



wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 01:44 AM GMT

PDB ID : 1XFX
Title : Crystal structure of anthrax edema factor (EF) in complex with calmodulin
in the presence of 10 millimolar exogenously added calcium chloride
Authors : Shen, Y.; Zhukovskaya, N.L.; Guo, Q.; Florian, J.; Tang, W.J.
Deposited on : 2004-09-15
Resolution : 3.20 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

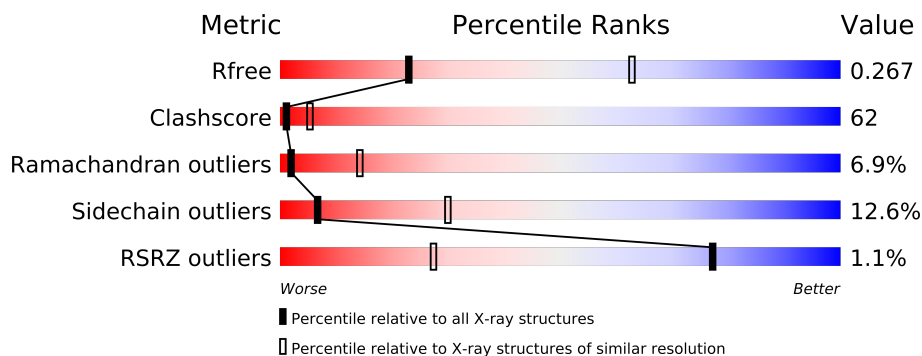
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.20 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}	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	777	
1	B	777	
1	C	777	
1	D	777	
1	E	777	
1	F	777	
2	O	149	
2	P	149	
2	Q	149	
2	R	149	
2	S	149	
2	T	149	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 42858 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 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	Se	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	Se 9	0	0	0
2	Q	146	Total 1146	C 702	N 186	O 249	Se 9	0	0	0
2	R	146	Total 1146	C 702	N 186	O 249	Se 9	0	0	0
2	S	146	Total 1146	C 702	N 186	O 249	Se 9	0	0	0
2	T	146	Total 1146	C 702	N 186	O 249	Se 9	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	0	MSE	MET	MODIFIED RESIDUE	UNP P62158
O	36	MSE	MET	MODIFIED RESIDUE	UNP P62158
O	51	MSE	MET	MODIFIED RESIDUE	UNP P62158
O	71	MSE	MET	MODIFIED RESIDUE	UNP P62158
O	72	MSE	MET	MODIFIED RESIDUE	UNP P62158
O	76	MSE	MET	MODIFIED RESIDUE	UNP P62158
O	109	MSE	MET	MODIFIED RESIDUE	UNP P62158
O	124	MSE	MET	MODIFIED RESIDUE	UNP P62158
O	144	MSE	MET	MODIFIED RESIDUE	UNP P62158
O	145	MSE	MET	MODIFIED RESIDUE	UNP P62158
P	0	MSE	MET	MODIFIED RESIDUE	UNP P62158
P	36	MSE	MET	MODIFIED RESIDUE	UNP P62158
P	51	MSE	MET	MODIFIED RESIDUE	UNP P62158
P	71	MSE	MET	MODIFIED RESIDUE	UNP P62158
P	72	MSE	MET	MODIFIED RESIDUE	UNP P62158
P	76	MSE	MET	MODIFIED RESIDUE	UNP P62158
P	109	MSE	MET	MODIFIED RESIDUE	UNP P62158
P	124	MSE	MET	MODIFIED RESIDUE	UNP P62158
P	144	MSE	MET	MODIFIED RESIDUE	UNP P62158
P	145	MSE	MET	MODIFIED RESIDUE	UNP P62158
Q	0	MSE	MET	MODIFIED RESIDUE	UNP P62158
Q	36	MSE	MET	MODIFIED RESIDUE	UNP P62158
Q	51	MSE	MET	MODIFIED RESIDUE	UNP P62158
Q	71	MSE	MET	MODIFIED RESIDUE	UNP P62158
Q	72	MSE	MET	MODIFIED RESIDUE	UNP P62158
Q	76	MSE	MET	MODIFIED RESIDUE	UNP P62158
Q	109	MSE	MET	MODIFIED RESIDUE	UNP P62158
Q	124	MSE	MET	MODIFIED RESIDUE	UNP P62158
Q	144	MSE	MET	MODIFIED RESIDUE	UNP P62158

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	145	MSE	MET	MODIFIED RESIDUE	UNP P62158
R	0	MSE	MET	MODIFIED RESIDUE	UNP P62158
R	36	MSE	MET	MODIFIED RESIDUE	UNP P62158
R	51	MSE	MET	MODIFIED RESIDUE	UNP P62158
R	71	MSE	MET	MODIFIED RESIDUE	UNP P62158
R	72	MSE	MET	MODIFIED RESIDUE	UNP P62158
R	76	MSE	MET	MODIFIED RESIDUE	UNP P62158
R	109	MSE	MET	MODIFIED RESIDUE	UNP P62158
R	124	MSE	MET	MODIFIED RESIDUE	UNP P62158
R	144	MSE	MET	MODIFIED RESIDUE	UNP P62158
R	145	MSE	MET	MODIFIED RESIDUE	UNP P62158
S	0	MSE	MET	MODIFIED RESIDUE	UNP P62158
S	36	MSE	MET	MODIFIED RESIDUE	UNP P62158
S	51	MSE	MET	MODIFIED RESIDUE	UNP P62158
S	71	MSE	MET	MODIFIED RESIDUE	UNP P62158
S	72	MSE	MET	MODIFIED RESIDUE	UNP P62158
S	76	MSE	MET	MODIFIED RESIDUE	UNP P62158
S	109	MSE	MET	MODIFIED RESIDUE	UNP P62158
S	124	MSE	MET	MODIFIED RESIDUE	UNP P62158
S	144	MSE	MET	MODIFIED RESIDUE	UNP P62158
S	145	MSE	MET	MODIFIED RESIDUE	UNP P62158
T	0	MSE	MET	MODIFIED RESIDUE	UNP P62158
T	36	MSE	MET	MODIFIED RESIDUE	UNP P62158
T	51	MSE	MET	MODIFIED RESIDUE	UNP P62158
T	71	MSE	MET	MODIFIED RESIDUE	UNP P62158
T	72	MSE	MET	MODIFIED RESIDUE	UNP P62158
T	76	MSE	MET	MODIFIED RESIDUE	UNP P62158
T	109	MSE	MET	MODIFIED RESIDUE	UNP P62158
T	124	MSE	MET	MODIFIED RESIDUE	UNP P62158
T	144	MSE	MET	MODIFIED RESIDUE	UNP P62158
T	145	MSE	MET	MODIFIED RESIDUE	UNP P62158

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

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

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

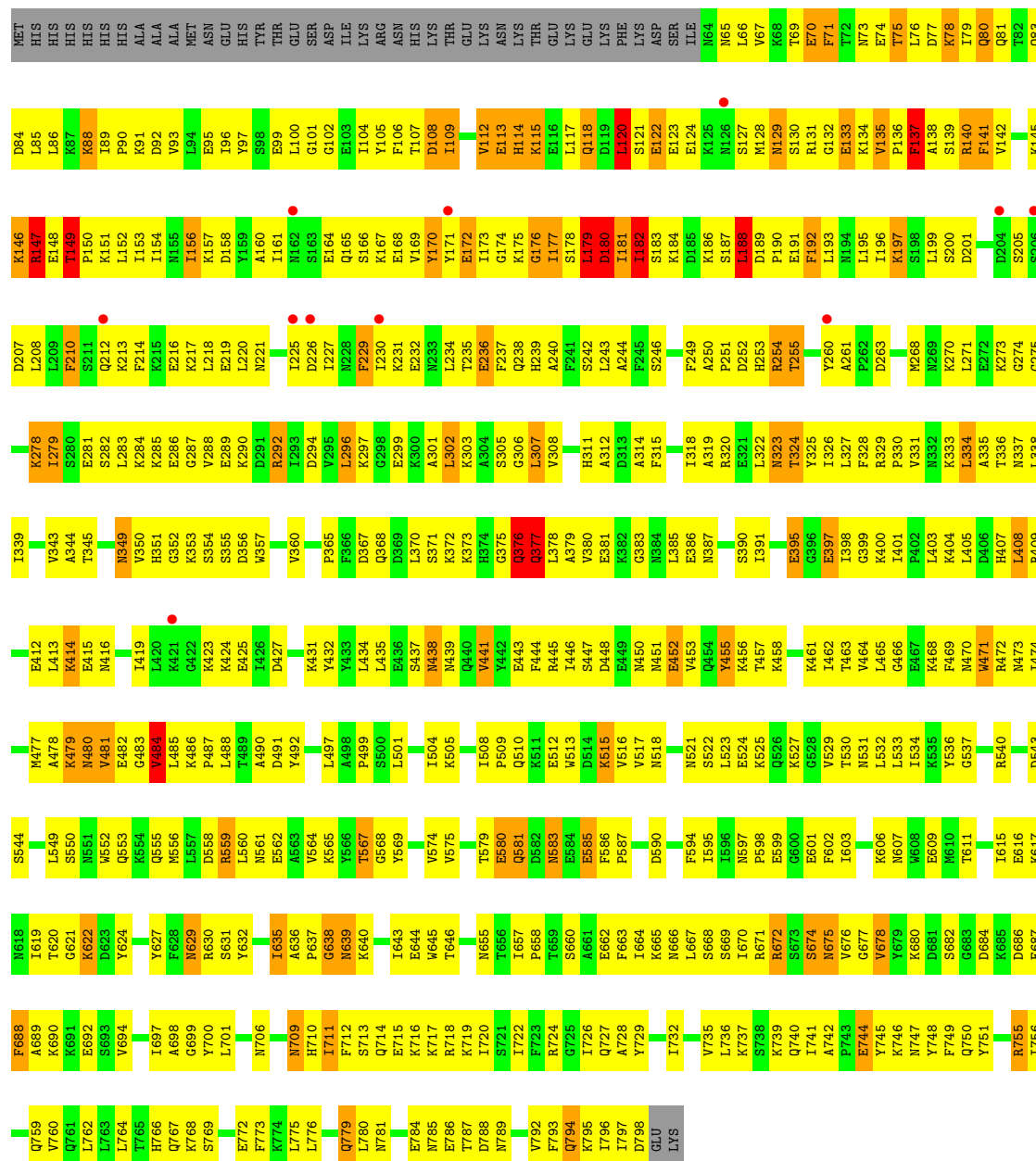
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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



• Molecule 1: Calmodulin-sensitive adenylate cyclase

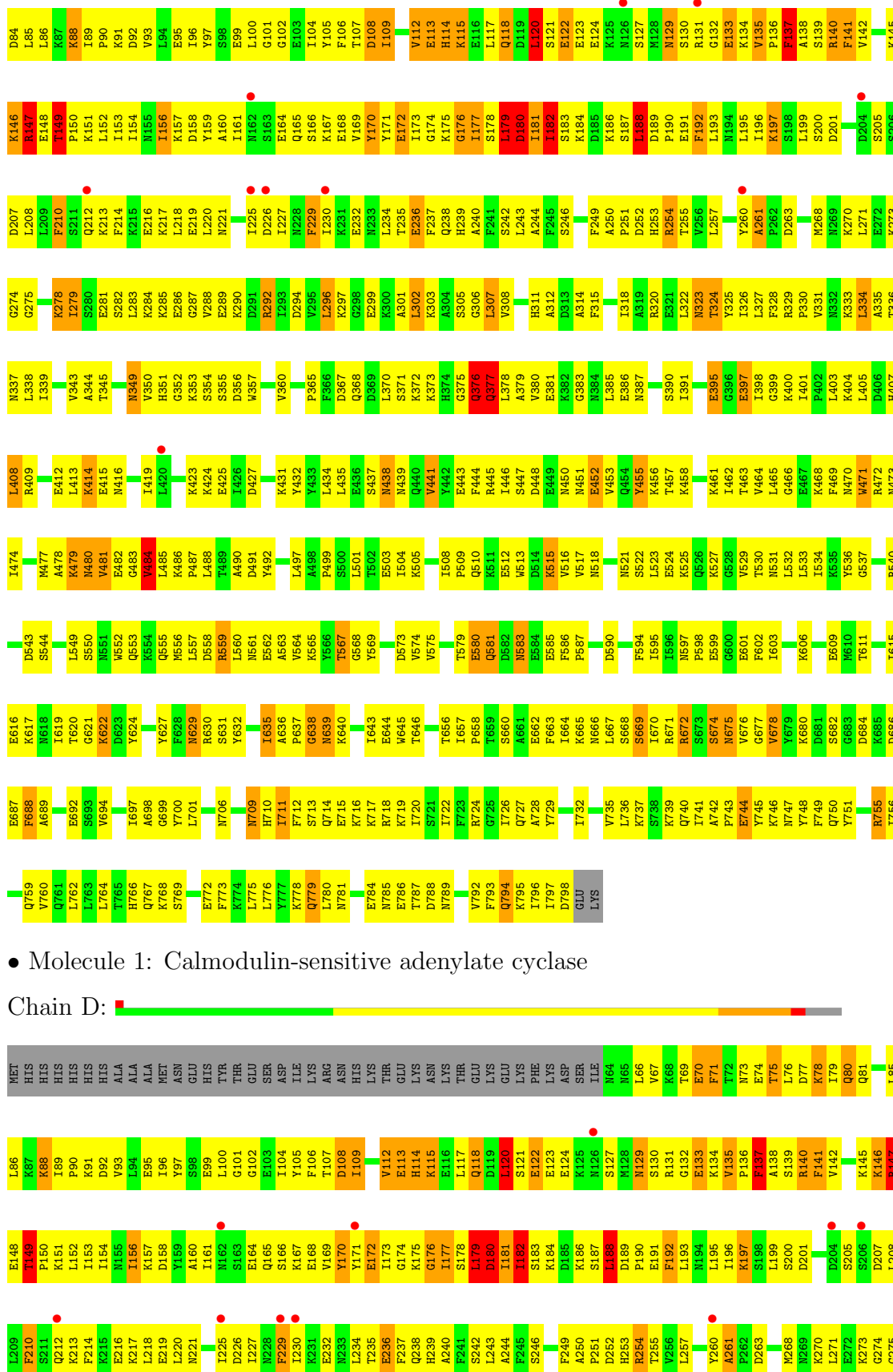
Chain B:

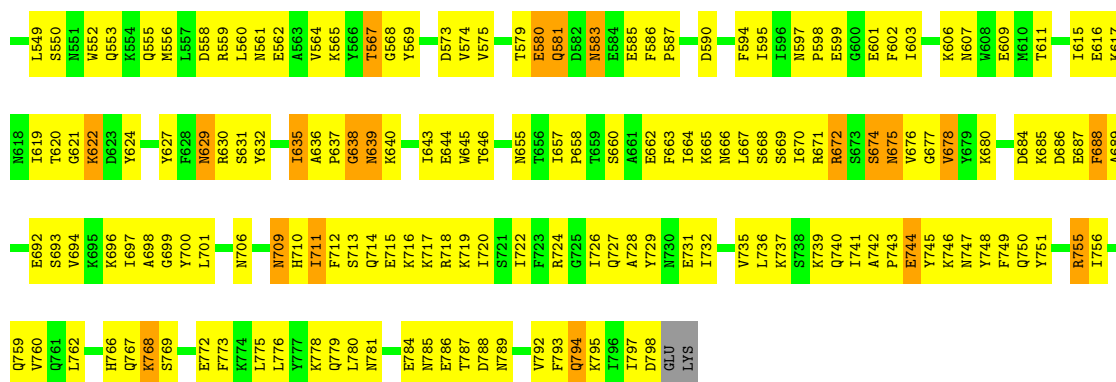


• Molecule 1: Calmodulin-sensitive adenylate cyclase

Chain C:

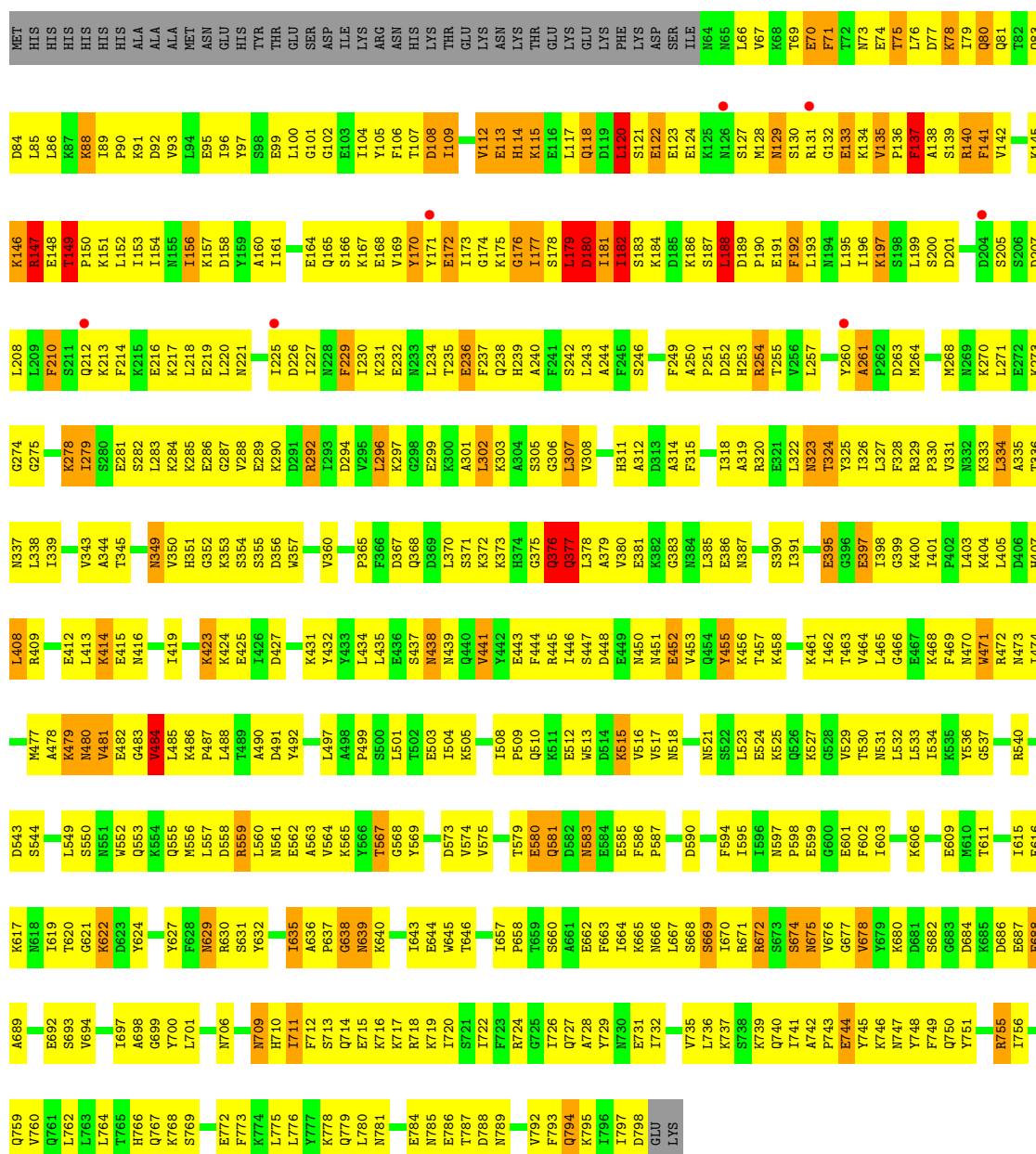




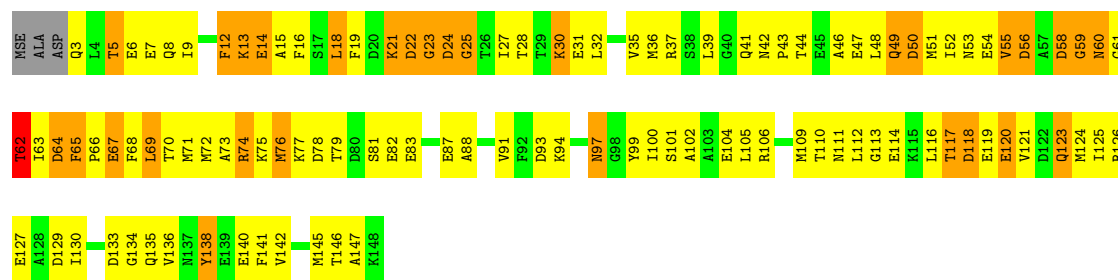


● Molecule 1: Calmodulin-sensitive adenylate cyclase

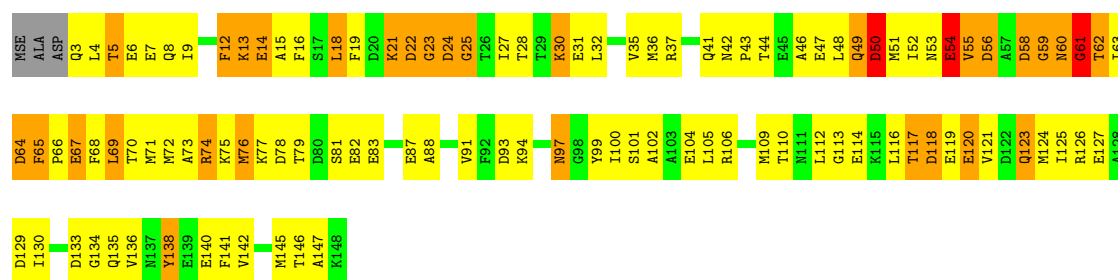
Chain F:



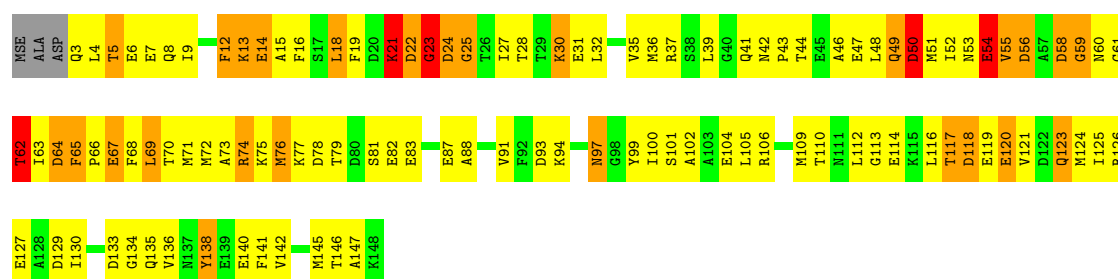
- Molecule 2: Calmodulin 2

Chain O: 

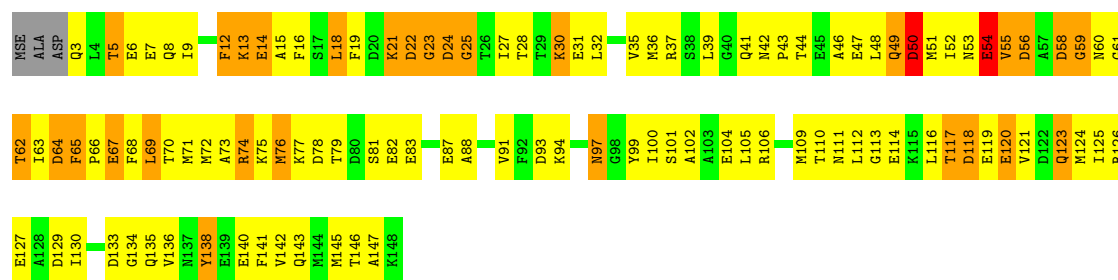
- Molecule 2: Calmodulin 2

Chain P: 

- Molecule 2: Calmodulin 2

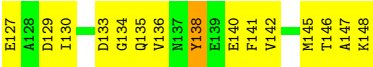
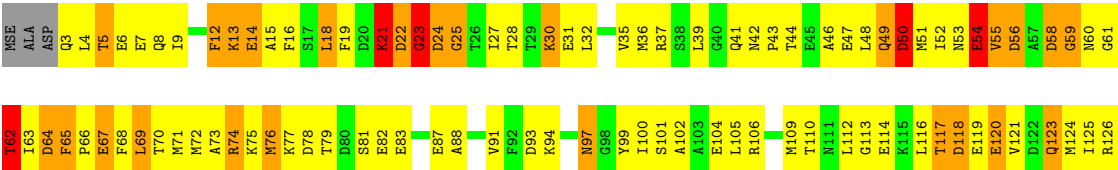
Chain Q: 

- Molecule 2: Calmodulin 2

Chain R: 

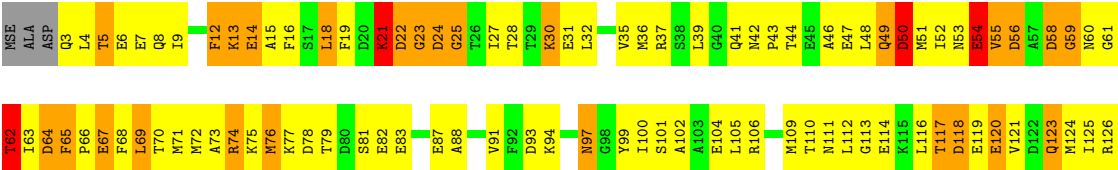
- Molecule 2: Calmodulin 2

Chain S: 



• Molecule 2: Calmodulin 2

Chain T:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	318.30Å 183.76Å 141.52Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	17.45 – 3.20 17.45 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.1 (17.45-3.20) 96.1 (17.45-3.20)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.03	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 3.21Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.262 , 0.278 0.251 , 0.267	Depositor DCC
R_{free} test set	6479 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	97.1	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 37.4	EDS
Estimated twinning fraction	0.479 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.480 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.478 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.480 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.479 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 132318 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	42858	wwPDB-VP
Average B, all atoms (Å ²)	87.0	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.

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	0.58	1/6104 (0.0%)	0.81	13/8208 (0.2%)
1	B	0.58	1/6104 (0.0%)	0.81	13/8208 (0.2%)
1	C	0.57	1/6104 (0.0%)	0.81	13/8208 (0.2%)
1	D	0.58	1/6104 (0.0%)	0.81	13/8208 (0.2%)
1	E	0.57	1/6104 (0.0%)	0.81	13/8208 (0.2%)
1	F	0.57	1/6104 (0.0%)	0.81	12/8208 (0.1%)
2	O	0.66	1/1149 (0.1%)	0.86	2/1526 (0.1%)
2	P	0.69	2/1149 (0.2%)	0.88	4/1526 (0.3%)
2	Q	0.64	1/1149 (0.1%)	0.86	4/1526 (0.3%)
2	R	0.66	1/1149 (0.1%)	0.86	4/1526 (0.3%)
2	S	0.65	1/1149 (0.1%)	0.86	3/1526 (0.2%)
2	T	0.67	2/1149 (0.2%)	0.86	3/1526 (0.2%)
All	All	0.59	14/43518 (0.0%)	0.82	97/58404 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	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	3
2	Q	0	3
2	R	0	3
2	S	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	T	0	3
All	All	0	22

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	61	GLY	C-O	7.82	1.36	1.23
2	S	62	THR	CB-CG2	6.71	1.74	1.52
2	R	62	THR	CB-CG2	6.62	1.74	1.52
2	T	62	THR	CB-CG2	6.50	1.73	1.52
2	O	62	THR	CB-CG2	6.42	1.73	1.52

The worst 5 of 97 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	188	LEU	N-CA-C	-11.99	78.63	111.00
1	F	188	LEU	N-CA-C	-11.96	78.71	111.00
1	A	188	LEU	N-CA-C	-11.95	78.73	111.00
1	C	188	LEU	N-CA-C	-11.95	78.75	111.00
1	D	188	LEU	N-CA-C	-11.94	78.75	111.00

There are no chirality outliers.

5 of 22 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 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5992	0	6010	720	1
1	B	5992	0	6010	721	1
1	C	5992	0	6010	724	1
1	D	5992	0	6010	718	0
1	E	5992	0	6010	708	0
1	F	5992	0	6010	715	1
2	O	1146	0	1071	180	0
2	P	1146	0	1071	182	0
2	Q	1146	0	1071	184	0
2	R	1146	0	1071	185	0
2	S	1146	0	1071	192	0
2	T	1146	0	1071	183	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	4	0	0	0	0
4	P	4	0	0	0	0
4	Q	4	0	0	0	0
4	R	4	0	0	0	0
4	S	4	0	0	0	0
4	T	4	0	0	0	0
All	All	42858	0	42486	5285	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 62.

The worst 5 of 5285 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:S:62:THR:CG2	2:S:62:THR:CB	1.74	1.60
1:B:179:LEU:O	1:B:183:SER:HB2	1.21	1.35
1:A:179:LEU:O	1:A:183:SER:HB2	1.21	1.35
1:E:179:LEU:O	1:E:183:SER:HB2	1.21	1.32
1:D:179:LEU:O	1:D:183:SER:HB2	1.20	1.32

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	Distance(Å)	Clash(Å)
1:A:682:SER:O	1:B:682:SER:O[2.555]	2.16	0.04
1:C:682:SER:O	1:F:682:SER:O[4.556]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	733/777 (94%)	526 (72%)	161 (22%)	46 (6%)	2	18
1	B	733/777 (94%)	525 (72%)	159 (22%)	49 (7%)	2	16
1	C	733/777 (94%)	526 (72%)	159 (22%)	48 (6%)	2	17
1	D	733/777 (94%)	523 (71%)	162 (22%)	48 (6%)	2	17
1	E	733/777 (94%)	522 (71%)	164 (22%)	47 (6%)	2	17
1	F	733/777 (94%)	526 (72%)	158 (22%)	49 (7%)	2	16
2	O	144/149 (97%)	110 (76%)	21 (15%)	13 (9%)	1	8
2	P	144/149 (97%)	108 (75%)	22 (15%)	14 (10%)	1	7
2	Q	144/149 (97%)	109 (76%)	23 (16%)	12 (8%)	1	9
2	R	144/149 (97%)	108 (75%)	24 (17%)	12 (8%)	1	9
2	S	144/149 (97%)	109 (76%)	23 (16%)	12 (8%)	1	9
2	T	144/149 (97%)	110 (76%)	22 (15%)	12 (8%)	1	9
All	All	5262/5556 (95%)	3802 (72%)	1098 (21%)	362 (7%)	2	14

5 of 362 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	THR
1	A	80	GLN
1	A	135	VAL
1	A	137	PHE
1	A	180	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	664/705 (94%)	585 (88%)	79 (12%)	8	33
1	B	664/705 (94%)	585 (88%)	79 (12%)	8	33
1	C	664/705 (94%)	585 (88%)	79 (12%)	8	33
1	D	664/705 (94%)	584 (88%)	80 (12%)	7	32
1	E	664/705 (94%)	585 (88%)	79 (12%)	8	33
1	F	664/705 (94%)	585 (88%)	79 (12%)	8	33
2	O	123/117 (105%)	103 (84%)	20 (16%)	3	15
2	P	123/117 (105%)	104 (85%)	19 (15%)	4	18
2	Q	123/117 (105%)	103 (84%)	20 (16%)	3	15
2	R	123/117 (105%)	104 (85%)	19 (15%)	4	18
2	S	123/117 (105%)	103 (84%)	20 (16%)	3	15
2	T	123/117 (105%)	103 (84%)	20 (16%)	3	15
All	All	4722/4932 (96%)	4129 (87%)	593 (13%)	7	30

5 of 593 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	255	THR
1	E	141	PHE
2	R	69	LEU
1	D	324	THR
1	D	629	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 229 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	785	ASN
1	D	639	ASN
2	O	8	GLN
1	D	80	GLN
1	D	438	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 30 ligands modelled in this entry, 30 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	735/777 (94%)	-0.03	10 (1%) 72 22	34, 87, 140, 151	0
1	B	735/777 (94%)	-0.04	11 (1%) 70 21	35, 87, 141, 153	0
1	C	735/777 (94%)	-0.04	10 (1%) 72 22	34, 87, 141, 153	0
1	D	735/777 (94%)	-0.03	10 (1%) 72 22	35, 87, 140, 152	0
1	E	735/777 (94%)	-0.04	11 (1%) 70 21	34, 87, 140, 153	0
1	F	735/777 (94%)	-0.03	7 (0%) 79 29	34, 87, 140, 153	0
2	O	146/149 (97%)	-0.18	0 100 100	27, 74, 127, 141	0
2	P	146/149 (97%)	-0.16	0 100 100	28, 74, 127, 141	0
2	Q	146/149 (97%)	-0.18	0 100 100	29, 74, 127, 141	0
2	R	146/149 (97%)	-0.17	0 100 100	28, 74, 127, 141	0
2	S	146/149 (97%)	-0.18	0 100 100	29, 74, 127, 141	0
2	T	146/149 (97%)	-0.16	0 100 100	29, 74, 127, 141	0
All	All	5286/5556 (95%)	-0.06	59 (1%) 77 27	27, 83, 140, 153	0

The worst 5 of 59 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	225	ILE	3.6
1	B	225	ILE	3.6
1	B	126	ASN	3.5
1	D	230	ILE	3.5
1	B	204	ASP	3.5

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	CA	T	711	1/1	0.20	0.92	84,84,84,84	0
3	MG	F	905	1/1	0.24	0.78	22,22,22,22	0
3	MG	A	900	1/1	0.26	0.75	28,28,28,28	0
4	CA	P	703	1/1	0.19	0.66	88,88,88,88	0
4	CA	R	807	1/1	0.19	0.53	38,38,38,38	0
3	MG	B	901	1/1	0.23	0.41	28,28,28,28	0
4	CA	R	808	1/1	0.24	0.40	44,44,44,44	0
4	CA	R	707	1/1	0.18	0.34	85,85,85,85	0
3	MG	E	904	1/1	0.22	0.01	23,23,23,23	0
4	CA	O	801	1/1	0.18	-0.03	36,36,36,36	0
4	CA	S	709	1/1	0.17	-0.09	83,83,83,83	0
4	CA	T	812	1/1	0.20	-0.14	48,48,48,48	0
4	CA	P	803	1/1	0.17	-0.31	36,36,36,36	0
3	MG	C	902	1/1	0.17	-0.35	23,23,23,23	0
4	CA	S	810	1/1	0.17	-0.38	44,44,44,44	0
4	CA	O	701	1/1	0.13	-0.43	83,83,83,83	0
4	CA	Q	806	1/1	0.18	-0.44	46,46,46,46	0
4	CA	O	802	1/1	0.17	-0.49	44,44,44,44	0
4	CA	P	804	1/1	0.17	-0.51	46,46,46,46	0
3	MG	D	903	1/1	0.17	-0.53	27,27,27,27	0
4	CA	S	809	1/1	0.15	-0.64	37,37,37,37	0
4	CA	Q	805	1/1	0.15	-0.66	38,38,38,38	0
4	CA	T	811	1/1	0.14	-0.92	43,43,43,43	0
4	CA	Q	705	1/1	0.09	-1.12	86,86,86,86	0
4	CA	O	702	1/1	0.10	-1.21	84,84,84,84	0
4	CA	Q	706	1/1	0.09	-1.25	84,84,84,84	0
4	CA	R	708	1/1	0.09	-1.38	85,85,85,85	0
4	CA	P	704	1/1	0.08	-1.39	82,82,82,82	0
4	CA	T	712	1/1	0.10	-1.73	85,85,85,85	0
4	CA	S	710	1/1	0.11	-2.85	87,87,87,87	0

6.5 Other polymers ⓘ

There are no such residues in this entry.