



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:31 PM GMT

PDB ID : 1XFY  
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](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

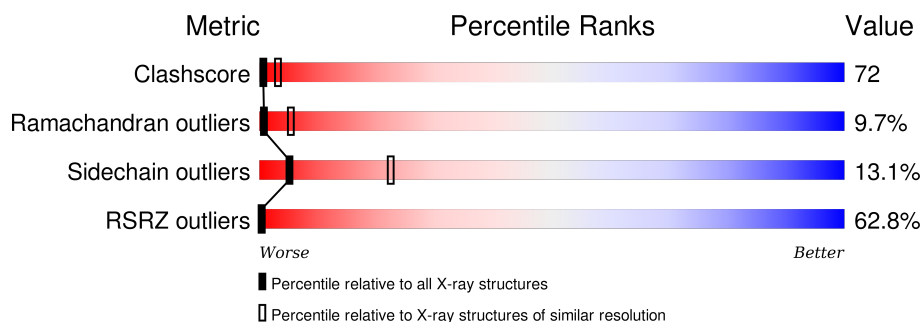
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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	<div> <div>59%</div> <div> <div>23%</div> <div>56%</div> <div>14%</div> <div>• 5%</div> </div> </div>
1	B	777	<div> <div>59%</div> <div> <div>23%</div> <div>56%</div> <div>14%</div> <div>• 5%</div> </div> </div>
1	C	777	<div> <div>64%</div> <div> <div>23%</div> <div>56%</div> <div>14%</div> <div>• 5%</div> </div> </div>
1	D	777	<div> <div>59%</div> <div> <div>23%</div> <div>56%</div> <div>14%</div> <div>• 5%</div> </div> </div>
1	E	777	<div> <div>61%</div> <div> <div>23%</div> <div>56%</div> <div>14%</div> <div>• 5%</div> </div> </div>
1	F	777	<div> <div>59%</div> <div> <div>23%</div> <div>56%</div> <div>14%</div> <div>• 5%</div> </div> </div>
2	O	149	<div> <div>58%</div> <div> <div>17%</div> <div>64%</div> <div>16%</div> <div>••</div> </div> </div>

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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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CA	P	803	-	-	-	X

## 2 Entry composition [i](#)

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

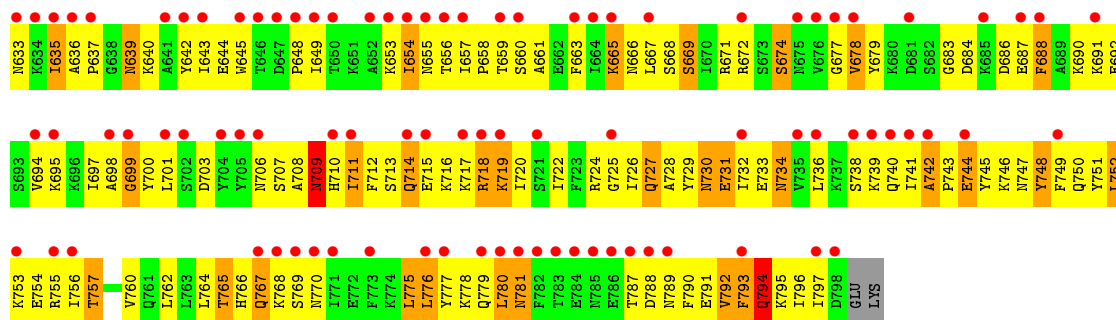
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

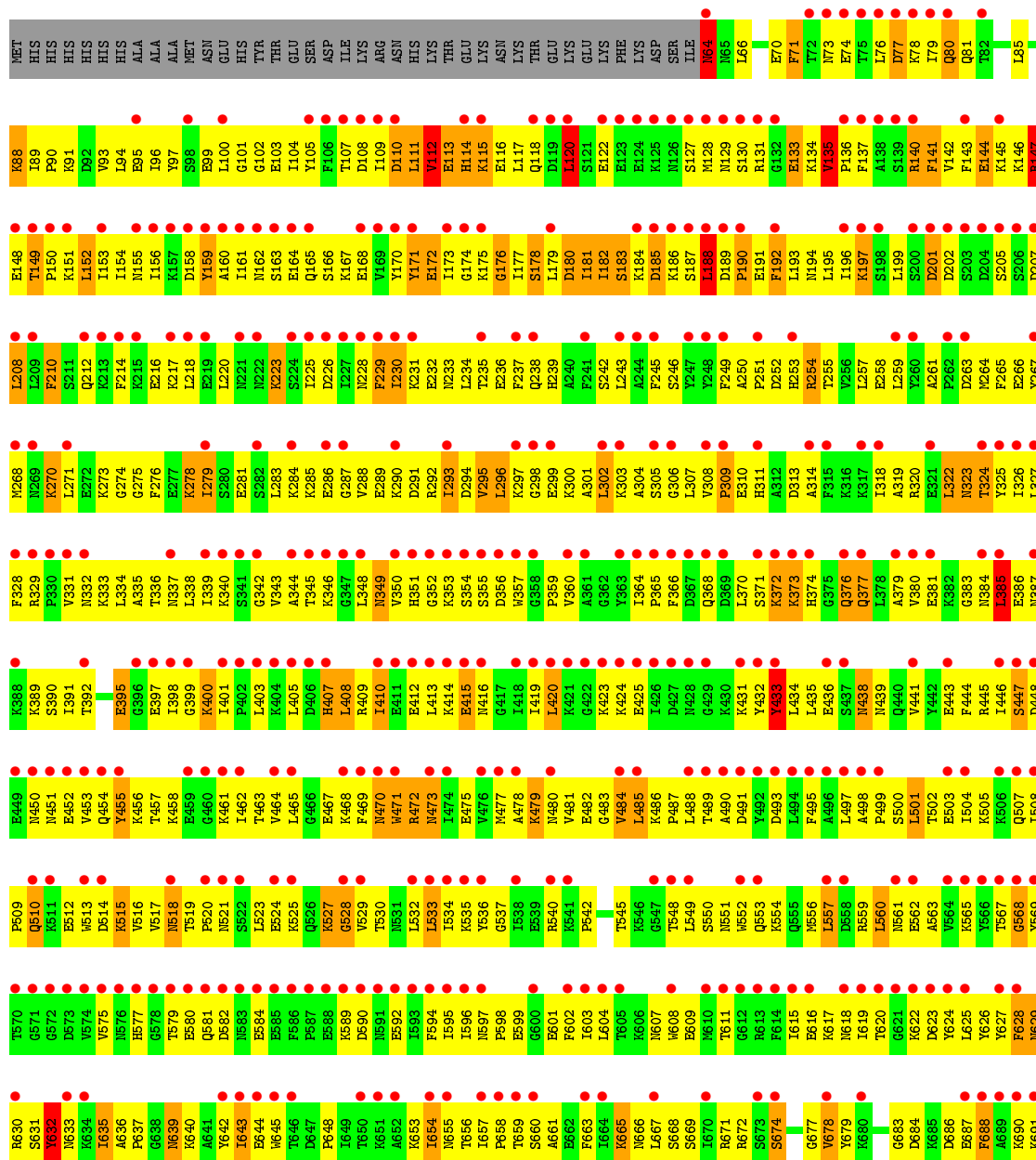
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

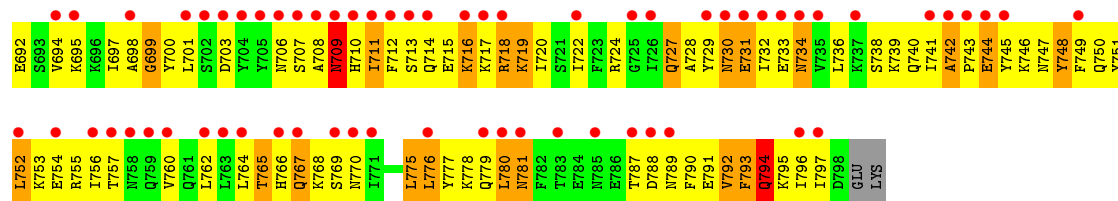




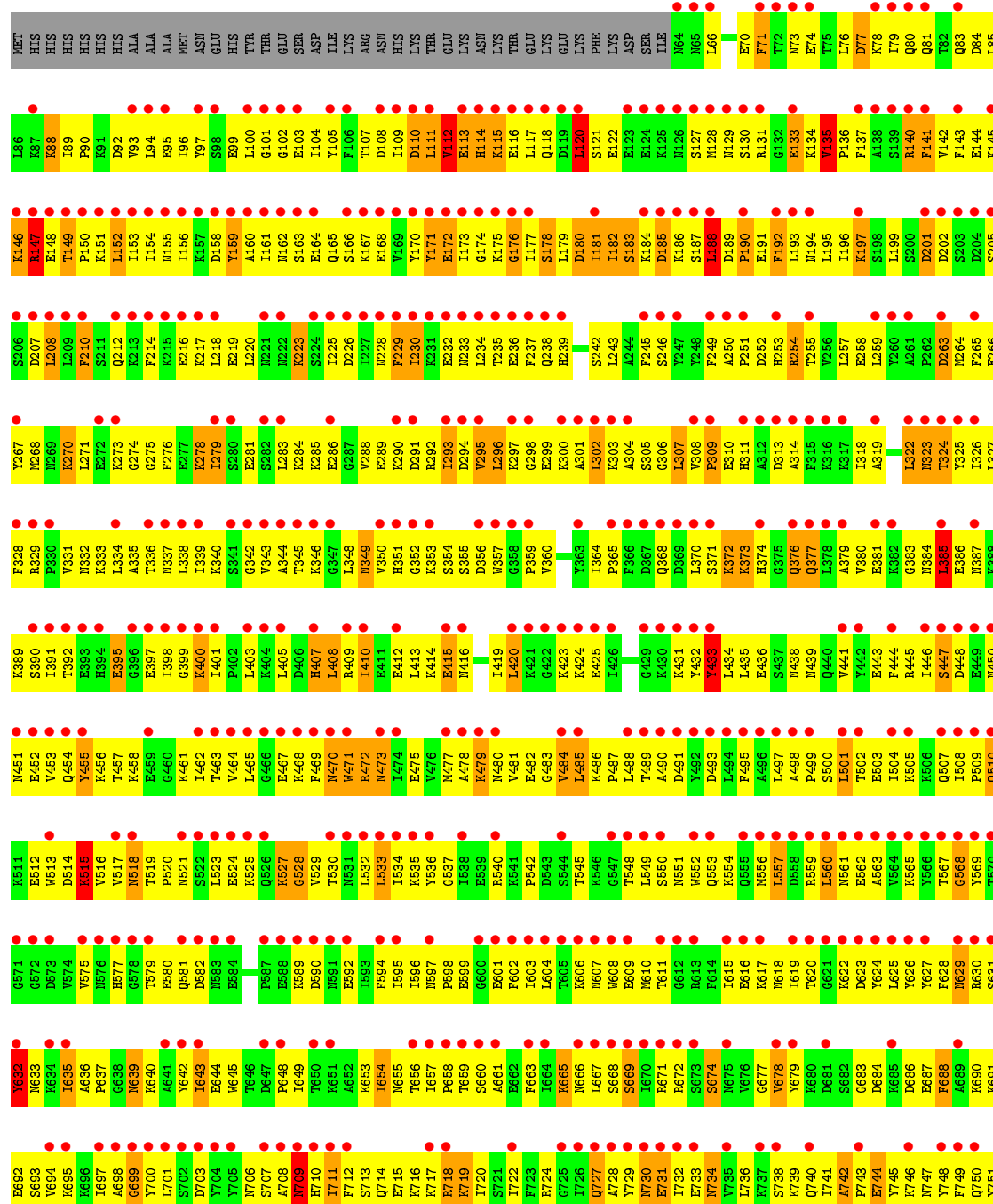
• Molecule 1: Calmodulin-sensitive adenylate cyclase

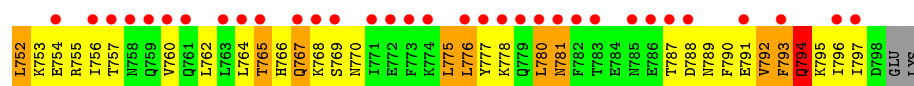




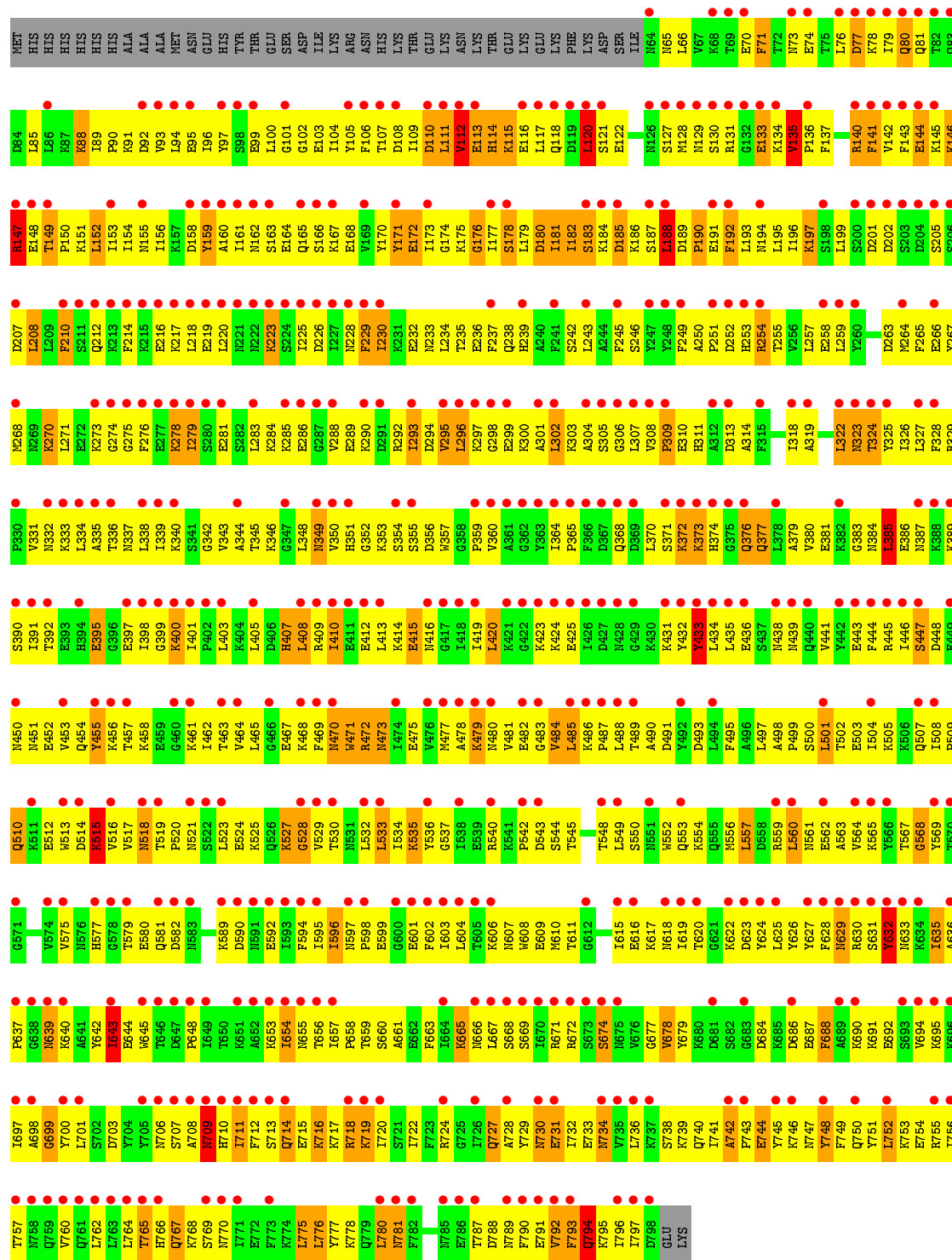


● Molecule 1: Calmodulin-sensitive adenylylate cyclase

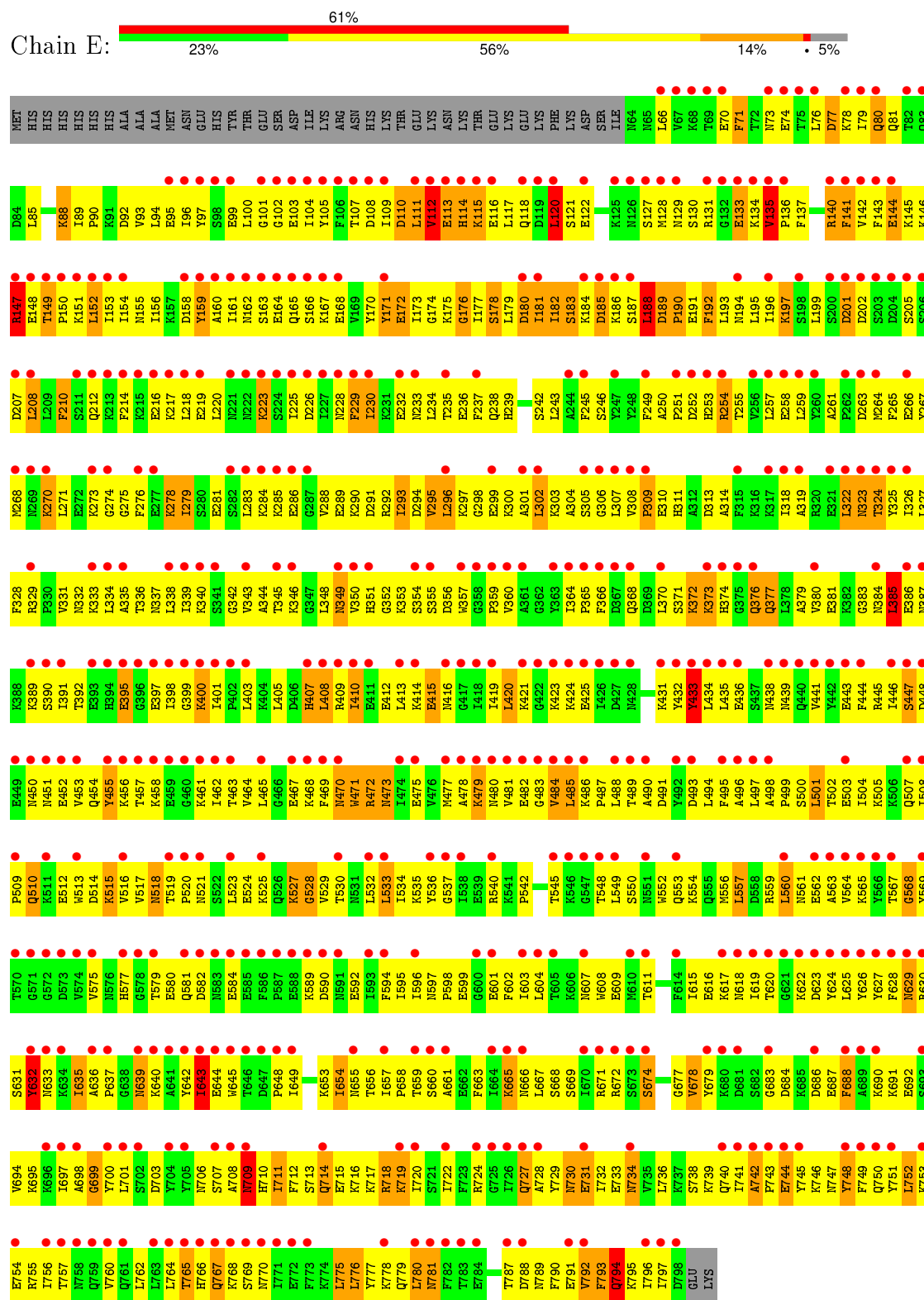




● Molecule 1: Calmodulin-sensitive adenylate cyclase

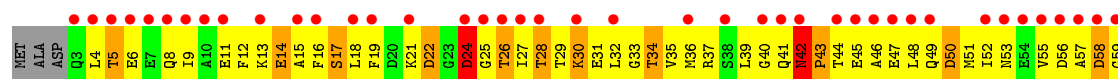


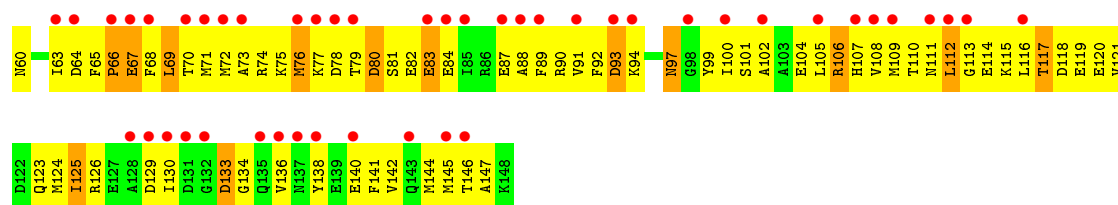
## Chain E:



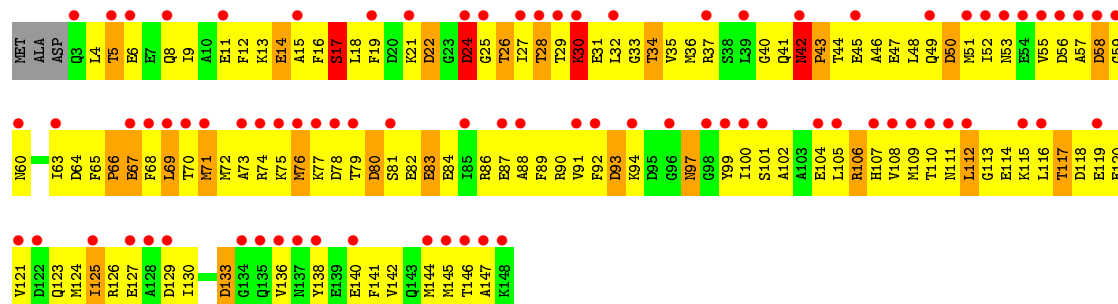
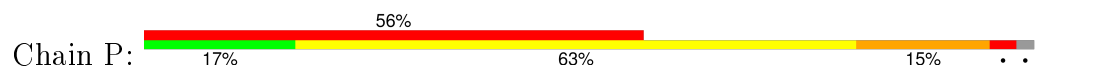
Chain F:



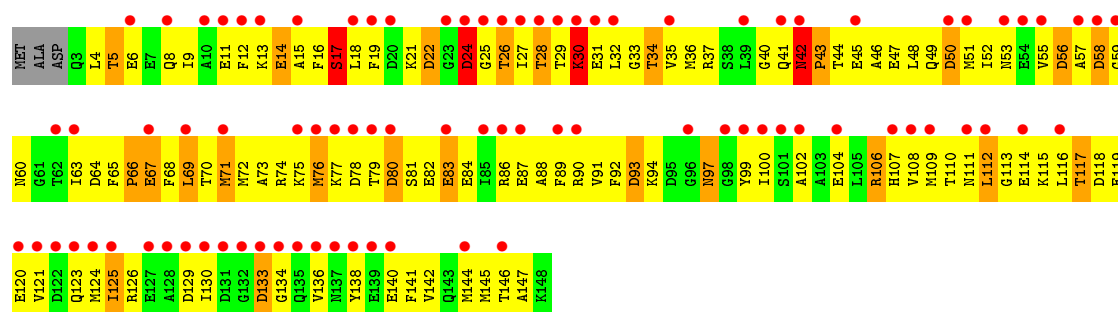
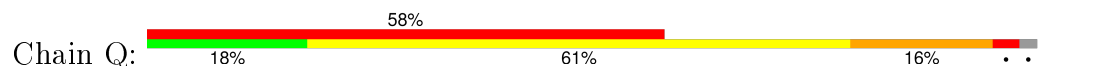




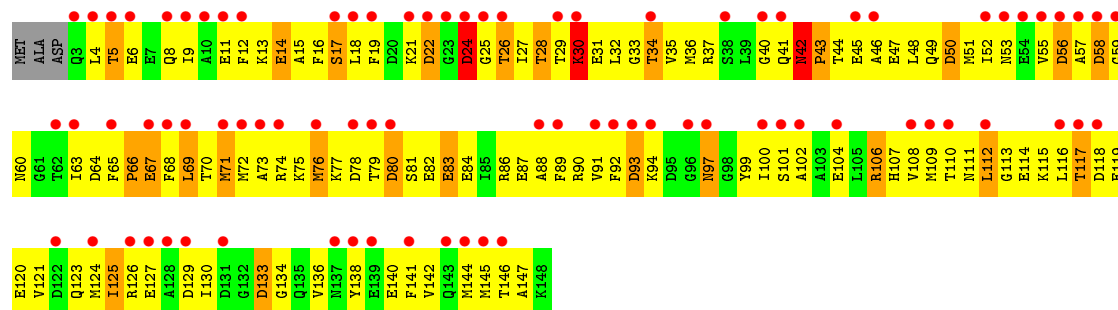
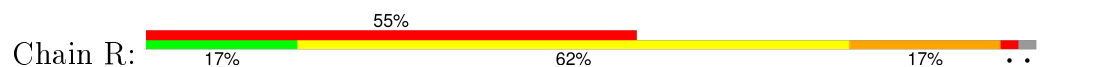
• Molecule 2: Calmodulin 2



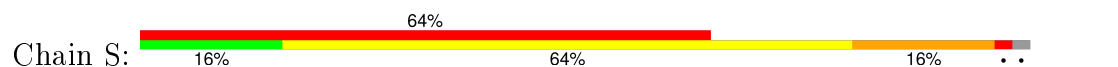
• Molecule 2: Calmodulin 2

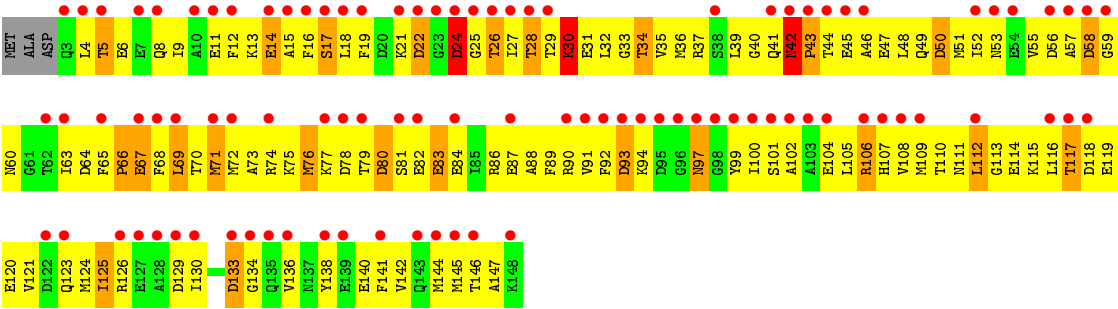


• Molecule 2: Calmodulin 2

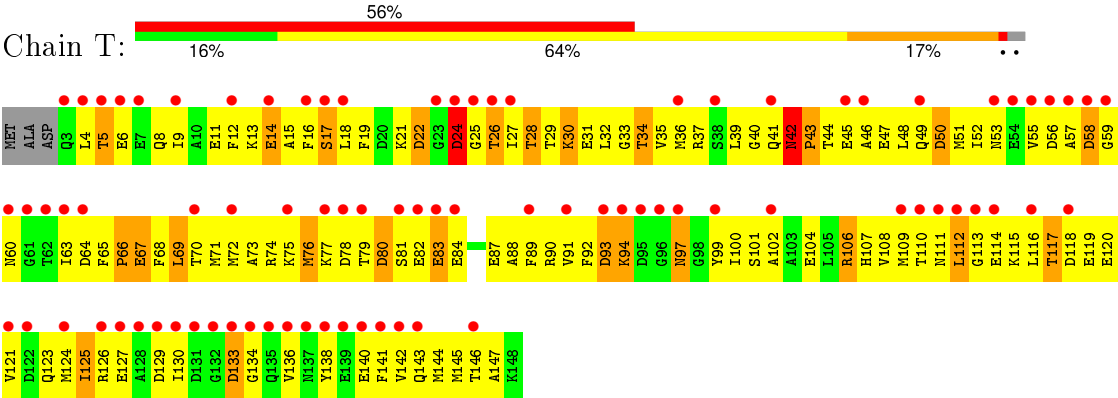


• Molecule 2: Calmodulin 2





● Molecule 2: Calmodulin 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	315.62Å 182.04Å 141.02Å 90.00° 89.93° 90.00°	Depositor
Resolution (Å)	10.00 – 3.30 29.82 – 3.26	Depositor EDS
% Data completeness (in resolution range)	93.9 (10.00-3.30) 91.8 (29.82-3.26)	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 0.273 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	101.4	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 56.2	EDS
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
L-test for twinning <sup>1</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	2 of 118338 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	42846	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</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	0.54	0/6104	0.84	15/8208 (0.2%)
1	B	0.54	0/6104	0.85	15/8208 (0.2%)
1	C	0.54	0/6104	0.85	17/8208 (0.2%)
1	D	0.54	1/6104 (0.0%)	0.85	17/8208 (0.2%)
1	E	0.54	0/6104	0.85	16/8208 (0.2%)
1	F	0.54	0/6104	0.85	16/8208 (0.2%)
2	O	0.54	0/1158	0.85	4/1553 (0.3%)
2	P	0.54	0/1158	0.86	4/1553 (0.3%)
2	Q	0.54	0/1158	0.85	4/1553 (0.3%)
2	R	0.55	0/1158	0.85	4/1553 (0.3%)
2	S	0.54	0/1158	0.85	4/1553 (0.3%)
2	T	0.53	0/1158	0.85	4/1553 (0.3%)
All	All	0.54	1/43572 (0.0%)	0.85	120/58566 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	190	PRO	N-CA	-5.69	1.37	1.47

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	160	ALA	N-CA-C	9.55	136.80	111.00
1	F	160	ALA	N-CA-C	9.55	136.78	111.00
1	E	160	ALA	N-CA-C	9.54	136.76	111.00
1	A	160	ALA	N-CA-C	9.54	136.75	111.00
1	D	160	ALA	N-CA-C	9.53	136.74	111.00

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	866	0
1	B	5992	0	6010	875	0
1	C	5992	0	6010	855	0
1	D	5992	0	6010	863	0
1	E	5992	0	6010	863	0
1	F	5992	0	6010	862	0
2	O	1146	0	1071	195	0
2	P	1146	0	1071	195	0
2	Q	1146	0	1071	189	0
2	R	1146	0	1071	196	0
2	S	1146	0	1071	196	0
2	T	1146	0	1071	192	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	6152	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 72.

The worst 5 of 6152 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	1	5
1	B	733/777 (94%)	492 (67%)	171 (23%)	70 (10%)	1	6
1	C	733/777 (94%)	494 (67%)	171 (23%)	68 (9%)	1	6
1	D	733/777 (94%)	493 (67%)	170 (23%)	70 (10%)	1	6
1	E	733/777 (94%)	492 (67%)	171 (23%)	70 (10%)	1	6
1	F	733/777 (94%)	490 (67%)	172 (24%)	71 (10%)	1	5
2	O	144/149 (97%)	92 (64%)	39 (27%)	13 (9%)	1	6
2	P	144/149 (97%)	89 (62%)	39 (27%)	16 (11%)	0	3
2	Q	144/149 (97%)	90 (62%)	37 (26%)	17 (12%)	0	3
2	R	144/149 (97%)	90 (62%)	38 (26%)	16 (11%)	0	3
2	S	144/149 (97%)	90 (62%)	39 (27%)	15 (10%)	1	4
2	T	144/149 (97%)	90 (62%)	40 (28%)	14 (10%)	1	5
All	All	5262/5556 (95%)	3492 (66%)	1257 (24%)	513 (10%)	1	5

5 of 513 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	ASP
1	A	111	LEU
1	A	113	GLU

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Mol	Chain	Res	Type
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%)	580 (87%)	84 (13%)	5	24
1	B	664/705 (94%)	576 (87%)	88 (13%)	5	21
1	C	664/705 (94%)	578 (87%)	86 (13%)	5	22
1	D	664/705 (94%)	577 (87%)	87 (13%)	5	22
1	E	664/705 (94%)	578 (87%)	86 (13%)	5	22
1	F	664/705 (94%)	579 (87%)	85 (13%)	5	23
2	O	123/127 (97%)	106 (86%)	17 (14%)	4	20
2	P	123/127 (97%)	106 (86%)	17 (14%)	4	20
2	Q	123/127 (97%)	106 (86%)	17 (14%)	4	20
2	R	123/127 (97%)	106 (86%)	17 (14%)	4	20
2	S	123/127 (97%)	106 (86%)	17 (14%)	4	20
2	T	123/127 (97%)	106 (86%)	17 (14%)	4	20
All	All	4722/4992 (95%)	4104 (87%)	618 (13%)	5	22

5 of 618 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	182	ILE
1	E	71	PHE
2	R	28	THR
1	D	254	ARG
1	D	479	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 191 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	64	ASN
1	D	655	ASN
2	P	8	GLN
1	D	239	HIS
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 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 [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, 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%)	3.13	461 (62%) 0 0	24, 83, 143, 153	0
1	B	735/777 (94%)	3.05	459 (62%) 0 0	25, 83, 143, 153	0
1	C	735/777 (94%)	3.16	495 (67%) 0 0	25, 83, 143, 153	0
1	D	735/777 (94%)	3.04	461 (62%) 0 0	25, 83, 143, 153	0
1	E	735/777 (94%)	3.00	471 (64%) 0 0	24, 83, 142, 152	0
1	F	735/777 (94%)	3.03	455 (61%) 0 0	27, 83, 143, 154	0
2	O	146/149 (97%)	2.86	87 (59%) 0 0	22, 74, 121, 134	0
2	P	146/149 (97%)	2.62	83 (56%) 0 0	20, 75, 121, 135	0
2	Q	146/149 (97%)	2.48	86 (58%) 0 0	21, 75, 121, 134	0
2	R	146/149 (97%)	2.73	82 (56%) 0 0	20, 75, 120, 134	0
2	S	146/149 (97%)	2.81	95 (65%) 0 0	21, 76, 121, 134	0
2	T	146/149 (97%)	2.83	83 (56%) 0 0	21, 75, 120, 134	0
All	All	5286/5556 (95%)	3.01	3318 (62%) 0 0	20, 80, 142, 154	0

The worst 5 of 3318 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	468	LYS	24.7
1	D	204	ASP	23.5
1	C	205	SER	22.5
2	P	78	ASP	20.1
1	A	230	ILE	19.5

### 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 [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
4	CA	P	803	1/1	0.49	0.46	-0.15	32,32,32,32	0
4	CA	T	812	1/1	0.40	0.24	-1.48	35,35,35,35	0
4	CA	P	804	1/1	0.67	0.25	-1.49	34,34,34,34	0
4	CA	T	811	1/1	0.79	0.25	-1.50	28,28,28,28	0
4	CA	O	802	1/1	0.05	0.14	-1.58	33,33,33,33	0
4	CA	O	801	1/1	0.59	0.12	-1.63	33,33,33,33	0
4	CA	S	809	1/1	0.29	0.20	-1.96	29,29,29,29	0
4	CA	Q	806	1/1	0.41	0.15	-2.12	35,35,35,35	0
4	CA	S	810	1/1	0.55	0.28	-2.36	40,40,40,40	0
4	CA	R	808	1/1	0.30	0.22	-2.78	36,36,36,36	0
4	CA	R	807	1/1	0.37	0.14	-3.81	30,30,30,30	0
4	CA	Q	805	1/1	0.65	0.21	-4.89	29,29,29,29	0
3	MG	B	901	1/1	0.37	0.30	-	16,16,16,16	0
3	MG	A	900	1/1	0.53	0.29	-	23,23,23,23	0
3	MG	C	902	1/1	0.33	0.57	-	23,23,23,23	0
3	MG	F	905	1/1	0.92	0.27	-	17,17,17,17	0
3	MG	E	904	1/1	-0.23	0.34	-	23,23,23,23	0
3	MG	D	903	1/1	0.39	0.32	-	21,21,21,21	0

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

There are no such residues in this entry.