



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 04:34 am BST

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

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

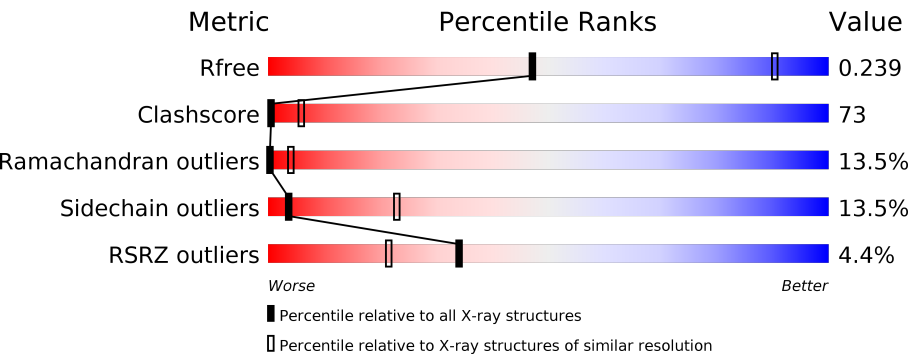
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	<div><div>5%</div><div>20%</div><div>56%</div><div>17%</div><div>• 5%</div></div>
1	B	777	<div><div>5%</div><div>19%</div><div>57%</div><div>17%</div><div>• 5%</div></div>
1	C	777	<div><div>5%</div><div>19%</div><div>57%</div><div>17%</div><div>• 5%</div></div>
1	D	777	<div><div>4%</div><div>19%</div><div>57%</div><div>17%</div><div>• 5%</div></div>
1	E	777	<div><div>5%</div><div>20%</div><div>56%</div><div>17%</div><div>• 5%</div></div>
1	F	777	<div><div>5%</div><div>19%</div><div>57%</div><div>16%</div><div>• 5%</div></div>

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Mol	Chain	Length	Quality of chain
2	H	146	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>15%</div><div>64%</div><div>19%</div><div></div></div></div>
2	I	146	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>16%</div><div>64%</div><div>19%</div><div></div></div></div>
2	J	146	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>16%</div><div>64%</div><div>18%</div><div></div></div></div>
2	K	146	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>16%</div><div>64%</div><div>18%</div><div></div></div></div>
2	L	146	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>15%</div><div>66%</div><div>18%</div><div></div></div></div>
2	M	146	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>16%</div><div>64%</div><div>19%</div><div></div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 42906 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Calmodulin-sensitive adenylate cyclase.

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

There are 54 discrepancies between the modelled and reference sequences:

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

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

- Molecule 2 is a protein called Calmodulin.

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

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

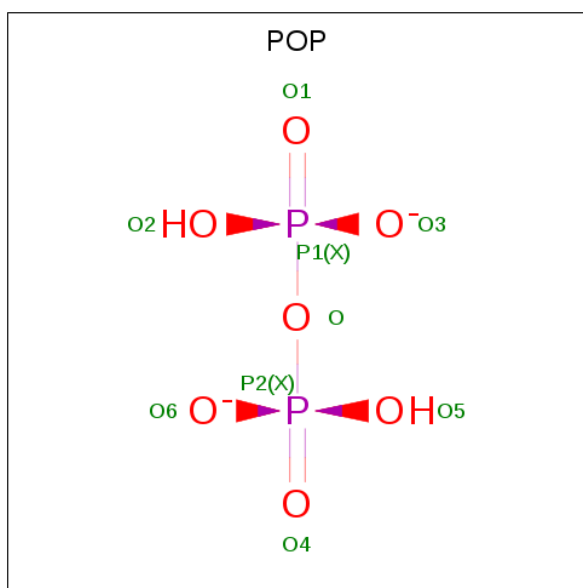
There are 12 discrepancies between the modelled and reference sequences:

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

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

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

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



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

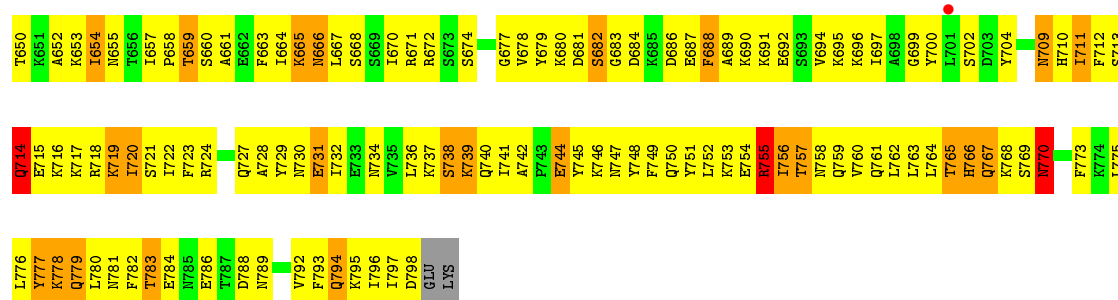
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

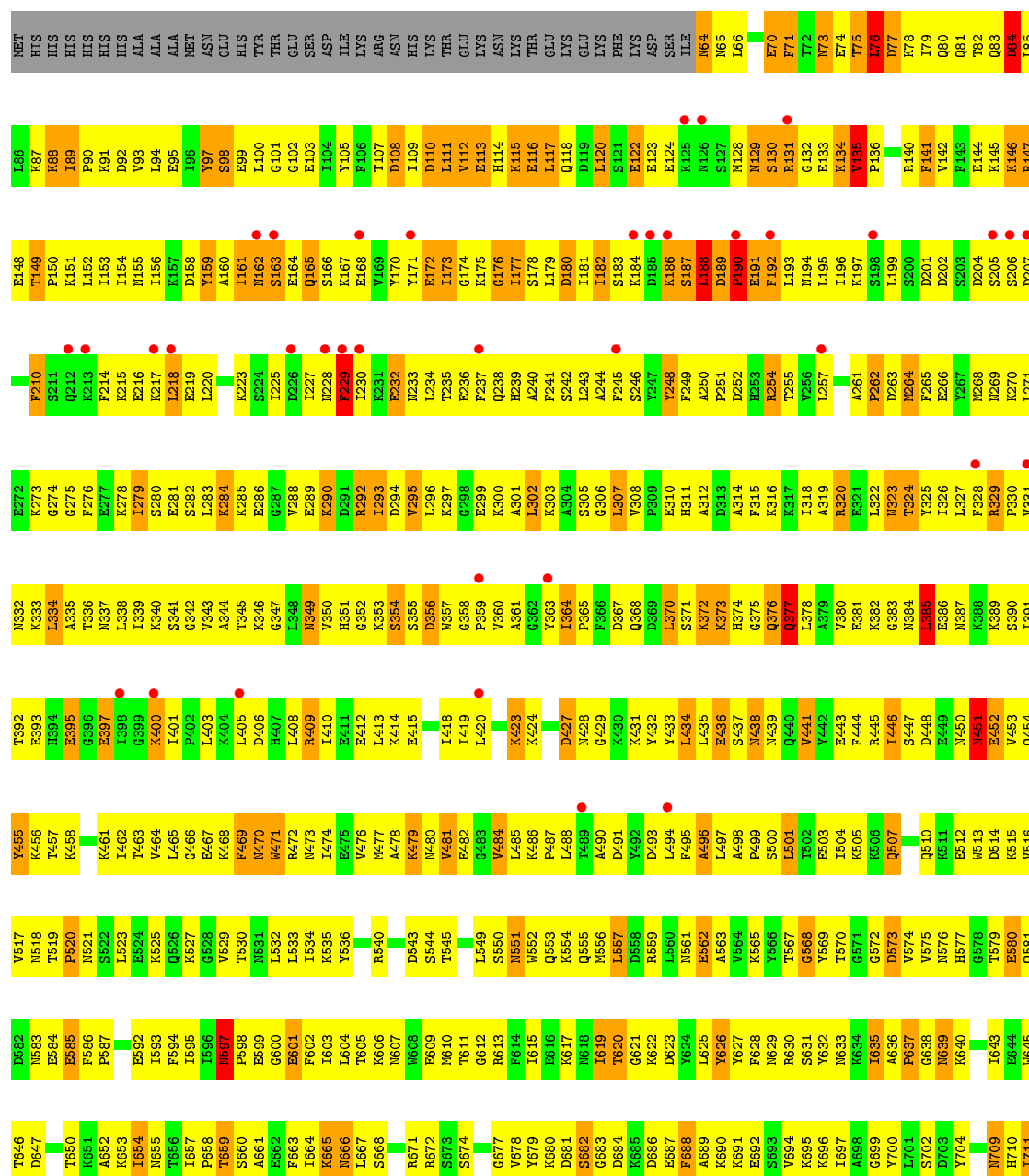
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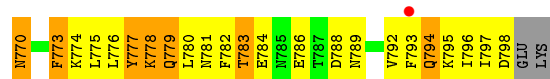
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	3	Total	Ca	0	0
			3	3		



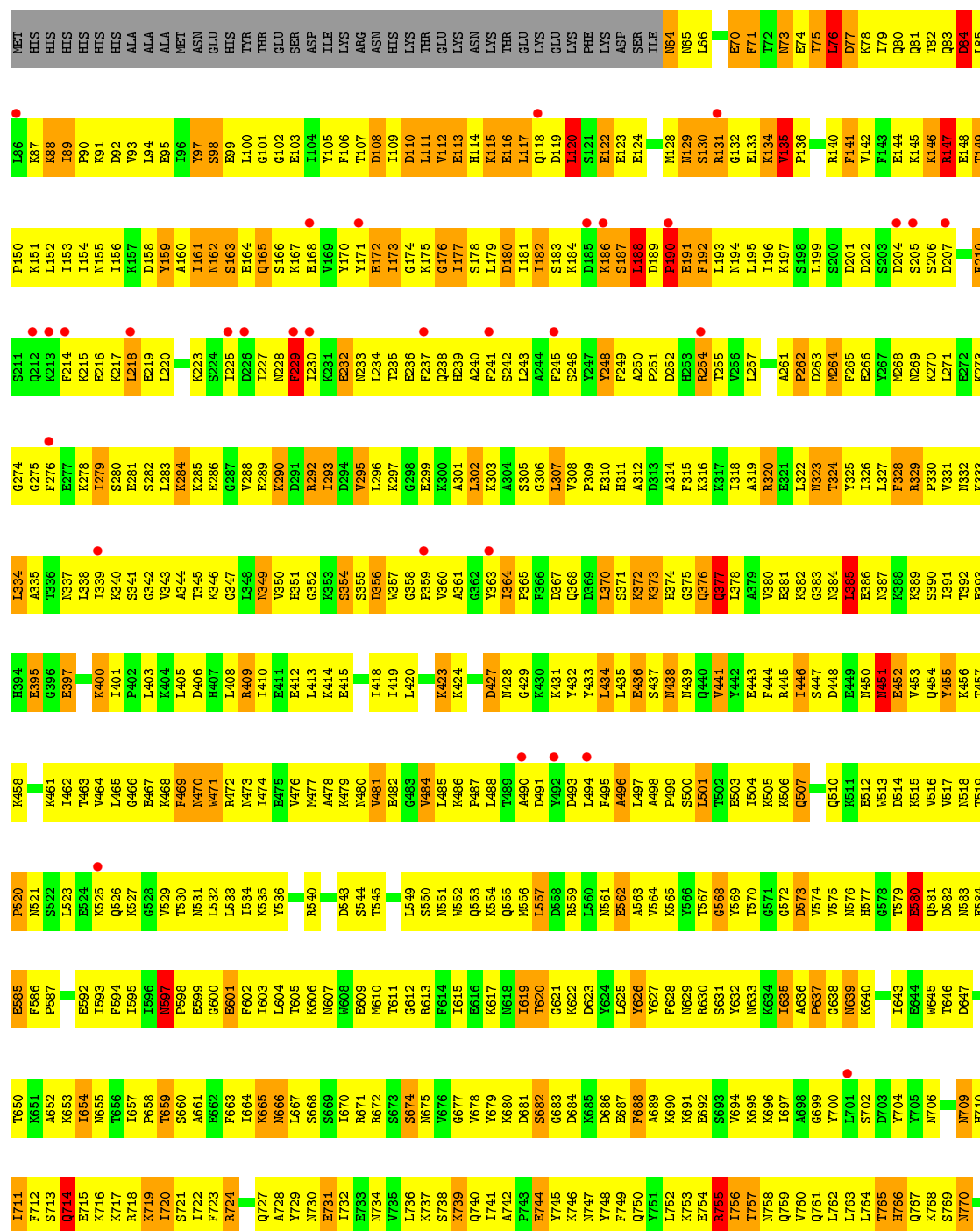
• Molecule 1: Calmodulin-sensitive adenylate cyclase





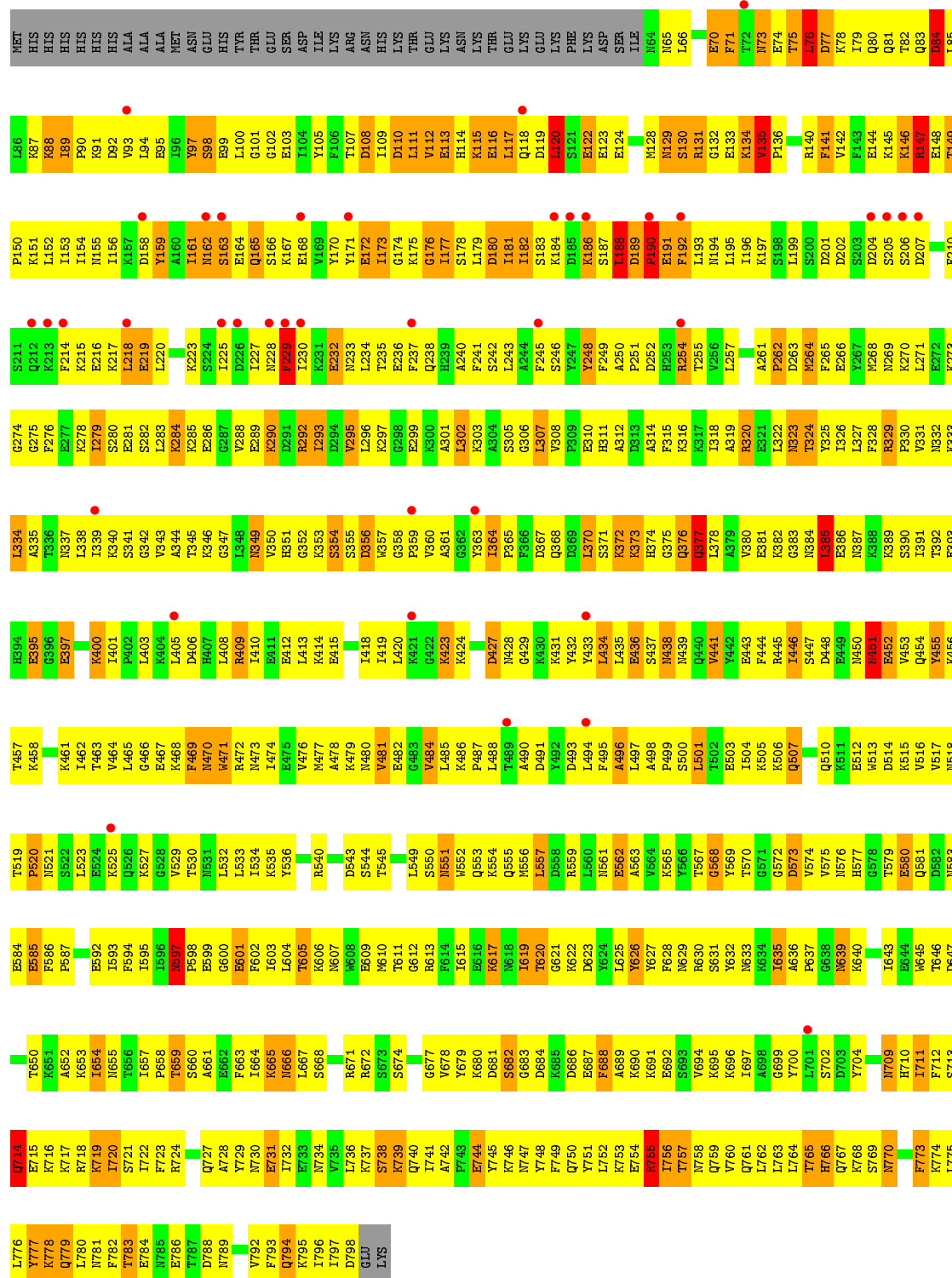


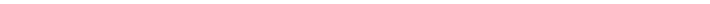
• Molecule 1: Calmodulin-sensitive adenylate cyclase

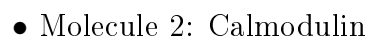


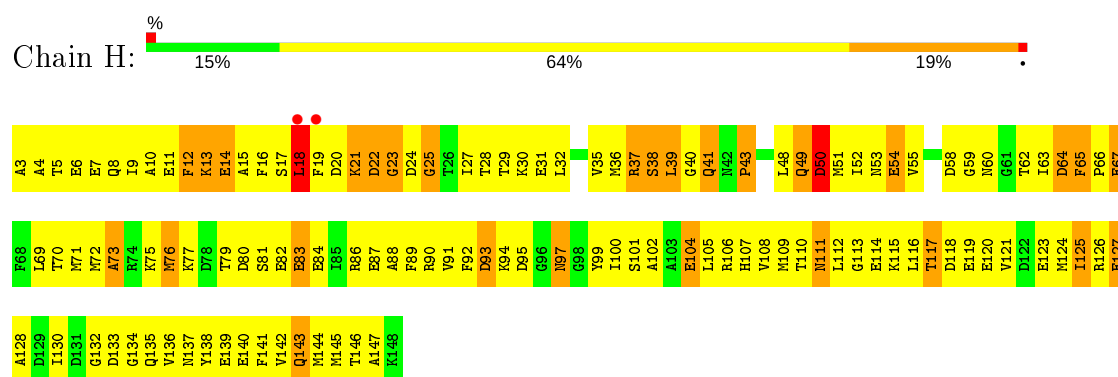


● Molecule 1: Calmodulin-sensitive adenylate cyclase

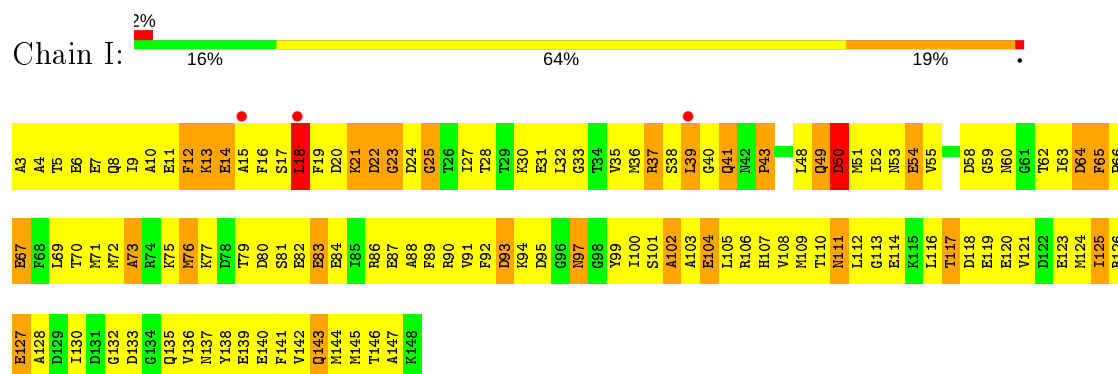


Chain F: 

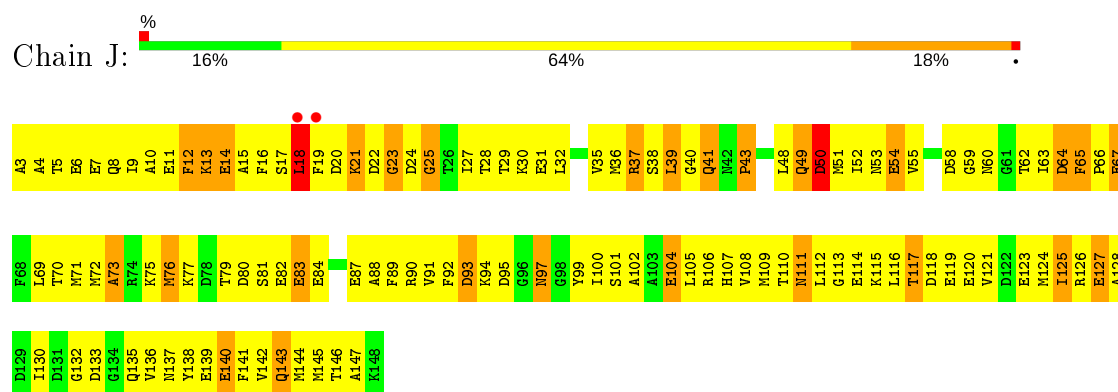




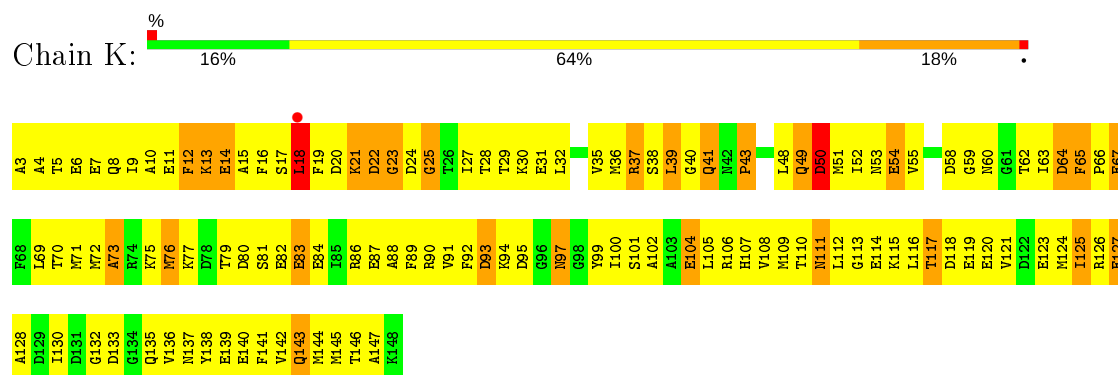
• Molecule 2: Calmodulin



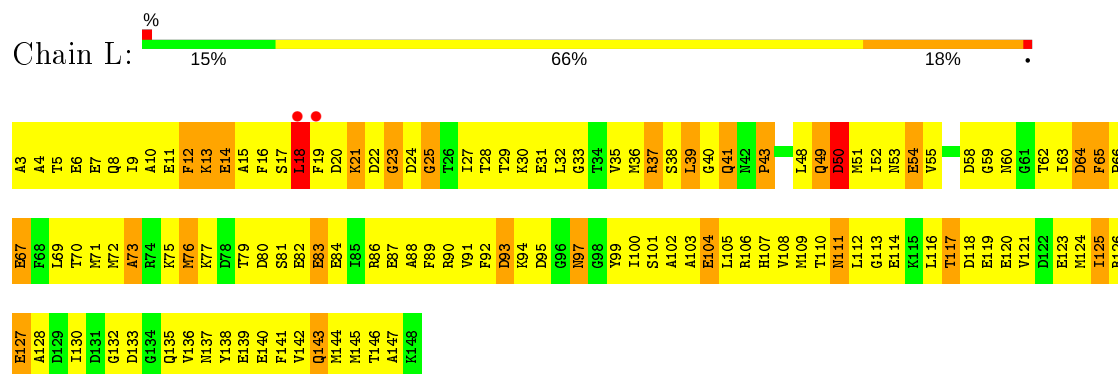
• Molecule 2: Calmodulin



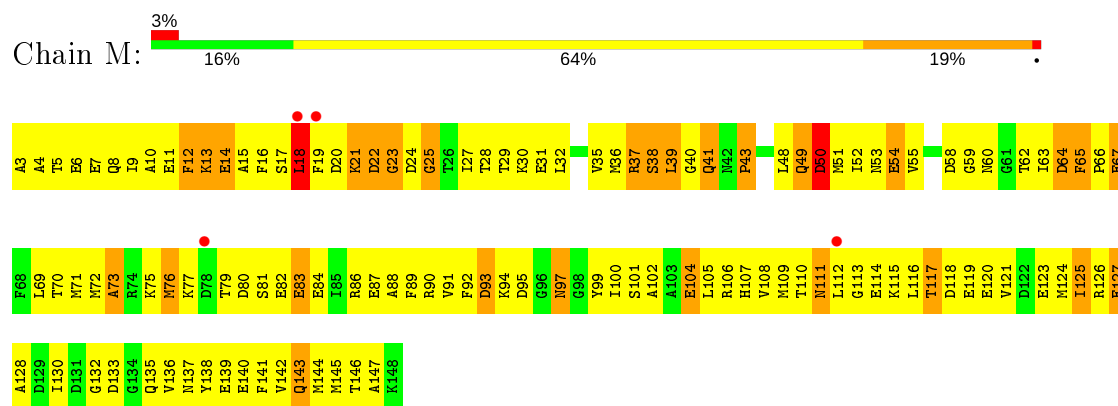
• Molecule 2: Calmodulin



• Molecule 2: Calmodulin



• Molecule 2: Calmodulin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	317.51Å 183.35Å 141.81Å 90.00° 90.05° 90.00°	Depositor
Resolution (Å)	29.87 – 3.60 44.04 – 3.52	Depositor EDS
% Data completeness (in resolution range)	86.2 (29.87-3.60) 93.3 (44.04-3.52)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 3.57Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.286 , 0.307 0.225 , 0.239	Depositor DCC
R_{free} test set	4714 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	119.9	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 70.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.458 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.458 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.450 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.450 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.458 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	42906	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MG, POP

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	0.57	4/6104 (0.1%)	0.80	19/8208 (0.2%)
1	B	0.52	2/6104 (0.0%)	0.77	11/8208 (0.1%)
1	C	0.52	1/6104 (0.0%)	0.78	14/8208 (0.2%)
1	D	0.52	1/6104 (0.0%)	0.78	10/8208 (0.1%)
1	E	0.52	1/6104 (0.0%)	0.77	12/8208 (0.1%)
1	F	0.52	0/6104	0.79	16/8208 (0.2%)
2	H	0.54	0/1158	0.72	0/1553
2	I	0.54	0/1158	0.71	0/1553
2	J	0.53	0/1158	0.71	0/1553
2	K	0.53	0/1158	0.71	0/1553
2	L	0.54	0/1158	0.72	0/1553
2	M	0.53	0/1158	0.72	0/1553
All	All	0.53	9/43572 (0.0%)	0.77	82/58566 (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

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	159	TYR	CA-CB	-13.07	1.25	1.53
1	A	159	TYR	CB-CG	-7.80	1.40	1.51
1	A	159	TYR	N-CA	7.25	1.60	1.46
1	E	159	TYR	CB-CG	-6.22	1.42	1.51
1	D	159	TYR	CB-CG	-5.77	1.43	1.51

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	F	188	LEU	C-N-CA	-10.45	95.58	121.70
1	C	159	TYR	N-CA-C	10.02	138.04	111.00
1	F	159	TYR	N-CA-C	10.01	138.03	111.00
1	E	159	TYR	N-CA-C	9.74	137.31	111.00
1	F	433	TYR	C-N-CA	-9.48	98.00	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	ASP	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5992	0	6010	891	0
1	B	5992	0	6010	886	0
1	C	5992	0	6010	882	0
1	D	5992	0	6010	880	0
1	E	5992	0	6010	872	0
1	F	5992	0	6010	882	0
2	H	1146	0	1075	194	0
2	I	1146	0	1075	189	0
2	J	1146	0	1075	194	0
2	K	1146	0	1075	198	0
2	L	1146	0	1075	190	0
2	M	1146	0	1075	193	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	9	0	0	0	0
4	B	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	9	0	0	0	0
4	D	9	0	0	0	0
4	E	9	0	0	0	0
4	F	9	0	0	0	0
5	H	3	0	0	0	0
5	I	3	0	0	0	0
5	J	3	0	0	0	0
5	K	3	0	0	0	0
5	L	3	0	0	0	0
5	M	3	0	0	0	0
All	All	42906	0	42510	6245	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 73.

The worst 5 of 6245 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:697:ILE:HD13	1:B:732:ILE:HD13	1.21	1.20
1:A:697:ILE:HD13	1:A:732:ILE:HD13	1.23	1.16
1:E:697:ILE:HD13	1:E:732:ILE:HD13	1.22	1.14
1:B:188:LEU:HD23	1:B:188:LEU:H	0.97	1.11
1:A:533:LEU:HD23	2:H:112:LEU:HD21	1.32	1.11

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	733/777 (94%)	466 (64%)	168 (23%)	99 (14%)	0	4
1	B	733/777 (94%)	463 (63%)	171 (23%)	99 (14%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	733/777 (94%)	463 (63%)	172 (24%)	98 (13%)	0	4
1	D	733/777 (94%)	467 (64%)	168 (23%)	98 (13%)	0	4
1	E	733/777 (94%)	464 (63%)	170 (23%)	99 (14%)	0	4
1	F	733/777 (94%)	466 (64%)	168 (23%)	99 (14%)	0	4
2	H	144/146 (99%)	86 (60%)	37 (26%)	21 (15%)	0	3
2	I	144/146 (99%)	87 (60%)	37 (26%)	20 (14%)	0	4
2	J	144/146 (99%)	87 (60%)	38 (26%)	19 (13%)	0	4
2	K	144/146 (99%)	87 (60%)	38 (26%)	19 (13%)	0	4
2	L	144/146 (99%)	87 (60%)	38 (26%)	19 (13%)	0	4
2	M	144/146 (99%)	87 (60%)	37 (26%)	20 (14%)	0	4
All	All	5262/5538 (95%)	3310 (63%)	1242 (24%)	710 (14%)	0	4

5 of 710 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	664/705 (94%)	577 (87%)	87 (13%)	4	23
1	B	664/705 (94%)	576 (87%)	88 (13%)	4	23
1	C	664/705 (94%)	575 (87%)	89 (13%)	4	23
1	D	664/705 (94%)	571 (86%)	93 (14%)	3	21
1	E	664/705 (94%)	577 (87%)	87 (13%)	4	23
1	F	664/705 (94%)	578 (87%)	86 (13%)	4	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	123/123 (100%)	105 (85%)	18 (15%)	3	20
2	I	123/123 (100%)	105 (85%)	18 (15%)	3	20
2	J	123/123 (100%)	105 (85%)	18 (15%)	3	20
2	K	123/123 (100%)	105 (85%)	18 (15%)	3	20
2	L	123/123 (100%)	105 (85%)	18 (15%)	3	20
2	M	123/123 (100%)	105 (85%)	18 (15%)	3	20
All	All	4722/4968 (95%)	4084 (86%)	638 (14%)	4	23

5 of 638 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	190	PRO
1	E	65	ASN
2	K	50	ASP
1	D	292	ARG
1	D	473	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 227 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	323	ASN
1	E	80	GLN
2	K	8	GLN
1	D	349	ASN
1	D	581	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 carbohydrates in this entry.

5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	POP	C	903	-	6,8,8	0.93	0	13,13,13	1.39	3 (23%)
4	POP	D	904	-	6,8,8	0.93	0	13,13,13	1.39	3 (23%)
4	POP	A	901	-	6,8,8	0.92	0	13,13,13	1.39	3 (23%)
4	POP	F	906	-	6,8,8	0.93	0	13,13,13	1.40	3 (23%)
4	POP	E	905	-	6,8,8	0.93	0	13,13,13	1.39	3 (23%)
4	POP	B	902	-	6,8,8	0.93	0	13,13,13	1.39	3 (23%)

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

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

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	906	POP	O5-P2-O4	-2.66	100.26	110.68
4	C	903	POP	O5-P2-O4	-2.66	100.28	110.68
4	B	902	POP	O5-P2-O4	-2.66	100.28	110.68
4	D	904	POP	O5-P2-O4	-2.66	100.28	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	905	POP	O5-P2-O4	-2.65	100.31	110.68

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	0.16	36 (4%)	29 18	28, 83, 137, 147	0
1	B	735/777 (94%)	0.16	37 (5%)	28 18	27, 83, 138, 147	0
1	C	735/777 (94%)	0.19	38 (5%)	27 17	28, 83, 138, 147	0
1	D	735/777 (94%)	0.11	33 (4%)	33 21	27, 84, 137, 147	0
1	E	735/777 (94%)	0.14	39 (5%)	26 16	28, 83, 138, 147	0
1	F	735/777 (94%)	0.17	36 (4%)	29 18	27, 84, 137, 147	0
2	H	146/146 (100%)	0.01	2 (1%)	75 61	26, 72, 130, 135	0
2	I	146/146 (100%)	-0.03	3 (2%)	63 48	27, 71, 130, 135	0
2	J	146/146 (100%)	-0.03	2 (1%)	75 61	26, 72, 130, 135	0
2	K	146/146 (100%)	-0.02	1 (0%)	87 78	27, 71, 129, 135	0
2	L	146/146 (100%)	0.01	2 (1%)	75 61	25, 71, 129, 135	0
2	M	146/146 (100%)	0.02	4 (2%)	54 38	25, 71, 130, 135	0
All	All	5286/5538 (95%)	0.13	233 (4%)	34 21	25, 81, 136, 147	0

The worst 5 of 233 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	185	ASP	10.4
1	B	229	PHE	9.3
1	C	205	SER	9.1
1	A	230	ILE	8.6
1	F	185	ASP	8.2

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 ⓘ

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	POP	C	903	9/9	0.76	0.21	74,83,88,88	0
4	POP	B	902	9/9	0.78	0.28	76,85,88,89	0
4	POP	F	906	9/9	0.79	0.18	74,84,86,86	0
4	POP	A	901	9/9	0.80	0.18	76,84,85,86	0
4	POP	D	904	9/9	0.84	0.16	75,82,86,88	0
3	MG	F	905	1/1	0.88	0.27	14,14,14,14	0
5	CA	I	804	1/1	0.90	0.18	50,50,50,50	0
4	POP	E	905	9/9	0.92	0.12	77,85,87,88	0
5	CA	M	711	1/1	0.93	0.19	86,86,86,86	0
5	CA	L	709	1/1	0.93	0.18	75,75,75,75	0
3	MG	A	900	1/1	0.93	0.33	11,11,11,11	0
3	MG	B	901	1/1	0.94	0.28	10,10,10,10	0
5	CA	H	701	1/1	0.94	0.15	77,77,77,77	0
5	CA	K	707	1/1	0.95	0.20	73,73,73,73	0
5	CA	I	703	1/1	0.95	0.17	73,73,73,73	0
5	CA	J	806	1/1	0.95	0.21	44,44,44,44	0
5	CA	I	803	1/1	0.95	0.14	24,24,24,24	0
5	CA	H	802	1/1	0.95	0.21	51,51,51,51	0
5	CA	M	812	1/1	0.95	0.24	48,48,48,48	0
5	CA	M	811	1/1	0.95	0.14	33,33,33,33	0
5	CA	K	808	1/1	0.95	0.21	47,47,47,47	0
3	MG	E	904	1/1	0.96	0.38	9,9,9,9	0
3	MG	C	902	1/1	0.96	0.24	5,5,5,5	0
3	MG	D	903	1/1	0.97	0.30	8,8,8,8	0
5	CA	H	801	1/1	0.97	0.12	29,29,29,29	0
5	CA	J	805	1/1	0.97	0.15	28,28,28,28	0
5	CA	L	810	1/1	0.97	0.21	51,51,51,51	0
5	CA	K	807	1/1	0.98	0.12	34,34,34,34	0
5	CA	L	809	1/1	0.98	0.15	28,28,28,28	0
5	CA	J	705	1/1	0.99	0.23	72,72,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.