Full wwPDB X-ray Structure Validation Report (i)

May 18, 2020 – 05:00 am BST

PDB ID	:	6XWV
Title	:	Crystal structure of drosophila melanogaster CENP-C bound to CAL1
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Deposited on	:	2020-01-24
Resolution	:	2.27 Å(reported)

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

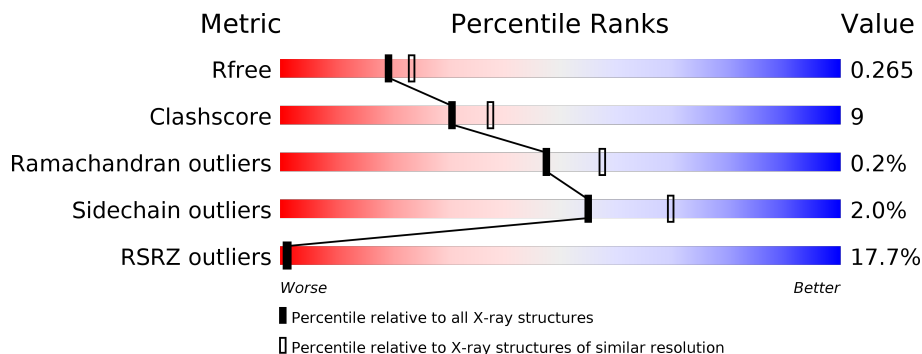|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.27 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	Percentile Ranks	Value
Rfree		0.265
Clashscore		9
Ramachandran outliers		0.2%
Sidechain outliers		2.0%
RSRZ outliers		17.7%

Worse ← → Better

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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 <=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	1411	2% / 7% • 91%
1	B	1411	% / 7% • 91%
1	C	1411	% / 8% • 91%
1	D	1411	2% / 7% • 91%
2	E	979	% / •• 98%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4229 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	133	Total 1041	C 659	N 178	O 197	S 7	0	0	0
1	B	125	Total 985	C 625	N 165	O 188	S 7	0	0	0
1	C	131	Total 1025	C 650	N 175	O 193	S 7	0	0	0
1	D	123	Total 969	C 617	N 160	O 185	S 7	0	0	0

- Molecule 2 is a protein called Ryanodine Receptor 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	24	Total 191	C 126	N 35	O 30	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total 6	O 6	0	0
3	E	1	Total 1	O 1	0	0
3	B	3	Total 3	O 3	0	0
3	C	3	Total 3	O 3	0	0
3	D	5	Total 5	O 5	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Calmodulin

Chain A:

GLY GLN ALA SER ILE LEU ARG ARG SER GLY LYS LYS LEU GLN HIS SER LYS GLN SER VAL GLN LYS SER ASN LYS GLU GLN ILE ILE ALA PRO TYR GLU ASN GLU ASP TYR ASP SER ASP GLU GLU PRO ILE TYR ASN GLU GLU TYR GLY LYS GLU GLU GLU SER ASN LYS ASN

VAL THR ARG ARG LYS SER ASP LYS ASP MET ALA SER HIS THR LEU GLU CYS ILE GLU GLY PRO ASP PRO ASN TRP ASN SER SER CYS ASN LYS GLU ARG GLU ASN HIS GLU ASN ALA LYS SER GLU ASP LEU ASN ARG SER GLN LYS LEU SER

ASN PRO ARG ASN ALA GLY THR LYS SER ALA LEU ASN ARG GLU GLU GLY GLU CYS SER GLU ASP SER VAL MET GLU SER LEU ARG VAL ASN THR PRO PRO ILE ASP GLN ASN ASP SER ASP VAL PRO ARG ASN SER PRO ARG THR LEU

LEU SER ASP VAL PRO THR SER ALA ARG ALA LEU LEU GLU PHE LEU GLN ARG GLN ASN SER MET LYS SER ARG PRO ASP GLU SER ALA ASP VAL VAL PHE LYS SER PRO LEU ALA PRO ALA ARG ALA SER LYS GLY LYS GLU VAL ASP LYS LYS

LEU ALA LYS MET PRO VAL ALA GLU LEU ASN THR GLY ILE ARG ARG SER LYS ARG GLY GLN VAL PRO LEU GLN MET SER CYS HIS THR MET ASP PRO SER LYS PHE ASN PHE MET GLY PHE ILE GLU GLU ARG SER LYS SER THR LYS GLY ASN LEU

SER LYS ALA LYS ALA SER ALA THR LYS PRO LYS THR VAL GLN LYS ASN LEU PRO ASP ARG GLY LEU CYS SER SER PRO ARG ILE GLU LYS LEU PRO GLY ALA ILE PRO SER GLU LEU GLY SER LEU THR TRP GLU GLU VAL GLN

ALA GLU ALA GLY VAL PRO LYS VAL LYS ARG GLY ARG PRO LYS LYS ALA VAL GLY VAL GLN THR ASP THR GLU GLU ARG PRO GLU GLU PRO GLU PRO MET ILE SER LEU ALA PRO ASP THR SER GLN GLU GLU PRO ASP VAL PRO ASP GLU GLN ALA PRO TYR THR GLU

ALA ALA LEU GLY PRO VAL VAL PHE SER THR PRO LEU ARG | D1274 E1275 Q1276 E1277 E1278 | K1282 | L1287 | V1290 G1291 D1292 A1293 P1294 P1295 | S1296 A1297 | SER MET SER ASP | E1302 N1303 A1304 S1305 | S1308 A1309 | D1321 | E1329 | L1333 G1334 | R1337 F1338 K1339 P1340 Y1341 Q1342 K1343 R1344 S1345 M1346

L1357 V1358 Q1359 | L1368 A1369 V1370 G1371 E1372 E1373 K1374 | S1378 V1379 L1380 R1381 | D1384 | D1389 R1390 | Y1394 | Q1397 N1398 | K1402 | L1406 M1407 C1408 I1409 R1410 | SER

- Molecule 1: Calmodulin

Chain B: 7% · 91%

MET SER LYS SER PRO GLN ASN ASP ASP THR LEU GLU LEU ASP ILE LEU SER GLN PRO VAL LYS ASP LYS GLU ARG PHE ALA ALA PHE MET MET ARG LYS LEU ALA GLU GLU LYS PRO ALA GLN ASN ASP ASN LEU PHE GLY ASN LYS PHE LEU GLU LYS ASP PHE LEU ASP GLU PHE GLU VAL PRO

LEU ILE LYS LYS SER GLN ALA LYS PRO LYS SER LEU LEU PRO GLU VAL GLN PRO LEU GLY GLU LEU VAL SER LYS ASP SER ALA THR GLY LYS VAL ASN GLU PRO PRO VAL ASP GLN ALA PRO ASN GLU ASN VAL PRO ARG ARG PRO THR LEU SER PRO ASN ASN ARG ARG

SER MET ARG SER GLY ASN VAL PRO GLY SER ASP LYS LEU ARG ARG HIS ALA ILE ARG ARG ARG SER CYS GLY ARG LEU LEU PRO GLY PHE GLU GLU THR VAL ASN LEU THR ARG SER ILE SER PRO VAL ASN PHE LEU PRO GLU ILE SER THR PRO CYS THR

GLU LYS GLN LYS GLU GLU VAL ALA LYS ASN THR ARG VAL GLU THR ASP LYS PRO ALA GLU LYS PRO MET GLU LEU SER GLU GLU PRO GLU GLY GLU ASN PRO LEU GLN LEU ARG THR TYR THR MET GLY LYS PRO ALA ARG ASN ILE LEU ALA GLU ILE GLN ILE CYS LYS GLU ARG

GLN SER SER PHE HIS LYS ASN VAL LEU GLN LEU ASP SER TYR SER GLY ARG ALA PRO TYR SER ARG PRO THR PRO SER PRO SER VAL ALA GLY LEU ARG ALA THR TYR THR MET GLU LYS PRO ALA GLY GLN LEU LEU LEU SER PRO HIS ARG TYR ASP THR PRO SER

LYS MET PRO VAL VAL LYS ALA LYS ARG PHE ASN GLN GLU LEU MET VAL PRO ASP THR PRO GLU ARG SER HIS ASP PRO ALA TRP GLN SER GLU GLU PRO GLN PRO GLU PHE VAL VAL PRO GLU THR GLN PRO ASP LEU GLU GLU LEU VAL GLN THR SER ARG SER ALA ILE SER

PRO ILE VAL VAL ILE ASN THR SER ASN SER ASN ARG VAL ARG ARG ASP ALA VAL MET ALA LYS SER VAL PRO THR SER PRO VAL THR LEU LYS ALA THR PRO PRO ILE ALA SER PRO ARG ALA ALA ALA PRO GLN SER ILE SER ILE ALA GLN LEU PRO ARG VAL GLU

GLU ASN ASP MET ALA ILE MET THR ASP ASP SER GLU SER GLU ASP HIS PRO SER VAL PRO LEU LEU ALA PRO MET LYS VAL PRO THR SER PRO VAL THR LEU ARG ARG LEU ARG SER ASN ARG ALA ALA ALA THR ILE GLU SER GLN GLU GLU SER MET ARG LEU ASN LEU HIS LYS

SER VAL ASN ALA LYS LYS SER SER LYS PRO ARG THR ILE PRO LEU ASN ALA PRO SER VAL ILE PRO PHE ALA GLU GLU LEU THR ARG MET SER ASN TYR GLU ILE GLU ASP LEU LYS ARG SER LEU GLU ILE TYR PRO LEU ASN GLY HIS ARG

ASN HIS ARG SER GLU LYS LEU ILE LEU GLU GLU GLU ILE GLN ARG GLU GLU LEU ARG ARG ASN LEU MET ASP GLU ALA GLU GLU LEU PRO LYS GLU GLN SER ASP ASP SER ASN GLU ASP TYR ILE PRO VAL PRO LYS THR GLN GLU SER LEU ARG LYS SER ASN ASP ARG SER

GLN GLY ARG ARG PRO ARG SER THR ARG ASP LEU PRO MET THR GLU LEU VAL ASN TYR SER LEU GLY LEU GLN THR LEU GLU THR ARG ARG LYS SER SER ASP GLY ARG CYS LEU TYR THR LYS SER SER ASP HIS GLU ASP SER ASN LEU SER PRO VAL

LYS LEU PRO ARG LEU SER ILE ILE VAL PRO PRO VAL SER LEU ARG TYR SER GLN SER GLN GLN ASN LEU ASP ILE VAL LEU MET ALA PRO ASP PHE HIS ASP SER VAL ASN SER ASP ALA ILE ILE ALA PRO PRO PRO GLY TYR VAL VAL ASN THR ARG GLY ARG SER THR SER ARG LYS ASN ASP LEU VAL PRO PRO PRO GLY GLY TYR GLU GLY GLY LYS ASP ASN ASP LEU VAL ASP GLU PRO ILE GLY TYR GLU GLY GLN GLU GLU GLU HIS ASP GLU ARG PRO SER GLN ILE PRO ARG CYS THR ALA GLU LEU GLN GLN SER THR GLN ASN GLY

ARG ARG ALA MET GLU ASN ALA GLN ASN LEU VAL PRO PRO PRO ILE GLU TYR VAL GLU GLU ASN ARG ASN ASN GLU GLN SER ARG ARG SER THR LYS ASN GLY LEU LEU VAL ASP ARG ASN THR HIS ASP GLU ILE ALA VAL TYR CYS GLU PRO PRO GLU PRO GLU GLU TYR ASP ASP ASP HIS

GLY GLN ALA ILE LEU ARG SER ARG SER LYS LYS GLU GLN HIS LYS GLN VAL GLN SER ASN LYS GLU GLN GLU SER ARG SER THR LYS ASN GLY LEU VAL ASP ARG PRO SER TYR ASN ASN ILE TYR ASN GLU GLU LYS SER GLN GLN ASN LYS ASN

VAL THR ARG ARG SER ASP MET ALA HIS THR LEU GLU CYS ILE GLU GLY PRO ASP PRO ASN TRP ASN SER CYS ASN LYS GLN ASN ARG ASN HIS GLN ASN ALA SER ASP LYS GLU ASN ASP ARG SER GLU LYS SER LEU SER

ASN PRO ARG GLN ALA ASN ALA VAL GLY THR GLU LYS SER VAL ALA LEU SER ASN ARG GLY GLU CYS THR GLU LYS SER SER ARG PRO ASP GLU MET GLY SER LEU ARG VAL ASN THR PRO THR PRO ILE ASP GLN ASN SER ASP VAL PRO SER ARG ASN SER PRO SER ARG THR LEU

LEU SER ASP ASP VAL PRO SER THR SER ARG ALA ALA LEU LEU GLU PHE LEU GLN ARG SER GLN ASN MET SER LYS SER ARG PRO ASP GLU SER SER ASP VAL PHE LYS PRO LEU ALA PRO ARG ALA LYS SER LYS LYS GLY LYS SER GLU VAL ASP LYS LEU LYS

LEU ALA LYS MET PRO VAL GLU GLU ALA GLU GLU LEU ASN THR GLY ILE ARG ARG SER LYS ARG GLY VAL PRO LEU GLN MET SER TRP CYS HIS THR MET ASP SER LYS PHE ASN PHE MET SER GLY PHE ILE GLU GLU PRO ARG SER LYS ASN SER SER THR LYS LYS GLY ASN LEU

SER LYS ALA LYS ALA SER ALA THR LYS PRO LYS PRO THR VAL GLU LYS ASN LEU PRO ASP ASN ARG GLY PRO LEU CYS SER SER THR PRO ARG ILE SER LEU LYS LEU PRO GLY ALA ILE PRO HIS SER GLU SER LEU GLY LEU SER THR LEU TRP GLU GLU THR GLU VAL GLN

ALA GLU ALA VAL LYS VAL LYS LYS ARG GLY ARG PRO LYS LYS VAL GLY GLY VAL GLN THR ASP THR GLU LEU ALA GLU ASP PRO GLU GLY PRO GLU PRO MET ILE SER VAL ALA PRO LEU THR SER ASP GLN GLU GLU PRO ASP VAL PRO ASP ASP GLN GLN ALA PRO TYR THR GLU

Chain C: 8% . 91%

MET SER LYS PRO GLN ASN ASP ASP THR LEU GLU LEU ASP ILE LEU SER GLN PRO VAL LYS ASP LEU ARG PHE ALA PHE MET MET ARG LEU ALA GLU LYS PRO ALA GLN ASP ASN LEU PHE GLY ASN PHE LYS LEU ASP PHE GLU LEU ASP GLU VAL PRO

LEU ILE LYS SER GLN GLN LYS PRO LYS SER LEU GLU PRO ASP VAL GLN GLN PRO LEU GLY LEU LEU VAL ASP SER LYS ASN ALA ALA THR GLU LYS VAL ASN GLU GLU PRO VAL ASP GLN ALA ASN ASP SER GLU VAL PRO ARG ASP ARG SER PRO ASN ASN ARG

SER MET ARG ARG GLY ASN VAL PRO GLY ASP SER GLU ARG LEU ARG HIS ALA ILE ARG ARG SER ASN CYS GLY GLN LEU LEU PRO ALA PHE GLU LEU THR VAL SER ILE SER SER PRO VAL ASN PHE LEU PRO GLU ILE SER LEU THR PRO CYS THR

GLU LYS GLN LYS GLU GLU VAL ALA LYS ASN THR ARG GLU VAL GLU THR ARG ARG LYS ASP ALA SER GLY CYS GLN ARG GLN GLN LEU LEU LEU PRO ALA VAL LEU ALA ALA GLU ILE GLN GLN ILE ILE CYS LYS GLU ARG

GLN SER PHE HIS LYS ASN VAL LEU GLN LEU ASP TYR SER GLY ARG ALA PRO TYR SER ARG PRO PRO THR PRO SER PRO SER VAL ALA GLY LEU ARG ARG THR TYR MET GLU LYS GLY PRO ALA PRO GLY GLN LEU LEU SER PRO HIS ARG TYR ASP THR PRO SER

LYS MET PRO VAL LYS LYS ALA LYS ARG PHE ASN GLN LEU MET GLU PRO VAL ASP GLU THR PRO GLU GLN ARG GLN SER HIS ASP PRO ALA TRP GLN SER GLU GLN PRO PHE VAL VAL PRO GLN THR GLN PRO ASP LEU GLU LEU VAL GLN THR LEU ARG SER ALA ILE SER

PRO ILE VAL VAL ILE ASN SER ASN ASN ARG VAL ARG ASP ALA VAL ALA MET LYS SER VAL PRO THR SER PRO VAL THR ALA LEU SER SER PRO ILE ALA PRO SER PRO ARG ARG SER ALA ALA ALA SER PRO GLN LYS ILE SER GLU ALA GLN LEU PRO ARG VAL GLU

GLU ASN MET ASP ALA ILE MET THR THR ASP GLU SER GLU HIS SER THR VAL PRO LEU LEU ASN ALA PRO SER GLY GLY ASN THR THR ARG GLN ARG ARG ARG LEU ARG SER ASN ALA ALA ARG ALA ILE GLU GLN SER GLU SER MET ARG LEU ASN LEU HIS LYS

SER VAL ASN LYS LYS PRO ARG LYS THR ALA ILE PRO ASN LYS ALA PRO SER ALA PRO ILE ASN GLY GLU GLN PHE ALA ARG GLU GLU THR MET SER ASN GLU ILE LEU ASP LEU ARG LYS ASN SER LEU GLU ILE TYR LEU GLY HIS ARG

ASN HIS ARG SER GLU LYS LEU ILE LEU LEU GLU GLU GLU ILE GLN ARG GLU LEU ARG ARG ASN LEU MET ASP GLU GLU ALA GLU GLY LEU PRO LYS GLN SER SER SER ASP SER ASN GLU ASP TYR ILE LEU PRO VAL PRO ARG LEU ARG LYS SER ASP ARG SER

GLN GLY ARG ARG PRO SER ARG SER THR ARG ARG ASP LEU PRO MET THR THR GLU LEU VAL ASN TYR LEU GLY LEU SER GLN THR LEU GLU ARG ARG SER LYS ASP GLY LYS ARG LEU SER TYR LEU LYS GLY SER ASP SER ASP HIS SER ASP ARG SER PRO VAL

LYS LEU PRO ARG LEU SER LYS ILE SER ILE GLN ILE VAL PRO PRO PRO VAL SER LEU ARG TYR SER GLN LEU GLN ASN LEU PRO CYS SER GLY LYS PHE ASP PHE ASN VAL MET ALA ALA PRO ASP PHE HIS ASP VAL ASN SER ALA ILE GLU ILE ALA PRO

PRO PRO GLU VAL TYR VAL ASN THR ARG GLY ARG SER THR GLY ARG LYS SER LYS ASN ASP LEU PRO PRO GLY TYR GLY GLY GLN HIS ASP ARG PRO ARG CYS THR ALA LYS GLU GLN GLN SER THR GLN ASN GLY

ARG ARG ALA MET GLU ASN GLU VAL PRO PRO ILE GLY TYR VAL GLU GLU ASN ARG ASN GLN GLU ARG SER LYS ASN GLY LEU VAL ARG ASN THR HIS ASN ALA VAL GLU TYR CYS GLU PRO PRO GLU TYR ASP SER ASP HIS

GLY GLN ALA SER ILE LEU ARG SER GLY LYS LEU GLN HIS SER LYS GLN SER VAL GLN LYS ASN LYS GLU GLN ILE ALA PRO SER TYR GLU ASN GLU TYR GLY LYS GLU GLN GLN ASN LYS ASN

VAL THR ARG LYS SER ASP GLU MET ALA HIS THR LEU GLU CYS ILE GLU GLY PRO ASN TRP ASN SER CYS ASN LYS GLN ASN ARG HIS GLN ASN ALA LYS SER GLU LYS ASN ASP ALA ARG SER LYS GLN LYS LEU SER

ASN PRO ARG GLN ASN ALA VAL GLY THR GLU LYS SER ALA LEU SER ASN ARG GLY GLU GLN CYS THR GLU LYS SER ARG ASP VAL MET GLY GLU LEU ARG ASN THR PRO PRO ILE ASP GLN ASN SER ASP GLU ALA ARG SER LYS GLN LYS THR LEU

LEU SER ASP VAL PRO SER THR SER ARG ALA ALA LEU GLU PHE LEU GLU ARG SER ASN MET SER GLU ALA ASP VAL PHE LYS PRO ALA ALA ALA ARG ALA LYS SER GLY LYS GLU VAL ASP LEU LYS

LEU ALA LYS MET PRO VAL GLU ALA GLU LEU ASN THR THR GLY ILE ARG SER LYS ARG GLN GLN MET SER TRP CYS HIS MET ASP PRO SER LYS PHE ASN PHE MET SER GLY PHE GLU ARG SER ASN SER THR LYS GLY ASN LEU

SER LYS ALA LYS ALA THR LYS SER ARG THR LYS PRO THR VAL GLU LYS ASN LEU PRO ASP ARG GLY LEU CYS SER SER THR PRO ARG ILE SER LEU PRO ARG MET ILE SER LEU PRO GLY ILE GLU GLY ARG SER PRO ARG THR LYS GLY ASN LEU

ALA GLU ALA GLY LYS VAL PRO LYS SER ARG GLY ARG PRO LYS ALA VAL GLY VAL GLN THR ASP GLU GLU ALA PRO GLY ILE HIS SER ASP SER LEU GLY LEU SER LEU THR LEU TRP GLU GLU GLU VAL GLN

D1274 E1277 K1282 W1286 L1287 R1288 G1289 V1290 G1291 D1292 A1293 P1294 P1295 S1296 A1304 N1310 L1333 G1334 Y1335 M1336 Y1341 M1346 K1347 V1351 H1352 L1357 E1362 V1370 G1371

E1372 E1373 K1374 E1375 V1376 H1377 R1381 D1389 R1393 Y1394 N1398 A1399 L1406 M1407 R1410 S1411

- Molecule 1: Calmodulin

2%

Chain D:
7% •
91%

MET SER LYS PRO GLN ASN ASN ASP THR LEU GLU LEU ASP ASP ILE LEU SER GLN PRO VAL LYS ASP LYS GLU ARG PHE ALA ALA PHE MET MET ARG LYS LEU ALA GLU GLN ASN ASP LEU ASN ASN PHE GLY ASN PHE LEU LYS ASP PHE ASP GLU VAL PRO

LEU ILE LYS LYS GLN SER GLN ALA LYS PRO LYS SER SER LYS LEU PRO GLU VAL GLN PRO GLU LEU GLY LEU GLU LEU VAL SER LYS ASN SER ALA THR GLY VAL LYS VAL ASN GLU PRO PRO VAL ASP GLN ALA PRO ASN GLU ASN VAL PRO PRO ARG ARG SER PRO THR LEU SER PRO ASN ASN ARG

SER MET ARG SER GLY ASN VAL PRO GLY SER SER ASP LYS SER LEU ARG ARG HIS ALA ILE ARG ARG SER ARG SER CYS ARG GLN GLN LEU LEU PRO GLU PHE GLU GLU THR VAL ASN LEU THR ARG SER ILE SER PRO VAL ASN PHE LEU PRO GLU ILE SER SER THR PRO CYS THR

GLU LYS GLN GLU GLU GLU VAL VAL ALA LYS ASN THR THR ARG VAL GLU THR ASP LYS PRO ALA GLU LYS PRO MET GLU LEU SER GLN PRO GLU GLN ASN PRO LEU GLN LYS THR SER ALA ARG ASN PRO ILE LEU ALA GLU ILE GLU GLN ILE CYS LYS GLU ARG

GLN SER SER PHE HIS LYS ASN VAL LEU LEU ASP LEU GLN ASP TYR SER GLY ALA PRO SER ARG PRO TYR SER ARG PRO THR PRO SER PRO SER PRO VAL ALA GLU LEU ARG THR TYR MET GLU LYS GLY PRO ALA PRO GLY LEU LEU LEU SER PRO HIS ARG TYR ASP THR PRO SER

LYS MET PRO VAL LYS VAL LYS ARG ASN GLN LEU MET VAL PRO ASP THR PRO GLU LEU ARG GLN SER ASP PRO ALA TRP GLN SER GLU GLN PRO GLU VAL PHE VAL PRO THR GLN PRO ASP LEU GLY LEU GLU VAL LEU LEU SER ARG ALA ILE SER

PRO ILE VAL VAL ILE ASN THR SER ASN ASN ARG VAL ARG ASP ALA ALA MET SER VAL THR SER PRO VAL THR ALA LEU SER PRO ILE ALA PRO SER ARG ALA ALA SER PRO GLN LYS ILE LEU PRO ARG VAL GLU

GLU ASN MET ASP ALA ILE MET THR ASP ASP GLU SER GLU HIS PRO SER THR VAL PRO LEU ASN ALA PRO GLY GLY ASN THR ARG GLN ARG ARG SER ASN ARG ALA ALA ILE GLU GLN GLU SER MET ARG LEU LEU HIS LYS

SER VAL ASN ALA LYS LYS LYS SER LYS PRO ARG LYS THR ILE PRO ASN ALA PRO ALA PRO ILE GLY GLU PHE ALA ARG GLU LEU THR ARG MET SER ASN TYR ILE LEU ASP ARG LYS ARG SER LEU GLU ILE TYR LEU GLY HIS ARG

ASN HIS ARG SER GLU LYS LEU ILE LEU GLU GLU ILE GLN ARG GLU LEU ARG ASN LEU MET ASP GLU ALA GLU GLY LEU PRO LYS GLN SER ASP ASP ASN GLU ASP TYR ILE PRO VAL PRO LYS SER GLN SER ARG SER SER ASP ARG SER

GLN GLY ARG GLY ARG PRO ARG SER THR ARG ARG ASP LEU PRO MET THR GLU LEU VAL ASN TYR LEU GLY SER GLN THR LEU GLU ARG LYS SER ASP LYS ARG CYS LEU TYR THR LYS GLY SER SER ASP GLU ASP ASP SER LEU SER PRO VAL

LYS LEU PRO ARG LEU SER LYS SER ILE ILE GLN ILE VAL PRO VAL PRO PRO VAL SER ARG LEU ARG TYR SER SER GLN ASN LEU PRO CYS SER GLY LYS PHE ASP PHE ASN VAL VAL MET ALA ALA PRO ASP PHE HIS ASP SER ASN SER ALA ILE GLU ILE ALA PRO

PRO PRO PRO GLU TYR VAL VAL ASN THR ARG GLY ARG SER THR SER GLY ARG LYS SER ASN LYS ASN ASP LEU VAL LEU PRO PRO GLY TYR GLU GLN GLY GLU GLU HIS ASP ARG PRO GLN GLN PRO ARG CYS THR ALA LYS GLU GLN GLN SER THR GLN ASN GLY

ARG ARG ALA MET GLU ASN GLU VAL PRO PRO ILE GLU TYR VAL GLU ASN ARG ASN GLN SER ARG SER THR LYS ASN GLY LEU VAL ASP ASN THR HIS ALA VAL GLU TYR CYS GLY PRO PRO GLU PRO TYR ASP SER ASP HIS

GLY GLN ALA SER ILE LEU ARG SER GLY LYS GLU GLN HIS SER LYS GLN SER VAL GLN SER ASN LYS GLN ILE ILE ALA PRO SER TYR GLU ASN ASN GLU TYR ASP TYR ASP GLU GLU ILE TYR GLU GLU TYR GLY LYS GLU GLU SER ASN LYS ASN

VAL THR ARG LYS SER LYS ASP LYS SER GLY MET ALA HIS THR LEU GLU GLU CYS ILE GLU GLY ASP PRO ASN GLN TRP ASN SER SER CYS ASN LYS GLN ARG ASN HIS GLN ASN ALA LYS SER GLU GLN ASP LEU ALA ASN SER LYS SER GLN LEU SER

ASN PRO ARG GLN ASN ALA VAL GLY THR GLU LYS SER VAL ALA LEU ASN SER ASN ARG GLU GLU CYS THR GLU LYS SER ARG ASP ASP MET GLU SER GLU LEU ARG VAL ASN THR THR PRO ILE ASP GLN SER ASP VAL PRO ASN ARG PRO SER PRO SER ARG THR LEU

LEU SER ASP ASP VAL PRO SER THR SER ARG ALA ALA LEU GLU PHE LEU GLN ARG GLN ASN SER MET SER GLU PRO PRO GLU SER GLU ALA ASP VAL PHE LYS SER PRO LEU ALA PRO ARG ALA SER LYS GLY LYS GLU GLU VAL ASP LEU LYS

LEU ALA LYS MET PRO VAL GLU ALA GLU GLU LEU ASN THR THR GLY ILE ARG SER LYS ARG GLN VAL LEU PRO LEU MET SER TRP CYS HIS THR MET ASP PRO SER LYS PHE ASN PHE MET SER GLY PHE ILE GLU PRO ARG SER ASN SER THR LYS GLY ASN LEU

SER LYS ALA LYS ALA SER ALA THR LYS PRO THR VAL GLU LYS ASN LEU PRO ASN ARG LEU LEU CYS SER THR PRO ARG SER GLU LYS PRO ALA ILE PRO HIS SER LEU GLU LEU THR LEU TRP GLU GLU GLU VAL GLN

ALA GLU ALA GLU LYS VAL PRO LYS LYS ARG GLY ARG PRO LYS LYS ALA VAL GLY GLY VAL GLN THR ASP THR GLU ALA GLU PRO GLU PRO GLU PRO GLU PRO MET ILE SER SER VAL ALA PRO LEU THR SER ASP GLN GLU GLU PRO ASP PRO ASP GLN GLN ALA PRO TYR THR GLU

ALA ALA LEU GLY PRO VAL VAL PHE SER THR PRO LEU ARG **D1274** **E1277** **E1278** **A1279** **S1280** **T1281** **Q1285** **W1286** **G1289** **V1290** GLY ASP ALA PRO PRO SER ALA SER MET SER ASP GLU ASN ALA SER **V1306** SER THR **I1313** **F1314** **Y1315** **Q1316** **V1317** **D1318** **G1319** **I1320** **D1321** **Y1322** **A1323** **F1324** **K1328** **E1329** **M1332**

L1333 **G1334** **R1337** **Y1341** **Q1342** **A1349** **K1350** **V1351** **H1352** **P1353** **L1354** **K1355** **L1356** **L1357** **V1358** **N1364** **V1365** **E1366** **V1370** **V1379** **I1388** **Y1394** **N1398** **L1406** **M1407** **C1408** **I1409** **R1410** **S1411**

- **Molecule 2: Ryanodine Receptor 2**

Chain E:

MET ALA ASN ALA VAL VAL ASP GLU GLU THR LEU GLU ALA MET VAL TYR GLY ARG SER LYS ALA TRP SER SER LYS MET ALA ASP PHE ALA LEU GLU ASP GLY MET ILE ASP VAL ALA GLU PHE ASP ASN LEU PHE HIS GLY LEU ASP ALA GLU ASP PRO ASP LEU ASP VAL ALA

LYS GLU ALA VAL GLU ASP ASN VAL PRO ASP GLU ALA LYS MET GLY HIS ILE ALA ASN THR SER VAL THR LEU MET GLY ILE LEU ILE LEU CYS ALA ASN GLU ASP ASN GLU ALA LYS ALA GLU GLU ILE GLU ILE LEU ASN GLN THR VAL PRO VAL VAL GLU GLU HIS LYS ARG LYS

TRP GLU GLU ALA GLY LEU ASP ARG ILE ASP GLU THR PHE ASP GLU LYS GLN ILE GLU HIS HIS VAL GLY ARG TRP MET ARG ARG HIS ASN SER VAL TYR GLU LEU ALA SER PRO LYS TYR LEU PRO PRO HIS HIS ASN SER ILE SER ASP GLU SER ARG ASP THR VAL LEU MET HIS SER ILE

ASP THR ALA ARG TYR ILE GLN GLN SER ARG ARG ASN ALA HIS MET THR ASN LYS ASN MET SER THR ILE LYS MET TYR ARG ARG HIS ASN SER VAL TYR GLU LEU GLU ALA SER PRO LYS ASP GLU ARG LYS ILE ASN SER ARG ILE GLU ASP THR GLY PHE GLY CYS ASP GLU HIS SER ILE SER ARG

ARG GLU ARG GLU ARG GLN LEU ALA TYR LEU ALA SER THR PRO MET GLN CYS VAL TYR SER GLY GLY HIS GLN ARG GLU HIS HIS MET ARG ARG LYS ASN LEU ARG ARG ILE ASN SER TRP MET PHE ASP ALA SER SER GLU GLN ASP THR PHE GLY CYS ASP

ARG ARG HIS TYR ALA LEU SER SER TYR VAL GLN SER PRO TYR GLY ARG GLY GLU GLN ARG GLU HIS HIS MET ALA SER ARG MET THR HIS MET ARG GLN GLN HIS PHE ASP GLU MET GLU MET ASP LEU ARG ARG PRO ARG LEU PRO GLU ASN GLU CYS SER CYS SER GLY HIS

ASN SER ASP ARG LEU CYS ASN SER ASN VAL ILE HIS ILE ASN SER SER SER PRO TYR GLY ARG TRP VAL VAL GLU ASN ARG ASN HIS LEU THR GLN GLU THR GLN LYS THR ARG LYS ASN LEU PRO MET ASP ALA ARG LYS VAL SER HIS PRO VAL CYS SER GLY HIS

GLU GLN LYS PRO LEU SER SER LYS ALA THR SER VAL LEU SER LYS LEU VAL LEU LEU SER GLU LYS TYR MET GLN GLN MET PHE ASP SER SER GLU SER ASP GLU ASN ALA LEU LEU LYS LYS GLY LEU CYS SER ASP ALA ARG LYS VAL SER GLN PRO VAL MET THR PHE PRO ASN ALA ALA

GLY LYS ILE ILE THR HIS PRO THR SER SER SER ALA LYS LYS SER ALA PRO LYS ARG GLY ILE ARG GLU THR ARG PRO LEU ASN GLY GLU GLN ILE GLU GLU SER PRO THR ALA ASN ASN PRO ILE GLU SER SER THR TYR LEU PRO VAL ALA HIS MET LYS SER VAL SER ILE ASP SER SER SER SER GLY THR SER

ALA THR PHE GLY SER PRO ALA LYS LYS SER ALA PRO LYS ARG GLY ILE ARG GLU GLU THR PRO LEU ASN GLY ILE GLN LEU SER THR ILE ASP ASP GLU LYS ALA SER LEU MET GLU VAL LYS VAL ALA HIS MET LYS SER VAL ILE ASP GLY ARG SER PHE ASP ARG ASN

LYS ASP PHE MET HIS ASN SER SER THR SER LYS ALA VAL LYS SER GLN GLU VAL ILE PRO SER ILE THR ASN ILE GLU LYS SER THR LEU GLU LYS ALA LYS THR PHE HIS ASP MET ASN SER ASN THR GLY ALA THR PRO ILE GLU SER LEU GLU LYS LEU VAL ALA ALA LYS LYS

LYS GLN SER VAL ARG LYS THR GLY ALA THR GLY LYS PRO SER SER THR ARG LEU LYS SER GLU LYS THR ARG THR THR GLU GLU GLU VAL ARG GLU GLU ASP VAL SER GLU VAL LEU ALA LYS PRO LYS PRO GLN GLN CYS SER THR

THR ALA SER ILE LYS GLY LEU GLY ASP GLY ALA ALA ASP SER ASN ASP ASP ALA CYS TYR ARG VAL LEU PRO LYS ARG GLY VAL LYS ARG ALA VAL VAL SER THR THR GLU GLU GLU LYS THR ALA THR ASN SER SER PRO THR SER LEU GLU GLU MET GLY SER PRO ALA GLU LYS SER MET SER VAL PHE

ASN ASN GLN SER VAL ALA CYS ASN SER THR ALA LEU ALA ASN ASP THR ALA CYS TYR ARG VAL ALA ALA VAL LEU PRO LYS ARG GLY VAL LYS THR ALA THR ASN SER SER SER PRO THR SER LEU SER GLU GLU MET GLY SER PRO THR

GLY GLY ASP PRO ASP CYS THR VAL VAL THR SER THR THR GLY CYS GLU PRO PRO ALA SER GLU ARG GLN GLU ILE PRO ALA THR ILE LYS ILE THR LYS ARG GLY ILE LEU LEU HIS SER PRO SER ALA PRO GLU GLY GLY ALA SER PHE **T890** **L891** **T892** **E893** **Q894** **G895** **I899** **L909** **K910**

Y911 **H912** **I913** GLY SER ARG SER PHE ASP SER ARG HIS SER VAL TYR TYR GLN PRO THR PRO GLN LEU ALA ALA ALA LEU SER ALA PRO GLN ASP ALA GLN ASN ILE GLY ASN ILE SER GLY SER SER ALA SER ASP ASP ASP ILE PHE GLU GLN ILE ASN ARG TYR GLY THR VAL TYR SER

ILE LEU GLU ASN ASN SER GLY ASP LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	86.27Å 86.44Å 88.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.08 – 2.27 29.10 – 2.27	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.08-2.27) 92.1 (29.10-2.27)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 2.26Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.237 , 0.266 0.237 , 0.265	Depositor DCC
R_{free} test set	1961 reflections (6.33%)	wwPDB-VP
Wilson B-factor (Å^2)	40.5	Xtriage
Anisotropy	1.016	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 49.6	EDS
L-test for twinning [2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.000 for -l,-k,-h 0.000 for k,h,-l 0.000 for k,l,h 0.000 for l,h,k	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4229	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9248e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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)

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	0.36	0/1058	0.71	4/1425 (0.3%)
1	B	0.48	1/1000 (0.1%)	0.82	6/1345 (0.4%)
1	C	0.36	0/1042	0.56	1/1403 (0.1%)
1	D	0.36	0/984	0.67	1/1325 (0.1%)
2	E	0.24	0/195	0.42	0/262
All	All	0.39	1/4279 (0.0%)	0.69	12/5760 (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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1390	ARG	CZ-NH1	5.92	1.40	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1390	ARG	NE-CZ-NH2	-11.31	114.64	120.30
1	A	1381	ARG	CG-CD-NE	9.18	131.08	111.80
1	A	1339	LYS	CA-CB-CG	8.01	131.02	113.40
1	B	1278	GLU	CB-CA-C	6.60	123.60	110.40
1	B	1315	TYR	CA-CB-CG	6.33	125.42	113.40
1	B	1352	HIS	N-CA-C	5.93	127.02	111.00
1	D	1277	GLU	CA-CB-CG	5.64	125.80	113.40
1	B	1390	ARG	CD-NE-CZ	5.54	131.36	123.60
1	C	1277	GLU	CA-CB-CG	-5.44	101.43	113.40
1	A	1381	ARG	CA-CB-CG	5.37	125.22	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1406	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	1381	ARG	CB-CG-CD	-5.14	98.25	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1390	ARG	Sidechain

5.2 Too-close contacts (i)

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	1041	0	1021	18	0
1	B	985	0	962	24	0
1	C	1025	0	1009	12	0
1	D	969	0	943	22	0
2	E	191	0	192	5	0
3	A	6	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	5	0	0	0	0
3	E	1	0	0	0	0
All	All	4229	0	4127	77	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 9.

All (77) 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:1352:HIS:HE1	1:B:1411:SER:N	1.74	0.86
1:B:1352:HIS:HE1	1:B:1411:SER:H	1.27	0.80
1:D:1352:HIS:CD2	1:D:1353:PRO:HD2	2.22	0.75
1:D:1352:HIS:ND1	1:D:1410:ARG:HB3	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1352:HIS:CE1	1:B:1411:SER:N	2.57	0.73
1:D:1354:LEU:HB3	1:D:1388:ILE:HB	1.73	0.71
1:B:1343:LYS:HD3	1:B:1343:LYS:H	1.58	0.67
1:D:1352:HIS:CE1	1:D:1411:SER:O	2.48	0.67
1:B:1352:HIS:CE1	1:B:1411:SER:H	2.09	0.66
1:B:1369:ALA:HB3	1:B:1372:GLU:HG3	1.80	0.63
2:E:892:THR:HG23	2:E:895:GLY:H	1.64	0.63
1:D:1352:HIS:NE2	1:D:1411:SER:O	2.32	0.63
1:A:1390:ARG:HH11	1:A:1390:ARG:HG3	1.63	0.62
1:D:1356:LEU:HD22	1:D:1406:LEU:HD21	1.80	0.61
1:D:1349:ALA:HB1	1:D:1352:HIS:O	2.01	0.60
1:C:1346:MET:O	1:C:1347:LYS:HD3	2.02	0.60
1:C:1370:VAL:HG23	1:C:1371:GLY:H	1.66	0.60
1:D:1281:THR:O	1:D:1285:GLN:HG3	2.03	0.57
1:C:1352:HIS:ND1	1:C:1411:SER:O	2.37	0.57
1:A:1274:ASP:O	1:A:1278:GLU:HG3	2.05	0.56
1:D:1319:GLY:O	1:D:1342:GLN:NE2	2.33	0.55
1:D:1352:HIS:HE1	1:D:1411:SER:N	2.05	0.55
1:B:1352:HIS:ND1	1:B:1353:PRO:O	2.40	0.54
1:B:1353:PRO:HD3	1:B:1390:ARG:HH21	1.74	0.53
1:B:1401:ASP:OD2	1:B:1401:ASP:N	2.35	0.53
1:B:1278:GLU:O	1:B:1282:LYS:HG2	2.09	0.53
1:A:1321:ASP:HB2	1:A:1337:ARG:HB3	1.91	0.53
1:B:1288:ARG:HD3	1:B:1360:PHE:CE2	2.45	0.52
1:A:1390:ARG:HH11	1:A:1390:ARG:CG	2.23	0.52
1:D:1329:GLU:HG2	1:D:1332:MET:SD	2.51	0.50
1:A:1402:LYS:NZ	1:B:1276:GLN:HB2	2.27	0.49
1:C:1295:PRO:O	1:C:1310:ASN:HB3	2.12	0.49
1:C:1346:MET:HG2	1:C:1393:ARG:HB3	1.94	0.49
1:C:1362:GLU:HB3	1:C:1399:ALA:HB3	1.95	0.49
1:C:1362:GLU:HG3	1:C:1381:ARG:HG2	1.94	0.48
1:C:1346:MET:HA	1:C:1394:TYR:O	2.12	0.48
1:D:1321:ASP:HB2	1:D:1337:ARG:HB3	1.95	0.48
1:A:1344:ARG:NH2	1:A:1394:TYR:OH	2.46	0.48
2:E:912:HIS:O	1:C:1410:ARG:NH2	2.47	0.48
1:B:1343:LYS:N	1:B:1343:LYS:HD3	2.25	0.48
1:D:1341:TYR:HA	1:D:1398:ASN:O	2.14	0.48
1:B:1316:GLN:HA	1:B:1320:ILE:O	2.14	0.47
1:D:1329:GLU:CG	1:D:1332:MET:SD	3.02	0.47
1:D:1324:PHE:CD1	1:D:1334:GLY:HA3	2.50	0.47
1:B:1321:ASP:HB2	1:B:1337:ARG:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1343:LYS:HA	1:A:1397:GLN:HA	1.96	0.47
1:B:1315:TYR:N	1:B:1322:TYR:O	2.46	0.46
1:A:1378:SER:HB3	1:B:1306:VAL:HG21	1.98	0.46
1:A:1295:PRO:HG2	1:A:1309:ALA:HB1	1.98	0.45
1:C:1286:TRP:CD1	1:C:1287:LEU:HD23	2.52	0.45
1:A:1346:MET:HA	1:A:1394:TYR:O	2.18	0.44
1:A:1358:VAL:HA	1:A:1406:LEU:HD12	1.99	0.44
1:A:1341:TYR:HA	1:A:1398:ASN:O	2.17	0.44
1:D:1352:HIS:CE1	1:D:1411:SER:N	2.85	0.44
1:B:1349:ALA:HB1	1:B:1352:HIS:O	2.18	0.44
1:D:1364:ASN:OD1	1:D:1379:VAL:HG12	2.17	0.44
1:D:1354:LEU:HD23	1:D:1355:LYS:N	2.34	0.43
1:B:1346:MET:O	1:B:1347:LYS:HG2	2.19	0.43
1:D:1356:LEU:CD2	1:D:1406:LEU:HD21	2.45	0.43
1:A:1303:ASN:HD21	1:A:1305:SER:HB2	1.84	0.43
1:A:1276:GLN:HG2	1:B:1361:GLY:HA2	1.99	0.43
1:A:1290:VAL:HG13	1:A:1290:VAL:O	2.18	0.43
1:A:1303:ASN:ND2	1:A:1305:SER:HB2	2.34	0.43
1:C:1341:TYR:HA	1:C:1398:ASN:O	2.18	0.42
1:D:1366:GLU:O	1:D:1394:TYR:HA	2.20	0.42
1:B:1352:HIS:HA	1:B:1353:PRO:HD3	1.76	0.42
1:B:1366:GLU:O	1:B:1394:TYR:HA	2.20	0.42
1:D:1352:HIS:HE1	1:D:1410:ARG:C	2.23	0.42
2:E:895:GLY:O	2:E:899:ILE:HG12	2.21	0.41
2:E:909:LEU:HA	2:E:909:LEU:HD23	1.77	0.41
1:B:1324:PHE:CD1	1:B:1334:GLY:HA3	2.56	0.41
2:E:892:THR:HG23	2:E:895:GLY:N	2.33	0.41
1:C:1407:MET:HE3	1:C:1407:MET:HB2	1.86	0.41
1:D:1329:GLU:CD	1:D:1332:MET:SD	2.99	0.41
1:A:1402:LYS:HE2	1:A:1402:LYS:HB2	1.69	0.40
1:A:1380:LEU:HD22	1:A:1384:ASP:HB3	2.03	0.40
1:B:1352:HIS:HE1	1:B:1410:ARG:C	2.24	0.40

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	129/1411 (9%)	124 (96%)	4 (3%)	1 (1%)	19	22
1	B	121/1411 (9%)	119 (98%)	2 (2%)	0	100	100
1	C	127/1411 (9%)	121 (95%)	6 (5%)	0	100	100
1	D	119/1411 (8%)	117 (98%)	2 (2%)	0	100	100
2	E	22/979 (2%)	22 (100%)	0	0	100	100
All	All	518/6623 (8%)	503 (97%)	14 (3%)	1 (0%)	47	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1372	GLU

5.3.2 Protein sidechains (i)

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	110/1275 (9%)	107 (97%)	3 (3%)	44	59
1	B	105/1275 (8%)	102 (97%)	3 (3%)	42	56
1	C	109/1275 (8%)	106 (97%)	3 (3%)	43	57
1	D	103/1275 (8%)	103 (100%)	0	100	100
2	E	17/861 (2%)	17 (100%)	0	100	100
All	All	444/5961 (7%)	435 (98%)	9 (2%)	55	70

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1308	SER
1	A	1381	ARG
1	A	1389	ASP

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Mol	Chain	Res	Type
1	B	1310	ASN
1	B	1315	TYR
1	B	1343	LYS
1	C	1282	LYS
1	C	1346	MET
1	C	1389	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1352	HIS
1	C	1316	GLN
1	D	1397	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	133/1411 (9%)	1.00	24 (18%)	1	1	39, 62, 111, 152	0
1	B	125/1411 (8%)	0.99	21 (16%)	1	2	41, 67, 114, 141	0
1	C	131/1411 (9%)	1.03	21 (16%)	1	2	41, 64, 126, 147	0
1	D	123/1411 (8%)	1.07	22 (17%)	1	1	43, 74, 123, 154	0
2	E	24/979 (2%)	1.10	7 (29%)	0	0	48, 61, 83, 114	0
All	All	536/6623 (8%)	1.03	95 (17%)	1	1	39, 67, 118, 154	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1293	ALA	8.8
1	B	1315	TYR	8.6
1	D	1352	HIS	8.0
1	C	1292	ASP	7.9
1	A	1373	GLU	6.4
1	C	1370	VAL	6.1
1	A	1370	VAL	6.0
1	B	1305	SER	5.9
1	B	1352	HIS	5.7
1	B	1291	GLY	5.2
1	C	1351	VAL	5.2
1	D	1328	LYS	5.1
1	C	1291	GLY	5.1
1	C	1304	ALA	5.0
1	C	1289	GLY	4.9
1	D	1315	TYR	4.8
1	D	1351	VAL	4.6
1	A	1406	LEU	4.4
2	E	890	THR	4.4
1	A	1407	MET	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	1371	GLY	4.3
1	D	1289	GLY	4.1
1	B	1411	SER	4.1
2	E	895	GLY	3.8
2	E	892	THR	3.8
1	C	1371	GLY	3.7
1	B	1351	VAL	3.6
1	A	1408	CYS	3.6
1	A	1293	ALA	3.5
1	B	1357	LEU	3.5
1	A	1390	ARG	3.4
1	A	1302	GLU	3.4
1	D	1411	SER	3.4
2	E	894	GLN	3.3
1	D	1357	LEU	3.3
1	C	1376	VAL	3.3
1	A	1294	PRO	3.2
1	C	1407	MET	3.2
1	A	1333	LEU	3.2
1	B	1290	VAL	3.1
1	D	1286	TRP	3.1
1	A	1359	GLN	3.1
1	A	1381	ARG	3.0
1	C	1294	PRO	3.0
1	A	1374	LYS	2.9
1	B	1409	ILE	2.8
1	B	1408	CYS	2.8
1	D	1322	TYR	2.8
1	A	1296	SER	2.8
1	A	1357	LEU	2.8
2	E	893	GLU	2.8
1	B	1385	MET	2.8
1	C	1357	LEU	2.8
1	D	1280	SER	2.8
1	B	1278	GLU	2.8
1	D	1358	VAL	2.7
1	D	1317	VAL	2.7
1	A	1334	GLY	2.7
1	B	1289	GLY	2.7
1	D	1329	GLU	2.6
1	D	1370	VAL	2.6
1	A	1329	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	1390	ARG	2.6
1	A	1372	GLU	2.6
1	A	1358	VAL	2.6
1	B	1406	LEU	2.5
1	C	1334	GLY	2.4
1	D	1409	ILE	2.4
1	D	1407	MET	2.4
2	E	891	LEU	2.4
1	C	1377	HIS	2.3
1	B	1330	LYS	2.3
1	B	1275	GLU	2.3
1	B	1356	LEU	2.3
1	C	1290	VAL	2.3
1	D	1278	GLU	2.3
1	A	1291	GLY	2.3
1	D	1313	ILE	2.3
1	A	1282	LYS	2.2
1	C	1295	PRO	2.2
1	B	1329	GLU	2.2
1	B	1359	GLN	2.2
1	D	1408	CYS	2.2
1	D	1353	PRO	2.2
1	D	1410	ARG	2.2
1	C	1333	LEU	2.2
1	C	1336	MET	2.2
1	C	1373	GLU	2.1
1	C	1374	LYS	2.1
1	A	1287	LEU	2.0
1	A	1368	LEU	2.0
1	C	1406	LEU	2.0
1	B	1407	MET	2.0
1	D	1290	VAL	2.0
2	E	911	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.