



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 06:20 PM BST

PDB ID : 4V40
Title : BETA-GALACTOSIDASE
Authors : Jacobson, R.H.; Zhang, X.; Dubose, R.F.; Matthews, B.W.
Deposited on : 1994-07-18
Resolution : 2.50 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

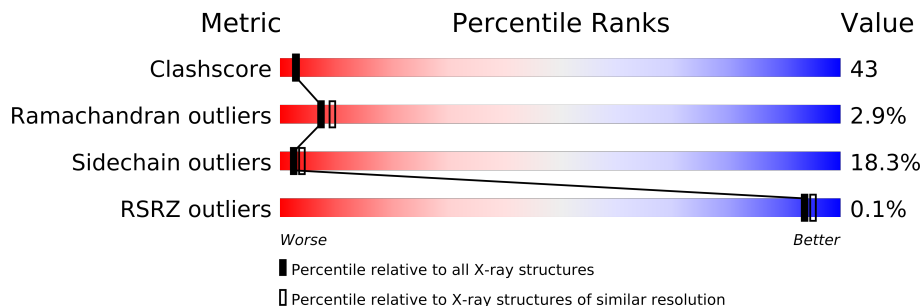
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : stable23397
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23397

1 Overall quality at a glance

The reported resolution of this entry is 2.50 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))
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1023	
1	B	1023	
1	C	1023	
1	D	1023	
1	E	1023	
1	F	1023	
1	G	1023	
1	H	1023	
1	I	1023	
1	J	1023	
1	K	1023	
1	L	1023	
1	M	1023	
1	N	1023	
1	O	1023	
1	P	1023	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	A	1101	-	X
2	MG	B	1101	-	X
2	MG	C	1101	-	X
2	MG	D	1101	-	X
2	MG	D	1102	-	X
2	MG	E	1101	-	X
2	MG	F	1101	-	X
2	MG	G	1101	-	X
2	MG	H	1101	-	X
2	MG	I	1101	-	X
2	MG	J	1101	-	X
2	MG	M	1101	-	X
2	MG	O	1101	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 132654 atoms, of which 0 are hydrogen and 0 are deuterium.

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 BETA-GALACTOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	B	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	C	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	D	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	E	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	F	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	G	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	H	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	I	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	J	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	K	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	L	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	M	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	N	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	O	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	P	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	P	2	Total 2	Mg 2	0	0
2	G	2	Total 2	Mg 2	0	0
2	J	2	Total 2	Mg 2	0	0
2	D	2	Total 2	Mg 2	0	0
2	K	2	Total 2	Mg 2	0	0
2	E	2	Total 2	Mg 2	0	0
2	H	2	Total 2	Mg 2	0	0
2	B	2	Total 2	Mg 2	0	0
2	I	2	Total 2	Mg 2	0	0
2	C	2	Total 2	Mg 2	0	0
2	A	2	Total 2	Mg 2	0	0
2	N	2	Total 2	Mg 2	0	0
2	O	2	Total 2	Mg 2	0	0
2	L	2	Total 2	Mg 2	0	0
2	F	2	Total 2	Mg 2	0	0
2	M	1	Total 1	Mg 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	88	Total 88	O 88	0	0
3	B	96	Total 96	O 96	0	0
3	C	91	Total 91	O 91	0	0

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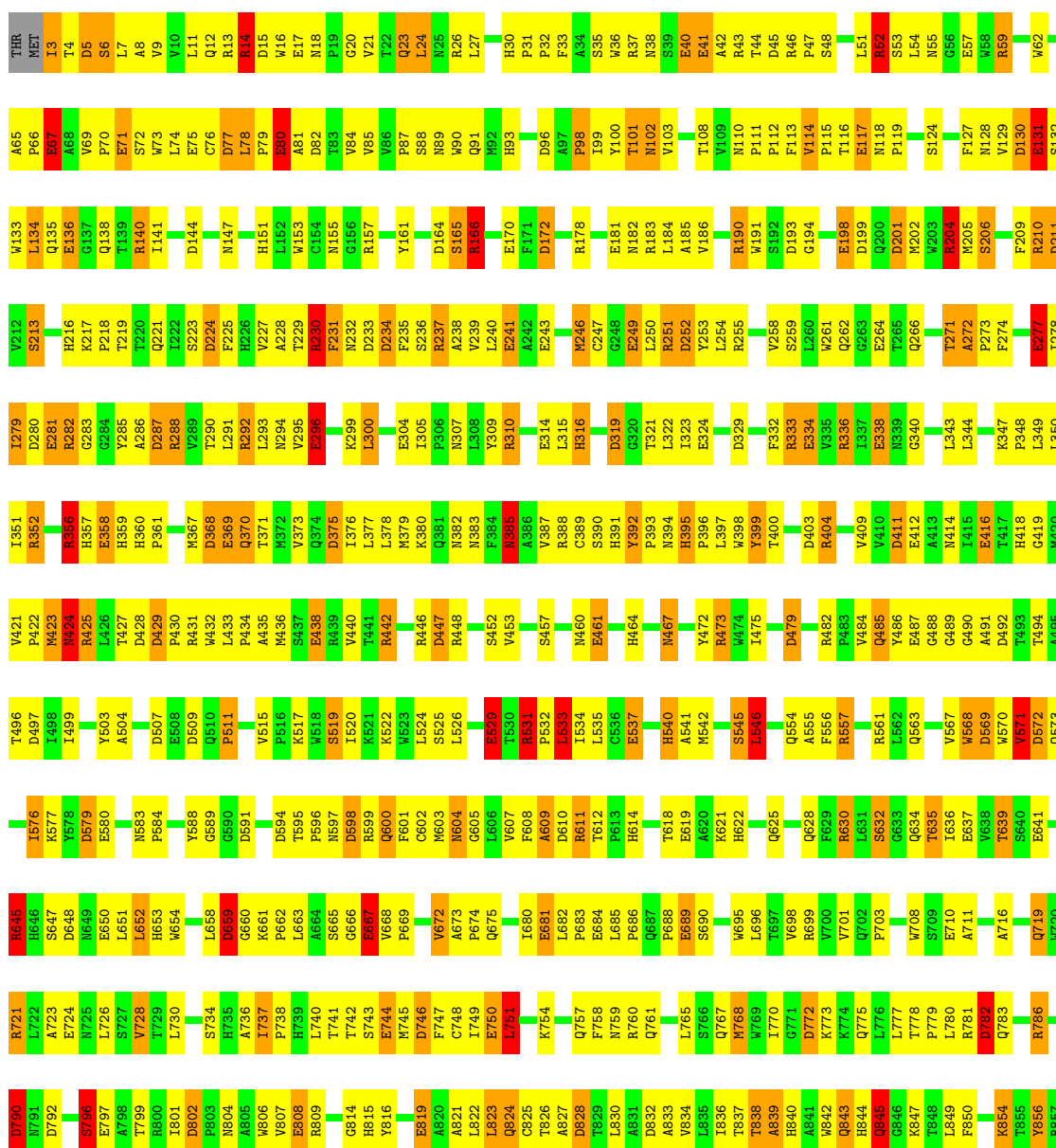
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	97	Total 97	O 97	0	0
3	E	94	Total 94	O 94	0	0
3	F	91	Total 91	O 91	0	0
3	G	95	Total 95	O 95	0	0
3	H	92	Total 92	O 92	0	0
3	I	90	Total 90	O 90	0	0
3	J	97	Total 97	O 97	0	0
3	K	87	Total 87	O 87	0	0
3	L	84	Total 84	O 84	0	0
3	M	79	Total 79	O 79	0	0
3	N	94	Total 94	O 94	0	0
3	O	95	Total 95	O 95	0	0
3	P	85	Total 85	O 85	0	0

3 Residue-property plots

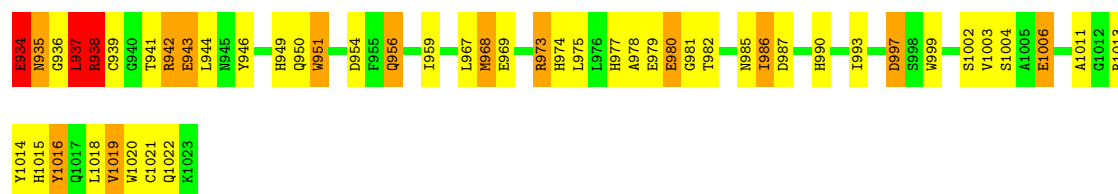
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: BETA-GALACTOSIDASE

Chain A:

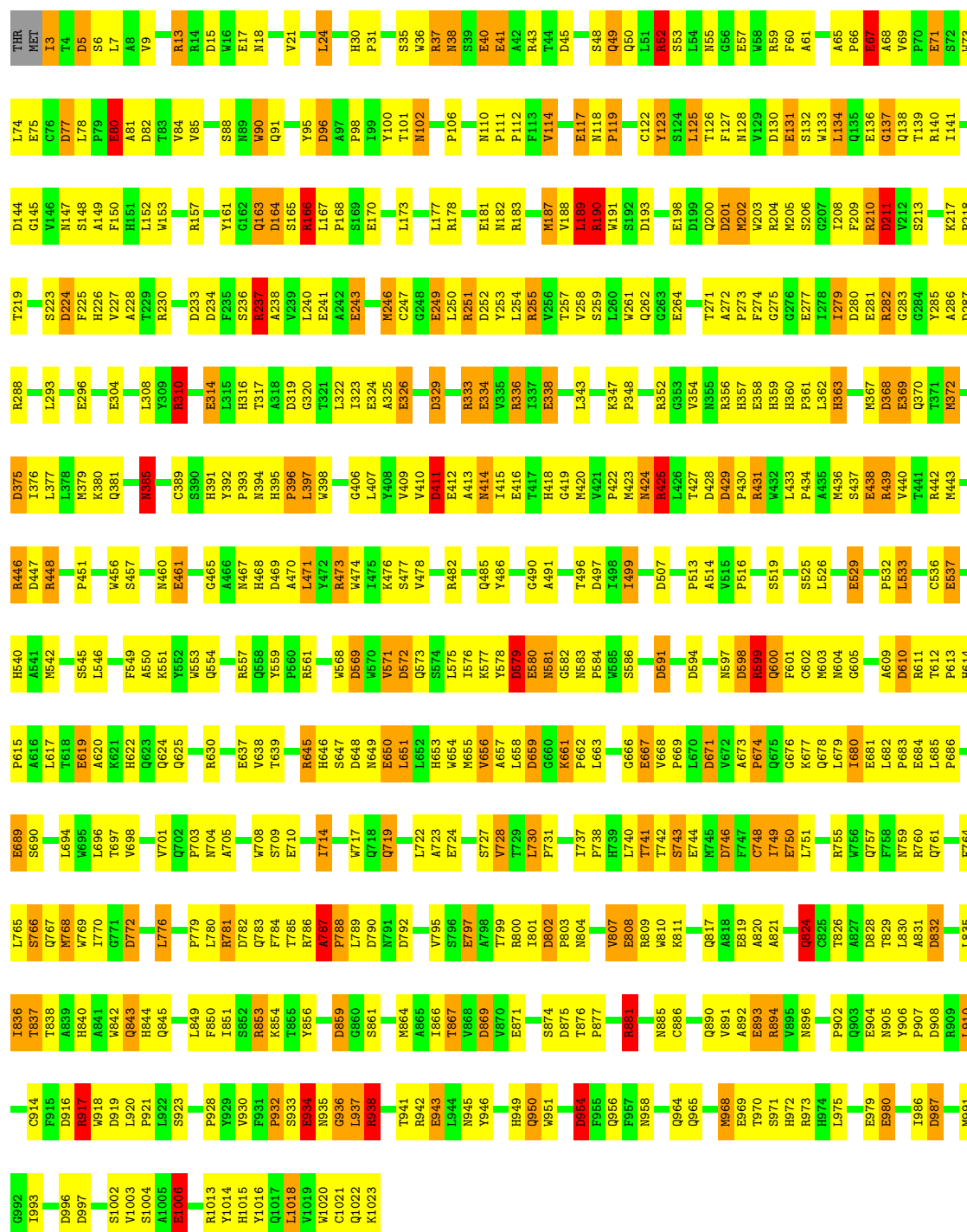


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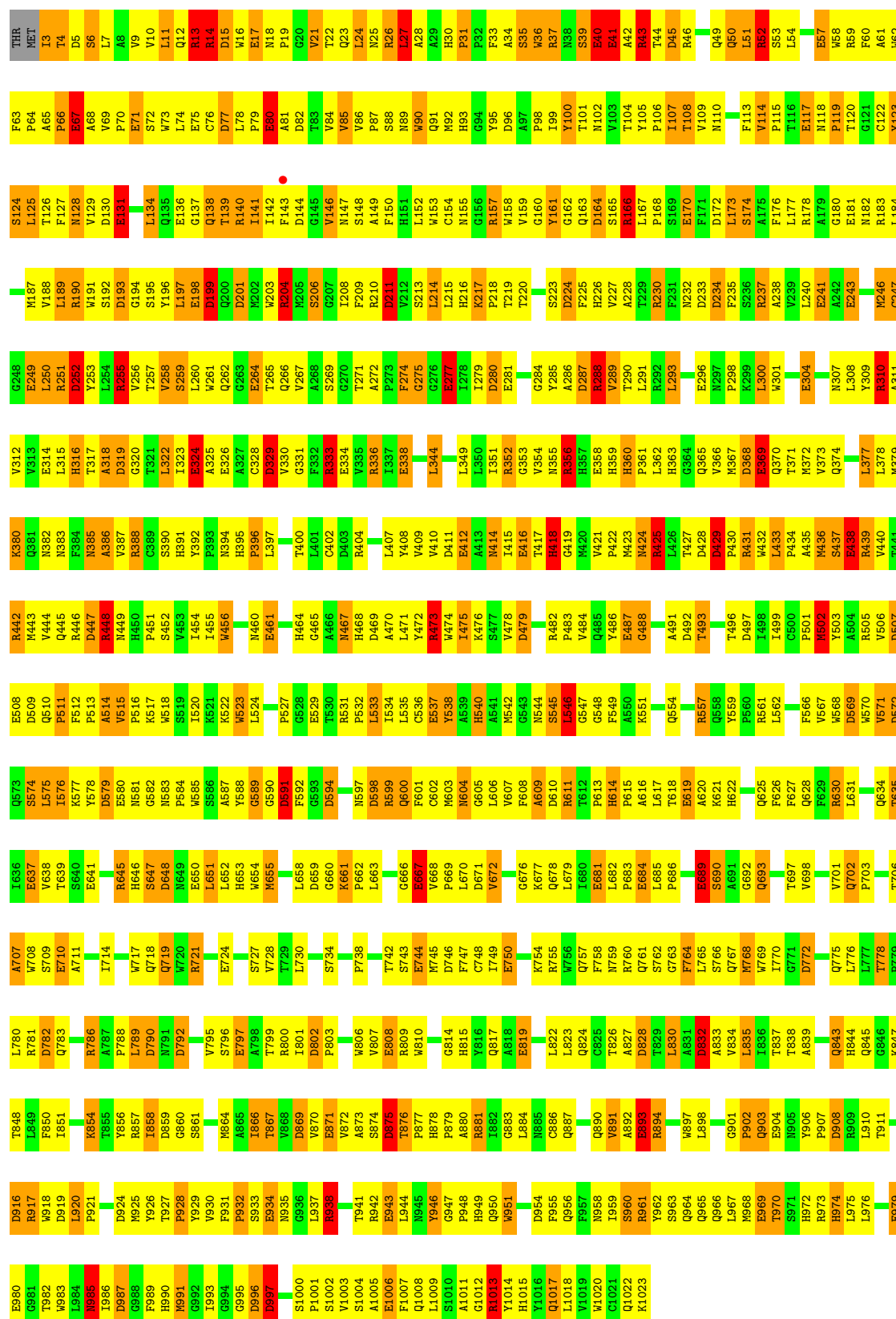
Chain C:



Chain D:

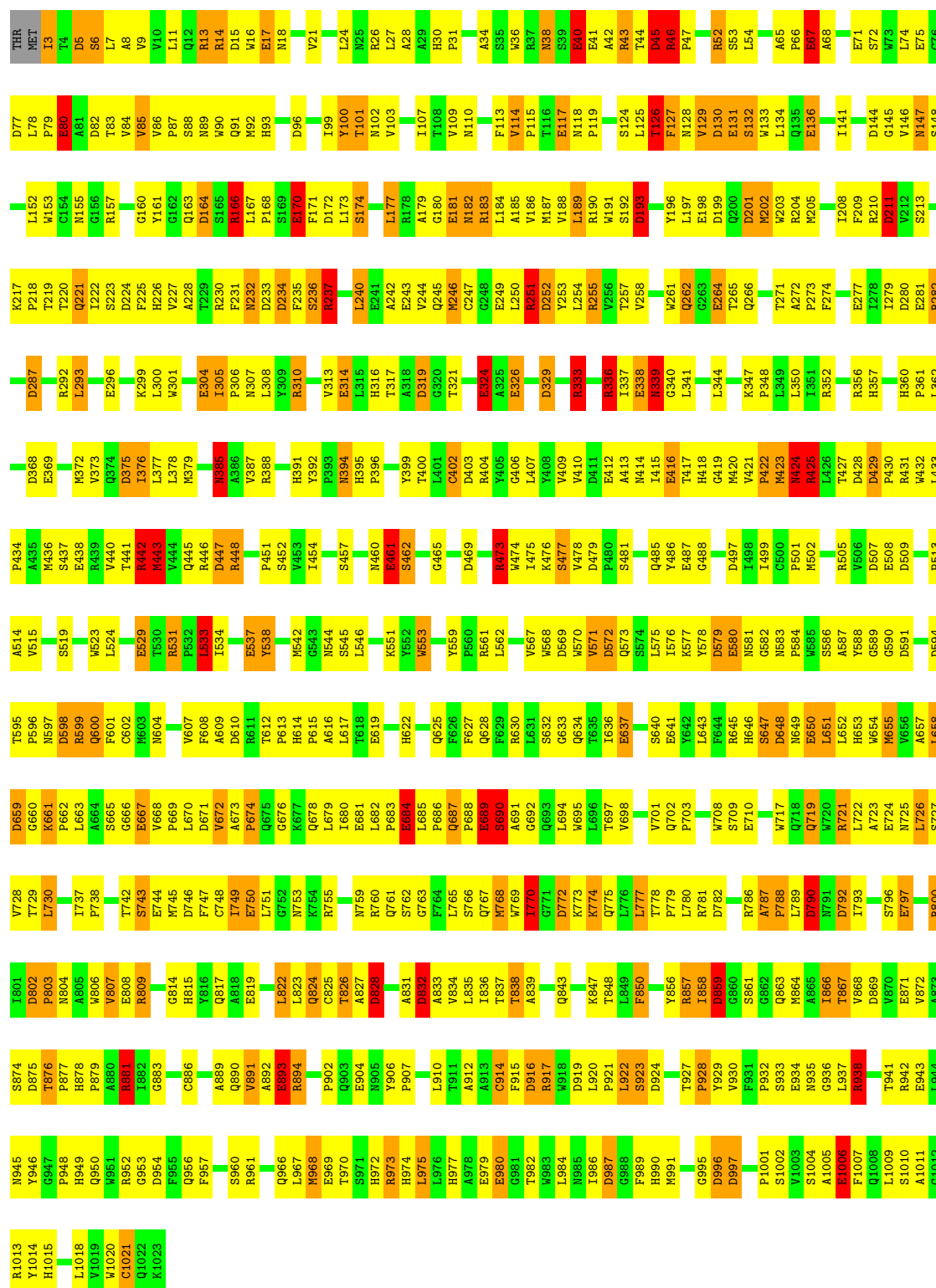


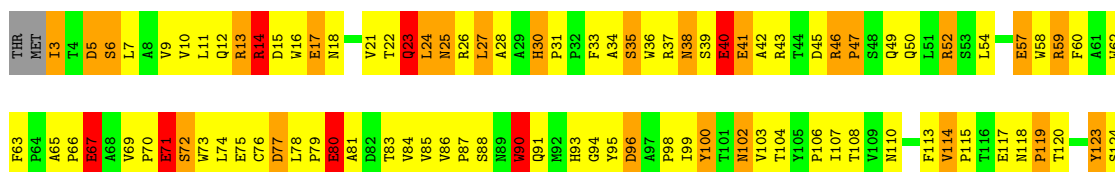
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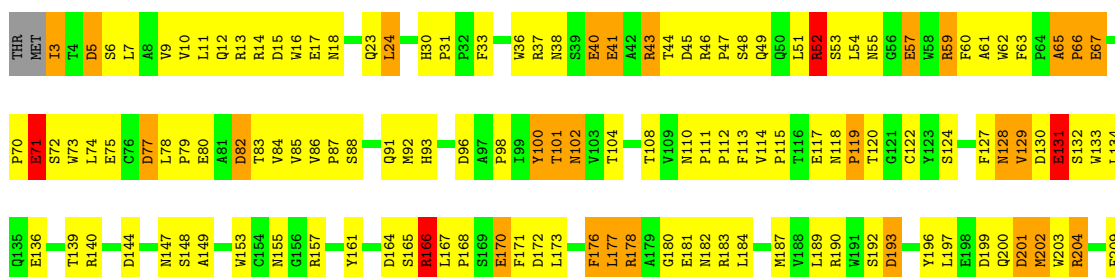
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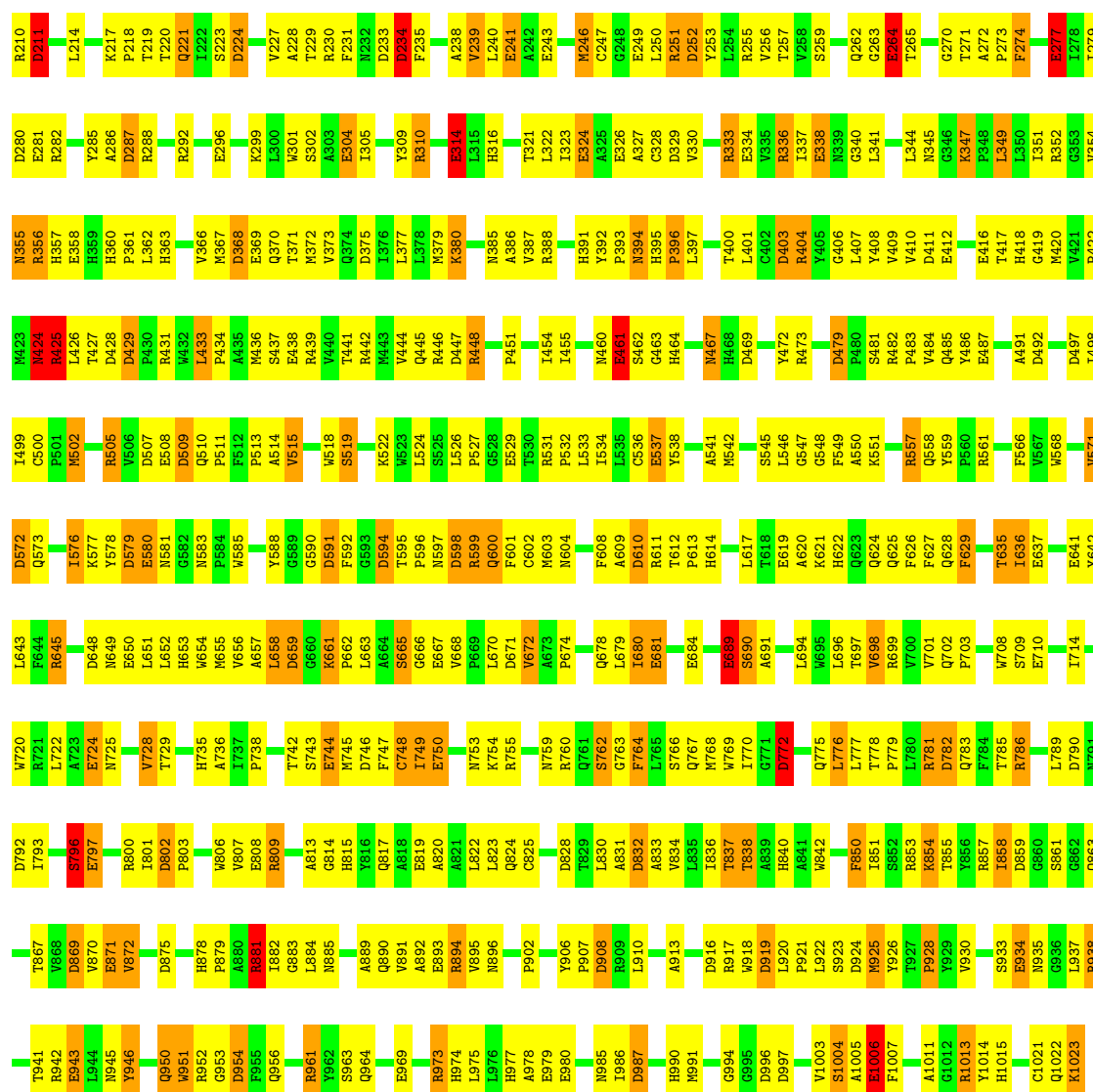
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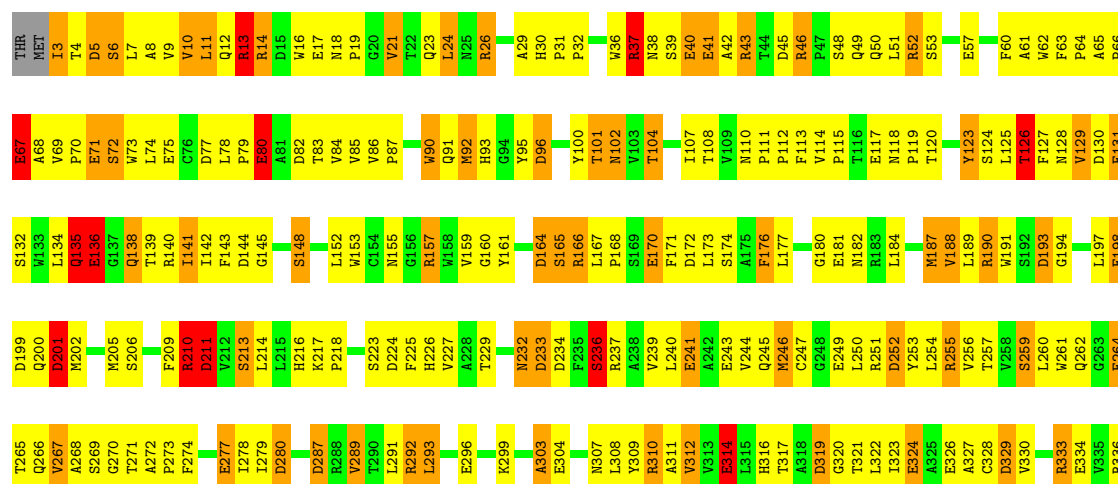


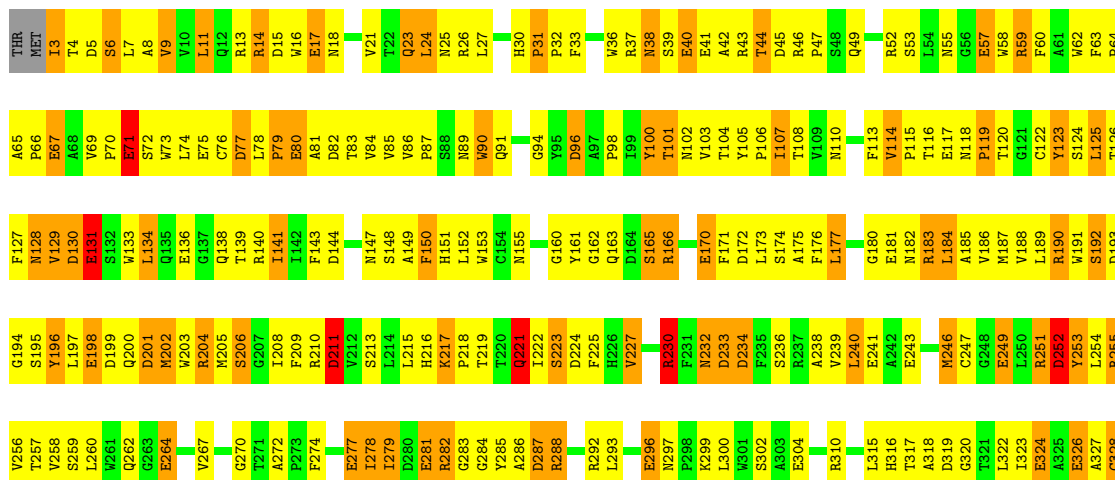




• Molecule 1: BETA-GALACTOSIDASE

Chain K:





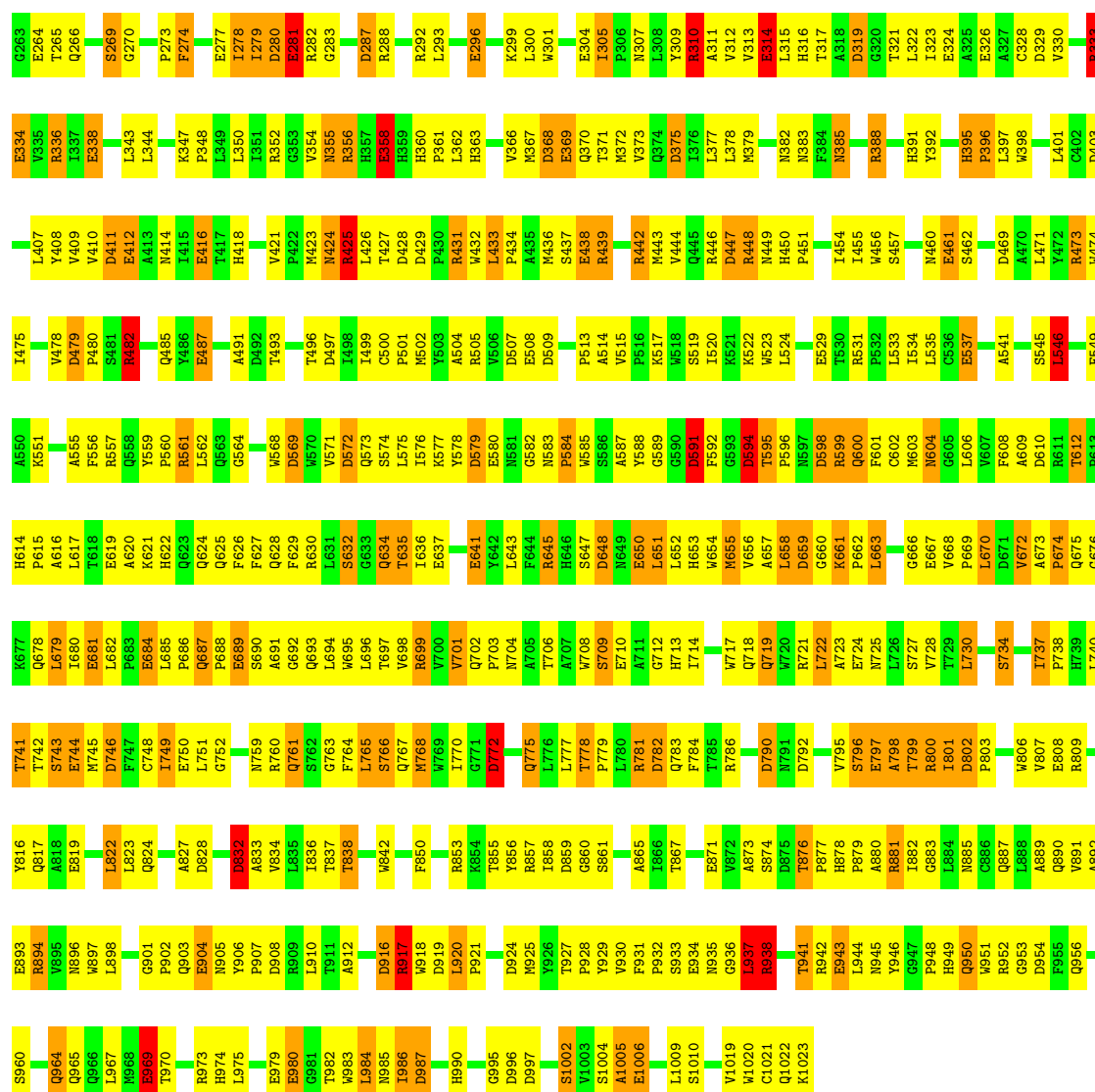


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A311	M373	A435	I498	Y559	K621	E681	L752	L822	L884	G947	Q1008
V312	Q374	M436	I499	P560	K622	L682	R755	L885	L885	G948	L1009
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A318	Q380	R442	R505	Y568	Q628	R689	R763	T829	R891	F954	H1015
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G320	N382	V444	D507	D569	R630	L686	L765	A831	E893	Q956	Q1017
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E326	C389	H450	P513	L575	L636	R699	G771	T837	G901	Y962	
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C328	R391	S452	V515	K577	V638	V701		A839	Q903	Q964	
D329	Y392	S453	P516	V578	T639	Q702	Q775	H840	E904	Q965	
V330	P393	I454	K517	D579	S640	P703	L776	A841	N905	Q966	
G331	N394	L455	W518	E580	E641	W704	L777	Q842	Y906	L967	
F332	H395	N456	S519	N581	Y642	A705	T778	Q843	P907	N968	
R333	P396	S457	I520	G582	L643	T706	P779	H844	D908	E969	
E334	L397		K521	N583	F644	A707	L780	Q845	R898	T970	
V335	W398	N460	K522	P584	R645	W708	R781	G846	L910	S971	
R336	Y399	E461	W523	N585	H466	S709	D782	K847	T911	H972	
L337	T400	S462	L524	S586	Q783	E710	Q783	T848	A912	N973	
E338		G463	S525	A587	D648	A711	E710	L849	A913	H974	
N339	D403	H464	L526	V588	T649	H712	T785	F850	C914	L975	
G340	R404	G465	E529	G589	E650	H713	R786	L851	F915	L976	
	Y405	A466	T530	G590	L651	I714	A787	S852	D916	E979	
	G406	D467	R531	F592	L652	W717	P788	K853	R917	G980	
	L407	H468	R531	G593	H653	Q718	D790	T854	D919	G981	
	Y408	D469	P532	D594	W654	Q719	N791	Y855	L920	T982	
	V409	A470	L533	D594	M655	W720	D792	R857	P921	N983	
	V410	L471	I534	N597	V656		T793	L858	L922	L984	
	D411	Y472	L535	N598	A657	A723	E796	D859	S923	N985	
	E412	R473	C536	R599	D659	E724	E797	G860	D924	N986	
	A413	Y474	E537	Q600	G660	Y538	R796	T867	N925	D987	
	N414	I475	Y538	P601	K661	S727	E797	V868	Y926	G988	
	G353	S477	A539	C502	P662	L730	R800	M864	T927	F989	
	V354	V478	H540	A541	L663	L730	L801	A865	P928	H990	
	N355	D478	M542	M603	A664	S734	D802	L866	Y929	N991	
	R356	D479	G543	N604	G665		P803	T867	V930	G992	
	H357	P480	N544	G605	G666		N804	V868		I993	
	M420	S481	M544	L606	E667	P738	A805	D869	S933	G994	
	V421	R482	S545	V607	V668	W739	W806	S870	E934	G995	
	R359	P483	L546	F608	P669	L740	R807	E871	N935	D996	
	H360	V484	G547	A609	L670	T741	E808	S874	G936	D997	
	L362	Q485	G548	D610	D671	T742	R809	D875	L937	S998	
	G363	Y486	F549	R611	V672	S743	W810	S875	N938	N999	
	G364	G488	A550	T612	G673	E744	R814	R876	C939	P1000	
	Q365	T427	K551	P613	A673	W745	H815	P877	G940	P1001	
	V366	G489	Y552	H614	P674	D746	H816	H878	T941	S1002	
	K367	D428	W553	P615	Q675	F747	Y816	P879	Q942	V1003	
	D368	D429	Q554	A616	G676	Q817	Y817	A880	E943	L134	
	E369	P430	A491	D492	K677	C748	A818	R881	L944	A1005	
	R431	R431									
	W432		F556	T618	Q678	I749					

• Molecule 1: BETA-GALACTOSIDASE

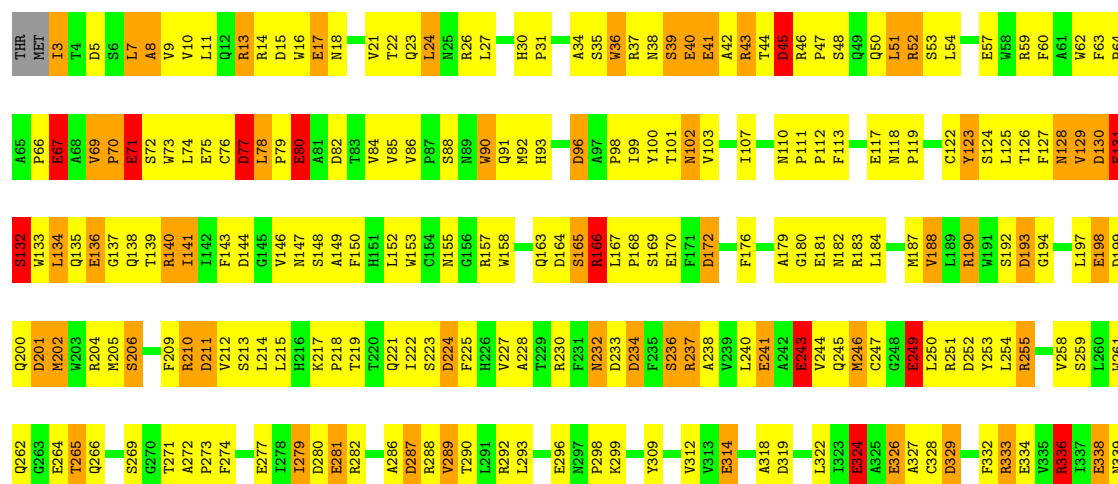
Chain N:

THR	A65	E136	D201	THR
MET	P66	G137	M202	
I3	E67	Q138	R203	
T4	A68	T139	W204	
D5	P69	R140	M205	
S6	V70	S141	S206	
L7	E71	I142	G207	
A8	S72	F143	I208	
V9	W73	D144	P209	
L10	A74	G145	R210	
L11	E75	V146	D211	
Q12	G76	N147	T212	
R13	D77	S148	S213	
R14	L78	L152	L214	
D15	P79	W153	K217	
D16	E80	C154	P218	
E17	A81	M155	T219	
N18	D82	G156	T220	
P19	T83	R157	Q221	
Q20	V84	G160	L222	
G21	H85	Y161	S223	
V22	N89	G162	D224	
Q23	W90	H163	F225	
L24	Q91	Q163	H226	
N25	R95	D164	V227	
R26	Y96	S165	A228	
A29	D96	R166	T229	
H30	P100	L167	R230	
P31	T101	G168	F231	
T101	N102	S169	M232	
M102	V103	E170	D233	
V103	W109	F171	D234	
V109	N110	D172	S235	
N38	S39	L173	T237	
E40	E40	F176	A238	
E41	A42	L177	V239	
A42	R43	R178	L240	
T44	G180	A179	E241	
D45	E181	G181	G242	
R46	N118	E182	E243	
P47	P119	R183	V244	
S48	T120	L184	Q245	
Q49	G121	A185	N246	
Q50	C122	V186	G247	
L51	Y123	M187	C248	
L51	S124	V188	E249	
S53	L125	L189	R251	
L54	T126	R190	D252	
	F127	W191	V253	
E57	N128	S192	L254	
W58	V129	D193	R255	
R59	D130	G194	V256	
F60	P101	S195	T257	
A61	S132	E198	L260	
W62	W133	D199	W261	
F63	L134	A355	Q262	
P64	Q135			



• Molecule 1: BETA-GALACTOSIDASE

Chain O:



G340	G341	L341	L342	L343	L344	L351	R352	G353	V354	N355	R356	R357	R358	R359	R360	R361	R362	R363	R364	R365	R366	R367	R368	R369	R370	R371	R372	R373	R374	R375	R376	R377	R378	R379	R380	R381	R382	R383	R384	R385	R386	R387	R388	R391	R392	R393	R394	R395	R396	R397	L401	C402	D403	L407	R408	R409	R410																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
D411	E412	A413	N414	I415	E416	T417	H418	G419	M420	N421	R422	R423	R424	R425	R426	R427	R428	R429	R430	R431	R432	R433	R434	R435	R436	R437	R438	R439	R440	R441	R442	R443	R444	R445	R446	R447	R448	R449	R450	R451	R452	R453	R454	R455	R456	N460	R461	R462	R463	R464	R465	R466	R467	R468	L471	R472	R473	R474																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
L475	R476	S477	V478	D479	V484	Q485	Y486	N487	G488	G489	D492	T496	D497	L498	G499	C500	P501	R505	R506	R507	R508	R509	R510	R511	R512	R513	R514	R515	R516	R517	R518	R519	R520	R521	R522	R523	R524	R525	G528	R529	R530	R531	R532	R533	R534	R535	R536	R537	R538	R539	R540	R541	R542	R543	R544	R545																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
L546	G547	G548	G549	A550	R551	Y552	W553	Q554	A555	F556	R557	Q558	Y559	P560	R561	L562	G565	F566	W568	D569	W570	W571	D572	Q573	R574	R575	R576	R577	R578	R579	R580	R581	R582	R583	R584	R585	R586	R587	R588	R589	R590	R591	R592	R593	R594	R595	R596	R597	R598	R599	R600	P601	C602	M603	A604	R605	R606	R607	R608	R609	R610																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
R611	T612	F613	H614	L615	L616	T617	T618	E619	A620	R621	Q622	Q623	Q624	Q625	Q626	Q627	G628	G629	G630	G631	G632	G633	G634	G635	G636	G637	G638	G639	G640	G641	G642	G643	G644	G645	G646	G647	G648	G649	G650	G651	G652	G653	G654	G655	G656	G657	G658	G659	G660	G661	G662	G663	G664	G665	G666	G667	G668	G669	G670	G671	G672	G673	G674	G675	G676	G677	G678	G679	G680																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
R681	L682	P683	G684	L685	P686	Q687	P688	P689	S690	Q691	Q692	Q693	Q694	Q695	Q696	Q697	Q698	Q699	Q700	Q701	Q702	Q703	Q704	Q705	Q706	Q707	Q708	Q709	Q710	Q711	Q712	Q713	Q714	Q715	Q716	Q717	Q718	Q719	Q720	Q721	Q722	Q723	Q724	Q725	Q726	Q727	Q728	Q729	Q730	Q731	Q732	Q733	Q734	Q735	Q736	Q737	Q738	Q739	Q740	Q741	Q742	Q743	Q744	Q745	Q746	Q747	Q748	Q749	Q750																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
L749	E750	G751	G752	N753	R754	R755	F756	N757	R758	R759	R760	R761	R762	R763	R764	R765	R766	R767	R768	R769	R770	R771	R772	R773	R774	R775	R776	R777	R778	R779	R780	R781	R782	R783	R784	R785	R786	R787	R788	R789	R790	R791	R792	R793	R794	R795	R796	R797	R798	R799	R800	R801	R802	R803	R804	R805	R806	R807	R808	R809	R810	R811	R812	R813	R814	R815	R816	R817	R818	R819	R820	R821	R822	R823	R824	R825	R826	R827	R828	R829	R830	R831	R832	R833	R834	R835	R836	R837	R838	R839	R840	R841	R842	R843	R844	R845	R846	R847	R848	R849	R850	R851	R852	R853	R854	R855	R856	R857	R858	R859	R860	R861	R862	R863	R864	R865	R866	R867	R868	R869	R870	R871	R872	R873	R874	R875	R876	R877	R878	R879	R880	R881	R882	R883	R884	R885	R886	R887	R888	R889	R890	R891	R892	R893	R894	R895	R896	R897	R898	R899	R900	R901	R902	R903	R904	R905	R906	R907	R908	R909	R910	R911	R912	R913	R914	R915	R916	R917	R918	R919	R920	R921	R922	R923	R924	R925	R926	R927	R928	R929	R930	R931	R932	R933	R934	R935	R936	R937	R938	R939	R940	R941	R942	R943	R944	R945	R946	R947	R948	R949	R950	R951	R952	R953	R954	R955	R956	R957	R958	R959	R960	R961	R962	R963	R964	R965	R966	R967	R968	R969	R970	R971	R972	R973	R974	R975	R976	R977	R978	R979	R980	R981	R982	R983	R984	R985	R986	R987	R988	R989	R990	R991	R992	R993	R994	R995	R996	R997	R998	R999	V1000	A1001	A1002	A1003	A1004	A1005	A1006	A1007	A1008	A1009	A1010	A1011	A1012	A1013	A1014	A1015	A1016	A1017	A1018	A1019	A1020	A1021	A1022	A1023	A1024	A1025	A1026	A1027	A1028	A1029	A1030	A1031	A1032	A1033	A1034	A1035	A1036	A1037	A1038	A1039	A1040	A1041	A1042	A1043	A1044	A1045	A1046	A1047	A1048	A1049	A1050	A1051	A1052	A1053	A1054	A1055	A1056	A1057	A1058	A1059	A1060	A1061	A1062	A1063	A1064	A1065	A1066	A1067	A1068	A1069	A1070	A1071	A1072	A1073	A1074	A1075	A1076	A1077	A1078	A1079	A1080	A1081	A1082	A1083	A1084	A1085	A1086	A1087	A1088	A1089	A1090	A1091	A1092	A1093	A1094	A1095	A1096	A1097	A1098	A1099	A1100	A1101	A1102	A1103	A1104	A1105	A1106	A1107	A1108	A1109	A1110	A1111	A1112	A1113	A1114	A1115	A1116	A1117	A1118	A1119	A1120	A1121	A1122	A1123	A1124	A1125	A1126	A1127	A1128	A1129	A1130	A1131	A1132	A1133	A1134	A1135	A1136	A1137	A1138	A1139	A1140	A1141	A1142	A1143	A1144	A1145	A1146	A1147	A1148	A1149	A1150	A1151	A1152	A1153	A1154	A1155	A1156	A1157	A1158	A1159	A1160	A1161	A1162	A1163	A1164	A1165	A1166	A1167	A1168	A1169	A1170	A1171	A1172	A1173	A1174	A1175	A1176	A1177	A1178	A1179	A1180	A1181	A1182	A1183	A1184	A1185	A1186	A1187	A1188	A1189	A1190	A1191	A1192	A1193	A1194	A1195	A1196	A1197	A1198	A1199	A1200	A1201	A1202	A1203	A1204	A1205	A1206	A1207	A1208	A1209	A1210	A1211	A1212	A1213	A1214	A1215	A1216	A1217	A1218	A1219	A1220	A1221	A1222	A1223	A1224	A1225	A1226	A1227	A1228	A1229	A1230	A1231	A1232	A1233	A1234	A1235	A1236	A1237	A1238	A1239	A1240	A1241	A1242	A1243	A1244	A1245	A1246	A1247	A1248	A1249	A1250	A1251	A1252	A1253	A1254	A1255	A1256	A1257	A1258	A1259	A1260	A1261	A1262	A1263	A1264	A1265	A1266	A1267	A1268	A1269	A1270	A1271	A1272	A1273	A1274	A1275	A1276	A1277	A1278	A1279	A1280	A1281	A1282	A1283	A1284	A1285	A1286	A1287	A1288	A1289	A1290	A1291	A1292	A1293	A1294	A1295	A1296	A1297	A1298	A1299	A1300	A1301	A1302	A1303	A1304	A1305	A1306	A1307	A1308	A1309	A1310	A1311	A1312	A1313	A1314	A1315	A1316	A1317	A1318	A1319	A1320	A1321	A1322	A1323	A1324	A1325	A1326	A1327	A1328	A1329	A1330	A1331	A1332	A1333	A1334	A1335	A1336	A1337	A1338	A1339	A1340	A1341	A1342	A1343	A1344	A1345	A1346	A1347	A1348	A1349	A1350	A1351	A1352	A1353	A1354	A1355	A1356	A1357	A1358	A1359	A1360	A1361	A1362	A1363	A1364	A1365	A1366	A1367	A1368	A1369	A1370	A1371	A1372	A1373	A1374	A1375	A1376	A1377	A1378	A1379	A1380	A1381	A1382	A1383	A1384	A1385	A1386	A1387	A1388	A1389	A1390	A1391	A1392	A1393	A1394	A1395	A1396	A1397	A1398	A1399	A1400	A1401	A1402	A1403	A1404	A1405	A1406	A1407	A1408	A1409	A1410	A1411	A1412	A1413	A1414	A1415	A1416	A1417	A1418	A1419	A1420	A1421	A1422	A1423	A1424	A1425	A1426	A1427	A1428	A1429	A1430	A1431	A1432	A1433	A1434	A1435	A1436	A1437	A1438	A1439	A1440	A1441	A1442	A1443	A1444	A1445	A1446	A1447	A1448	A1449	A1450	A1451	A1452	A1453	A1454	A1455	A1456	A1457	A1458	A1459	A1460	A1461	A1462	A1463	A1464	A1465	A1466	A1467	A1468	A1469	A1470	A1471	A1472	A1473	A1474	A1475	A1476	A1477	A1478	A1479	A1480	A1481	A1482	A1483	A1484	A1485	A1486	A1487	A1488	A1489	A1490	A1491	A1492	A1493	A1494	A1495	A1496	A1497	A1498	A1499	A1500	A1501	A1502	A1503	A1504	A1505	A1506	A1507	A1508	A1509	A1510	A1511	A1512	A1513	A1514	A1515	A1516	A1517	A1518	A1519	A1520	A1521	A1522	A1523	A1524	A1525	A1526	A1527	A1528	A1529	A1530	A1531	A1532	A1533	A1534	A1535	A1536	A1537	A1538	A1539	A1540	A1541	A1542	A1543	A1544	A1545	A1546	A1547	A1548	A1549	A1550	A1551	A1552	A1553	A1554	A1555	A1556	A1557	A1558	A1559	A1560	A1561	A1562	A1563	A1564	A1565	A1566	A1567	A1568	A1569	A1570	A1571	A1572	A1573	A1574	A1575	A1576	A1577	A1578	A1579	A1580	A1581	A1582	A1583	A1584	A1585	A1586	A1587	A1588	A1589	A1590	A1591	A1592	A1593	A1594	A1595	A1596	A1597	A1598	A1599	A1600	A1601	A1602	A1603	A1604	A1605	A1606	A1607	A1608	A1609	A1610	A1611	A1612	A1613	A1614	A1615	A1616	A1617	A1618	A1619	A1620	A1621	A1622	A1623	A1624	A1625	A1626	A1627	A1628	A1629	A1630	A1631	A1632	A1633	A1634	A1635	A1636	A1637	A1638	A1639	A1640	A1641	A1642	A1643	A1644	A1645	A1646	A1647	A1648	A1649	A1650	A1651	A1652	A1653	A1654	A1655	A1656	A1657	A1658	A1659	A1660	A1661	A1662	A1663	A1664	A1665	A1666	A1667	A1668	A1669	A1670	A1671	A1672	A1673	A1674	A1675	A1676	A1677	A1678	A1679	A1680	A1681	A1682	A1683	A1684	A1685	A1686	A1687	A1688	A1689	A1690	A1691	A1692	A1693	A1694	A1695	A1696	A1697	A1698	A1699	A1700	A1701	A1702	A1703	A1704	A1705	A1706	A1707	A1708	A1709	A1710	A1711	A1712	A1713	A1714	A1715	A1716	A1717	A1718	A1719	A1720	A1721	A1722	A1723	A1724	A1725	A1726	A1727	A1728	A1729	A1730	A1731	A1732	A1733	A1734	A1735	A1736	A1737	A1738	A1739	A1740	A1741	A1742	A1743	A1744	A1745	A1746	A1747	A1748	A1749	A1750	A1751	A1752	A1753	A1754	A1755	A1756	A1757	A1758	A1759	A1760	A1761	A1762	A1763	A1764	A1765	A1766	A1767	A1768	A1769	A1770	A1771	A1772	A1773	A1774	A1775	A1776	A1777	A1778	A1779	A1780	A1781	A1782	A1783	A1784	A1785	A1786	A1787	A1788	A1789	A1790	A179

L1009	L1010	R1013	Y1014	H1015	Y1016	Q1017	L1018	W1019	W1020	C1021	Q1022	K1023																																																	
L884	N885	C886	Q887	L888	A889	Q890	N891	A892	R893	N894	N895	N896	N897	L898	N898	G899	L900	S901	P902	Q903	E904	N905	Y906	P907	D908	R909	L910	T911	R912	R913	C914	F915	D916	R917	N918	D919	L920	P921	L922	S923	D924	Y926	T927	P928	Y929	V930	F931	P932	S933	E934	N935	G936	L937	R938	C939	G940	T941	R942	E943		
Q817	A818	E819	L822	L823	Q824	D828	T829	L830	A831	D832	A833	L834	L835	T836	T837	T838	A839	H840	A841	H842	H843	H844	Q845	G846	R847	T848	L849	F850	R853	R854	T855	Y856	R857	L858	D859	G860	S861	G862	Q863	M864	A865	T867	V868	P869	V870	E871	S874	D875	L876	T877	C878	I879	A881	P882	H883	R884	R881				
R755	Q687	P688	E689	S690	L694	M695	L696	T697	V698	R699	V700	V701	Q702	P703	N704	A705	T706	A707	W708	S709	E710	A711	G712	H713	I714	S715	A716	W717	L722	A723	E724	N725	L726	S727	R728	T729	L730	H735	A736	I737	P738	H739	L740	T741	T742	S743	E744	N745	D746	R809	W810	K811	I812	A813	G814	H815	Y816				
Q625	F626	F629	R630	L631	S632	G633	Q634	T635	I636	R637	V638	Q639	T640	S641	E642	Y643	F644	R645	H646	S647	D648	N649	E650	L651	L652	H653	M654	M655	V656	A657	D658	S659	G660	K661	P662	L663	A664	G666	E667	V668	P669	L670	D671	V672	A673	P674	K677	Q678	L679	I680	E681	I682	P683	E684	L685	P686					
R561	L562	Q563	F566	V567	M568	D569	W570	P571	D572	Q573	Y574	S575	L576	K577	E578	D579	E580	N583	P584	W585	S586	A587	G590	D591	F592	G593	D594	T595	P596	N597	D598	R599	Q600	F601	M602	M603	N604	L606	V607	F608	A609	D610	R611	T612	P613	A616	L617	F618	E619	A620	Y621	K621	H622	Q623	Q624						
Q370	V373	Q374	D375	L376	L377	L378	M379	K380	Q381	N382	N383	F384	N385	A386	V387	R388	C389	S390	R391	Y392	P393	N394	H395	P396	L397	W398	Y399	T400	L401	C402	H403	R404	L407	Y408	V409	V410	D411	E412	L413	M414	T415	E416	T417	R418	C419	M420	V421	P422	M423	M424	R425	L426	G364	Q365	V366	D367	P430	R431			
Y309	R310	A311	V312	D313	E314	L315	H316	T317	Q318	D319	N320	L322	I323	A324	V325	R326	A327	C328	D329	V330	G331	F332	H333	E334	V335	L337	E338	L341	L342	L343	L344	N345	L407	Y408	V409	V410	D411	E412	L350	M413	R352	G353	V354	N355	R356	H357	C419	M420	V421	H359	H360	P361	M424	R425	L426	G364	Q365	V366	D367	P430	R431

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.90Å 207.50Å 509.90Å 90.00° 94.70° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50 92.62 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.50) 39.3 (92.62-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.00Å)	Xtriage
Refinement program	TNT V. 5-D	Depositor
R, R_{free}	0.174 , (Not available) 0.175 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 68.0	EDS
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 590207 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	132654	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.16	51/8440 (0.6%)	1.52	139/11516 (1.2%)
1	B	1.17	54/8440 (0.6%)	1.51	130/11516 (1.1%)
1	C	1.18	56/8440 (0.7%)	1.50	132/11516 (1.1%)
1	D	1.16	55/8440 (0.7%)	1.52	148/11516 (1.3%)
1	E	1.16	55/8440 (0.7%)	1.56	145/11516 (1.3%)
1	F	1.18	45/8440 (0.5%)	1.53	144/11516 (1.3%)
1	G	1.16	58/8440 (0.7%)	1.51	151/11516 (1.3%)
1	H	1.16	56/8440 (0.7%)	1.57	150/11516 (1.3%)
1	I	1.13	53/8440 (0.6%)	1.52	140/11516 (1.2%)
1	J	1.12	48/8440 (0.6%)	1.48	134/11516 (1.2%)
1	K	1.09	53/8440 (0.6%)	1.45	115/11516 (1.0%)
1	L	1.13	53/8440 (0.6%)	1.54	134/11516 (1.2%)
1	M	1.16	55/8440 (0.7%)	1.58	142/11516 (1.2%)
1	N	1.14	51/8440 (0.6%)	1.49	127/11516 (1.1%)
1	O	1.11	54/8440 (0.6%)	1.49	141/11516 (1.2%)
1	P	1.17	57/8440 (0.7%)	1.60	151/11516 (1.3%)
All	All	1.15	854/135040 (0.6%)	1.52	2223/184256 (1.2%)

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	1	0
1	B	1	0
1	D	2	1
1	E	1	0
1	F	2	0
1	G	2	0
1	H	1	0

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	1	0
1	J	1	0
1	L	1	0
1	M	2	0
1	P	2	0
All	All	17	1

The worst 5 of 854 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	358	GLU	CD-OE2	11.52	1.38	1.25
1	F	75	GLU	CD-OE1	10.30	1.36	1.25
1	K	358	GLU	CD-OE2	9.34	1.35	1.25
1	B	650	GLU	CD-OE1	9.31	1.35	1.25
1	F	326	GLU	CD-OE2	9.01	1.35	1.25

The worst 5 of 2223 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	881	ARG	NE-CZ-NH2	-14.45	113.08	120.30
1	B	166	ARG	NE-CZ-NH2	-14.23	113.19	120.30
1	N	561	ARG	NE-CZ-NH2	-14.06	113.27	120.30
1	L	425	ARG	NE-CZ-NH2	13.74	127.17	120.30
1	L	997	ASP	CB-CG-OD2	-13.64	106.02	118.30

5 of 17 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	90	TRP	CA
1	B	718	GLN	CA
1	D	95	TYR	CA
1	D	914	CYS	CA
1	E	118	ASN	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	473	ARG	Sidechain

5.2 Close contacts ⓘ

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8198	0	7796	540	0
1	B	8198	0	7796	546	0
1	C	8198	0	7796	446	0
1	D	8198	0	7796	551	0
1	E	8198	0	7795	892	0
1	F	8198	0	7796	579	0
1	G	8198	0	7796	641	0
1	H	8198	0	7796	882	0
1	I	8198	0	7796	618	0
1	J	8198	0	7795	507	0
1	K	8198	0	7796	781	0
1	L	8198	0	7796	792	0
1	M	8198	0	7796	1078	0
1	N	8198	0	7795	630	0
1	O	8198	0	7796	659	0
1	P	8198	0	7796	1151	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
2	M	1	0	0	0	0
2	N	2	0	0	0	0
2	O	2	0	0	0	0
2	P	2	0	0	0	0
3	A	88	0	0	7	0
3	B	96	0	0	14	0
3	C	91	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	97	0	0	13	0
3	E	94	0	0	20	0
3	F	91	0	0	9	0
3	G	95	0	0	13	0
3	H	92	0	0	18	0
3	I	90	0	0	15	0
3	J	97	0	0	9	0
3	K	87	0	0	9	0
3	L	84	0	0	12	0
3	M	79	0	0	17	0
3	N	94	0	0	19	0
3	O	95	0	0	12	0
3	P	85	0	0	21	0
All	All	132654	0	124733	11096	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 43.

The worst 5 of 11096 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:7:LEU:HD13	1:E:74:LEU:HD11	1.23	1.17
1:D:572:ASP:HB3	1:D:603:MET:HG2	1.25	1.16
1:C:427:THR:HA	1:C:436:MET:HE1	1.21	1.16
1:A:770:ILE:HD11	1:A:1022:GLN:HG2	1.18	1.15
1:I:316:HIS:HA	1:I:323:ILE:HD13	1.24	1.13

There are no symmetry-related clashes.

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	1019/1023 (100%)	909 (89%)	92 (9%)	18 (2%)	13 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1019/1023 (100%)	914 (90%)	85 (8%)	20 (2%)	11	17
1	C	1019/1023 (100%)	919 (90%)	81 (8%)	19 (2%)	12	19
1	D	1019/1023 (100%)	910 (89%)	98 (10%)	11 (1%)	21	34
1	E	1019/1023 (100%)	842 (83%)	135 (13%)	42 (4%)	4	5
1	F	1019/1023 (100%)	892 (88%)	101 (10%)	26 (3%)	8	11
1	G	1019/1023 (100%)	893 (88%)	101 (10%)	25 (2%)	9	12
1	H	1019/1023 (100%)	845 (83%)	140 (14%)	34 (3%)	6	7
1	I	1019/1023 (100%)	884 (87%)	111 (11%)	24 (2%)	9	13
1	J	1019/1023 (100%)	887 (87%)	118 (12%)	14 (1%)	16	27
1	K	1019/1023 (100%)	855 (84%)	131 (13%)	33 (3%)	6	8
1	L	1019/1023 (100%)	838 (82%)	146 (14%)	35 (3%)	6	7
1	M	1019/1023 (100%)	836 (82%)	127 (12%)	56 (6%)	3	2
1	N	1019/1023 (100%)	875 (86%)	117 (12%)	27 (3%)	8	11
1	O	1019/1023 (100%)	889 (87%)	102 (10%)	28 (3%)	8	10
1	P	1019/1023 (100%)	797 (78%)	164 (16%)	58 (6%)	3	2
All	All	16304/16368 (100%)	13985 (86%)	1849 (11%)	470 (3%)	7	9

5 of 470 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	ASP
1	A	277	GLU
1	A	389	CYS
1	A	541	ALA
1	A	659	ASP

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	873/875 (100%)	723 (83%)	150 (17%)	3	5
1	B	873/875 (100%)	709 (81%)	164 (19%)	2	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	873/875 (100%)	754 (86%)	119 (14%)	5	10
1	D	873/875 (100%)	729 (84%)	144 (16%)	3	6
1	E	873/875 (100%)	686 (79%)	187 (21%)	1	2
1	F	873/875 (100%)	735 (84%)	138 (16%)	4	6
1	G	873/875 (100%)	717 (82%)	156 (18%)	2	4
1	H	873/875 (100%)	693 (79%)	180 (21%)	2	3
1	I	873/875 (100%)	716 (82%)	157 (18%)	2	4
1	J	873/875 (100%)	755 (86%)	118 (14%)	6	10
1	K	873/875 (100%)	722 (83%)	151 (17%)	3	5
1	L	873/875 (100%)	704 (81%)	169 (19%)	2	3
1	M	873/875 (100%)	677 (78%)	196 (22%)	1	2
1	N	873/875 (100%)	717 (82%)	156 (18%)	2	4
1	O	873/875 (100%)	715 (82%)	158 (18%)	2	4
1	P	873/875 (100%)	665 (76%)	208 (24%)	1	1
All	All	13968/14000 (100%)	11417 (82%)	2551 (18%)	2	4

5 of 2551 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	523	TRP
1	J	277	GLU
1	P	71	GLU
1	H	724	GLU
1	I	293	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 370 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	262	GLN
1	I	950	GLN
1	O	1008	GLN
1	H	460	ASN
1	I	38	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 31 ligands modelled in this entry, 31 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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	1021/1023 (99%)	-0.94	0 100 100	2, 24, 54, 79	0
1	B	1021/1023 (99%)	-0.97	0 100 100	2, 23, 54, 81	0
1	C	1021/1023 (99%)	-0.94	0 100 100	4, 21, 52, 80	0
1	D	1021/1023 (99%)	-0.96	0 100 100	4, 25, 56, 81	0
1	E	1021/1023 (99%)	-0.84	1 (0%) 93 95	8, 34, 61, 86	0
1	F	1021/1023 (99%)	-0.92	0 100 100	2, 23, 55, 78	0
1	G	1021/1023 (99%)	-0.94	0 100 100	3, 27, 58, 82	0
1	H	1021/1023 (99%)	-0.79	1 (0%) 93 95	6, 33, 61, 89	0
1	I	1021/1023 (99%)	-0.91	0 100 100	4, 30, 59, 80	0
1	J	1021/1023 (99%)	-0.90	0 100 100	8, 28, 56, 85	0
1	K	1021/1023 (99%)	-0.79	2 (0%) 93 94	10, 35, 64, 92	0
1	L	1021/1023 (99%)	-0.76	0 100 100	6, 35, 63, 84	0
1	M	1021/1023 (99%)	-0.71	1 (0%) 93 95	12, 39, 65, 80	0
1	N	1021/1023 (99%)	-0.85	0 100 100	9, 30, 59, 89	0
1	O	1021/1023 (99%)	-0.90	0 100 100	11, 31, 60, 81	0
1	P	1021/1023 (99%)	-0.41	12 (1%) 75 77	14, 43, 69, 89	0
All	All	16336/16368 (99%)	-0.85	17 (0%) 93 95	2, 30, 60, 92	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	313	VAL	3.6
1	P	81	ALA	3.6
1	P	141	ILE	3.3
1	P	143	PHE	3.1
1	P	70	PRO	2.8

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MG	F	1101	1/1	0.19	9.20	35,35,35,35	0
2	MG	C	1101	1/1	0.17	8.22	23,23,23,23	0
2	MG	G	1101	1/1	0.17	8.11	32,32,32,32	0
2	MG	A	1101	1/1	0.14	6.08	37,37,37,37	0
2	MG	I	1101	1/1	0.13	4.97	33,33,33,33	0
2	MG	B	1101	1/1	0.14	4.05	25,25,25,25	0
2	MG	O	1101	1/1	0.12	4.01	40,40,40,40	0
2	MG	E	1101	1/1	0.16	3.84	39,39,39,39	0
2	MG	J	1101	1/1	0.14	3.68	34,34,34,34	0
2	MG	H	1101	1/1	0.13	3.31	27,27,27,27	0
2	MG	D	1101	1/1	0.12	2.52	28,28,28,28	0
2	MG	D	1102	1/1	0.12	2.37	42,42,42,42	0
2	MG	M	1101	1/1	0.14	2.35	56,56,56,56	0
2	MG	N	1101	1/1	0.11	1.86	32,32,32,32	0
2	MG	L	1101	1/1	0.13	1.26	31,31,31,31	0
2	MG	N	1102	1/1	0.13	0.43	26,26,26,26	0
2	MG	C	1102	1/1	0.09	0.33	28,28,28,28	0
2	MG	K	1101	1/1	0.08	-0.35	34,34,34,34	0
2	MG	E	1102	1/1	0.08	-0.50	32,32,32,32	0
2	MG	P	1101	1/1	0.11	-0.58	49,49,49,49	0
2	MG	A	1102	1/1	0.07	-1.15	37,37,37,37	0
2	MG	O	1102	1/1	0.07	-1.21	15,15,15,15	0
2	MG	H	1102	1/1	0.06	-1.30	22,22,22,22	0
2	MG	L	1102	1/1	0.04	-1.95	28,28,28,28	0
2	MG	K	1102	1/1	0.04	-2.02	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MG	I	1102	1/1	0.05	-2.03	33,33,33,33	0
2	MG	B	1102	1/1	0.06	-2.45	23,23,23,23	0
2	MG	P	1102	1/1	0.04	-2.64	26,26,26,26	0
2	MG	J	1102	1/1	0.05	-2.93	29,29,29,29	0
2	MG	F	1102	1/1	0.06	-4.29	26,26,26,26	0
2	MG	G	1102	1/1	0.03	-5.05	18,18,18,18	0

6.5 Other polymers ⓘ

There are no such residues in this entry.