



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 06:30 AM UTC

PDB ID : 1XFY / pdb_00001xfy
Title : Crystal structure of anthrax edema factor (EF) in complex with calmodulin
Authors : Shen, Y.; Zhukovskaya, N.L.; Guo, Q.; Florian, J.; Tang, W.J.
Deposited on : 2004-09-15
Resolution : 3.30 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
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

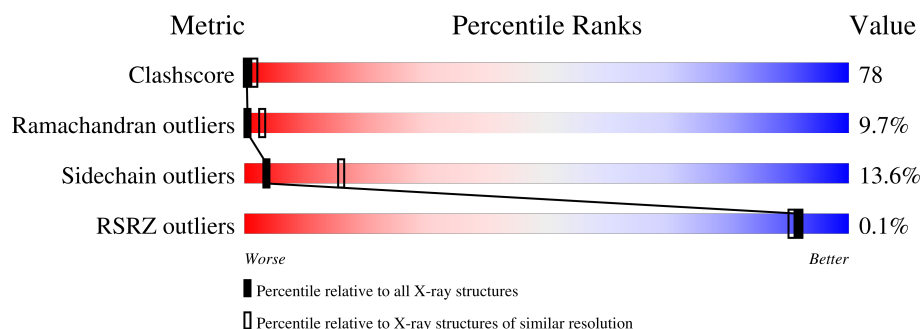
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

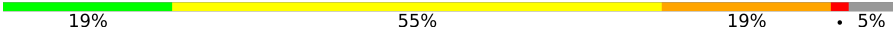
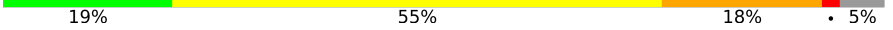
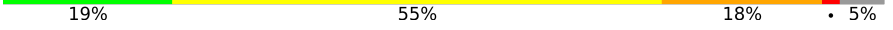
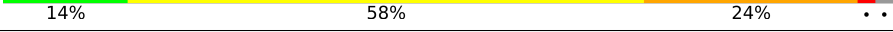
The reported resolution of this entry is 3.30 Å.

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	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	
1	F	777	
2	O	149	

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Mol	Chain	Length	Quality of chain
2	P	149	14%57%23%
2	Q	149	15%55%24%
2	R	149	13%58%25%
2	S	149	13%58%24%
2	T	149	%13%58%24%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 42846 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	-	initiating methionine	UNP P40136
A	25	HIS	-	expression tag	UNP P40136
A	26	HIS	-	expression tag	UNP P40136
A	27	HIS	-	expression tag	UNP P40136
A	28	HIS	-	expression tag	UNP P40136
A	29	HIS	-	expression tag	UNP P40136
A	30	HIS	-	expression tag	UNP P40136
A	31	ALA	-	cloning artifact	UNP P40136
A	32	ALA	-	cloning artifact	UNP P40136
B	24	MET	-	initiating methionine	UNP P40136
B	25	HIS	-	expression tag	UNP P40136
B	26	HIS	-	expression tag	UNP P40136
B	27	HIS	-	expression tag	UNP P40136
B	28	HIS	-	expression tag	UNP P40136
B	29	HIS	-	expression tag	UNP P40136
B	30	HIS	-	expression tag	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	-	initiating methionine	UNP P40136
C	25	HIS	-	expression tag	UNP P40136
C	26	HIS	-	expression tag	UNP P40136
C	27	HIS	-	expression tag	UNP P40136
C	28	HIS	-	expression tag	UNP P40136
C	29	HIS	-	expression tag	UNP P40136
C	30	HIS	-	expression tag	UNP P40136
C	31	ALA	-	cloning artifact	UNP P40136
C	32	ALA	-	cloning artifact	UNP P40136
D	24	MET	-	initiating methionine	UNP P40136
D	25	HIS	-	expression tag	UNP P40136
D	26	HIS	-	expression tag	UNP P40136
D	27	HIS	-	expression tag	UNP P40136
D	28	HIS	-	expression tag	UNP P40136
D	29	HIS	-	expression tag	UNP P40136
D	30	HIS	-	expression tag	UNP P40136
D	31	ALA	-	cloning artifact	UNP P40136
D	32	ALA	-	cloning artifact	UNP P40136
E	24	MET	-	initiating methionine	UNP P40136
E	25	HIS	-	expression tag	UNP P40136
E	26	HIS	-	expression tag	UNP P40136
E	27	HIS	-	expression tag	UNP P40136
E	28	HIS	-	expression tag	UNP P40136
E	29	HIS	-	expression tag	UNP P40136
E	30	HIS	-	expression tag	UNP P40136
E	31	ALA	-	cloning artifact	UNP P40136
E	32	ALA	-	cloning artifact	UNP P40136
F	24	MET	-	initiating methionine	UNP P40136
F	25	HIS	-	expression tag	UNP P40136
F	26	HIS	-	expression tag	UNP P40136
F	27	HIS	-	expression tag	UNP P40136
F	28	HIS	-	expression tag	UNP P40136
F	29	HIS	-	expression tag	UNP P40136
F	30	HIS	-	expression tag	UNP P40136
F	31	ALA	-	cloning artifact	UNP P40136
F	32	ALA	-	cloning artifact	UNP P40136

- Molecule 2 is a protein called Calmodulin 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	146	Total	C	N	O	S	0	0	0
			1146	702	186	249	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	146	Total 1146	C 702	N 186	O 249	S 9	0	0	0
2	Q	146	Total 1146	C 702	N 186	O 249	S 9	0	0	0
2	R	146	Total 1146	C 702	N 186	O 249	S 9	0	0	0
2	S	146	Total 1146	C 702	N 186	O 249	S 9	0	0	0
2	T	146	Total 1146	C 702	N 186	O 249	S 9	0	0	0

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

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

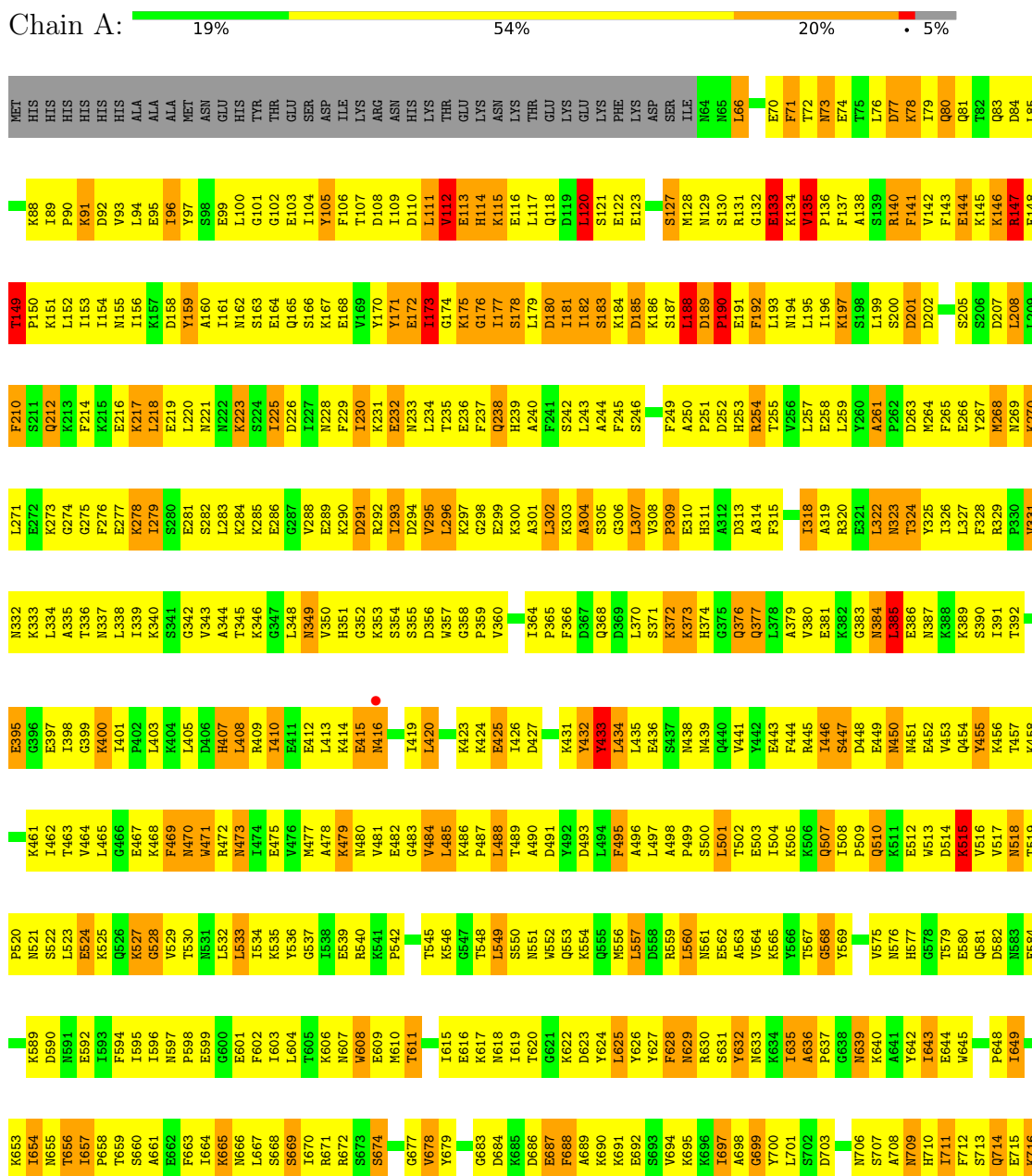
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	O	2	Total 2	Ca 2	0	0
4	P	2	Total 2	Ca 2	0	0
4	Q	2	Total 2	Ca 2	0	0
4	R	2	Total 2	Ca 2	0	0
4	S	2	Total 2	Ca 2	0	0
4	T	2	Total 2	Ca 2	0	0

3 Residue-property plots

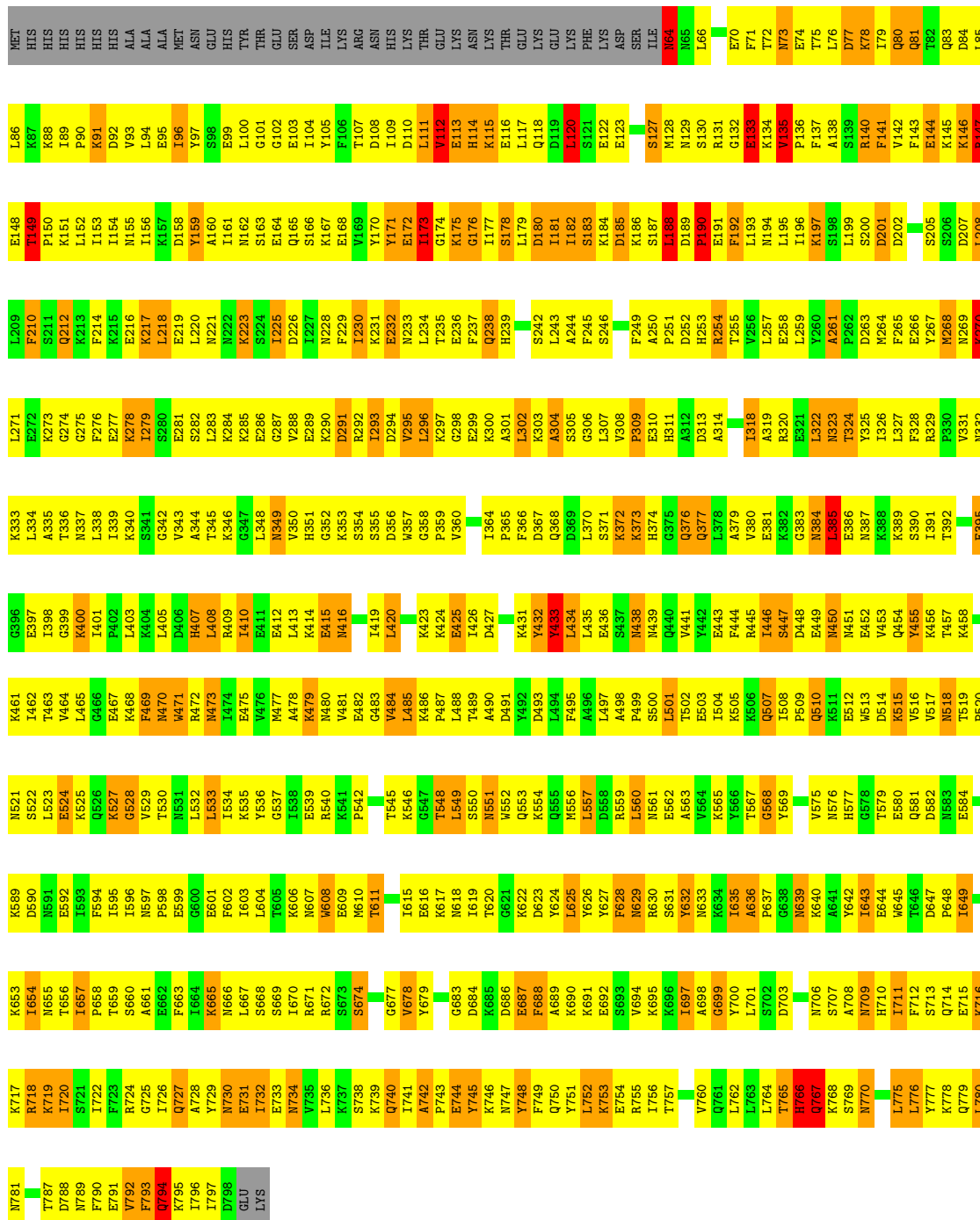
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

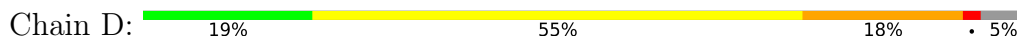
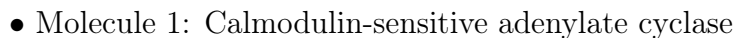


- Molecule 1: Calmodulin-sensitive adenylate cyclase

Chain B: 19% 55% 19% • 5%



Chain C: 19% 54% 19% • 5%



MET	HIS	L86	E148	L209	K272	A335	I398	T463	L523	E592	I657	S791	M789
HIS	HIS	K87	T149	F210	K273	T336	G399	V464	E524	I693	P658	I722	F790
HIS	HIS	K88	P150	S211	G274	N337	K400	L465	E525	I694	T659	F723	F791
HIS	HIS	I89	K151	K212	G275	L338	I401	G466	E526	I695	T660	F724	V792
HIS	HIS	P90	K152	K213	F276	L339	F402	E467	E527	I596	A661	F725	F793
HIS	HIS	K91	L153	K214	E277	K340	L403	K468	E528	N597	E662	I726	K794
HIS	HIS	D92	I154	K215	K278	S341	K404	F469	E529	P598	F663	I727	K795
ALA	ALA	V93	I155	E216	K279	G342	L405	N470	E530	E599	I664	A728	I796
ALA	ALA	L94	I156	K217	S280	V343	D406	N471	E531	G600	K665	I729	I797
MET	MET	E95	K157	E218	E281	K344	H407	N472	E532	E601	N666	F730	D798
ASN	ASN	I96	E158	E219	E282	T345	L408	N473	E533	F602	L667	F731	GLU
GLU	GLU	Y97	A159	L220	L283	K346	R409	L474	E534	L603	S668	I732	LVS
GLU	GLU	S98	Y159	L221	K284	G347	T410	E475	E535	L604	S669	I733	
HIS	HIS	E99	A160	N222	K285	L348	E411	N476	E536	T605	I670	M734	
TYR	TYR	L100	I161	K223	E286	N349	E412	N477	E537	K606	R671	V735	
THR	THR	G101	S163	K224	E287	V350	L413	N478	E538	K607	R672	L736	
GLU	GLU	G102	E164	K225	E288	H351	K414	N479	E539	M608	S673	S737	
SER	SER	E103	Q165	E289	E289	G352	E415	N480	E540	E609	S674	K738	
ASP	ASP	I104	Q166	K290	K290	K353	N416	N481	E541	N610	G677	K739	
ILE	ILE	Y105	K167	D291	D291	S354	E425	E482	E542	T611	G678	Q740	
LYS	LYS	F106	E168	L230	K292	S355	T419	G483	E543	D543	V678	I741	
ARG	ARG	T107	E169	K231	L293	V356	L420	N484	E544	S544	Y679	A742	
ASN	ASN	D108	Y170	E232	D294	K357	E427	L485	E545	E616	G683	F743	
HIS	HIS	I109	Y171	N233	V295	G358	K423	N486	E546	K617	D684	E744	
LYS	LYS	D110	Y172	L234	L296	P359	K424	P487	E547	N618	G685	Y745	
THR	THR	L111	L173	K297	K297	V360	E425	L488	E548	T619	D686	K746	
GLU	GLU	Y112	G174	E296	E296	T364	L426	N489	E549	T620	E687	N747	
LYS	LYS	E113	K175	E299	E299	P365	D427	N490	E550	G621	E687	Y748	
ASN	ASN	H114	Q176	K300	K300	F366	K431	D491	E551	N622	F688	F749	
LYS	LYS	K115	I177	A301	H239	F366	Y432	N492	E552	G623	A689	Q750	
THR	THR	E116	S178	L302	K303	K367	Y433	D493	E553	G624	G690	Y751	
GLU	GLU	L117	L179	K303	K303	Q368	Y434	L494	E554	L625	K691	L752	
LYS	LYS	Q118	D180	L243	A304	P369	L434	N495	E555	G626	E692	L753	
GLU	GLU	D119	I181	L435	S305	L370	L436	N496	E556	G627	S693	E754	
LYS	LYS	L120	I182	F245	G306	S371	E436	N497	E557	F628	V694	L755	
PHE	PHE	S121	K183	S246	L307	K372	S437	N498	E558	N629	K695	I756	
LYS	LYS	E122	K184		V308	K373	N438	P499	E559	R630	K696	I757	
ASP	ASP	E123	D185	F249	P309	H374	N439	S500	E560	S631	I697		
SER	SER		K186	A250	E310	G375	Q440	L501	E561	G632	A698	V760	
ILE	ILE	S127	K187	P251	H311	Q376	V441	T502	E562	N633	G699	Q761	
N64	N64	M128	L188	D252	A312	Q377	Y442	E503	E563	R634	Y700	L762	
N65	N65	N129	D189	H253	D313	L378	E443	E504	E564	L635	L701	L763	
L66	L66	S130	P190	R254	A314	A379	F444	E505	E565	A636	S702	L764	
E70	E70	R131	E191	T255		V380	P445	E506	E566	P637	D703	T765	
F71	F71	G132	F192	Y256	I318	E381	L446	Q507	E567	G638	N706	H766	
T72	T72	E133	L193	L257	A319	K382	S447	E508	E568	N639	S707	Q767	
N73	N73	K134	N194	E258		G383	D448	P509	E569	R640	A708	K768	
E74	E74	V135	L195	L259		N384	E449	Q510	E570	A641	H709	S769	
T75	T75	P136	I196	Y260	N323	E386	N450	E511	E571	G642	H710	N770	
L76	L76	F137	K197	A261	T324	E387	N451	E512	E572	E643	I711		
D77	D77	A138	S198	P262	Y325	N387	E452	E513	E573	E644	F712	L775	
K78	K78	S139	L199	D263	D263	K388	V453	E514	E574	E645	S713	L776	
F140	F140	R140	M284	M284	L327	K389	Q454	E515	E575	T579	Q714	L777	
I79	I79	F141	S200	F265	F328	S390	Y455	E516	E580	P648	S715	L778	
Q80	Q80	F142	D201	E266	K329	I391	K456	E517	E581	L649	E715	Q779	
Q81	Q81	F143	D202	Y267	P330	T392	T457	E518	D582		K716	L780	
T82	T82	E144	S205	M288	V331	T392	K458	T519	K653		K717	N781	
Q83	Q83	K145	S206	E269	N332	E395	K461	P520	E589	L654	R718		
D84	D84	K270	K333	K333	L334	G396	L462	N521	D590	N655	K719		
L85	L85	R147	L208	L271		E397		S522	E591	T656	I720	D788	

• Molecule 1: Calmodulin-sensitive adenylate cyclase

Chain E: 19% 54% 19% 5%

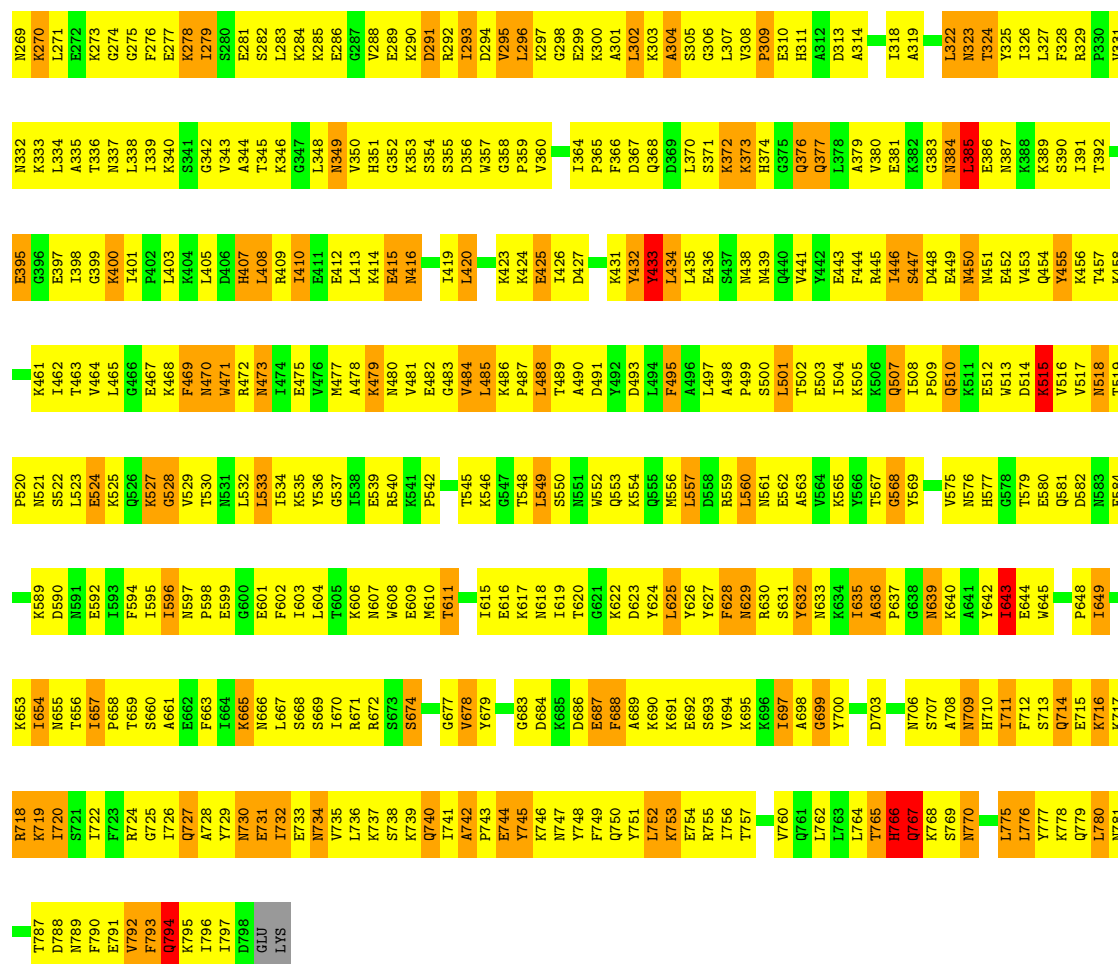
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E148	L209	K270	K333	G396	P520	K569	K653	K717	H781
L149	F210	L271	L334	E397	N521	K589	L654	R718	
P150	S211	E272	A335	I398	S522	D590	M655	R719	T787
K151	Q212	K273	T336	G399	S523	N591	T656	T720	D788
L152	K213	G274	N337	K400	E524	E593	L657	T721	N789
L153	F214	Q275	L338	I401	K525	E594	P658	T722	F790
L154	K215	F276	L339	P402	Q526	F594	T659	F723	E791
L155	E216	E277	K340	L403	K527	I595	S660	R724	V792
L156	K217	K278	S341	K404	G528	I596	A661	G725	F793
K157	L218	S280	G342	L405	V529	N597	E662	T726	Q794
L158	E219	K281	V343	D406	T530	P598	F663	Q727	K795
L159	L220	E282	A344	H407	N531	E599	E664	T728	I796
L160	L221	S283	T345	L408	L532	E600	K665	W729	I797
L161	N222	L283	K346	R409	L533	E601	M666	R730	
M162	K223	K284	G347	I410	F534	F602	L667	T731	
S163	S224	K285	E411	E411	I534	T603	S668	T732	
E164	I225	E286	L348	E412	K535	F604	E669	E733	
Q165	I226	G287	N349	V476	Y536	L604	S670	W734	
Q166	D226	V288	V350	M477	G537	T605	L670	W735	
S166	I227	H351	H351	A478	F538	K606	R671	V736	
K167	N228	E289	G352	K479	E539	M607	R672	L736	
E168	F229	K290	K353	N480	R540	M608	S673	T737	
V169	I230	D291	S354	V481	K541	E609	S674	W738	
Y170	K231	R292	S355	E482	M610	T611		T741	
E171	E232	I293	D356	G483	T545			T742	
E172	N233	D294	W357	V484	K546			T743	
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G174	T235	L296	P359	K423	T548			W745	
K175	E236	K297	V360	P486	M618			K746	
G176	F237	G298	I364	L488	S550			W747	
I177	Q238	E299	T364	T489	M551			T748	
S178	H239	K300	P365	A490	W552			F749	
L179	A240	A301	F366	D491	K553			Q750	
D180	F241	L302	D367	V492	D623			W751	
I181	S242	K303	K368	D493	K554			L752	
I182	L243	A304	D369	L494	Q555			W753	
S183	A244	S305	L370	F495	M556			T754	
K184	F245	G306	S371	A496	L557			R755	
D185	S246	L307	K372	L497	D558			T756	
K186		V308	K373	A498	R559			W757	
S187		P309	H374	P499	L560				
L188	A250	E310	G375	S500	N561			V760	
D189	P251	H311	Q376	L501	E562			L762	
P190	D252	H253	Q377	T502	A563			T763	
E191	H253	H253	L378	E503	V564			W765	
F192	R254	A314	A379	I504	K565			H766	
L193	T255	I318	V380	K505	Y566			Q767	
N194	L257	L318	E381	K506	T567			K768	
L195	E258	A319	G382	Q507	G568			S769	
I196	E259		G383	I508	Y569			W770	
K197	L259		N384	P509				T771	
S198	Y260		L385	Q510	V575			L772	
L199	A261		E386	K511	N576			W773	
S200	P262		N387	E512	H577			T774	
D201	D263		Y325	W513	T579			W775	
D202	M264		L326	E452	G578			L776	
	F265		L327	V453	T579			W777	
	E266		F328	K389	E580			K778	
			R329	S390	Q581			L780	
S205			I391	Q454	W581				
S206			T392	Y455	D582				
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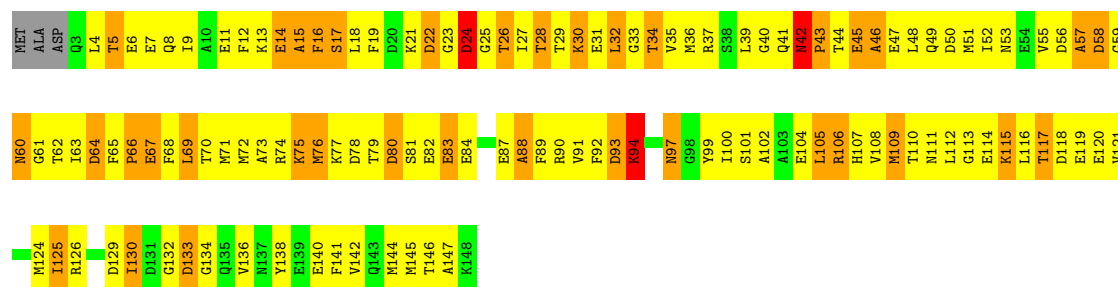
Chain F: 19% 55% 18% 5%

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HIS	K88	P150	Q211	
HIS	I89	K151	S212	
HIS	K90	L152	K213	
HIS	P91	L153	F214	
HIS	D92	L154	K215	
ALA	V93	L155	E216	
ALA	L94	L156	K217	
ALA	E95	K157	L218	
MET	I96	L159	E219	
ASN	Y97	L160	L220	
GLU	S98	L161	N221	
HIS	E99	L162	N222	
TYR	L100	M162	K223	
THR	G101	S163	S224	
GLU	G102	E164	I225	
SER	E103	Q165	D226	
ASP	I104	S166	I227	
ILE	Y105	K167	N228	
LYS	F106	E168	F229	
ARG	T107	V169	I230	
ASN	D108	Y170	K231	
HIS	I109	Y171	E232	
LYS	D110	E172	N233	
THR	L111	I173	L234	
GLU	V112	G174	T235	
LYS	K113	K175	E236	
ASN	H114	G176	F237	
LYS	K115	I177	Q238	
THR	E116	S178	H239	
GLU	L117	L179	A240	
LYS	Q118	D180	F241	
GLU	D119	I181	S242	
LYS	L120	I182	L243	
PHE	S121	S183	A244	
LYS	E122	K184	F245	
ASP	E123	D185	S246	
SER	S127	K186	Y247	
ILE	M128	S187	Y248	
N64	N129	L188	F249	
N65	S130	D189	A250	
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E70	G132	E191	D252	
F71	E133	F192	H253	
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D77	A139	S198	L259	
K78	S139	Y260	Y260	
W79	R140	L199	A261	
I79	F141	S200	P262	
Q80	V142	D201	D263	
O81	F143	D202	M264	
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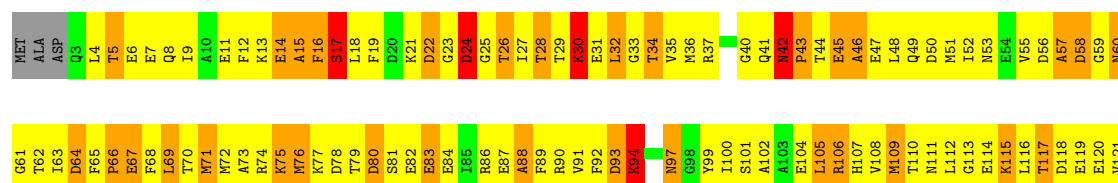
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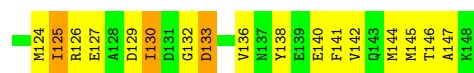
Chain O: 14% 58% 24% . .



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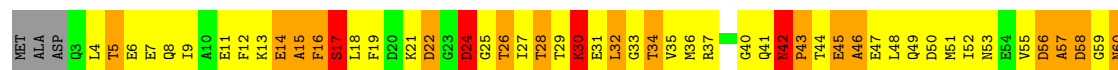
Chain P: 14% 57% 23% . .





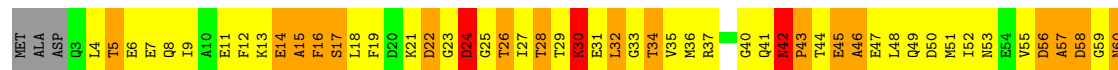
• Molecule 2: Calmodulin 2

Chain Q: 15% 55% 24% . .



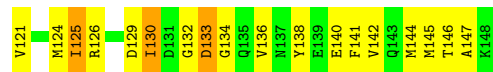
• Molecule 2: Calmodulin 2

Chain R: 13% 58% 25% . .



• Molecule 2: Calmodulin 2

Chain S: 13% 58% 24% . .



• Molecule 2: Calmodulin 2

Chain T: 13% 58% 24% . .



M60	M61	M62	M63	M64	M65	M66	M67	M68	M69	M70	M71	M72	M73	M74	M75	M76	M77	M78	M79	M80	M81	M82	M83	M84	M85	M86	M87	M88	M89	M90	M91	M92	M93	M94	M95	M96	M97	M98	M99	I100	I101	I102	I103	I104	I105	I106	I107	I108	I109	I110	I111	I112	I113	I114	I115	I116	I117	I118	I119	I120	I121	I122	I123	I124	I125	I126	I127	I128	I129	I130	I131	G132	G133	G134	G135	V136	V137	V138	E139	E140	F141	V142	Q143	M144	M145	T146	A147	K148
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	315.62Å 182.04Å 141.02Å 90.00° 89.93° 90.00°	Depositor
Resolution (Å)	10.00 – 3.30 10.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	93.9 (10.00-3.30) 93.8 (10.00-3.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.03	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.269 , 0.289 0.244 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	101.4	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 166.8	EDS
L-test for twinning ¹	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.448 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.448 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.448 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.448 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	42846	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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: CA, 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	0.69	7/6104 (0.1%)	1.28	89/8208 (1.1%)
1	B	0.69	7/6104 (0.1%)	1.30	86/8208 (1.0%)
1	C	0.69	6/6104 (0.1%)	1.29	93/8208 (1.1%)
1	D	0.70	7/6104 (0.1%)	1.29	91/8208 (1.1%)
1	E	0.70	7/6104 (0.1%)	1.29	93/8208 (1.1%)
1	F	0.69	6/6104 (0.1%)	1.29	85/8208 (1.0%)
2	O	0.65	0/1158	1.33	21/1553 (1.4%)
2	P	0.66	0/1158	1.33	21/1553 (1.4%)
2	Q	0.66	0/1158	1.33	19/1553 (1.2%)
2	R	0.66	0/1158	1.32	21/1553 (1.4%)
2	S	0.67	1/1158 (0.1%)	1.32	21/1553 (1.4%)
2	T	0.64	0/1158	1.33	21/1553 (1.4%)
All	All	0.69	41/43572 (0.1%)	1.29	661/58566 (1.1%)

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	190	PRO	N-CA	-7.62	1.37	1.47
1	F	433	TYR	N-CA	-7.36	1.36	1.46
1	C	433	TYR	N-CA	-7.30	1.36	1.46
1	A	433	TYR	N-CA	-7.28	1.36	1.46
1	B	433	TYR	N-CA	-7.28	1.36	1.46

The worst 5 of 661 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	22	ASP	N-CA-C	-13.06	90.94	110.14
2	O	22	ASP	N-CA-C	-13.03	90.99	110.14
2	P	22	ASP	N-CA-C	-12.93	91.14	110.14
2	R	22	ASP	N-CA-C	-12.88	91.21	110.14
2	S	22	ASP	N-CA-C	-12.88	91.21	110.14

There are no chirality outliers.

There are no planarity outliers.

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	938	0
1	B	5992	0	6010	934	0
1	C	5992	0	6010	918	0
1	D	5992	0	6010	935	0
1	E	5992	0	6010	924	0
1	F	5992	0	6010	923	0
2	O	1146	0	1071	211	0
2	P	1146	0	1071	209	0
2	Q	1146	0	1071	205	0
2	R	1146	0	1071	212	0
2	S	1146	0	1071	212	0
2	T	1146	0	1071	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	O	2	0	0	0	0
4	P	2	0	0	0	0
4	Q	2	0	0	0	0
4	R	2	0	0	0	0
4	S	2	0	0	0	0
4	T	2	0	0	0	0
All	All	42846	0	42486	6630	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 78.

The worst 5 of 6630 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:183:SER:O	1:A:187:SER:CB	1.70	1.39
1:D:183:SER:O	1:D:187:SER:CB	1.70	1.38
1:F:183:SER:O	1:F:187:SER:CB	1.70	1.37
1:E:183:SER:O	1:E:187:SER:CB	1.70	1.36
1:B:183:SER:O	1:B:187:SER:CB	1.70	1.35

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%)	490 (67%)	170 (23%)	73 (10%)	0	3
1	B	733/777 (94%)	492 (67%)	171 (23%)	70 (10%)	0	3
1	C	733/777 (94%)	494 (67%)	171 (23%)	68 (9%)	0	3
1	D	733/777 (94%)	493 (67%)	170 (23%)	70 (10%)	0	3
1	E	733/777 (94%)	492 (67%)	171 (23%)	70 (10%)	0	3
1	F	733/777 (94%)	490 (67%)	172 (24%)	71 (10%)	0	3
2	O	144/149 (97%)	92 (64%)	39 (27%)	13 (9%)	0	4
2	P	144/149 (97%)	89 (62%)	39 (27%)	16 (11%)	0	2
2	Q	144/149 (97%)	90 (62%)	37 (26%)	17 (12%)	0	1
2	R	144/149 (97%)	90 (62%)	38 (26%)	16 (11%)	0	2
2	S	144/149 (97%)	90 (62%)	39 (27%)	15 (10%)	0	2
2	T	144/149 (97%)	90 (62%)	40 (28%)	14 (10%)	0	3
All	All	5262/5556 (95%)	3492 (66%)	1257 (24%)	513 (10%)	0	3

5 of 513 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	ASP

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Mol	Chain	Res	Type
1	A	111	LEU
1	A	113	GLU
1	A	135	VAL
1	A	162	ASN

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%)	574 (86%)	90 (14%)	3	16
1	B	664/705 (94%)	575 (87%)	89 (13%)	4	16
1	C	664/705 (94%)	577 (87%)	87 (13%)	4	17
1	D	664/705 (94%)	577 (87%)	87 (13%)	4	17
1	E	664/705 (94%)	577 (87%)	87 (13%)	4	17
1	F	664/705 (94%)	576 (87%)	88 (13%)	4	17
2	O	123/127 (97%)	104 (85%)	19 (15%)	2	12
2	P	123/127 (97%)	104 (85%)	19 (15%)	2	12
2	Q	123/127 (97%)	104 (85%)	19 (15%)	2	12
2	R	123/127 (97%)	104 (85%)	19 (15%)	2	12
2	S	123/127 (97%)	104 (85%)	19 (15%)	2	12
2	T	123/127 (97%)	104 (85%)	19 (15%)	2	12
All	All	4722/4992 (95%)	4080 (86%)	642 (14%)	3	16

5 of 642 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	208	LEU
2	Q	45	GLU
1	F	324	THR
1	F	197	LYS
1	F	738	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 219 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	577	HIS
1	E	507	GLN
2	P	8	GLN
1	D	639	ASN
1	D	794	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 18 ligands modelled in this entry, 18 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 ⓘ

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	735/777 (94%)	-1.26	1 (0%) 92 90	24, 83, 143, 153	0
1	B	735/777 (94%)	-1.24	0 100 100	25, 83, 143, 153	0
1	C	735/777 (94%)	-1.24	2 (0%) 90 82	25, 83, 143, 153	0
1	D	735/777 (94%)	-1.28	1 (0%) 92 90	25, 83, 143, 153	0
1	E	735/777 (94%)	-1.27	0 100 100	24, 83, 142, 152	0
1	F	735/777 (94%)	-1.27	0 100 100	27, 83, 143, 154	0
2	O	146/149 (97%)	-1.23	0 100 100	22, 74, 121, 134	0
2	P	146/149 (97%)	-1.26	0 100 100	20, 75, 121, 135	0
2	Q	146/149 (97%)	-1.27	0 100 100	21, 75, 121, 134	0
2	R	146/149 (97%)	-1.23	0 100 100	20, 75, 120, 134	0
2	S	146/149 (97%)	-1.33	0 100 100	21, 76, 121, 134	0
2	T	146/149 (97%)	-1.23	1 (0%) 84 70	21, 75, 120, 134	0
All	All	5286/5556 (95%)	-1.26	5 (0%) 92 90	20, 80, 142, 154	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	207	ASP	3.4
1	C	162	ASN	3.0
2	T	25	GLY	2.5
1	C	455	TYR	2.4
1	A	416	ASN	2.2

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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	900	1/1	0.99	0.02	23,23,23,23	0
3	MG	B	901	1/1	1.00	0.01	16,16,16,16	0
3	MG	C	902	1/1	1.00	0.01	23,23,23,23	0
3	MG	D	903	1/1	1.00	0.02	21,21,21,21	0
3	MG	E	904	1/1	1.00	0.03	23,23,23,23	0
3	MG	F	905	1/1	1.00	0.03	17,17,17,17	0
4	CA	O	801	1/1	1.00	0.02	33,33,33,33	0
4	CA	O	802	1/1	1.00	0.01	33,33,33,33	0
4	CA	P	803	1/1	1.00	0.03	32,32,32,32	0
4	CA	P	804	1/1	1.00	0.02	34,34,34,34	0
4	CA	Q	805	1/1	1.00	0.03	29,29,29,29	0
4	CA	Q	806	1/1	1.00	0.01	35,35,35,35	0
4	CA	R	807	1/1	1.00	0.02	30,30,30,30	0
4	CA	R	808	1/1	1.00	0.01	36,36,36,36	0
4	CA	S	809	1/1	1.00	0.03	29,29,29,29	0
4	CA	S	810	1/1	1.00	0.01	40,40,40,40	0
4	CA	T	811	1/1	1.00	0.03	28,28,28,28	0
4	CA	T	812	1/1	1.00	0.02	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.