447	V448	G449	M450	P451	V452	P453	M454	A455	G456	G457	L458	R459	R460	V461	L462	V463	P464	T465	E466	G467	L468	S471	K472	I473	C474	S475	V476	S477	S478																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
A385	A386	A387	A388	A389	A390	A391	A392	A393	A394	A395	A396	A397	A398	A399	A400	A401	A402	A403	A404	A405	A406	A407	A408	A409	A410	A411	A412	A413	A414	A415	A416	A417	A418	A419	A420	A421	A422	A423	A424	A425	A426	A427	A428	A429	A430	A431	A432	A433	A434	A435	A436	A437	A438	A439	A440	A441	A442	A443	A444	A445	A446	A447	A448	A449	A450	A451	A452	A453	A454	A455	A456	A457	A458	A459	A460	A461	A462	A463	A464	A465	A466	A467	A468	A469	A470	A471	A472	A473	A474	A475	A476	A477	A478	A479	A480	A481	A482	A483	A484	A485	A486	A487	A488	A489	A490	A491	A492	A493	A494	A495	A496	A497	A498	A499	A500	A501	A502	A503	A504	A505	A506	A507	A508	A509	A510	A511	A512	A513	A514	A515	A516	A517	A518	A519	A520	A521	A522	A523	A524	A525	A526	A527	A528	A529	A530	A531	A532	A533	A534	A535	A536	A537	A538	A539	A540	A541	A542	A543	A544	A545	A546	A547	A548	A549	A550	A551	A552	A553	A554	A555	A556	A557	A558	A559	A560	A561	A562	A563	A564	A565	A566	A567	A568	A569	A570	A571	A572	A573	A574	A575	A576	A577	A578	A579	A580	A581	A582	A583	A584	A585	A586	A587	A588	A589	A590	A591	A592	A593	A594	A595	A596	A597	A598	A599	A600	A601	A602	A603	A604	A605	A606	A607	A608	A609	A610	A611	A612	A613	A614	A615	A616	A617	A618	A619	A620	A621	A622	A623	A624	A625	A626	A627	A628	A629	A630	A631	A632	A633	A634	A635	A636	A637	A638	A639	A640	A641	A642	A643	A644	A645	A646	A647	A648	A649	A650	A651	A652	A653	A654	A655	A656	A657	A658	A659	A660	A661	A662	A663	A664	A665	A666	A667	A668	A669	A670	A671	A672	A673	A674	A675	A676	A677	A678	A679	A680	A681	A682	A683	A684	A685	A686	A687	A688	A689	A690	A691	A692	A693	A694	A695	A696	A697	A698	A699	A700	A701	A702	A703	A704	A705	A706	A707	A708	A709	A710	A711	A712	A713	A714	A715	A716	A717	A718	A719	A720	A721	A722	A723	A724	A725	A726	A727	A728	A729	A730	A731	A732	A733	A734	A735	A736	A737	A738	A739	A740	A741	A742	A743	A744	A745	A746	A747	A748	A749	A750	A751	A752	A753	A754	A755	A756	A757	A758	A759	A760	A761	A762	A763	A764	A765	A766	A767	A768	A769	A770	A771	A772	A773	A774	A775	A776	A777	A778	A779	A780	A781	A782	A783	A784	A785	A786	A787	A788	A789	A790	A791	A792	A793	A794	A795	A796	A797	A798	A799	A800	A801	A802	A803	A804	A805	A806	A807	A808	A809	A810	A811	A812	A813	A814	A815	A816	A817	A818	A819	A820	A821	A822	A823	A824	A825	A826	A827	A828	A829	A830	A831	A832	A833	A834	A835	A836	A837	A838	A839	A840	A841	A842	A843	A844	A845	A846	A847	A848	A849	A850	A851	A852	A853	A854	A855	A856	A857	A858	A859	A860	A861	A862	A863	A864	A865	A866	A867	A868	A869	A870	A871	A872	A873	A874	A875	A876	A877	A878	A879	A880	A881	A882	A883	A884	A885	A886	A887	A888	A889	A890	A891	A892	A893	A894	A895	A896	A897	A898	A899	A900	A901	A902	A903	A904	A905	A906	A907	A908	A909	A910	A911	A912	A913	A914	A915	A916	A917	A918	A919	A920	A921	A922	A923	A924	A925	A926	A927	A928	A929	A930	A931	A932	A933	A934	A935	A936	A937	A938	A939	A940	A941	A942	A943	A944	A945	A946	A947	A948	A949	A950	A951	A952	A953	A954	A955	A956	A957	A958	A959	A960	A961	A962	A963	A964	A965	A966	A967	A968	A969	A970	A971	A972	A973	A974	A975	A976	A977	A978	A979	A980	A981	A982	A983	A984	A985	A986	A987	A988	A989	A990	A991	A992	A993	A994	A995	A996	A997	A998	A999	A1000			
K184	M244	Y304	A385	A386	A387	A388	A389	A390	A391	A392	A393	A394	A395	A396	A397	A398	A399	A400	A401	A402	A403	A404	A405	A406	A407	A408	A409	A410	A411	A412	A413	A414	A415	A416	A417	A418	A419	A420	A421	A422	A423	A424	A425	A426	A427	A428	A429	A430	A431	A432	A433	A434	A435	A436	A437	A438	A439	A440	A441	A442	A443	A444	A445	A446	A447	A448	A449	A450	A451	A452	A453	A454	A455	A456	A457	A458	A459	A460	A461	A462	A463	A464	A465	A466	A467	A468	A469	A470	A471	A472	A473	A474	A475	A476	A477	A478	A479	A480	A481	A482	A483	A484	A485	A486	A487	A488	A489	A490	A491	A492	A493	A494	A495	A496	A497	A498	A499	A500	A501	A502	A503	A504	A505	A506	A507	A508	A509	A510	A511	A512	A513	A514	A515	A516	A517	A518	A519	A520	A521	A522	A523	A524	A525	A526	A527	A528	A529	A530	A531	A532	A533	A534	A535	A536	A537	A538	A539	A540	A541	A542	A543	A544	A545	A546	A547	A548	A549	A550	A551	A552	A553	A554	A555	A556	A557	A558	A559	A560	A561	A562	A563	A564	A565	A566	A567	A568	A569	A570	A571	A572	A573	A574	A575	A576	A577	A578	A579	A580	A581	A582	A583	A584	A585	A586	A587	A588	A589	A590	A591	A592	A593	A594	A595	A596	A597	A598	A599	A600	A601	A602	A603	A604	A605	A606	A607	A608	A609	A610	A611	A612	A613	A614	A615	A616	A617	A618	A619	A620	A621	A622	A623	A624	A625	A626	A627	A628	A629	A630	A631	A632	A633	A634	A635	A636	A637	A638	A639	A640	A641	A642	A643	A644	A645	A646	A647	A648	A649	A650	A651	A652	A653	A654	A655	A656	A657	A658	A659	A660	A661	A662	A663	A664	A665	A666	A667	A668	A669	A670	A671	A672	A673	A674	A675	A676	A677	A678	A679	A680	A681	A682	A683	A684	A685	A686	A687	A688	A689	A690	A691	A692	A693	A694	A695	A696	A697	A698	A699	A700	A701	A702	A703	A704	A705	A706	A707	A708	A709	A710	A711	A712	A713	A714	A715	A716	A717	A718	A719	A720	A721	A722	A723	A724	A725	A726	A727	A728	A729	A730	A731	A732	A733	A734	A735	A736	A737	A738	A739	A740	A741	A742	A743	A744	A745	A746	A747	A748	A749	A750	A751	A752	A753	A754	A755	A756	A757	A758	A759	A760	A761	A762	A763	A764	A765	A766	A767	A768	A769	A770	A771	A772	A773	A774	A775	A776	A777	A778	A779	A780	A781	A782	A783	A784	A785	A786	A787	A788	A789	A790	A791	A792	A793	A794	A795	A796	A797	A798	A799	A800	A801	A802	A803	A804	A805	A806	A807	A808	A809	A810	A811	A812	A813	A814	A815	A816	A817	A818	A819	A820	A821	A822	A823	A824	A825	A826	A827	A828	A829	A830	A831	A832	A833	A834	A835	A836	A837	A838	A839	A840	A841	A842	A843	A844	A845	A846	A847	A848	A849	A850	A851	A852	A853	A854	A855	A856	A857	A858	A859	A860	A861	A862	A863	A864	A865	A866	A867	A868	A869	A870	A871	A872	A873	A874	A875	A876	A877	A878	A879	A880	A881	A882	A883	A884	A885	A886	A887	A888	A889	A890	A891	A892	A893	A894	A895	A896	A897	A898	A899	A900	A901	A902	A903	A904	A905	A906	A907	A908	A909	A910	A911	A912	A913	A914	A915	A916	A917	A918	A919	A920	A921	A922	A923	A924	A925	A926	A927	A928	A929	A930	A931	A932	A933	A934	A935	A936	A937	A938	A939	A940	A941	A942	A943	A944	A945	A946	A947	A948	A949	A950	A951	A952	A953	A954	A955	A956	A957	A958	A959	A960	A961	A962	A963	A964	A965	A966	A967	A968	A969	A970	A971	A972	A973	A974	A975	A976	A977	A978	A979	A980	A981	A982	A983	A984	A985	A986	A987	A988	A989	A990	A991	A992	A993	A994	A995	A996	A997	A998	A999	A1000

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.90Å 133.30Å 94.30Å 90.00° 102.70° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11073	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	1.93	77/3782 (2.0%)	3.42	363/5163 (7.0%)
1	B	1.93	77/3782 (2.0%)	3.42	364/5163 (7.1%)
1	C	1.93	77/3782 (2.0%)	3.42	362/5163 (7.0%)
All	All	1.93	231/11346 (2.0%)	3.42	1089/15489 (7.0%)

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	2	87
1	B	2	87
1	C	2	87
All	All	6	261

The worst 5 of 231 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	463	TYR	CD1-CE1	-20.38	1.08	1.39
1	A	463	TYR	CD1-CE1	-20.38	1.08	1.39
1	C	463	TYR	CD1-CE1	-20.36	1.08	1.39
1	C	463	TYR	CZ-OH	19.61	1.71	1.37
1	A	463	TYR	CZ-OH	19.60	1.71	1.37

The worst 5 of 1089 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	300	ARG	NE-CZ-NH1	-56.15	92.22	120.30
1	A	300	ARG	NE-CZ-NH1	-56.10	92.25	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	300	ARG	NE-CZ-NH1	-56.05	92.27	120.30
1	C	19	PHE	CD1-CE1-CZ	-44.96	66.15	120.10
1	A	19	PHE	CD1-CE1-CZ	-44.94	66.17	120.10

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	208	VAL	CA
1	A	404	ILE	CB
1	B	208	VAL	CA
1	B	404	ILE	CB
1	C	208	VAL	CA

5 of 261 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	PHE	Mainchain
1	A	15	LEU	Mainchain
1	A	17	ASP	Mainchain
1	A	2	THR	Mainchain
1	A	7	ARG	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	A	3690	0	3448	1687	135
1	B	3690	0	3414	2177	0
1	C	3690	0	3447	1369	135
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
All	All	11073	0	10309	3895	135

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 182.

The worst 5 of 3895 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:A:87:ILE:CD1	1:B:374:SER:HB3	1.16	1.63
1:B:445:GLY:CA	1:C:185:ASN:HD22	0.99	1.62
1:A:205:ILE:CG2	1:B:472:LYS:HG3	1.17	1.60
1:A:205:ILE:HG21	1:B:472:LYS:CG	1.31	1.59
1:B:278:THR:HA	1:C:380:VAL:CG2	1.28	1.59

The worst 5 of 135 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:A:151:PHE:C	1:C:25:SER:O[2_646]	0.53	1.67
1:A:149:PHE:CB	1:C:29:THR:OG1[2_646]	0.66	1.54
1:A:149:PHE:CD2	1:C:29:THR:CA[2_646]	0.70	1.50
1:A:165:TRP:O	1:C:27:THR:CA[2_646]	0.72	1.48
1:A:152:ILE:CA	1:C:26:THR:N[2_646]	0.76	1.44

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	476/478 (100%)	237 (50%)	117 (25%)	122 (26%)	0	0
1	B	476/478 (100%)	237 (50%)	117 (25%)	122 (26%)	0	0
1	C	476/478 (100%)	237 (50%)	117 (25%)	122 (26%)	0	0
All	All	1428/1434 (100%)	711 (50%)	351 (25%)	366 (26%)	0	0

5 of 366 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	7	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	16	THR
1	A	19	PHE
1	A	21	ARG

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	A	400/400 (100%)	256 (64%)	144 (36%)	0	1
1	B	400/400 (100%)	256 (64%)	144 (36%)	0	1
1	C	400/400 (100%)	256 (64%)	144 (36%)	0	1
All	All	1200/1200 (100%)	768 (64%)	432 (36%)	0	1

5 of 432 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	186	GLU
1	B	320	LEU
1	C	376	ASP
1	B	205	ILE
1	B	264	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	147	HIS
1	B	298	ASN
1	C	334	HIS
1	B	158	GLN
1	B	220	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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.