



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:30 PM GMT

PDB ID : 1XFV
Title : Crystal structure of anthrax edema factor (EF) in complex with calmodulin and 3' deoxy-ATP
Authors : Shen, Q.; Zhukovskaya, N.L.; Guo, Q.; Florian, J.; Tang, W.J.
Deposited on : 2004-09-15
Resolution : 3.35 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
<http://wwpdb.org/validation/2016/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 : 1.7 (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

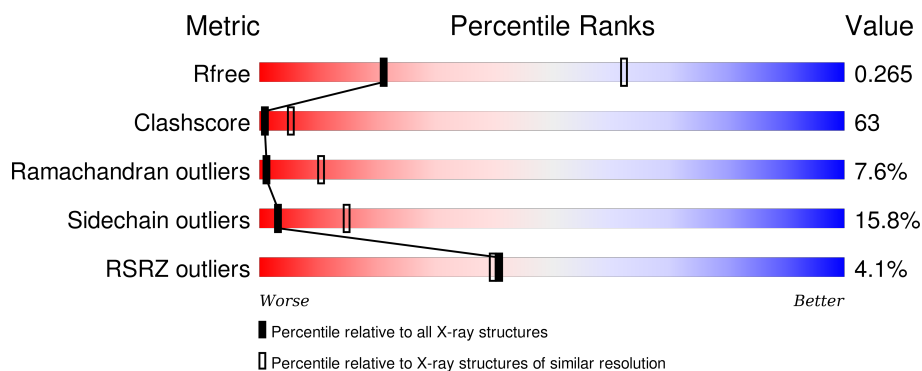
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

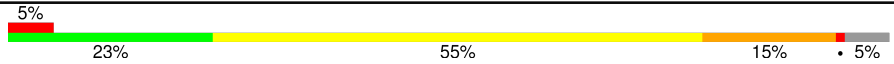
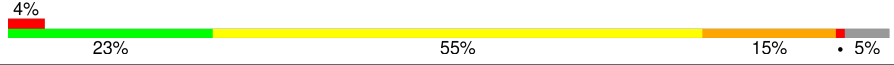
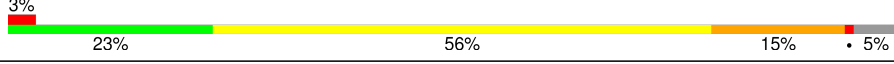
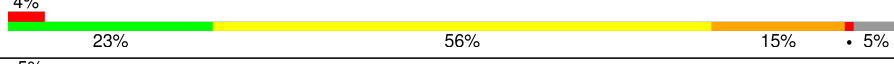
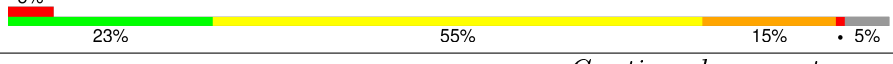
The reported resolution of this entry is 3.35 Å.

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}	91344	1005 (3.42-3.30)
Clashscore	102246	1076 (3.42-3.30)
Ramachandran outliers	100387	1059 (3.42-3.30)
Sidechain outliers	100360	1058 (3.42-3.30)
RSRZ outliers	91569	1010 (3.42-3.30)

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. 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	

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Mol	Chain	Length	Quality of chain
1	F	777	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>5%24%55%15%5%</div></div>
2	O	149	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%24%61%13%</div></div>
2	P	149	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%22%64%12%</div></div>
2	Q	149	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%23%62%13%</div></div>
2	R	149	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%21%63%13%</div></div>
2	S	149	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>3%22%63%13%</div></div>
2	T	149	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>2%23%62%13%</div></div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 43044 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 adenylylase.

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

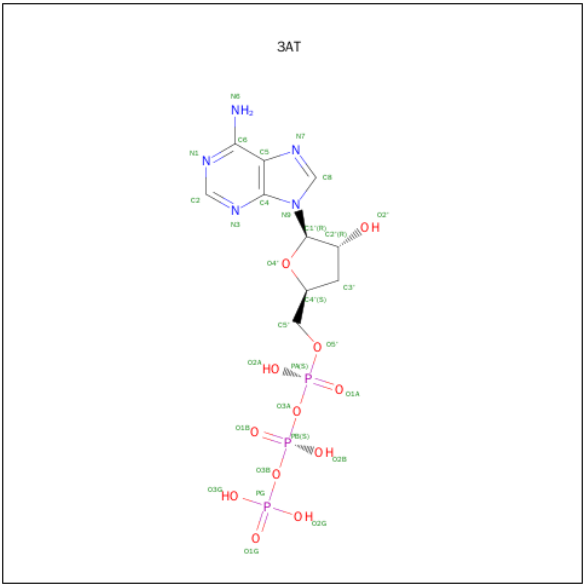
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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	2	Total 2	Mg 2	0	0
4	E	2	Total 2	Mg 2	0	0
4	B	2	Total 2	Mg 2	0	0
4	C	2	Total 2	Mg 2	0	0
4	A	2	Total 2	Mg 2	0	0
4	F	2	Total 2	Mg 2	0	0

- Molecule 5 is 3'-DEOXYADENOSINE-5'-TRIPHOSPHATE (three-letter code: 3AT) (formula: C₁₀H₁₆N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
5	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
5	C	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
5	D	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
5	E	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
5	F	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

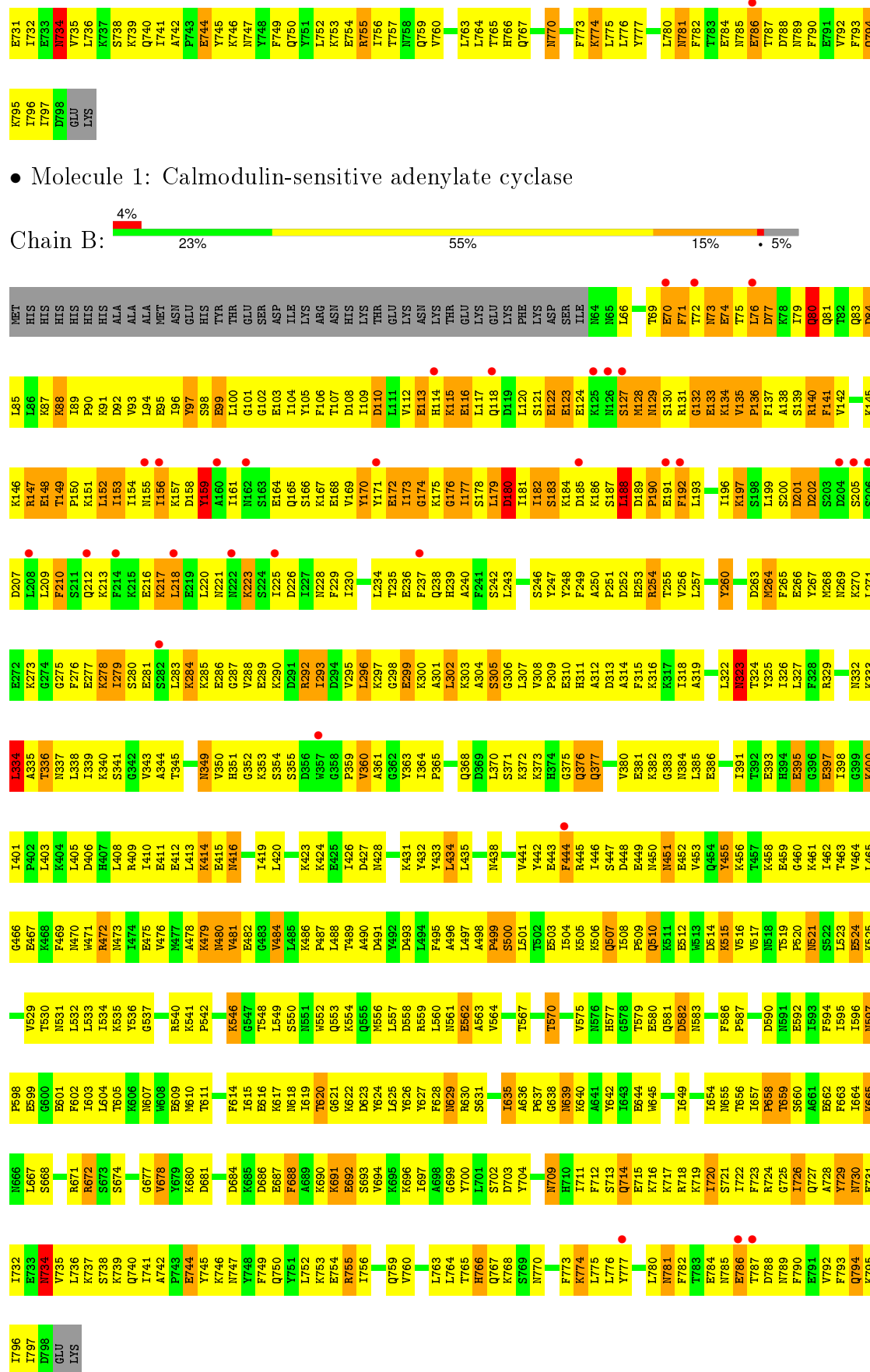
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			1	1		
6	B	1	Total	O	0	0
			1	1		
6	C	1	Total	O	0	0
			1	1		
6	D	1	Total	O	0	0
			1	1		

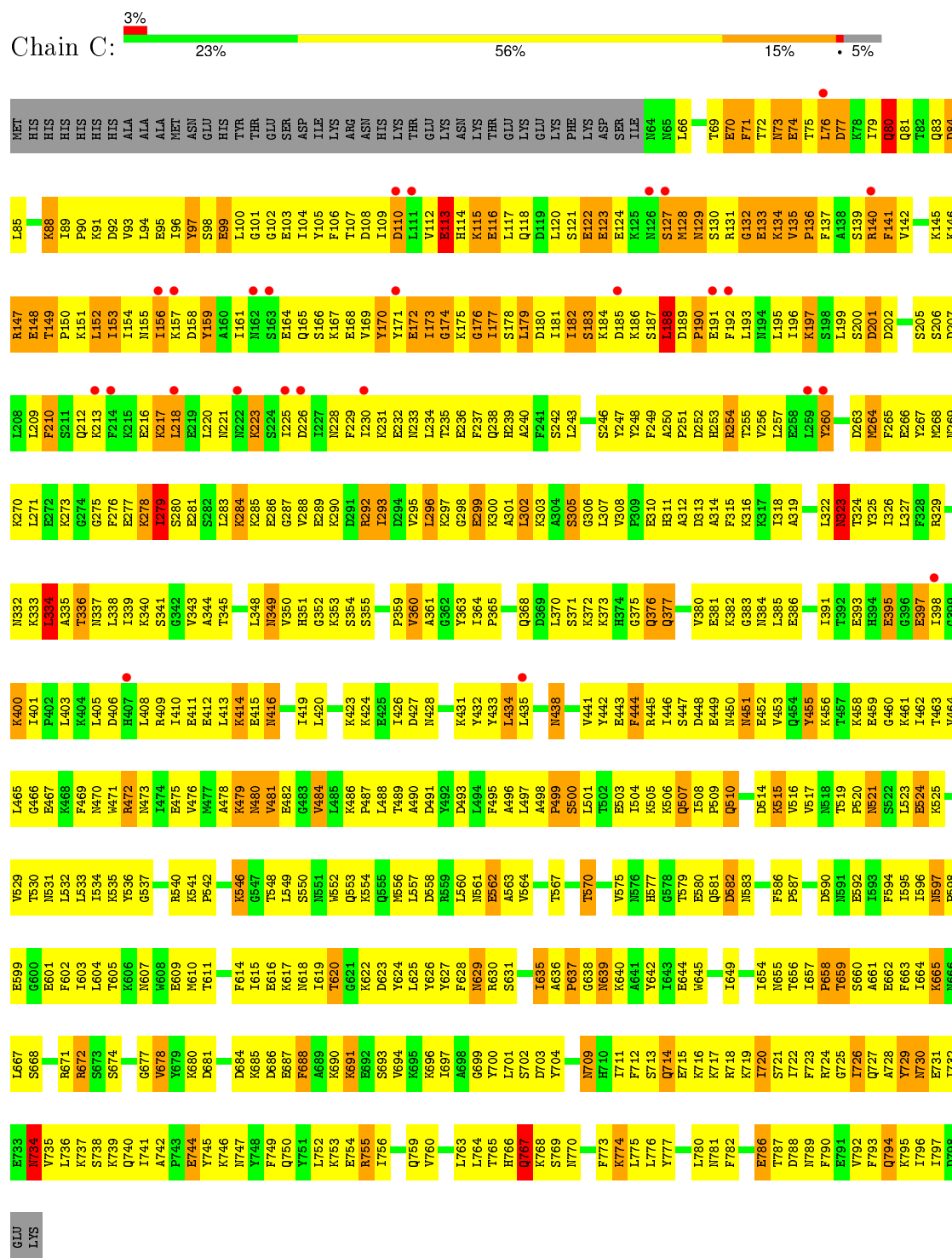
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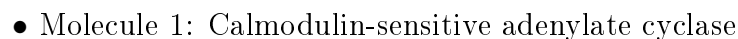
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	1	Total	O	0	0
			1	1		
6	F	1	Total	O	0	0
			1	1		

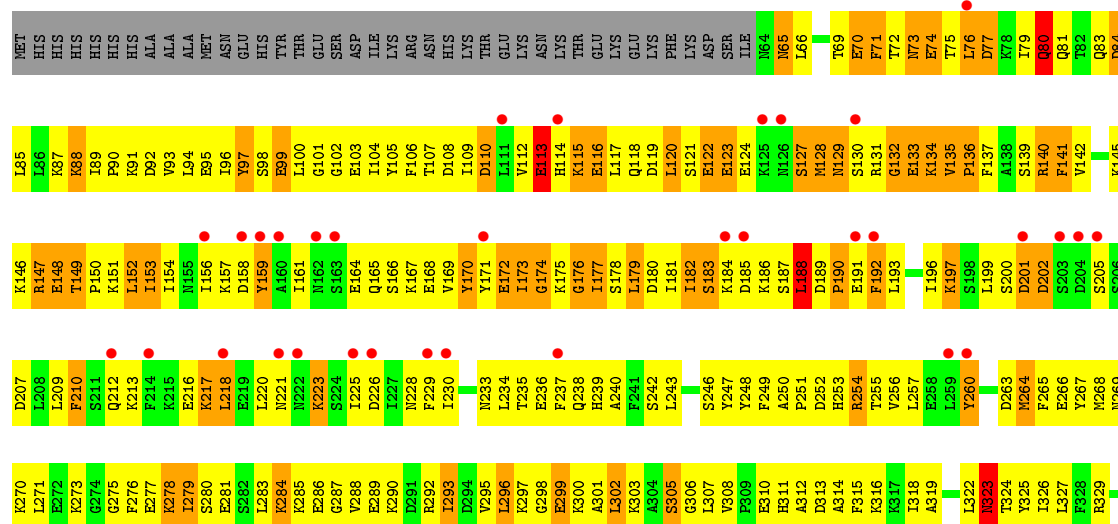


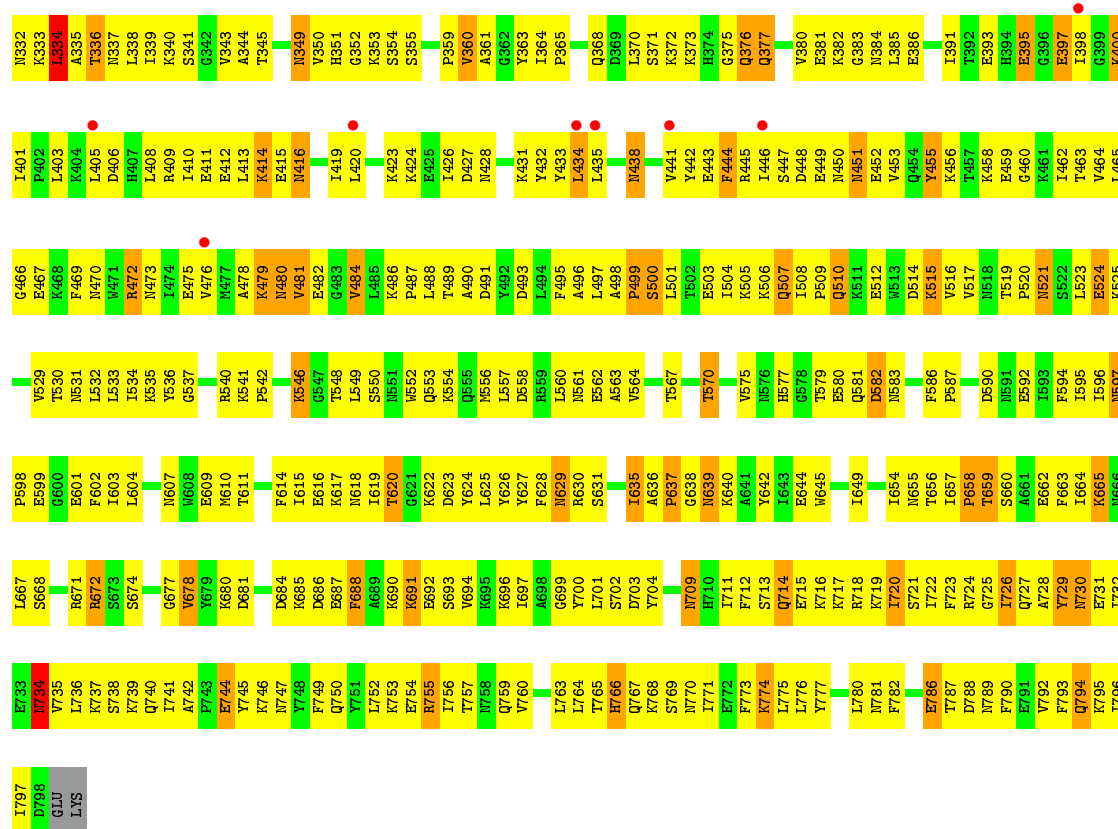
• Molecule 1: Calmodulin-sensitive adenylate cyclase



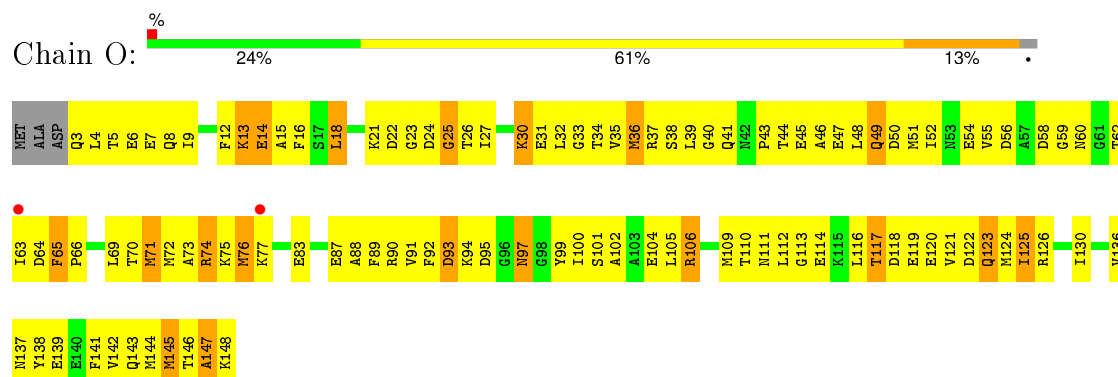


R147	L95	HIS	MET
E148	K98	HIS	
T149	I99	HIS	
P150	P90	HIS	
K151	K91	HIS	
L152	D92	HIS	
I153	V93	ALA	
T154	L94	ALA	
N155	E95	ALA	
I156	K157	MET	
K157	I96	ASN	
L158	Y97	GLU	
Y159	S98	GLU	
A160	E99	HIS	
I161	L100	TYR	
N162	G101	THR	
S163	G102	GLU	
E164	E103	SER	
K165	I104	ASP	
S166	Y105	ILE	
K167	F106	LYS	
E168	T107	ARG	
Y169	D108	ASN	
Y170	I109	ASN	
Y171	D110	LYS	
E172	L111	THR	
I173	Y112	GLU	
G174	E113	LYS	
K175	H114	ASN	
G176	K115	LYS	
I177	E116	THR	
S178	L117	GLU	
L179	Q118	LYS	
D180	D119	GLU	
I181	L120	LYS	
I182	S121	PRE	
S183	E122	LYS	
K184	E123	ASP	
D185	E124	SER	
K186	N125	ILE	
S187	K126	ILE	
L188	S127	P64	
D189	M128	P65	
P190	N129	L66	
E191	S130		
F192	R131	T69	
L193	G132	F71	
	E133	T72	
K197	K134	N73	
S198	V135	E74	
L199	P136	T75	
S200	F137	L76	
D201	A138	D77	
D202	S139	K78	
S203	R140	I79	
D204	F141	S80	
S205	V142	Q81	
S206		T82	
D207	K145	S83	
S208	K146	T84	

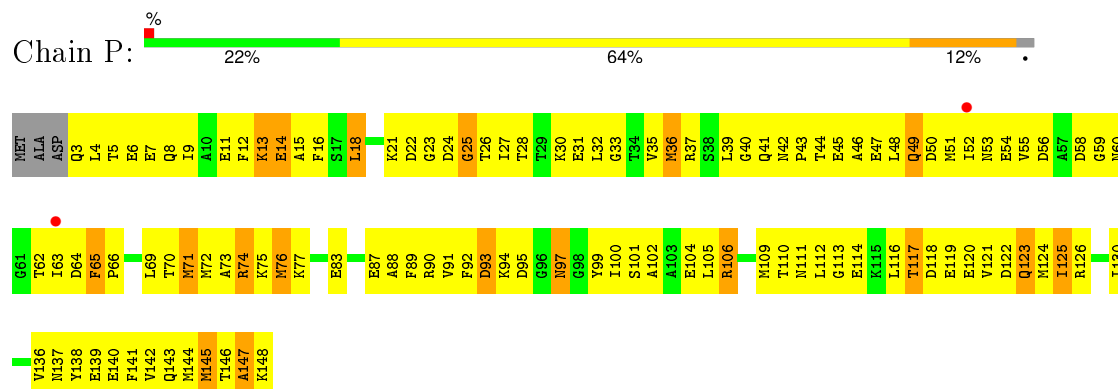




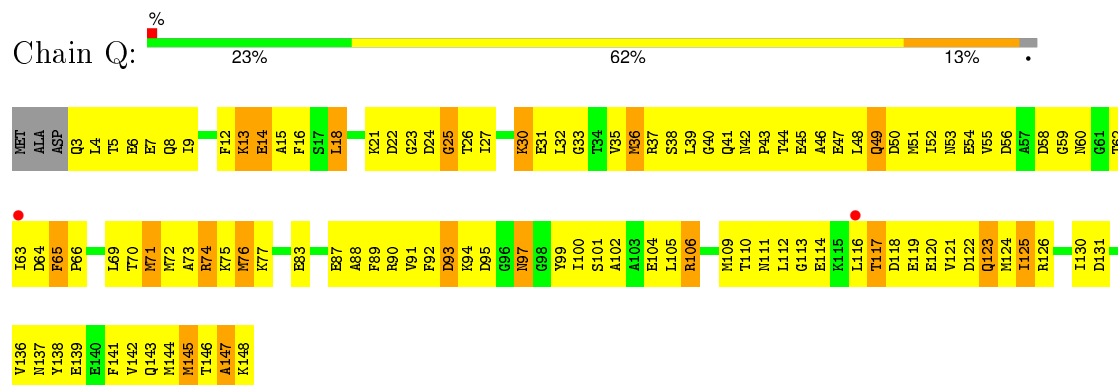
• Molecule 2: Calmodulin 2



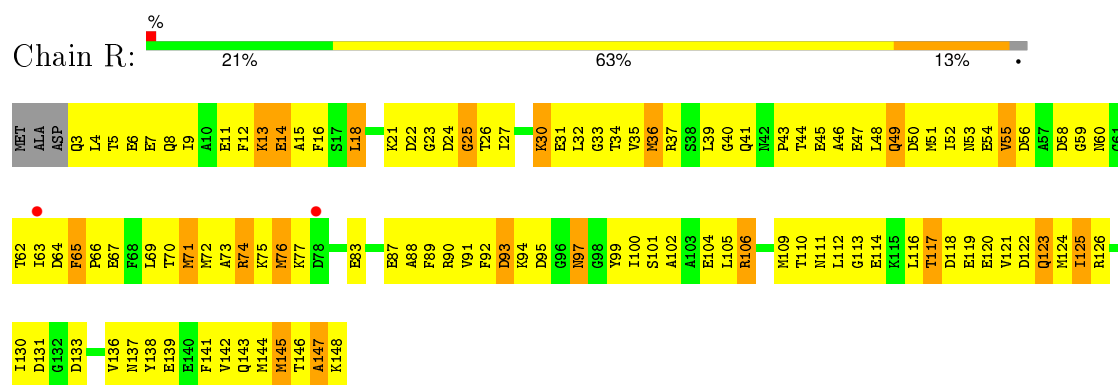
• Molecule 2: Calmodulin 2



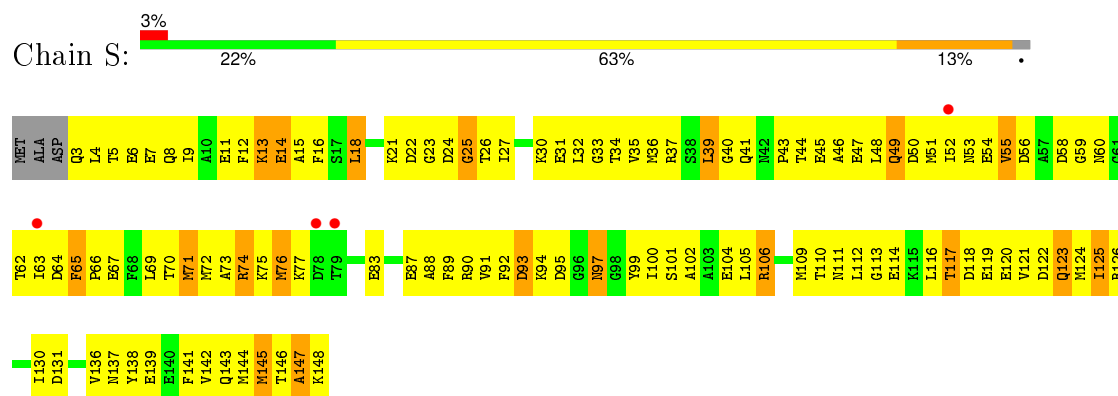
● Molecule 2: Calmodulin 2



● Molecule 2: Calmodulin 2



● Molecule 2: Calmodulin 2



● Molecule 2: Calmodulin 2



V132	D133
V136	M137
Y138	E139
E140	F141
V142	Q143
M144	M145
T146	A147
K148	

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	184.60Å 319.29Å 142.05Å 90.00° 90.22° 90.00°	Depositor
Resolution (Å)	29.57 – 3.35 35.51 – 3.35	Depositor EDS
% Data completeness (in resolution range)	92.6 (29.57-3.35) 91.6 (35.51-3.35)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 3.32Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.263 , 0.282 0.250 , 0.265	Depositor DCC
R_{free} test set	5479 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	97.5	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 56.3	EDS
Estimated twinning fraction	0.458 for -1/2*h+1/2*k,3/2*h+1/2*k,-l 0.458 for -1/2*h-1/2*k,-3/2*h+1/2*k,-l 0.440 for 1/2*h+1/2*k,3/2*h-1/2*k,-l 0.447 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.439 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 114975 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	43044	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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, 3AT

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	0.53	0/6104	0.82	13/8208 (0.2%)
1	B	0.54	0/6104	0.83	13/8208 (0.2%)
1	C	0.56	1/6104 (0.0%)	0.89	22/8208 (0.3%)
1	D	0.56	3/6104 (0.0%)	0.85	15/8208 (0.2%)
1	E	0.56	2/6104 (0.0%)	0.85	16/8208 (0.2%)
1	F	0.54	0/6104	0.84	12/8208 (0.1%)
2	O	0.53	0/1158	0.76	0/1553
2	P	0.54	0/1158	0.76	0/1553
2	Q	0.55	0/1158	0.75	0/1553
2	R	0.55	0/1158	0.76	0/1553
2	S	0.56	0/1158	0.76	0/1553
2	T	0.56	0/1158	0.76	0/1553
All	All	0.55	6/43572 (0.0%)	0.83	91/58566 (0.2%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	740	GLN	C-N	-5.88	1.20	1.34
1	C	766	HIS	C-N	-5.74	1.20	1.34
1	D	784	GLU	C-N	5.50	1.46	1.34
1	D	621	GLY	C-N	5.27	1.46	1.34
1	E	784	GLU	C-N	5.14	1.45	1.34

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	766	HIS	O-C-N	-15.18	98.42	122.70
1	C	767	GLN	CA-C-N	12.73	145.20	117.20
1	C	766	HIS	CG-ND1-CE1	9.42	121.39	108.20
1	C	766	HIS	ND1-CG-CD2	-8.71	93.81	106.00
1	C	767	GLN	O-C-N	-7.95	109.99	122.70

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	771	2
1	B	5992	0	6010	765	2
1	C	5992	0	6010	770	2
1	D	5992	0	6009	771	3
1	E	5992	0	6009	772	3
1	F	5992	0	6010	755	1
2	O	1146	0	1071	150	0
2	P	1146	0	1071	157	0
2	Q	1146	0	1071	155	0
2	R	1146	0	1071	157	0
2	S	1146	0	1071	162	0
2	T	1146	0	1071	157	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	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
5	A	30	0	12	1	0
5	B	30	0	12	1	0
5	C	30	0	12	1	0
5	D	30	0	12	1	0
5	E	30	0	12	1	0
5	F	30	0	12	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
All	All	43044	0	42556	5389	8

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 63.

The worst 5 of 5389 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:E:179:LEU:O	1:E:183:SER:CB	1.74	1.36
1:D:179:LEU:O	1:D:183:SER:CB	1.77	1.30
1:F:179:LEU:O	1:F:183:SER:CB	1.80	1.30
1:C:179:LEU:O	1:C:183:SER:CB	1.77	1.30
1:F:188:LEU:H	1:F:188:LEU:CD2	1.46	1.27

The worst 5 of 8 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:D:685:LYS:NZ	1:D:685:LYS:NZ[2_657]	2.03	0.17
1:A:75:THR:CG2	1:E:786:GLU:O[4_556]	2.09	0.11
1:B:786:GLU:O	1:D:75:THR:CG2[4_656]	2.12	0.08
1:F:75:THR:CG2	1:F:786:GLU:O[2_557]	2.13	0.07
1:B:75:THR:CG2	1:D:786:GLU:O[4_656]	2.14	0.06

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%)	497 (68%)	179 (24%)	57 (8%)	1	9
1	B	733/777 (94%)	494 (67%)	183 (25%)	56 (8%)	1	10
1	C	733/777 (94%)	491 (67%)	187 (26%)	55 (8%)	1	11
1	D	733/777 (94%)	492 (67%)	187 (26%)	54 (7%)	1	11
1	E	733/777 (94%)	490 (67%)	186 (25%)	57 (8%)	1	9
1	F	733/777 (94%)	492 (67%)	186 (25%)	55 (8%)	1	11
2	O	144/149 (97%)	103 (72%)	30 (21%)	11 (8%)	1	10
2	P	144/149 (97%)	103 (72%)	30 (21%)	11 (8%)	1	10
2	Q	144/149 (97%)	103 (72%)	30 (21%)	11 (8%)	1	10
2	R	144/149 (97%)	103 (72%)	29 (20%)	12 (8%)	1	8
2	S	144/149 (97%)	103 (72%)	30 (21%)	11 (8%)	1	10
2	T	144/149 (97%)	103 (72%)	30 (21%)	11 (8%)	1	10
All	All	5262/5556 (95%)	3574 (68%)	1287 (24%)	401 (8%)	1	10

5 of 401 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	GLY
1	A	183	SER
1	A	302	LEU
1	A	787	THR
1	B	137	PHE

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%)	562 (85%)	102 (15%)	3	16
1	B	664/705 (94%)	558 (84%)	106 (16%)	3	14
1	C	664/705 (94%)	560 (84%)	104 (16%)	3	15
1	D	664/705 (94%)	558 (84%)	106 (16%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	664/705 (94%)	558 (84%)	106 (16%)	3	14
1	F	664/705 (94%)	558 (84%)	106 (16%)	3	14
2	O	123/127 (97%)	103 (84%)	20 (16%)	3	14
2	P	123/127 (97%)	105 (85%)	18 (15%)	4	18
2	Q	123/127 (97%)	104 (85%)	19 (15%)	3	16
2	R	123/127 (97%)	103 (84%)	20 (16%)	3	14
2	S	123/127 (97%)	105 (85%)	18 (15%)	4	18
2	T	123/127 (97%)	104 (85%)	19 (15%)	3	16
All	All	4722/4992 (95%)	3978 (84%)	744 (16%)	3	15

5 of 744 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	156	ILE
1	D	786	GLU
2	R	13	LYS
1	D	201	ASP
1	D	444	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 225 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	770	ASN
1	D	581	GLN
2	O	49	GLN
1	D	64	ASN
1	D	376	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 30 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$
5	3AT	A	903	4	24,32,32	1.41	4 (16%)	26,50,50	1.37	4 (15%)
5	3AT	B	904	4	24,32,32	1.40	4 (16%)	26,50,50	1.35	4 (15%)
5	3AT	C	905	4	24,32,32	1.45	4 (16%)	26,50,50	1.37	4 (15%)
5	3AT	D	906	4	24,32,32	1.42	4 (16%)	26,50,50	1.34	4 (15%)
5	3AT	E	907	4	24,32,32	1.37	4 (16%)	26,50,50	1.31	4 (15%)
5	3AT	F	908	4	24,32,32	1.36	4 (16%)	26,50,50	1.33	4 (15%)

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
5	3AT	A	903	4	-	0/18/34/34	0/3/3/3
5	3AT	B	904	4	-	0/18/34/34	0/3/3/3
5	3AT	C	905	4	-	0/18/34/34	0/3/3/3
5	3AT	D	906	4	-	0/18/34/34	0/3/3/3
5	3AT	E	907	4	-	0/18/34/34	0/3/3/3
5	3AT	F	908	4	-	0/18/34/34	0/3/3/3

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	905	3AT	PG-O2G	-3.16	1.43	1.54
5	E	907	3AT	PG-O2G	-3.14	1.43	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	903	3AT	PG-O2G	-3.04	1.43	1.54
5	B	904	3AT	PG-O2G	-3.01	1.43	1.54
5	D	906	3AT	PG-O2G	-2.89	1.44	1.54

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	905	3AT	N3-C2-N1	-3.23	126.42	128.89
5	A	903	3AT	N3-C2-N1	-3.09	126.53	128.89
5	B	904	3AT	N3-C2-N1	-3.02	126.58	128.89
5	F	908	3AT	N3-C2-N1	-2.98	126.61	128.89
5	D	906	3AT	N3-C2-N1	-2.94	126.64	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	903	3AT	1	0
5	B	904	3AT	1	0
5	C	905	3AT	1	0
5	D	906	3AT	1	0
5	E	907	3AT	1	0
5	F	908	3AT	1	0

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%)	0.37	39 (5%) 30 30	26, 80, 136, 148	0
1	B	735/777 (94%)	0.30	32 (4%) 38 37	27, 80, 136, 148	0
1	C	735/777 (94%)	0.31	26 (3%) 48 47	27, 80, 136, 148	0
1	D	735/777 (94%)	0.32	29 (3%) 43 42	27, 80, 136, 150	0
1	E	735/777 (94%)	0.34	36 (4%) 33 32	26, 80, 136, 148	0
1	F	735/777 (94%)	0.36	41 (5%) 28 27	27, 80, 136, 148	0
2	O	146/149 (97%)	0.13	2 (1%) 78 79	33, 63, 124, 131	0
2	P	146/149 (97%)	0.13	2 (1%) 78 79	33, 63, 124, 131	0
2	Q	146/149 (97%)	0.12	2 (1%) 78 79	33, 62, 124, 131	0
2	R	146/149 (97%)	0.16	2 (1%) 78 79	33, 63, 124, 131	0
2	S	146/149 (97%)	0.15	4 (2%) 58 58	32, 62, 124, 131	0
2	T	146/149 (97%)	0.12	3 (2%) 67 67	33, 62, 124, 131	0
All	All	5286/5556 (95%)	0.30	218 (4%) 41 40	26, 76, 134, 150	0

The worst 5 of 218 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	126	ASN	8.7
1	D	162	ASN	7.9
1	A	222	ASN	7.8
1	D	171	TYR	7.5
1	B	126	ASN	7.3

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	3AT	A	903	30/30	0.92	0.24	-0.25	60,74,93,94	0
5	3AT	C	905	30/30	0.92	0.22	-0.32	62,73,94,95	0
5	3AT	B	904	30/30	0.92	0.23	-0.39	58,73,93,94	0
3	CA	T	812	1/1	0.98	0.16	-0.56	49,49,49,49	0
3	CA	Q	806	1/1	0.97	0.16	-0.62	57,57,57,57	0
3	CA	P	703	1/1	0.97	0.15	-0.66	62,62,62,62	0
5	3AT	E	907	30/30	0.93	0.22	-0.69	60,74,96,97	0
5	3AT	F	908	30/30	0.92	0.21	-0.71	61,75,94,95	0
3	CA	O	802	1/1	0.98	0.14	-0.84	52,52,52,52	0
5	3AT	D	906	30/30	0.92	0.21	-0.85	58,74,94,95	0
3	CA	T	811	1/1	0.95	0.17	-1.04	33,33,33,33	0
3	CA	S	809	1/1	0.95	0.16	-1.04	26,26,26,26	0
3	CA	S	709	1/1	0.96	0.11	-1.08	57,57,57,57	0
3	CA	O	801	1/1	0.98	0.16	-1.08	30,30,30,30	0
3	CA	R	807	1/1	0.97	0.14	-1.15	33,33,33,33	0
3	CA	R	808	1/1	0.98	0.11	-1.19	54,54,54,54	0
3	CA	Q	705	1/1	0.93	0.10	-1.20	55,55,55,55	0
3	CA	P	804	1/1	0.98	0.10	-1.29	52,52,52,52	0
3	CA	S	810	1/1	0.99	0.12	-1.44	56,56,56,56	0
3	CA	T	711	1/1	0.96	0.10	-1.44	55,55,55,55	0
3	CA	R	707	1/1	0.96	0.10	-1.64	62,62,62,62	0
3	CA	P	803	1/1	0.98	0.14	-1.71	31,31,31,31	0
3	CA	Q	805	1/1	0.95	0.17	-2.04	27,27,27,27	0
3	CA	O	701	1/1	0.93	0.06	-3.16	51,51,51,51	0
4	MG	C	903	1/1	0.93	0.15	-	9,9,9,9	0
4	MG	F	907	1/1	0.98	0.11	-	34,34,34,34	0
4	MG	E	906	1/1	0.97	0.14	-	26,26,26,26	0
4	MG	A	902	1/1	0.97	0.16	-	28,28,28,28	0
4	MG	F	906	1/1	0.97	0.15	-	11,11,11,11	0
4	MG	E	905	1/1	0.98	0.13	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	MG	D	905	1/1	0.97	0.10	-	43,43,43,43	0
4	MG	A	901	1/1	0.96	0.20	-	5,5,5,5	0
4	MG	B	902	1/1	0.94	0.21	-	17,17,17,17	0
4	MG	C	904	1/1	0.98	0.15	-	26,26,26,26	0
4	MG	D	904	1/1	0.95	0.17	-	8,8,8,8	0
4	MG	B	903	1/1	0.98	0.13	-	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.