



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:31 PM GMT

PDB ID : 1XFZ  
Title : Crystal structure of anthrax edema factor (EF) in complex with calmodulin  
in the presence of 1 millimolar exogenously added calcium chloride  
Authors : Shen, Y.; Zhukovskaya, N.L.; Guo, Q.; Florian, J.; Tang, W.J.  
Deposited on : 2004-09-15  
Resolution : 3.25 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

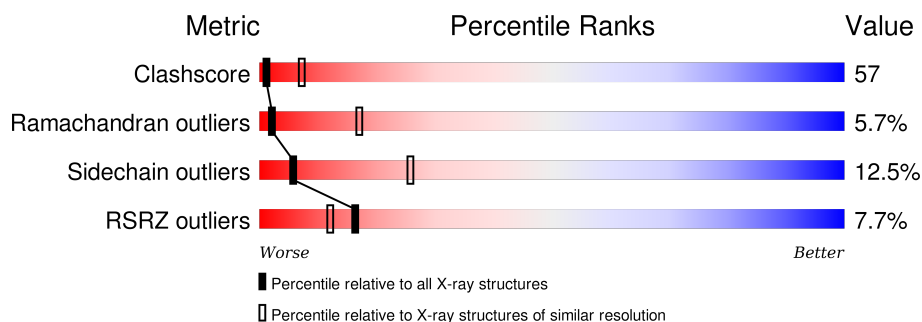
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)
RSRZ outliers	91569	1632 (3.32-3.20)

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

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	
2	Q	149	
2	R	149	
2	S	149	
2	T	149	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 42852 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

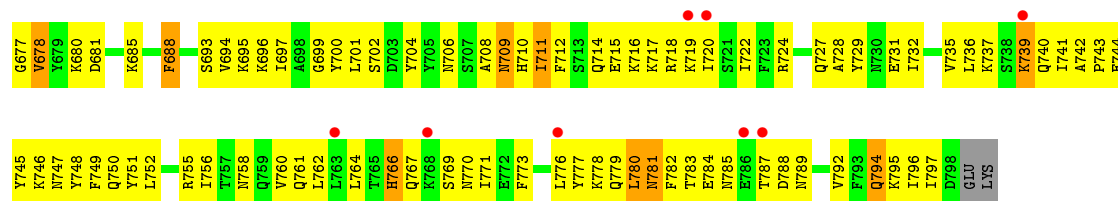
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	3	Total 3	Ca 3	0	0
3	Q	3	Total 3	Ca 3	0	0
3	T	3	Total 3	Ca 3	0	0
3	O	3	Total 3	Ca 3	0	0
3	R	3	Total 3	Ca 3	0	0
3	S	3	Total 3	Ca 3	0	0

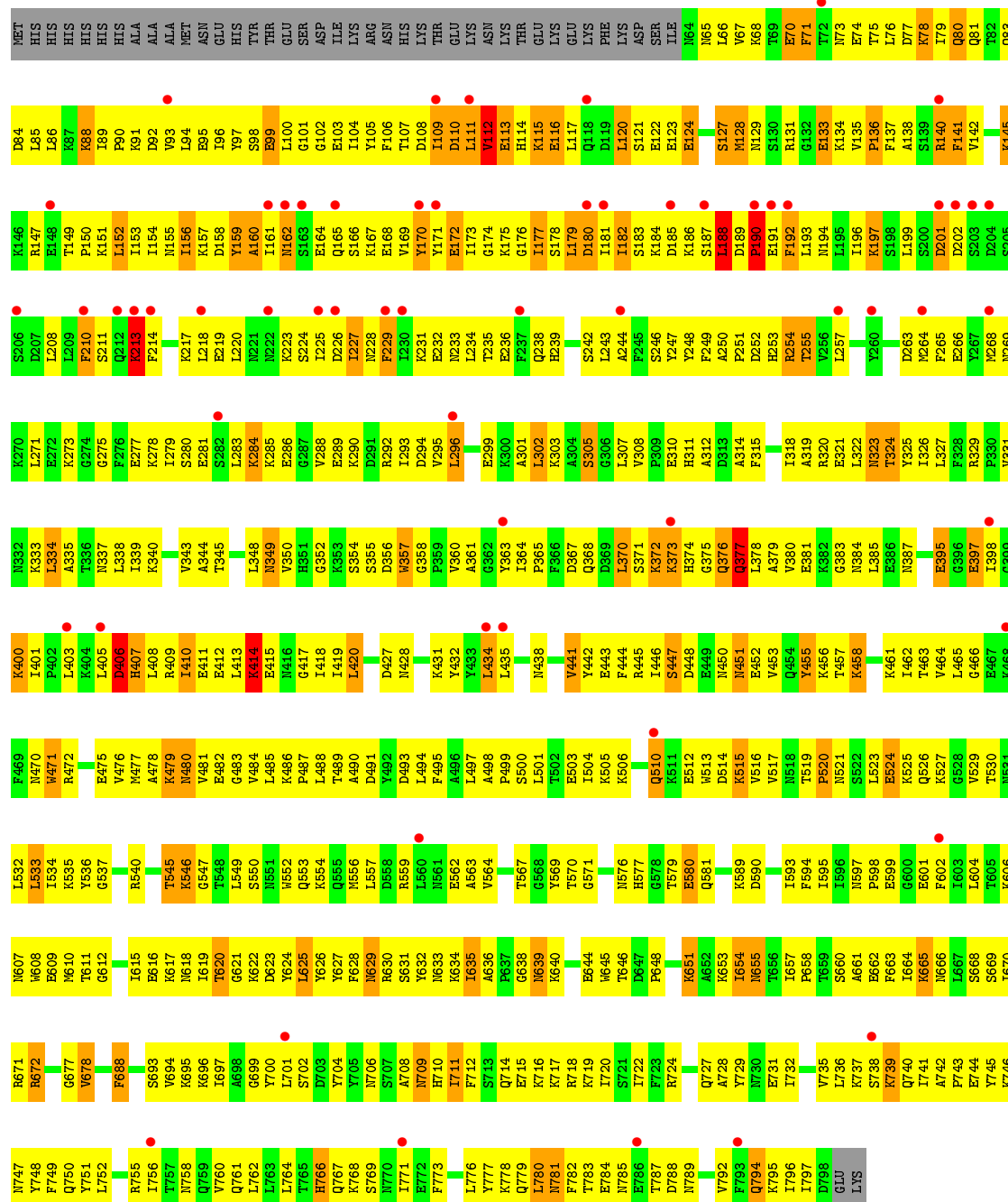
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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



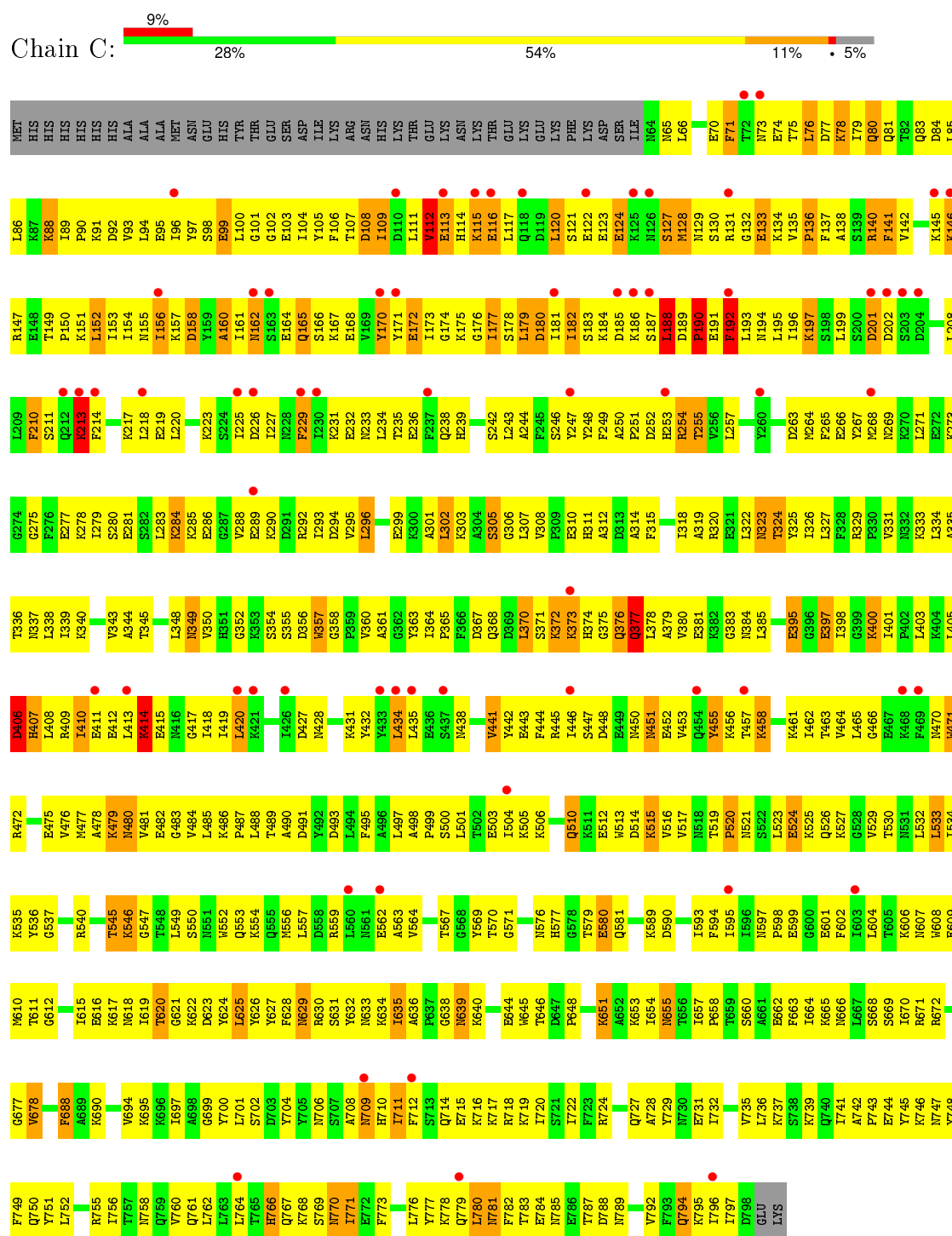


• Molecule 1: Calmodulin-sensitive adenylate cyclase

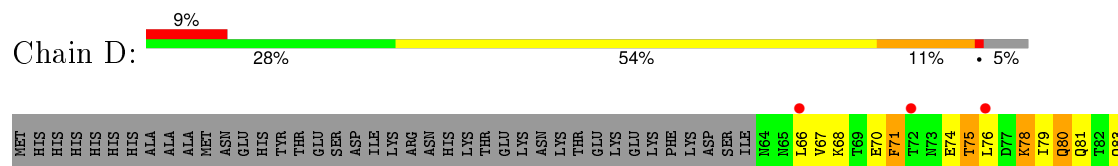


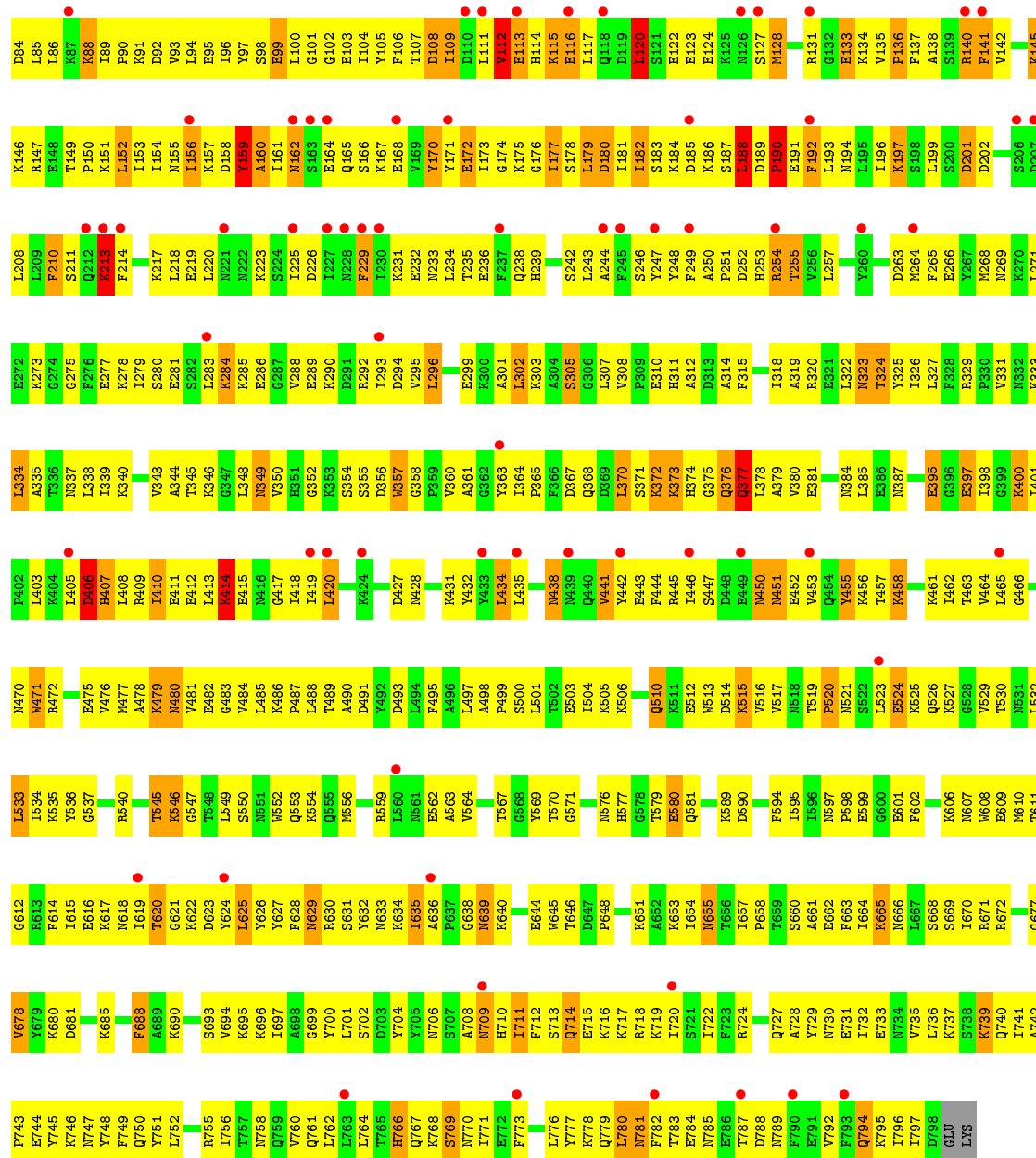
• Molecule 1: Calmodulin-sensitive adenylate cyclase



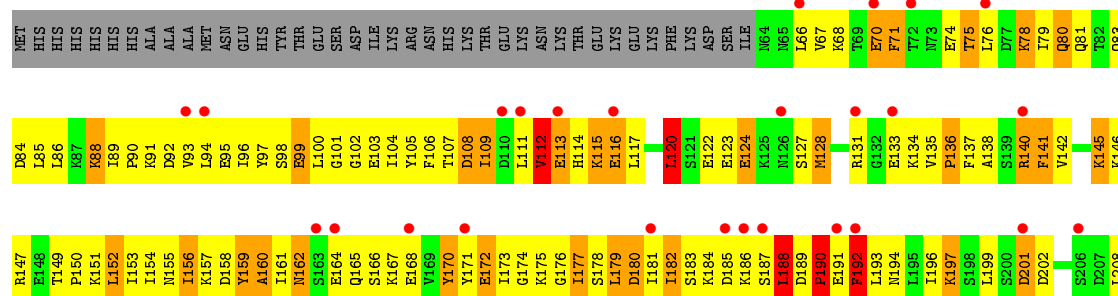


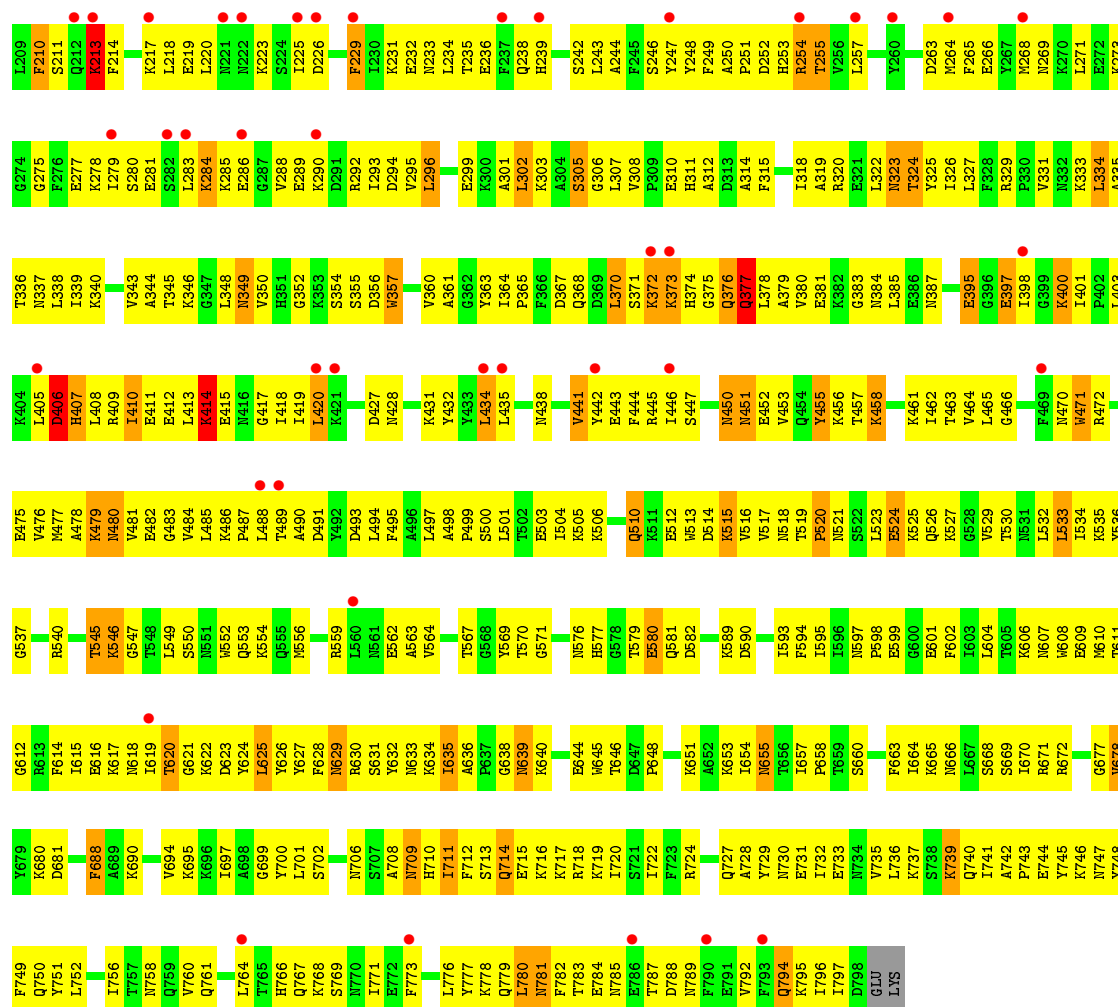
- Molecule 1: Calmodulin-sensitive adenylate cyclase



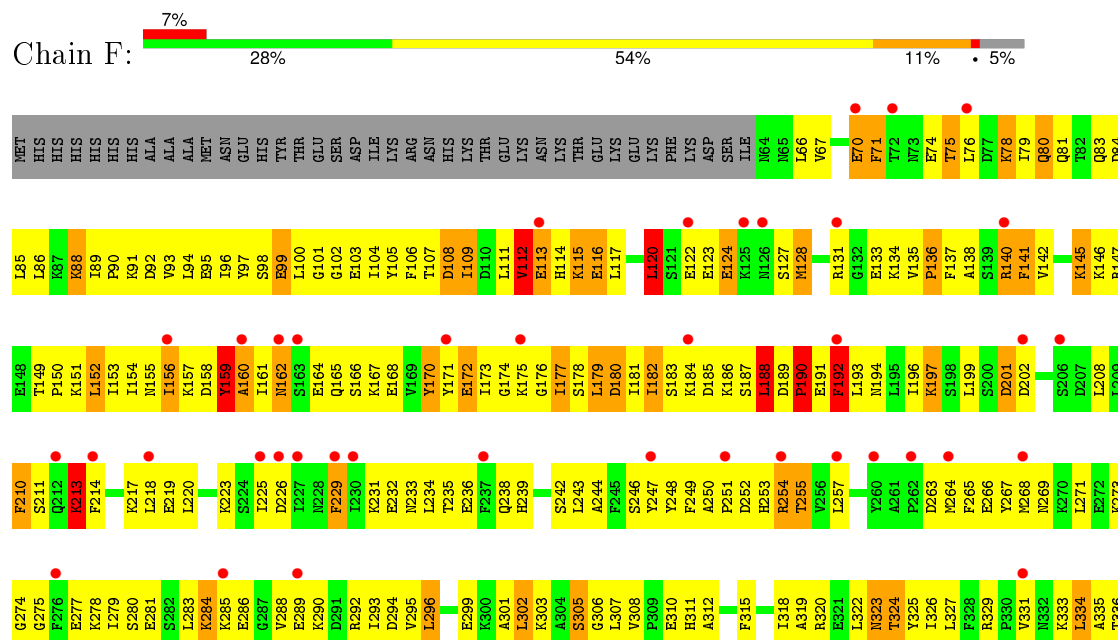


• Molecule 1: Calmodulin-sensitive adenylylate cyclase

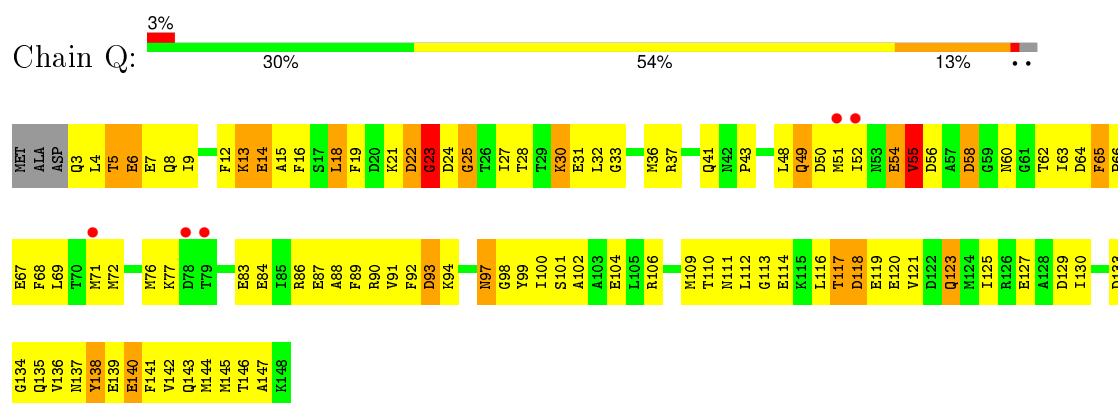




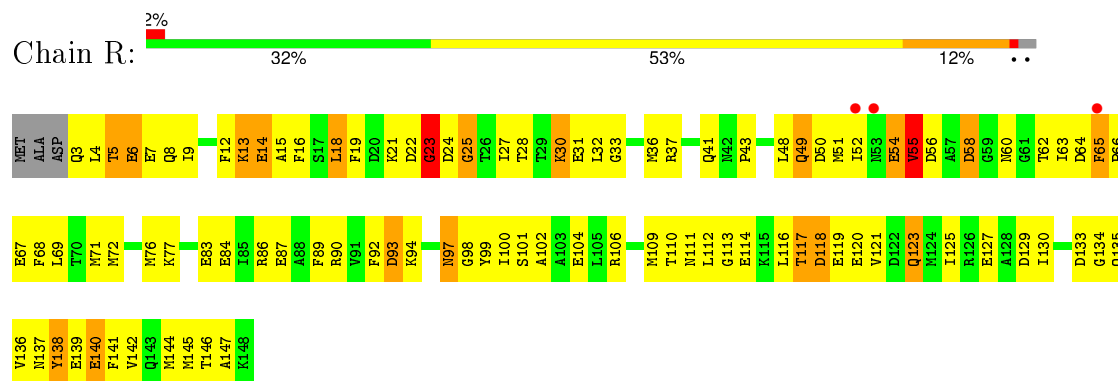
- Molecule 1: Calmodulin-sensitive adenylate cyclase



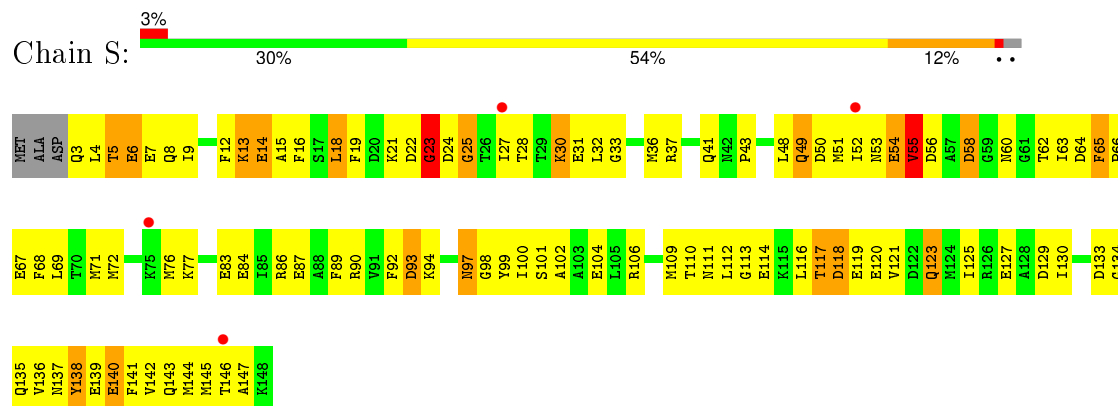




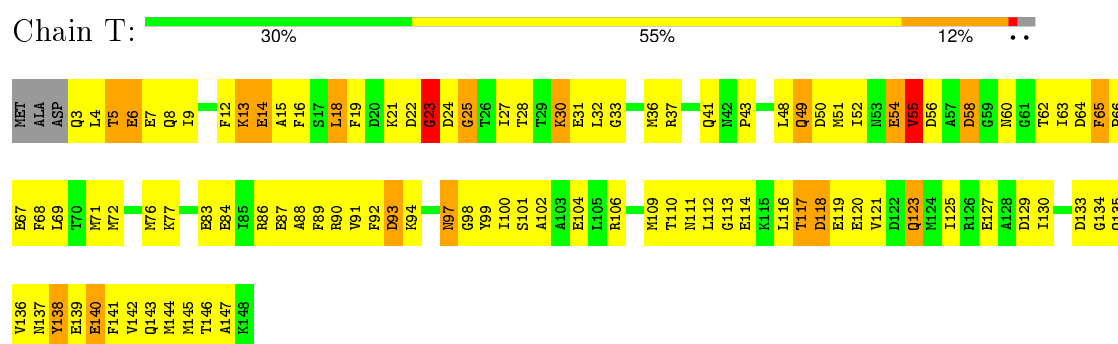
## • Molecule 2: Calmodulin 2



## • Molecule 2: Calmodulin 2



## • Molecule 2: Calmodulin 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	183.26Å 316.48Å 140.80Å 90.00° 89.91° 90.00°	Depositor
Resolution (Å)	29.99 – 3.25 39.65 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.0 (29.99-3.25) 93.3 (39.65-3.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 3.18Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.258 , 0.270 0.277 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	95.5	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 68.6	EDS
Estimated twinning fraction	0.467 for -1/2*h+1/2*k,3/2*h+1/2*k,-l 0.467 for -1/2*h-1/2*k,-3/2*h+1/2*k,-l 0.460 for 1/2*h+1/2*k,3/2*h-1/2*k,-l 0.460 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.469 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 128284 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	42852	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.52	1/6104 (0.0%)	0.77	13/8208 (0.2%)
1	B	0.52	2/6104 (0.0%)	0.77	13/8208 (0.2%)
1	C	0.53	2/6104 (0.0%)	0.78	12/8208 (0.1%)
1	D	0.52	0/6104	0.77	12/8208 (0.1%)
1	E	0.52	0/6104	0.78	13/8208 (0.2%)
1	F	0.51	0/6104	0.77	13/8208 (0.2%)
2	O	0.54	0/1158	0.73	1/1553 (0.1%)
2	P	0.53	0/1158	0.72	0/1553
2	Q	0.54	0/1158	0.72	1/1553 (0.1%)
2	R	0.54	0/1158	0.72	1/1553 (0.1%)
2	S	0.54	0/1158	0.72	1/1553 (0.1%)
2	T	0.53	0/1158	0.73	1/1553 (0.1%)
All	All	0.52	5/43572 (0.0%)	0.77	81/58566 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
2	O	0	1
2	P	0	1
2	Q	0	1
2	R	0	1
2	S	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	T	0	1
All	All	0	12

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	133	GLU	CG-CD	-7.09	1.41	1.51
1	A	133	GLU	CD-OE1	-6.43	1.18	1.25
1	B	133	GLU	CG-CD	-6.42	1.42	1.51
1	B	133	GLU	CD-OE1	-5.36	1.19	1.25
1	C	133	GLU	CD-OE1	-5.11	1.20	1.25

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	188	LEU	N-CA-C	-9.08	86.49	111.00
1	E	188	LEU	N-CA-C	-8.91	86.95	111.00
1	D	188	LEU	N-CA-C	-8.32	88.53	111.00
1	F	188	LEU	N-CA-C	-8.22	88.81	111.00
1	E	160	ALA	N-CA-C	8.01	132.62	111.00

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	170	TYR	Sidechain
1	B	170	TYR	Sidechain
1	C	170	TYR	Sidechain
1	D	170	TYR	Sidechain
1	E	170	TYR	Sidechain

## 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	669	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5992	0	6010	688	0
1	C	5992	0	6010	684	0
1	D	5992	0	6010	678	1
1	E	5992	0	6010	672	0
1	F	5992	0	6010	674	0
2	O	1146	0	1071	157	0
2	P	1146	0	1071	156	0
2	Q	1146	0	1071	155	0
2	R	1146	0	1071	156	0
2	S	1146	0	1071	151	0
2	T	1146	0	1071	152	0
3	O	3	0	0	0	0
3	P	3	0	0	0	0
3	Q	3	0	0	0	0
3	R	3	0	0	0	0
3	S	3	0	0	0	0
3	T	3	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
All	All	42852	0	42486	4849	2

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 57.

The worst 5 of 4849 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:414:LYS:HA	1:F:414:LYS:HZ2	1.13	1.13
1:B:655:ASN:HB3	1:B:758:ASN:HB3	1.31	1.12
1:A:127:SER:O	1:A:133:GLU:HG3	1.50	1.12
1:E:655:ASN:HB3	1:E:758:ASN:HB3	1.32	1.12
1:A:655:ASN:HB3	1:A:758:ASN:HB3	1.30	1.11

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:685:LYS:NZ	1:A:685:LYS:NZ[2_656]	2.09	0.11
1:D:685:LYS:NZ	1:D:685:LYS:NZ[2_657]	2.18	0.02

## 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%)	542 (74%)	150 (20%)	41 (6%)	2	17
1	B	733/777 (94%)	546 (74%)	144 (20%)	43 (6%)	2	16
1	C	733/777 (94%)	537 (73%)	151 (21%)	45 (6%)	2	15
1	D	733/777 (94%)	541 (74%)	148 (20%)	44 (6%)	2	15
1	E	733/777 (94%)	537 (73%)	153 (21%)	43 (6%)	2	16
1	F	733/777 (94%)	547 (75%)	142 (19%)	44 (6%)	2	15
2	O	144/149 (97%)	111 (77%)	26 (18%)	7 (5%)	3	21
2	P	144/149 (97%)	111 (77%)	26 (18%)	7 (5%)	3	21
2	Q	144/149 (97%)	112 (78%)	25 (17%)	7 (5%)	3	21
2	R	144/149 (97%)	113 (78%)	24 (17%)	7 (5%)	3	21
2	S	144/149 (97%)	111 (77%)	26 (18%)	7 (5%)	3	21
2	T	144/149 (97%)	113 (78%)	24 (17%)	7 (5%)	3	21
All	All	5262/5556 (95%)	3921 (74%)	1039 (20%)	302 (6%)	2	17

5 of 302 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	THR
1	A	180	ASP
1	A	192	PHE
1	A	458	LYS
1	A	510	GLN

### 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%)	581 (88%)	83 (12%)	6	26
1	B	664/705 (94%)	582 (88%)	82 (12%)	6	26
1	C	664/705 (94%)	582 (88%)	82 (12%)	6	26
1	D	664/705 (94%)	581 (88%)	83 (12%)	6	26
1	E	664/705 (94%)	582 (88%)	82 (12%)	6	26
1	F	664/705 (94%)	582 (88%)	82 (12%)	6	26
2	O	123/127 (97%)	107 (87%)	16 (13%)	5	24
2	P	123/127 (97%)	107 (87%)	16 (13%)	5	24
2	Q	123/127 (97%)	107 (87%)	16 (13%)	5	24
2	R	123/127 (97%)	107 (87%)	16 (13%)	5	24
2	S	123/127 (97%)	107 (87%)	16 (13%)	5	24
2	T	123/127 (97%)	107 (87%)	16 (13%)	5	24
All	All	4722/4992 (95%)	4132 (88%)	590 (12%)	6	26

5 of 590 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	158	ASP
1	E	67	VAL
2	R	14	GLU
1	D	210	PHE
1	D	451	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 198 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	794	GLN
1	D	709	ASN
2	O	143	GLN
1	D	323	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	510	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	735/777 (94%)	0.59	64 (8%) 13 8	33, 86, 135, 148	0
1	B	735/777 (94%)	0.60	60 (8%) 14 10	33, 87, 135, 148	0
1	C	735/777 (94%)	0.57	67 (9%) 11 8	34, 87, 136, 148	0
1	D	735/777 (94%)	0.59	69 (9%) 11 8	32, 87, 135, 148	0
1	E	735/777 (94%)	0.61	67 (9%) 11 8	34, 87, 136, 148	0
1	F	735/777 (94%)	0.55	57 (7%) 16 11	34, 87, 135, 148	0
2	O	146/149 (97%)	0.28	4 (2%) 58 48	37, 72, 130, 141	0
2	P	146/149 (97%)	0.33	5 (3%) 49 39	36, 72, 130, 141	0
2	Q	146/149 (97%)	0.35	5 (3%) 49 39	36, 72, 130, 141	0
2	R	146/149 (97%)	0.32	3 (2%) 67 57	36, 72, 130, 141	0
2	S	146/149 (97%)	0.33	4 (2%) 58 48	36, 72, 130, 141	0
2	T	146/149 (97%)	0.27	0 100 100	36, 72, 130, 140	0
All	All	5286/5556 (95%)	0.54	405 (7%) 16 12	32, 84, 135, 148	0

The worst 5 of 405 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	212	GLN	8.6
1	B	212	GLN	7.7
1	B	229	PHE	7.5
1	C	225	ILE	7.4
1	C	229	PHE	7.4

### 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 carbohydrates 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. 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, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	CA	R	808	1/1	0.95	0.20	-0.21	51,51,51,51	0
3	CA	P	804	1/1	0.86	0.24	-0.29	52,52,52,52	0
3	CA	S	810	1/1	0.97	0.24	-0.29	52,52,52,52	0
3	CA	P	803	1/1	0.99	0.19	-0.31	39,39,39,39	0
3	CA	O	802	1/1	0.97	0.19	-0.41	47,47,47,47	0
3	CA	Q	806	1/1	0.94	0.21	-0.43	50,50,50,50	0
3	CA	T	812	1/1	0.98	0.18	-0.79	51,51,51,51	0
3	CA	R	807	1/1	0.99	0.17	-0.99	40,40,40,40	0
3	CA	T	711	1/1	0.96	0.13	-1.10	65,65,65,65	0
3	CA	S	809	1/1	0.96	0.17	-1.14	37,37,37,37	0
3	CA	Q	805	1/1	0.97	0.13	-1.21	42,42,42,42	0
3	CA	O	801	1/1	0.99	0.16	-1.23	39,39,39,39	0
3	CA	S	709	1/1	0.95	0.08	-1.29	65,65,65,65	0
3	CA	P	703	1/1	0.95	0.11	-1.54	66,66,66,66	0
3	CA	R	707	1/1	0.97	0.11	-1.55	64,64,64,64	0
3	CA	Q	705	1/1	0.94	0.11	-1.56	66,66,66,66	0
3	CA	O	701	1/1	0.97	0.14	-1.60	66,66,66,66	0
3	CA	T	811	1/1	0.98	0.11	-1.96	40,40,40,40	0
4	MG	C	903	1/1	0.98	0.21	-	27,27,27,27	0
4	MG	A	901	1/1	0.99	0.23	-	26,26,26,26	0
4	MG	E	905	1/1	0.98	0.19	-	23,23,23,23	0
4	MG	D	904	1/1	0.97	0.29	-	29,29,29,29	0
4	MG	F	906	1/1	0.98	0.25	-	25,25,25,25	0
4	MG	B	902	1/1	0.89	0.20	-	28,28,28,28	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.