



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 06:30 AM UTC

PDB ID : 1Y0V / pdb_00001y0v
Title : Crystal structure of anthrax edema factor (EF) in complex with calmodulin and pyrophosphate
Authors : Shen, Y.; Zhukovskaya, N.L.; Guo, Q.; Florian, J.; Tang, W.-J.
Deposited on : 2004-11-16
Resolution : 3.60 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

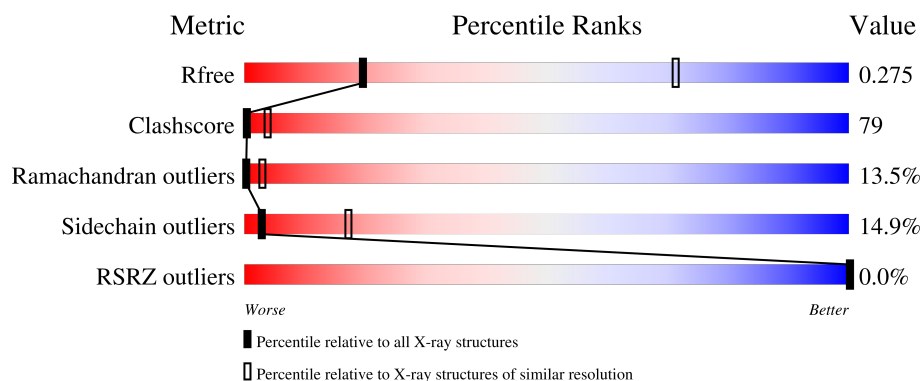
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



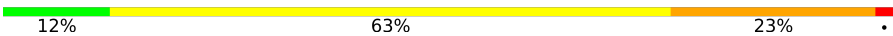
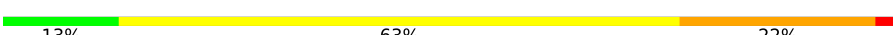
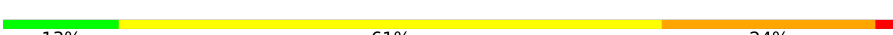
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	777	
1	B	777	
1	C	777	
1	D	777	
1	E	777	

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Mol	Chain	Length	Quality of chain
1	F	777	 16% 55% 21% 5%
2	H	146	 12% 63% 23%
2	I	146	 13% 62% 23%
2	J	146	 14% 62% 22%
2	K	146	 13% 62% 23%
2	L	146	 13% 63% 22%
2	M	146	 13% 61% 24%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 42906 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 Calmodulin-sensitive adenylate cyclase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	735	Total	C	N	O	S	0	0	0
			5992	3828	995	1163	6			
1	B	735	Total	C	N	O	S	0	0	0
			5992	3828	995	1163	6			
1	C	735	Total	C	N	O	S	0	0	0
			5992	3828	995	1163	6			
1	D	735	Total	C	N	O	S	0	0	0
			5992	3828	995	1163	6			
1	E	735	Total	C	N	O	S	0	0	0
			5992	3828	995	1163	6			
1	F	735	Total	C	N	O	S	0	0	0
			5992	3828	995	1163	6			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	MET	-	cloning artifact	UNP P40136
A	25	HIS	-	cloning artifact	UNP P40136
A	26	HIS	-	cloning artifact	UNP P40136
A	27	HIS	-	cloning artifact	UNP P40136
A	28	HIS	-	cloning artifact	UNP P40136
A	29	HIS	-	cloning artifact	UNP P40136
A	30	HIS	-	cloning artifact	UNP P40136
A	31	ALA	-	cloning artifact	UNP P40136
A	32	ALA	-	cloning artifact	UNP P40136
B	24	MET	-	cloning artifact	UNP P40136
B	25	HIS	-	cloning artifact	UNP P40136
B	26	HIS	-	cloning artifact	UNP P40136
B	27	HIS	-	cloning artifact	UNP P40136
B	28	HIS	-	cloning artifact	UNP P40136
B	29	HIS	-	cloning artifact	UNP P40136
B	30	HIS	-	cloning artifact	UNP P40136
B	31	ALA	-	cloning artifact	UNP P40136

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Chain	Residue	Modelled	Actual	Comment	Reference
B	32	ALA	-	cloning artifact	UNP P40136
C	24	MET	-	cloning artifact	UNP P40136
C	25	HIS	-	cloning artifact	UNP P40136
C	26	HIS	-	cloning artifact	UNP P40136
C	27	HIS	-	cloning artifact	UNP P40136
C	28	HIS	-	cloning artifact	UNP P40136
C	29	HIS	-	cloning artifact	UNP P40136
C	30	HIS	-	cloning artifact	UNP P40136
C	31	ALA	-	cloning artifact	UNP P40136
C	32	ALA	-	cloning artifact	UNP P40136
D	24	MET	-	cloning artifact	UNP P40136
D	25	HIS	-	cloning artifact	UNP P40136
D	26	HIS	-	cloning artifact	UNP P40136
D	27	HIS	-	cloning artifact	UNP P40136
D	28	HIS	-	cloning artifact	UNP P40136
D	29	HIS	-	cloning artifact	UNP P40136
D	30	HIS	-	cloning artifact	UNP P40136
D	31	ALA	-	cloning artifact	UNP P40136
D	32	ALA	-	cloning artifact	UNP P40136
E	24	MET	-	cloning artifact	UNP P40136
E	25	HIS	-	cloning artifact	UNP P40136
E	26	HIS	-	cloning artifact	UNP P40136
E	27	HIS	-	cloning artifact	UNP P40136
E	28	HIS	-	cloning artifact	UNP P40136
E	29	HIS	-	cloning artifact	UNP P40136
E	30	HIS	-	cloning artifact	UNP P40136
E	31	ALA	-	cloning artifact	UNP P40136
E	32	ALA	-	cloning artifact	UNP P40136
F	24	MET	-	cloning artifact	UNP P40136
F	25	HIS	-	cloning artifact	UNP P40136
F	26	HIS	-	cloning artifact	UNP P40136
F	27	HIS	-	cloning artifact	UNP P40136
F	28	HIS	-	cloning artifact	UNP P40136
F	29	HIS	-	cloning artifact	UNP P40136
F	30	HIS	-	cloning artifact	UNP P40136
F	31	ALA	-	cloning artifact	UNP P40136
F	32	ALA	-	cloning artifact	UNP P40136

- Molecule 2 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	146	Total	C	N	O	S	0	0	0
			1146	702	185	250	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	146	Total	C	N	O	S	0	0	0
			1146	702	185	250	9			
2	J	146	Total	C	N	O	S	0	0	0
			1146	702	185	250	9			
2	K	146	Total	C	N	O	S	0	0	0
			1146	702	185	250	9			
2	L	146	Total	C	N	O	S	0	0	0
			1146	702	185	250	9			
2	M	146	Total	C	N	O	S	0	0	0
			1146	702	185	250	9			

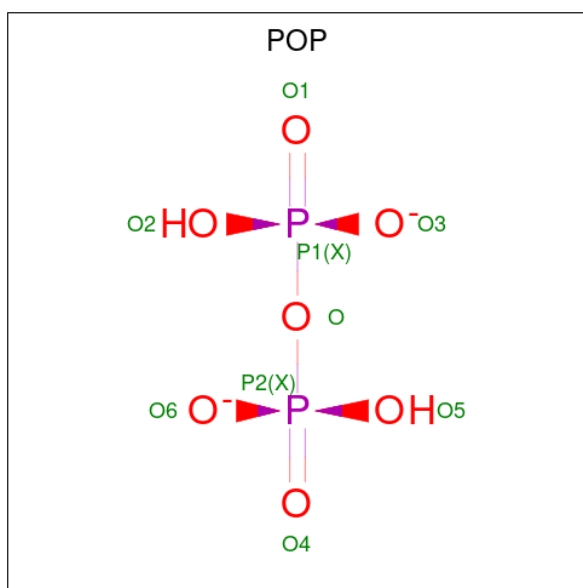
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	3	ALA	-	cloning artifact	UNP P62155
H	4	ALA	-	cloning artifact	UNP P62155
I	3	ALA	-	cloning artifact	UNP P62155
I	4	ALA	-	cloning artifact	UNP P62155
J	3	ALA	-	cloning artifact	UNP P62155
J	4	ALA	-	cloning artifact	UNP P62155
K	3	ALA	-	cloning artifact	UNP P62155
K	4	ALA	-	cloning artifact	UNP P62155
L	3	ALA	-	cloning artifact	UNP P62155
L	4	ALA	-	cloning artifact	UNP P62155
M	3	ALA	-	cloning artifact	UNP P62155
M	4	ALA	-	cloning artifact	UNP P62155

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

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

- Molecule 4 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: $\text{H}_2\text{O}_7\text{P}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			9	7	2		
4	B	1	Total	O	P	0	0
			9	7	2		
4	C	1	Total	O	P	0	0
			9	7	2		
4	D	1	Total	O	P	0	0
			9	7	2		
4	E	1	Total	O	P	0	0
			9	7	2		
4	F	1	Total	O	P	0	0
			9	7	2		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	3	Total	Ca	0	0
			3	3		
5	I	3	Total	Ca	0	0
			3	3		
5	J	3	Total	Ca	0	0
			3	3		
5	K	3	Total	Ca	0	0
			3	3		
5	L	3	Total	Ca	0	0
			3	3		

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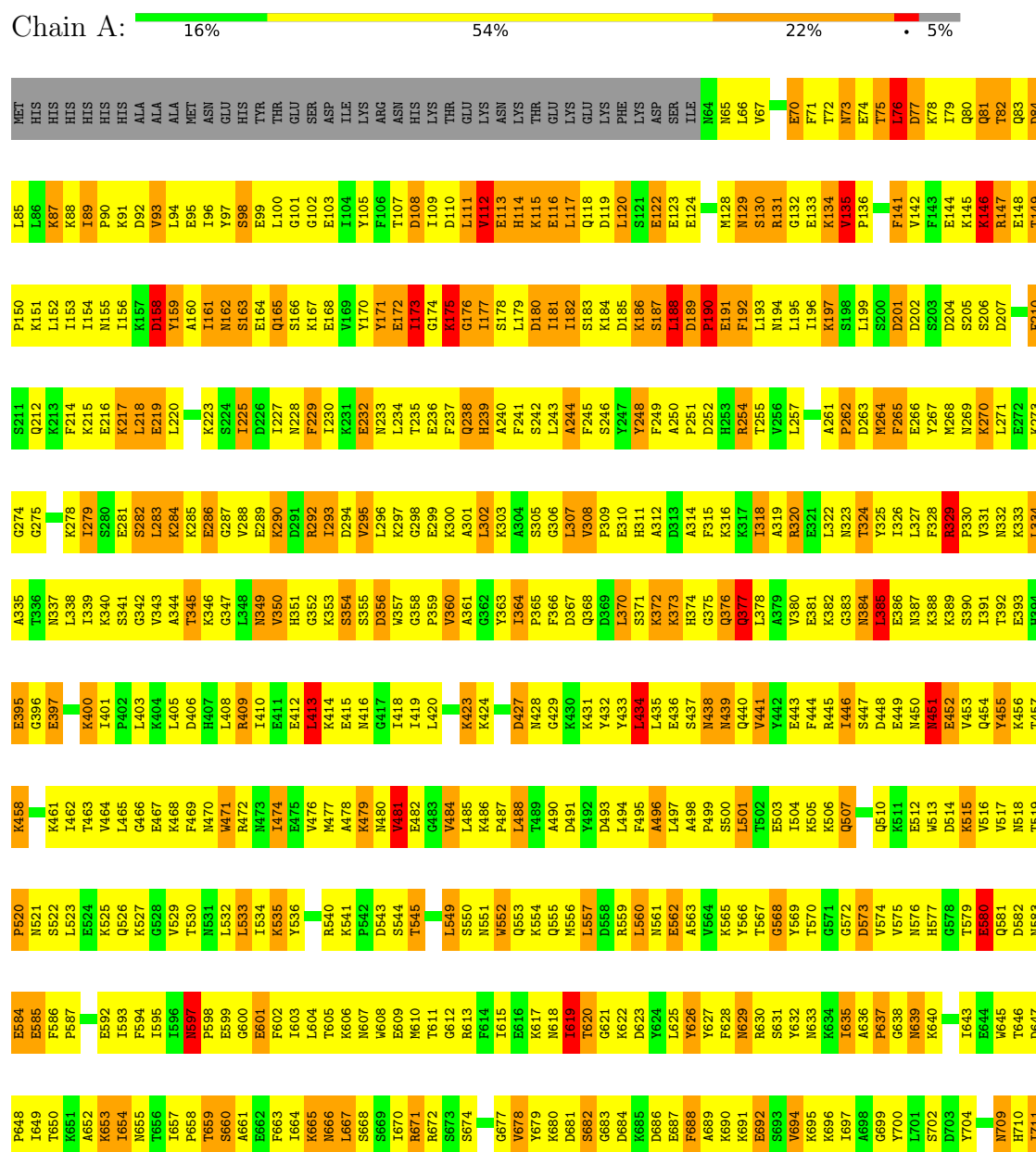
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	3	Total	Ca	0	0
			3	3		

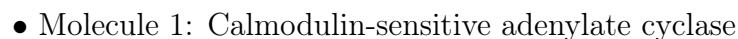
3 Residue-property plots

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

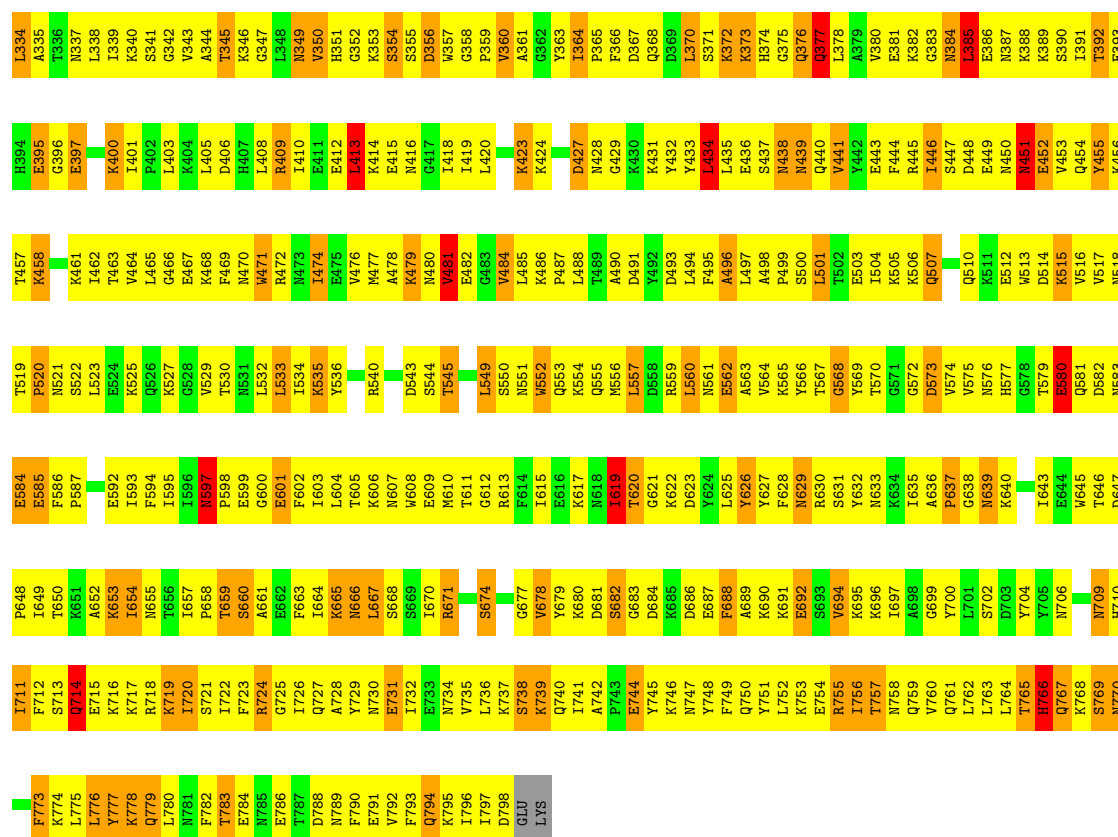
- Molecule 1: Calmodulin-sensitive adenylate cyclase



L85	L86	L87	L88	L89	P90	K91	D92	V93	E95	A160	I161	M162	S163	E99	L100	G101	K167	E168	V169	Y170	G176	I177	S178	H114	K115	E116	L117	Q118	D119	L185	S121	E122	E123	E124	M128	N129	S130	R131	G132	E133	K134	V135	P136	F141	V142	S203	D204	S205	S206	D207	F210																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
P150	K151	L152	L153	I154	M155	L156	K157	D158	Y159	A160	I161	M162	S163	E164	Q165	S166	K167	E168	V169	Y170	G176	I177	S178	H114	K115	E116	L117	Q118	D119	L185	S121	E122	E123	E124	M128	N129	S130	R131	G132	E133	K134	V135	P136	F141	V142	S203	D204	S205	S206	D207	F210																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
Q211	Q212	K213	F214	K215	E216	K217	L218	E219	L220	K223	S224	K225	I226	D227	N228	F229	K230	E231	K232	E233	E234	N235	L236	F237	Q238	H239	A240	L241	S242	L243	A244	L245	L246	L247	L248	L249	L250	P251	D252	H253	F254	T255	V256	L257	A261	E321	L322	K323	M324	T325	Y326	L327	M328	R329	P330	V331	E332	K333																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
Q274	Q275	E276	E277	K278	L279	S280	E281	S282	L283	K284	K285	E286	G287	V288	E289	K290	D291	R292	L293	D294	V295	L296	K297	G298	E299	K300	A301	L302	K303	A304	S305	G306	L307	Q308	P309	E310	H311	A312	D313	A314	F315	K316	K317	L318	A319	R320	E321	L322	K323	M324	T325	Y326	L327	M328	R329	P330	V331	E332	K333																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
L334	A335	T336	N337	L338	I339	K340	S341	G342	V343	A344	K345	E346	G347	N348	V350	K351	H352	G353	K354	S355	L356	G357	K358	P359	V360	A361	L362	K363	A364	S365	F366	L367	Q368	D369	L370	S371	K372	H373	G374	K375	Q376	Q377	L378	A379	V380	E381	K382	G383	M384	D385	E386	N387	K388	R389	S390	I391	T392	E393																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
H394	E395	G396	E397	K400	L401	P402	L403	L404	L405	D406	K407	L408	R409	L410	E411	G412	L413	K414	E415	N416	G417	L418	L419	L420	K423	A424	K425	D427	M428	G429	K430	K431	Y432	D433	L434	L435	E436	S437	M438	M439	Q440	V441	Y442	E443	P444	R445	T446	S447	D448	E449	M450	K451	E452	V453	Q454	Y455	K456																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
T457	K458	K461	L462	T463	V464	L465	G466	K467	K468	P469	M470	L471	R472	M473	L474	E475	V476	M477	A478	N479	L480	L481	E482	G483	V484	L485	K486	P487	L488	T489	A490	D491	Y492	D493	L494	F495	A496	L497	A498	P499	S500	L501	T502	E503	T504	K505	K506	Q507	Q510	K511	E512	N513	V514	K515	V516	Q517	N518																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
T519	P520	N521	S522	L523	E524	K525	Q526	S527	G528	V529	L530	N531	L532	L533	E534	F535	Y536	R540	K541	N542	D543	S544	T545	L549	S550	N551	K552	G553	K554	A555	M556	L557	T558	D559	L560	N561	E562	A563	V564	P565	K566	L567	E568	G569	T570	K571	E572	D573	V574	V575	N576	H577	G578	T579	E580	Q581	V582																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
N583	E584	E585	F586	P587	E589	L590	L591	L592	F593	L594	L595	L596	L597	L598	L599	L600	L601	L602	L603	L604	L605	L606	L607	L608	L609	L610	L611	L612	L613	L614	L615	L616	L617	L618	L619	L620	L621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
D647	T650	K651	A652	K653	L654	L655	L656	L657	L658	L659	S660	A661	E662	F663	L664	L665	L666	L667	S668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
N709	H710	F711	L712	S713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
S769	N770	F773	K774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000	L1001	L1002	L1003	L1004	L1005	L1006	L1007	L1008	L1009	L1010	L1011	L1012	L1013	L1014	L1015	L1016	L1017	L1018	L1019	L1020	L1021	L1022	L1023	L1024	L1025	L1026	L1027	L1028	L1029	L1030	L1031	L1032	L1033	L1034	L1035	L1036	L1037	L1038	L1039	L1040	L1041	L1042	L1043	L1044	L1045	L1046	L1047	L1048	L1049	L1050	L1051	L1052	L1053	L1054	L1055	L1056	L1057	L1058	L1059	L1060	L1061	L1062	L1063	L1064	L1065	L1066	L1067	L1068	L1069	L1070	L1071	L1072	L1073	L1074	L1075	L1076	L1077	L1078	L1079	L1080	L1081	L1082	L1083	L1084	L1085	L1086	L1087	L1088	L1089	L1090	L1091	L1092	L1093	L1094	L1095	L1096	L1097	L1098	L1099	L1100	L1101	L1102	L1103	L1104	L1105	L1106	L1107	L1108	L1109	L1110	L1111	L1112	L1113	L1114	L1115	L1116	L1117	L1118	L1119	L1120	L1121	L1122	L1123	L1124	L1125	L1126	L1127	L1128	L1129	L1130	L1131	L1132	L1133	L1134	L1135	L1136	L1137	L1138	L1139	L1140	L1141	L1142	L1143	L1144	L1145	L1146	L1147	L1148	L1149	L1150	L1151	L1152	L1153	L1154	L1155	L1156	L1157	L1158	L1159	L1160	L1161	L1162	L1163	L1164	L1165	L1166	L1167	L1168	L1169	L1170	L1171	L1172	L1173	L1174	L1175	L1176	L1177	L1178	L1179	L1180	L1181	L1182	L1183	L1184	L1185	L1186	L1187	L1188	L1189	L1190	L1191	L1192	L1193	L1194	L1195	L1196	L1197	L1198	L1199	L1200	L1201	L1202	L1203	L1204	L1205	L1206	L1207	L1208	L1209	L1210	L1211	L1212	L1213	L1214	L1215	L1216	L1217	L1218	L1219	L1220	L1221	L1222	L1223	L1224	L1225	L1226	L1227	L1228	L1229	L1230	L1231	L1232	L1233	L1234	L1235	L1236	L1237	L1238	L1239	L1240	L1241	L1242	L1243	L1244	L1245	L1246	L1247	L1248	L1249	L1250	L1251	L1252	L1253	L1254	L1255	L1256	L1257	L1258	L1259	L1260	L1261	L1262	L1263	L1264	L1265	L1266	L1267	L1268	L1269	L1270	L1271	L1272	L1273	L1274	L1275	L1276	L1277	L1278	L1279	L1280	L1281	L1282	L1283	L1284	L1285	L1286	L1287	L1288	L1289	L1290	L1291	L1292	L1293	L1294	L1295	L1296	L1297	L1298	L1299	L1300	L1301	L1302	L1303	L1304	L1305	L1306	L1307	L1308	L1309	L1310	L1311	L1312	L1313	L1314	L1315	L1316	L1317	L1318	L1319	L1320	L1321	L1322	L1323	L1324	L1325	L1326	L1327	L1328	L1329	L1330	L1331	L1332	L1333	L1334	L1335	L1336	L1337	L1338	L1339	L1340	L1341	L1342	L1343	L1344	L1345	L1346	L1347	L1348	L1349	L1350	L1351	L1352	L1353	L1354	L1355	L1356	L1357	L1358	L1359	L1360	L1361	L1362	L1363	L1364	L1365	L1366	L1367	L1368	L1369	L1370	L1371	L1372	L1373	L1374	L1375	L1376	L1377	L1378	L1379	L1380	L1381	L1382	L1383	L1384	L1385	L1386	L1387	L1388	L1389	L1390	L1391	L1392	L1393	L1394	L1395	L1396	L1397	L1398	L1399	L1400	L1401	L1402	L1403	L1404	L1405	L1406	L1407	L1408	L1409	L1410	L1411	L1412	L1413	L1414	L1415	L1416	L1417	L1418	L1419	L1420	L1421	L1422	L1423	L1424	L1425	L1426	L1427	L1428	L1429	L1430	L1431	L1432	L1433	L1434	L1435	L1436	L1437	L1438	L1439	L1440	L1441	L1442	L1443	L1444	L1445	L1446	L1447	L1448	L1449	L1450	L1451	L1452	L1453	L1454	L1455	L1456	L1457	L1458	L1459	L1460	L1461	L1462	L1463	L1464	L1465	L1466	L1467	L1468	L1469	L1470	L1471	L1472	L1473	L1474	L1475	L1476	L1477	L1478	L1479	L1480	L1481	L1482	L1483	L1484	L1485	L1486	L1487	L1488	L1489	L1490	L1491	L1492	L1493	L1494	L1495	L1496	L1497	L1498	L1499	L1500	L1501	L1502	L1503	L1504	L1505	L1506	L1507	L1508	L1509	L1510	L1511	L1512	L1513	L1514	L1515	L1516	L1517	L1518	L1519	L1520	L1521	L1522	L1523	L1524	L1525	L1526	L1527	L1528	L1529	L1530	L1531	L1532	L1533	L1534	L1535	L1536	L1537	L1538	L1539	L1540	L1541	L1542	L1543	L1544	L1545	L1546	L1547	L1548	L1549	L1550	L1551	L1552	L1553	L1554	L1555	L1556	L1557	L1558	L1559	L1560	L1561	L1562	L1563	L1564	L1565	L1566	L1567	L1568	L1569	L1570	L1571	L1572	L1573	L1574	L1575	L1576	L1577	L1578	L1579	L1

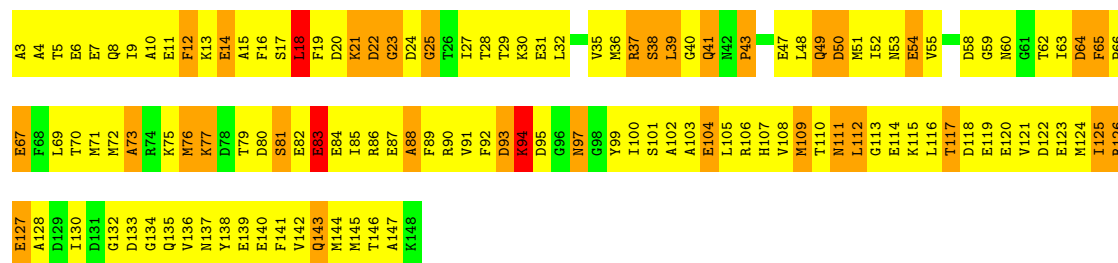


G274	K211	P150	L85	MET
G275	K212	K151	L86	HIS
G276	K213	L152	K87	HIS
G277	F214	I153	K88	HIS
K278	K215	I154	I89	HIS
I279	E216	I155	P90	HIS
K280	K217	I156	K91	HIS
E281	L218	K157	D92	ALA
E282	E219	D158	V93	ALA
K283	L220	Y159	L94	ALA
K284		A160	E95	MET
K285	K223	I161	I96	ASN
E286	E224	I162	Y97	GLU
G287	I225	S163	S98	HIS
V288	D226	E164	E99	TYR
E289	I227	Q165	L100	THR
K290	N228	S166	G101	GLU
D291	F229	K167	G102	SER
K292	L230	E168	E103	ASP
I293	K231	V169	I104	ILE
K294	D294	Y170	Y105	LYS
V295	N233	K171	F106	ARG
L296	L234	E172	T107	ASN
K297	T235	I173	D108	HIS
G298	E236	G174	I109	LYS
E299	F237	K175	D110	THR
K300	Q238	G176	L111	GLU
A301	H239	I177	V112	LVS
L302	A240	S178	E113	ASN
K303	F241	L179	H114	LVS
A304	S242	D180	K115	THR
S305	L243	I181	E116	GLU
G306	A244	I182	L117	LVS
L307	F245	S183	Q118	GLU
V308	S246	K184	D119	LVS
P309	Y247	D185	L120	PHE
E310	Y248	K186	S121	ASP
H311	F249	S187	E122	SER
A312	A250	L188	E123	SER
K313	P251	D189	E124	ILE
A314	D252	P190		N64
F315	H253	E191	M128	M65
K316	K254	F192	L129	L66
K317	T255	L193	S130	V67
I318	V256	L194	R131	
A319	L257	K195	G132	E70
R320		I196	E133	F71
E321	A261	K197	K134	T72
L322	P262	S198	V135	N73
N323	D263	L199	P136	T75
T324	M264	S200		T76
V325	F265	D201	F141	L76
I326	E266	D202	V142	D77
L327	Y267	S203	F143	K78
F328	M268	D204	I144	I79
R329	N269	S205	K145	Q80
P330	K270	S206	K146	Q81
V331	L271	D207	R147	T82
N332	E272		S148	Q83
K333	F273	E149	T149	D84



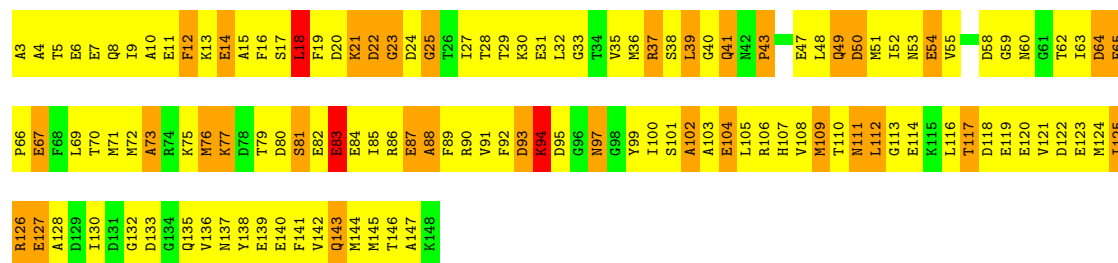
• Molecule 2: Calmodulin

Chain H: 12% 63% 23%

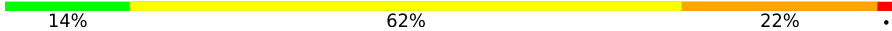


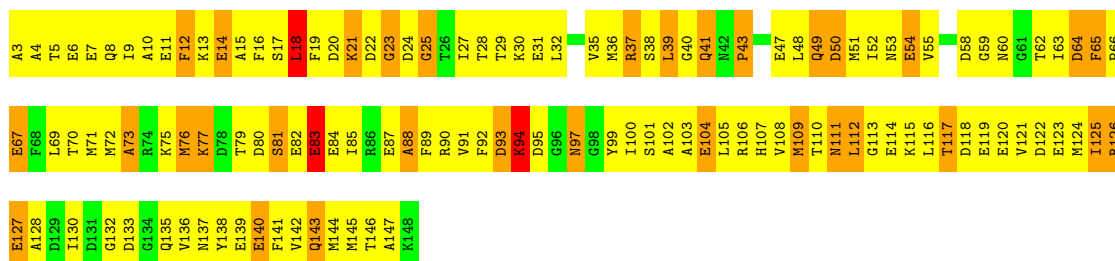
• Molecule 2: Calmodulin

Chain I: 13% 62% 23%

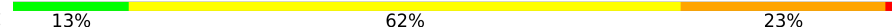


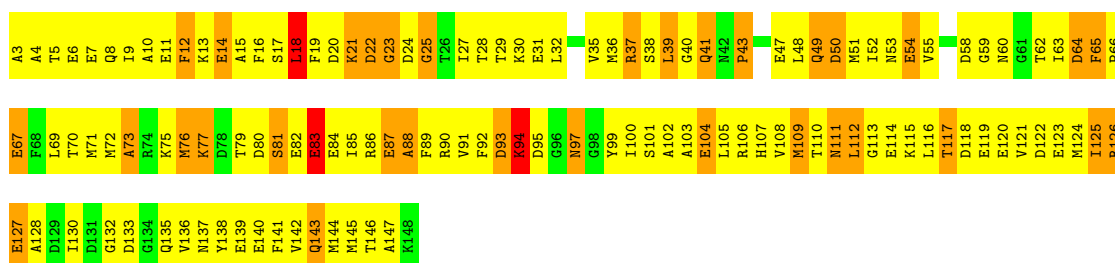
• Molecule 2: Calmodulin

Chain J:  14% 62% 22% .



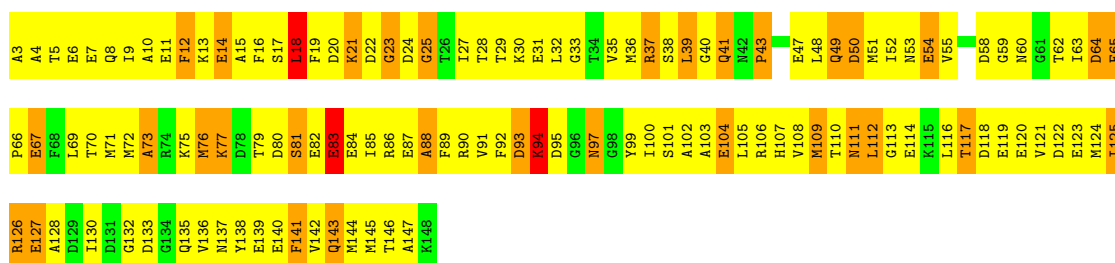
• Molecule 2: Calmodulin

Chain K:  13% 62% 23% .

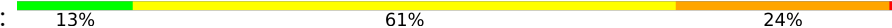


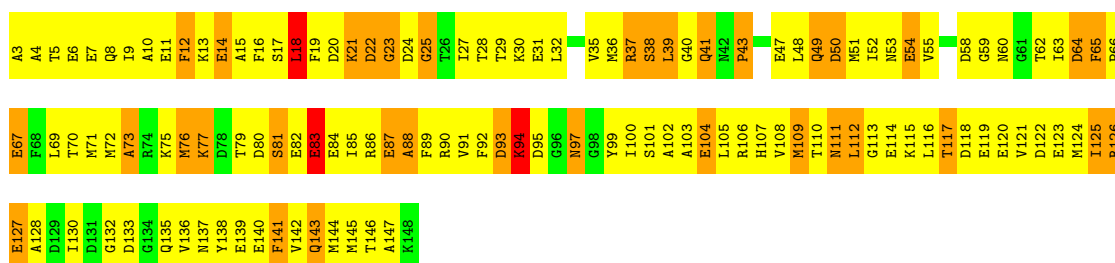
• Molecule 2: Calmodulin

Chain L:  13% 63% 22% .



• Molecule 2: Calmodulin

Chain M:  13% 61% 24% .



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	317.51Å 183.35Å 141.81Å 90.00° 90.05° 90.00°	Depositor
Resolution (Å)	29.87 – 3.60 29.87 – 3.60	Depositor EDS
% Data completeness (in resolution range)	86.2 (29.87-3.60) 95.7 (29.87-3.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 3.57Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.286 , 0.307 0.255 , 0.275	Depositor DCC
R_{free} test set	4714 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	119.9	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 217.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.458 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.458 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.450 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.450 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.458 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	42906	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, POP, 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	0.73	8/6104 (0.1%)	1.21	69/8208 (0.8%)
1	B	0.62	1/6104 (0.0%)	1.17	63/8208 (0.8%)
1	C	0.63	1/6104 (0.0%)	1.17	62/8208 (0.8%)
1	D	0.62	2/6104 (0.0%)	1.18	67/8208 (0.8%)
1	E	0.62	0/6104	1.17	65/8208 (0.8%)
1	F	0.62	2/6104 (0.0%)	1.20	67/8208 (0.8%)
2	H	0.66	0/1158	1.10	8/1553 (0.5%)
2	I	0.67	0/1158	1.11	9/1553 (0.6%)
2	J	0.66	0/1158	1.10	8/1553 (0.5%)
2	K	0.66	0/1158	1.11	9/1553 (0.6%)
2	L	0.66	0/1158	1.11	9/1553 (0.6%)
2	M	0.66	0/1158	1.10	10/1553 (0.6%)
All	All	0.65	14/43572 (0.0%)	1.17	446/58566 (0.8%)

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	0	1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	159	TYR	CA-CB	-24.28	1.25	1.53
1	A	159	TYR	N-CA	10.46	1.60	1.46
1	A	190	PRO	CA-C	7.78	1.63	1.52
1	C	766	HIS	N-CA	-7.21	1.36	1.46
1	D	766	HIS	N-CA	-7.03	1.36	1.46

The worst 5 of 446 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	ARG	N-CA-C	18.26	134.15	111.69
1	C	147	ARG	N-CA-C	17.84	133.63	111.69
1	B	147	ARG	N-CA-C	17.82	133.61	111.69
1	F	147	ARG	N-CA-C	17.60	133.34	111.69
1	E	147	ARG	N-CA-C	17.34	132.56	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	ASP	Peptide

5.2 Too-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 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	5992	0	6010	967	0
1	B	5992	0	6010	960	0
1	C	5992	0	6010	949	0
1	D	5992	0	6010	952	0
1	E	5992	0	6010	947	0
1	F	5992	0	6010	957	0
2	H	1146	0	1075	206	0
2	I	1146	0	1075	205	0
2	J	1146	0	1075	204	0
2	K	1146	0	1075	209	0
2	L	1146	0	1075	204	0
2	M	1146	0	1075	204	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	9	0	0	0	0
4	B	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	9	0	0	0	0
4	D	9	0	0	0	0
4	E	9	0	0	0	0
4	F	9	0	0	0	0
5	H	3	0	0	0	0
5	I	3	0	0	0	0
5	J	3	0	0	0	0
5	K	3	0	0	0	0
5	L	3	0	0	0	0
5	M	3	0	0	0	0
All	All	42906	0	42510	6746	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 79.

The worst 5 of 6746 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:697:ILE:HD13	1:B:732:ILE:HD13	1.21	1.20
1:A:697:ILE:HD13	1:A:732:ILE:HD13	1.23	1.16
2:I:36:MET:HE3	2:I:43:PRO:HG3	1.27	1.16
2:H:36:MET:HE3	2:H:43:PRO:HG3	1.26	1.15
1:E:697:ILE:HD13	1:E:732:ILE:HD13	1.22	1.14

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	733/777 (94%)	466 (64%)	168 (23%)	99 (14%)	0 3
1	B	733/777 (94%)	463 (63%)	171 (23%)	99 (14%)	0 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	733/777 (94%)	463 (63%)	172 (24%)	98 (13%)	0	3
1	D	733/777 (94%)	467 (64%)	168 (23%)	98 (13%)	0	3
1	E	733/777 (94%)	464 (63%)	170 (23%)	99 (14%)	0	3
1	F	733/777 (94%)	466 (64%)	168 (23%)	99 (14%)	0	3
2	H	144/146 (99%)	86 (60%)	37 (26%)	21 (15%)	0	3
2	I	144/146 (99%)	87 (60%)	37 (26%)	20 (14%)	0	3
2	J	144/146 (99%)	87 (60%)	38 (26%)	19 (13%)	0	3
2	K	144/146 (99%)	87 (60%)	38 (26%)	19 (13%)	0	3
2	L	144/146 (99%)	87 (60%)	38 (26%)	19 (13%)	0	3
2	M	144/146 (99%)	87 (60%)	37 (26%)	20 (14%)	0	3
All	All	5262/5538 (95%)	3310 (63%)	1242 (24%)	710 (14%)	0	3

5 of 710 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	THR
1	A	76	LEU
1	A	77	ASP
1	A	80	GLN
1	A	111	LEU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	664/705 (94%)	568 (86%)	96 (14%)	3	18
1	B	664/705 (94%)	566 (85%)	98 (15%)	3	17
1	C	664/705 (94%)	567 (85%)	97 (15%)	3	18
1	D	664/705 (94%)	565 (85%)	99 (15%)	3	17
1	E	664/705 (94%)	568 (86%)	96 (14%)	3	18
1	F	664/705 (94%)	568 (86%)	96 (14%)	3	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	123/123 (100%)	103 (84%)	20 (16%)	2	15
2	I	123/123 (100%)	103 (84%)	20 (16%)	2	15
2	J	123/123 (100%)	103 (84%)	20 (16%)	2	15
2	K	123/123 (100%)	103 (84%)	20 (16%)	2	15
2	L	123/123 (100%)	103 (84%)	20 (16%)	2	15
2	M	123/123 (100%)	103 (84%)	20 (16%)	2	15
All	All	4722/4968 (95%)	4020 (85%)	702 (15%)	3	17

5 of 702 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	573	ASP
1	F	682	SER
1	E	674	SER
1	E	562	GLU
1	F	309	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 257 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	8	GLN
2	J	49	GLN
1	C	581	GLN
1	C	521	ASN
2	K	49	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 30 ligands modelled in this entry, 24 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	POP	A	901	-	6,8,8	0.96	0	12,13,13	1.42	3 (25%)
4	POP	B	902	-	6,8,8	0.96	0	12,13,13	1.42	3 (25%)
4	POP	E	905	-	6,8,8	0.97	0	12,13,13	1.42	3 (25%)
4	POP	C	903	-	6,8,8	0.96	0	12,13,13	1.42	3 (25%)
4	POP	F	906	-	6,8,8	0.96	0	12,13,13	1.42	3 (25%)
4	POP	D	904	-	6,8,8	0.96	0	12,13,13	1.42	3 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	POP	A	901	-	-	2/6/6/6	-
4	POP	B	902	-	-	2/6/6/6	-
4	POP	E	905	-	-	2/6/6/6	-
4	POP	C	903	-	-	2/6/6/6	-
4	POP	F	906	-	-	2/6/6/6	-
4	POP	D	904	-	-	2/6/6/6	-

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	906	POP	O5-P2-O4	-2.71	100.26	110.83
4	C	903	POP	O5-P2-O4	-2.71	100.28	110.83
4	B	902	POP	O5-P2-O4	-2.71	100.28	110.83
4	D	904	POP	O5-P2-O4	-2.71	100.28	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	905	POP	O5-P2-O4	-2.70	100.31	110.83

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	901	POP	P1-O-P2-O6
4	B	902	POP	P1-O-P2-O6
4	C	903	POP	P1-O-P2-O6
4	D	904	POP	P1-O-P2-O6
4	E	905	POP	P1-O-P2-O6

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	735/777 (94%)	-1.19	0 100 100	28, 83, 137, 147	0
1	B	735/777 (94%)	-1.17	1 (0%) 92 85	27, 83, 138, 147	0
1	C	735/777 (94%)	-1.20	0 100 100	28, 83, 138, 147	0
1	D	735/777 (94%)	-1.19	0 100 100	27, 84, 137, 147	0
1	E	735/777 (94%)	-1.18	0 100 100	28, 83, 138, 147	0
1	F	735/777 (94%)	-1.20	1 (0%) 92 85	27, 84, 137, 147	0
2	H	146/146 (100%)	-1.24	0 100 100	26, 72, 130, 135	0
2	I	146/146 (100%)	-1.21	0 100 100	27, 71, 130, 135	0
2	J	146/146 (100%)	-1.30	0 100 100	26, 72, 130, 135	0
2	K	146/146 (100%)	-1.22	0 100 100	27, 71, 129, 135	0
2	L	146/146 (100%)	-1.20	0 100 100	25, 71, 129, 135	0
2	M	146/146 (100%)	-1.33	0 100 100	25, 71, 130, 135	0
All	All	5286/5538 (95%)	-1.20	2 (0%) 100 100	25, 81, 136, 147	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	185	ASP	2.7
1	B	114	HIS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	POP	A	901	9/9	0.97	0.08	76,84,85,86	0
4	POP	C	903	9/9	0.97	0.04	74,83,88,88	0
4	POP	B	902	9/9	0.98	0.03	76,85,88,89	0
4	POP	D	904	9/9	0.98	0.05	75,82,86,88	0
4	POP	E	905	9/9	0.98	0.05	77,85,87,88	0
4	POP	F	906	9/9	0.98	0.05	74,84,86,86	0
3	MG	B	901	1/1	0.99	0.06	10,10,10,10	0
3	MG	C	902	1/1	1.00	0.01	5,5,5,5	0
3	MG	D	903	1/1	1.00	0.01	8,8,8,8	0
3	MG	E	904	1/1	1.00	0.02	9,9,9,9	0
3	MG	F	905	1/1	1.00	0.01	14,14,14,14	0
3	MG	A	900	1/1	1.00	0.02	11,11,11,11	0
5	CA	H	701	1/1	1.00	0.01	77,77,77,77	0
5	CA	H	801	1/1	1.00	0.03	29,29,29,29	0
5	CA	H	802	1/1	1.00	0.01	51,51,51,51	0
5	CA	I	703	1/1	1.00	0.01	73,73,73,73	0
5	CA	I	803	1/1	1.00	0.04	24,24,24,24	0
5	CA	I	804	1/1	1.00	0.01	50,50,50,50	0
5	CA	J	705	1/1	1.00	0.01	72,72,72,72	0
5	CA	J	805	1/1	1.00	0.03	28,28,28,28	0
5	CA	J	806	1/1	1.00	0.01	44,44,44,44	0
5	CA	K	707	1/1	1.00	0.02	73,73,73,73	0
5	CA	K	807	1/1	1.00	0.02	34,34,34,34	0
5	CA	K	808	1/1	1.00	0.01	47,47,47,47	0
5	CA	L	709	1/1	1.00	0.02	75,75,75,75	0
5	CA	L	809	1/1	1.00	0.02	28,28,28,28	0
5	CA	L	810	1/1	1.00	0.02	51,51,51,51	0
5	CA	M	711	1/1	1.00	0.01	86,86,86,86	0
5	CA	M	811	1/1	1.00	0.01	33,33,33,33	0
5	CA	M	812	1/1	1.00	0.01	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.