



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 15, 2024 – 08:50 AM EDT

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 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

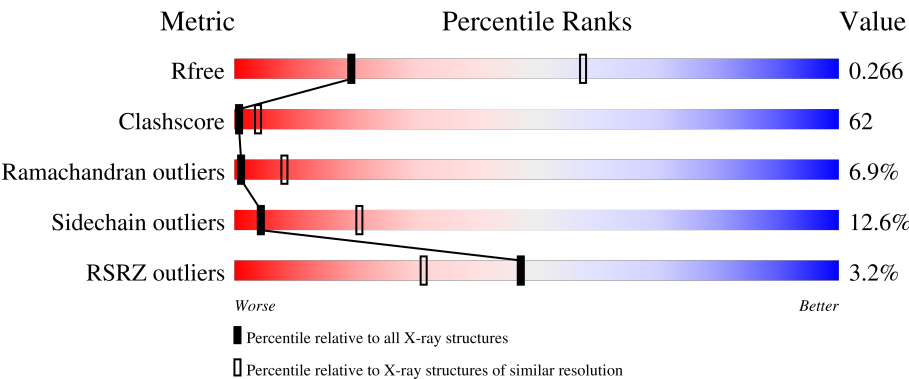
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 of 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>4%</div><div>29%</div><div>54%</div><div>10%</div><div>5%</div></div>
1	B	777	<div><div>3%</div><div>29%</div><div>54%</div><div>10%</div><div>5%</div></div>
1	C	777	<div><div>3%</div><div>29%</div><div>54%</div><div>10%</div><div>5%</div></div>
1	D	777	<div><div>4%</div><div>30%</div><div>53%</div><div>10%</div><div>5%</div></div>
1	E	777	<div><div>3%</div><div>29%</div><div>54%</div><div>10%</div><div>5%</div></div>

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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>4%29%54%10%5%</div></div>
2	O	149	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%24%53%20%..</div></div>
2	P	149	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%25%51%20%..</div></div>
2	Q	149	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%24%53%17%..</div></div>
2	R	149	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%23%54%19%..</div></div>
2	S	149	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%23%54%17%..</div></div>
2	T	149	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%23%54%18%..</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 42858 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	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	A	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
3	D	1	Total Mg 1 1	0	0

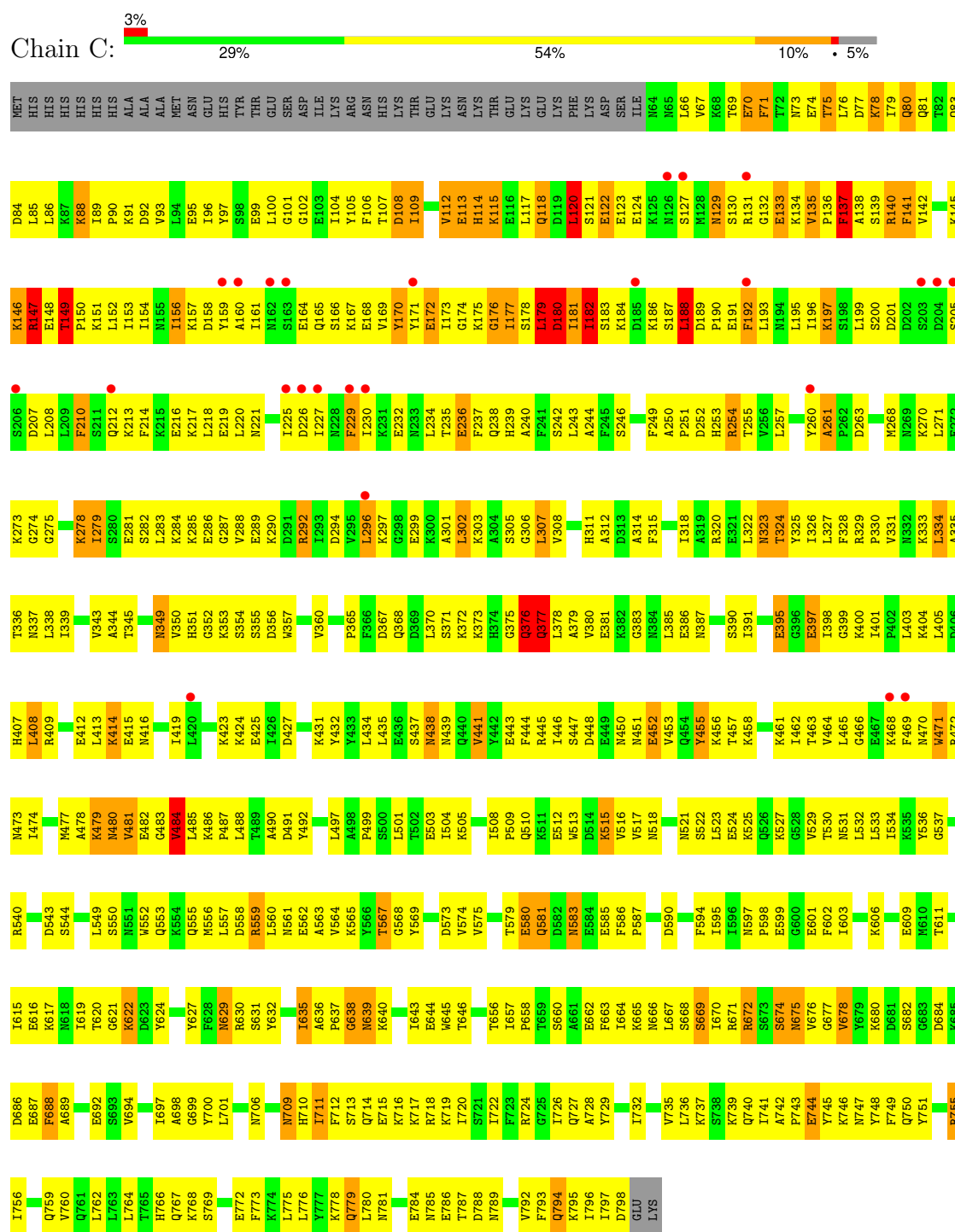
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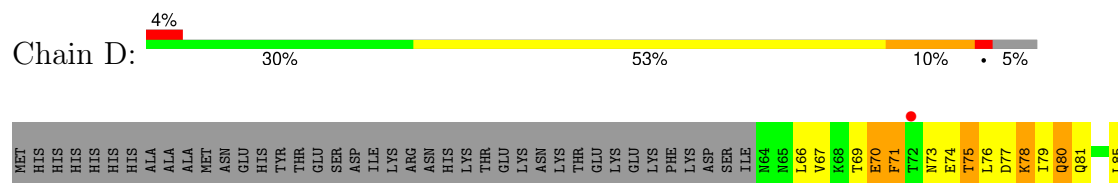
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total 1	Mg 1	0	0
3	F	1	Total 1	Mg 1	0	0

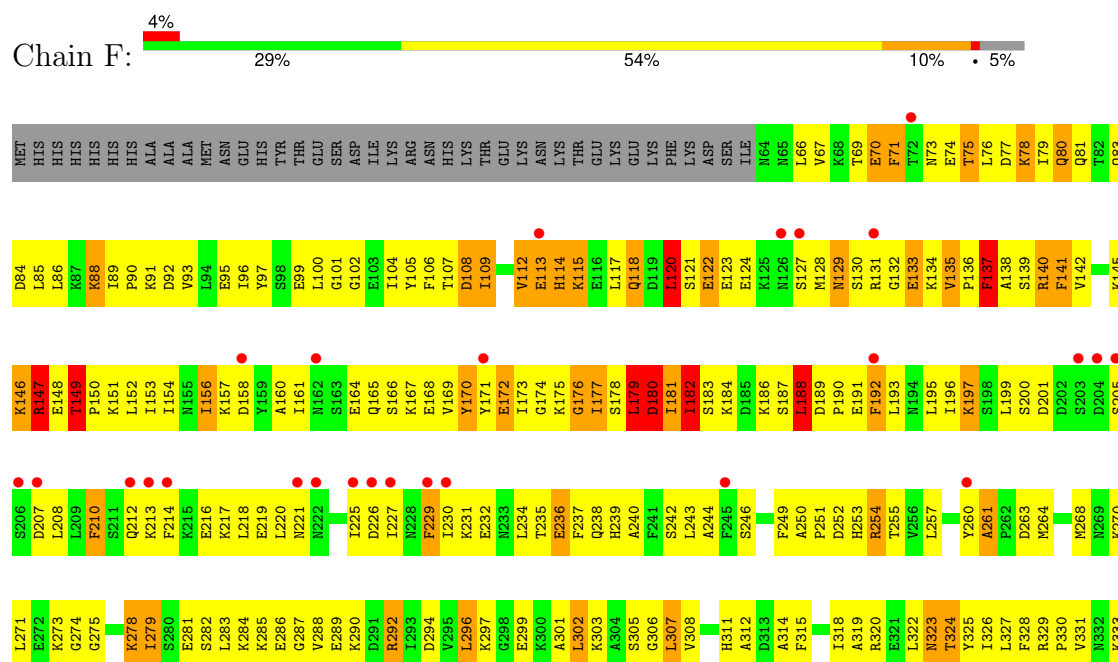
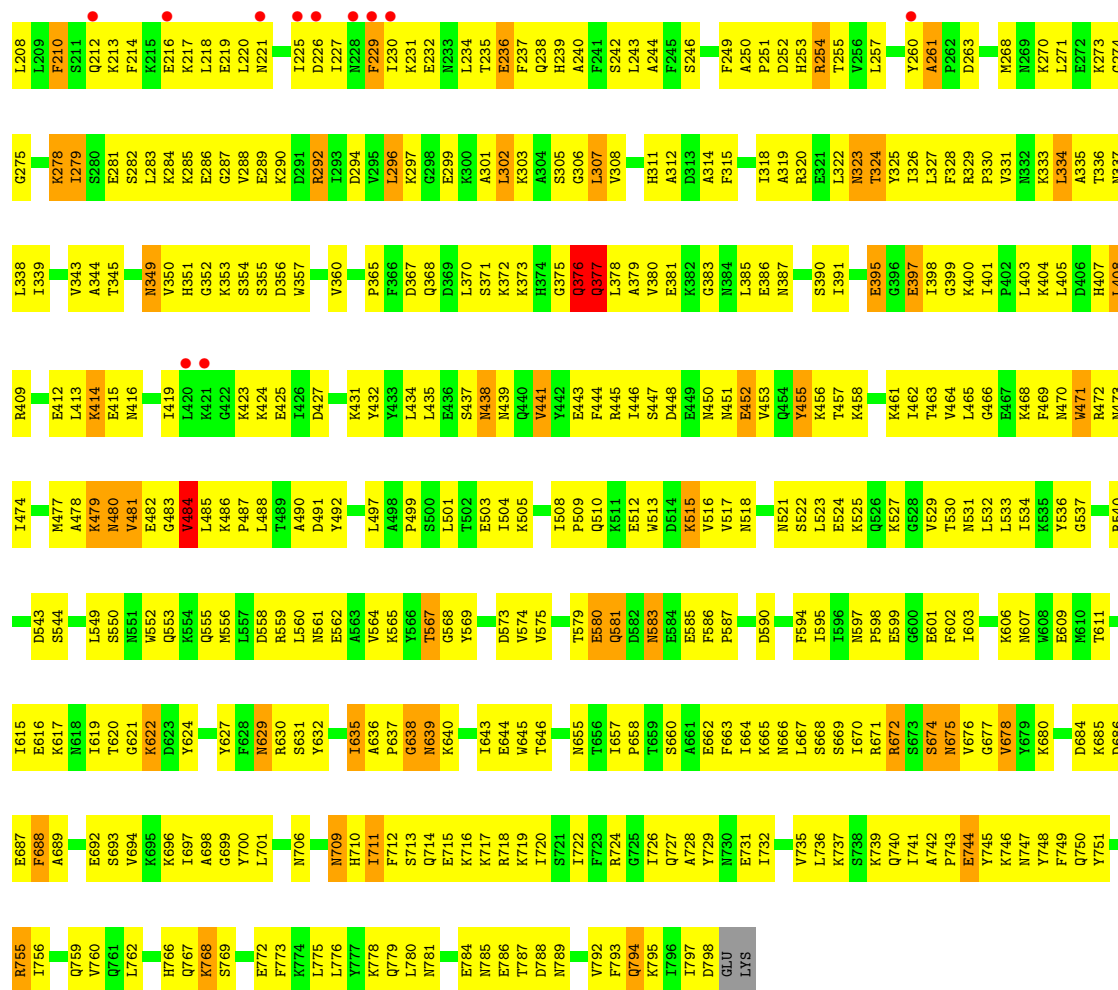
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

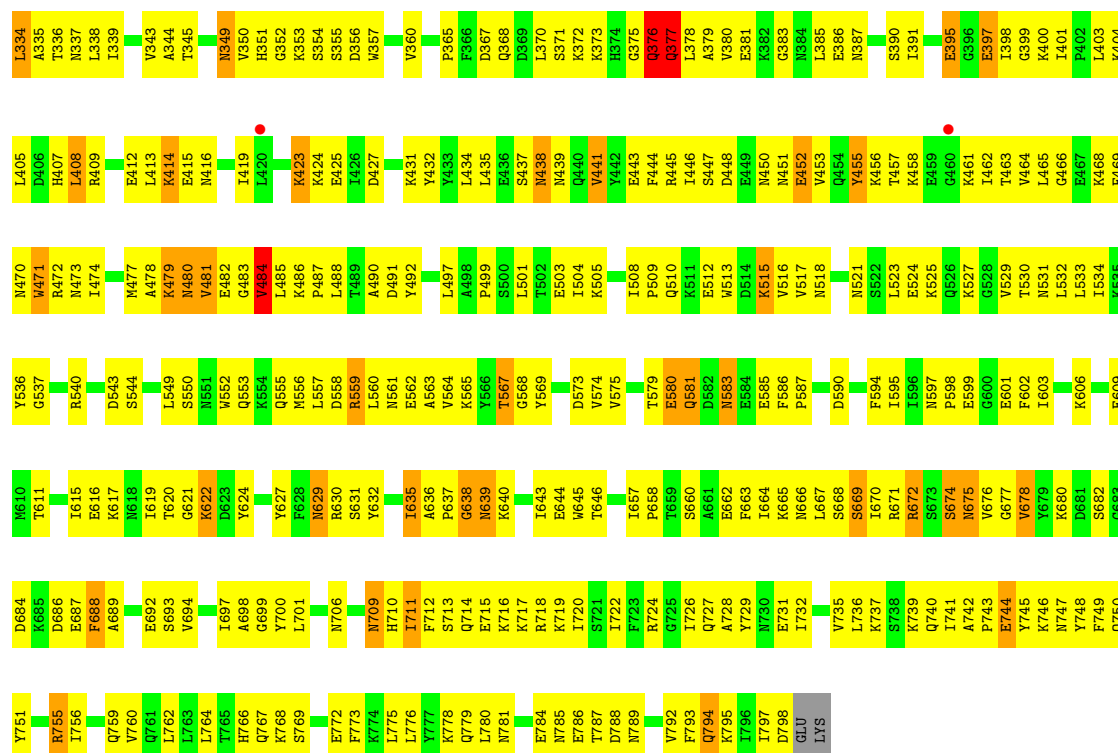
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	O	4	Total 4	Ca 4	0	0
4	P	4	Total 4	Ca 4	0	0
4	Q	4	Total 4	Ca 4	0	0
4	R	4	Total 4	Ca 4	0	0
4	S	4	Total 4	Ca 4	0	0
4	T	4	Total 4	Ca 4	0	0



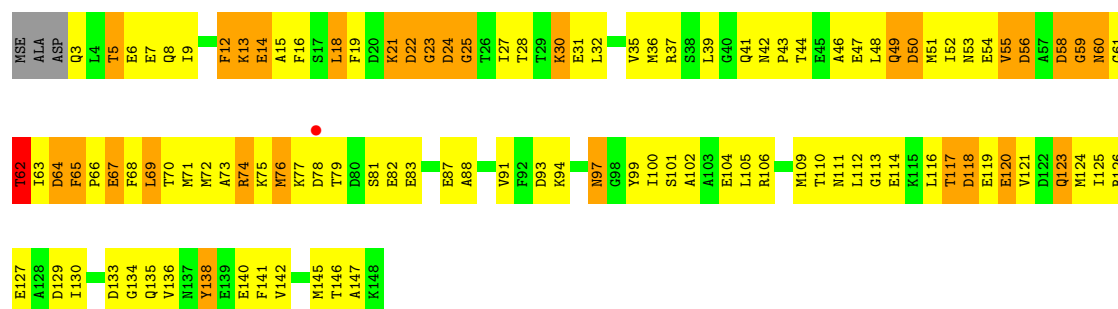
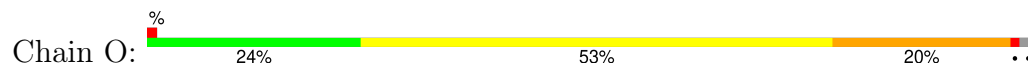
- Molecule 1: Calmodulin-sensitive adenylylate cyclase







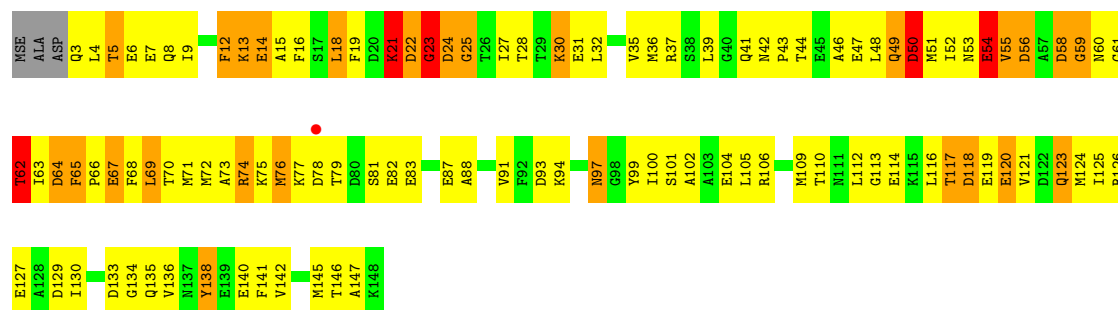
- Molecule 2: Calmodulin 2



- Molecule 2: Calmodulin 2



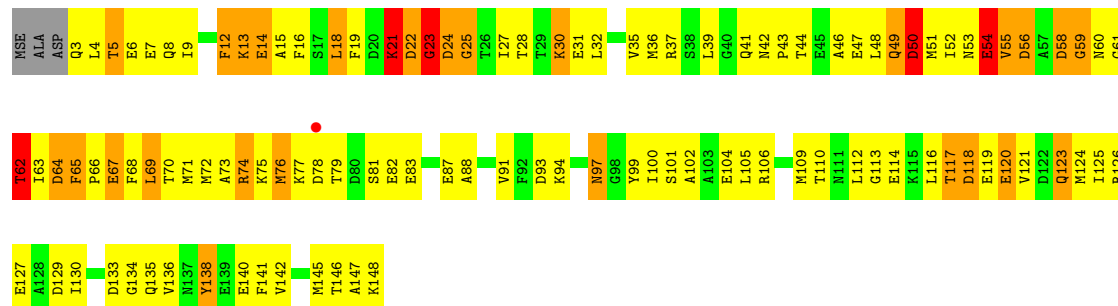
• Molecule 2: Calmodulin 2



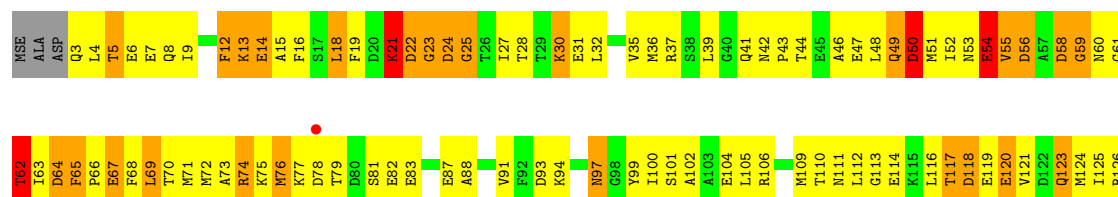
• Molecule 2: Calmodulin 2



• Molecule 2: Calmodulin 2



• Molecule 2: Calmodulin 2



E127	A128	D129	I130	D133	G134	Q135	V136	N137	Y138	E139	E140	F141	V142	Q143	M144	M145	T146	A147	R148
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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 , 0.266	Depositor DCC
R_{free} test set	6706 reflections (5.07%)	wwPDB-VP
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 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
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
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.

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

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 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	720	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 62.

The worst 5 of 5285 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)
2:S:62:THR:CB	2:S:62:THR:CG2	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	Interatomic distance (Å)	Clash overlap (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 [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%)	526 (72%)	161 (22%)	46 (6%)	1	10
1	B	733/777 (94%)	525 (72%)	159 (22%)	49 (7%)	1	9
1	C	733/777 (94%)	526 (72%)	159 (22%)	48 (6%)	1	10
1	D	733/777 (94%)	523 (71%)	162 (22%)	48 (6%)	1	10
1	E	733/777 (94%)	522 (71%)	164 (22%)	47 (6%)	1	10
1	F	733/777 (94%)	526 (72%)	158 (22%)	49 (7%)	1	9
2	O	144/149 (97%)	110 (76%)	21 (15%)	13 (9%)	1	4
2	P	144/149 (97%)	108 (75%)	22 (15%)	14 (10%)	0	3
2	Q	144/149 (97%)	109 (76%)	23 (16%)	12 (8%)	1	5
2	R	144/149 (97%)	108 (75%)	24 (17%)	12 (8%)	1	5
2	S	144/149 (97%)	109 (76%)	23 (16%)	12 (8%)	1	5
2	T	144/149 (97%)	110 (76%)	22 (15%)	12 (8%)	1	5
All	All	5262/5556 (95%)	3802 (72%)	1098 (21%)	362 (7%)	1	8

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%)	5	22
1	B	664/705 (94%)	585 (88%)	79 (12%)	5	22
1	C	664/705 (94%)	585 (88%)	79 (12%)	5	22
1	D	664/705 (94%)	584 (88%)	80 (12%)	5	22
1	E	664/705 (94%)	585 (88%)	79 (12%)	5	22
1	F	664/705 (94%)	585 (88%)	79 (12%)	5	22
2	O	123/117 (105%)	103 (84%)	20 (16%)	2	11
2	P	123/117 (105%)	104 (85%)	19 (15%)	2	13
2	Q	123/117 (105%)	103 (84%)	20 (16%)	2	11
2	R	123/117 (105%)	104 (85%)	19 (15%)	2	13
2	S	123/117 (105%)	103 (84%)	20 (16%)	2	11
2	T	123/117 (105%)	103 (84%)	20 (16%)	2	11
All	All	4722/4932 (96%)	4129 (87%)	593 (13%)	4	21

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

Mol	Chain	Res	Type
1	F	646	THR
2	T	5	THR
2	O	13	LYS
1	F	644	GLU
2	Q	49	GLN

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

Mol	Chain	Res	Type
1	D	387	ASN
2	R	49	GLN
1	E	165	GLN
2	Q	111	ASN

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Mol	Chain	Res	Type
1	F	655	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

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, 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%)	-0.01	32 (4%) 34 21	34, 87, 140, 151	0
1	B	735/777 (94%)	0.01	23 (3%) 49 32	35, 87, 141, 153	0
1	C	735/777 (94%)	0.03	25 (3%) 45 29	34, 87, 141, 153	0
1	D	735/777 (94%)	0.01	28 (3%) 40 26	35, 87, 140, 152	0
1	E	735/777 (94%)	0.01	26 (3%) 44 28	34, 87, 140, 153	0
1	F	735/777 (94%)	-0.03	28 (3%) 40 26	34, 87, 140, 153	0
2	O	137/149 (91%)	-0.21	1 (0%) 87 81	27, 74, 124, 135	0
2	P	137/149 (91%)	-0.17	2 (1%) 73 61	28, 74, 124, 135	0
2	Q	137/149 (91%)	-0.18	1 (0%) 87 81	29, 74, 124, 135	0
2	R	137/149 (91%)	-0.24	1 (0%) 87 81	28, 74, 125, 135	0
2	S	137/149 (91%)	-0.24	1 (0%) 87 81	29, 74, 125, 135	0
2	T	137/149 (91%)	-0.24	1 (0%) 87 81	29, 73, 124, 135	0
All	All	5232/5556 (94%)	-0.03	169 (3%) 47 31	27, 83, 140, 153	0

The worst 5 of 169 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	204	ASP	8.7
1	C	126	ASN	7.6
1	E	204	ASP	6.9
1	B	126	ASN	6.5
1	F	162	ASN	6.1

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 ⓘ

There are no monosaccharides 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	CA	S	710	1/1	0.38	0.11	87,87,87,87	0
4	CA	P	704	1/1	0.42	0.07	82,82,82,82	0
4	CA	Q	706	1/1	0.45	0.07	84,84,84,84	0
4	CA	O	702	1/1	0.63	0.09	84,84,84,84	0
4	CA	T	712	1/1	0.65	0.11	85,85,85,85	0
4	CA	R	708	1/1	0.77	0.14	85,85,85,85	0
4	CA	Q	705	1/1	0.90	0.13	86,86,86,86	0
4	CA	R	707	1/1	0.93	0.13	85,85,85,85	0
3	MG	F	905	1/1	0.94	0.21	22,22,22,22	0
4	CA	S	810	1/1	0.94	0.18	44,44,44,44	0
4	CA	P	804	1/1	0.94	0.17	46,46,46,46	0
4	CA	Q	806	1/1	0.95	0.20	46,46,46,46	0
3	MG	B	901	1/1	0.95	0.27	28,28,28,28	0
3	MG	D	903	1/1	0.95	0.18	27,27,27,27	0
3	MG	E	904	1/1	0.95	0.22	23,23,23,23	0
3	MG	A	900	1/1	0.95	0.19	28,28,28,28	0
4	CA	O	701	1/1	0.95	0.14	83,83,83,83	0
4	CA	T	711	1/1	0.96	0.16	84,84,84,84	0
4	CA	P	703	1/1	0.96	0.15	88,88,88,88	0
4	CA	T	812	1/1	0.96	0.18	48,48,48,48	0
4	CA	S	709	1/1	0.97	0.19	83,83,83,83	0
4	CA	O	802	1/1	0.97	0.20	44,44,44,44	0
3	MG	C	902	1/1	0.98	0.23	23,23,23,23	0
4	CA	R	807	1/1	0.98	0.16	38,38,38,38	0
4	CA	S	809	1/1	0.99	0.16	37,37,37,37	0
4	CA	P	803	1/1	0.99	0.18	36,36,36,36	0
4	CA	R	808	1/1	0.99	0.18	44,44,44,44	0
4	CA	O	801	1/1	0.99	0.17	36,36,36,36	0
4	CA	T	811	1/1	0.99	0.15	43,43,43,43	0
4	CA	Q	805	1/1	0.99	0.16	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.