Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:31 PM GMT

PDB ID	:	4IL1
Title	:	Crystal Structure of the Rat Calcineurin
Authors	:	Ye, Q.; Faucher, F.; Jia, Z.
Deposited on	:	2012-12-28
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

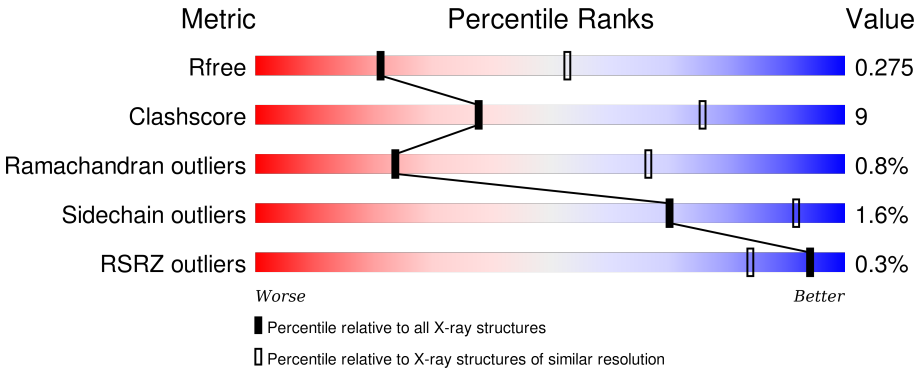
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 <=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	823	51% 13% 36%
1	B	823	52% 12% 36%
1	C	823	51% 13% • 36%
1	D	823	49% 14% • 36%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 17255 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, Calcineurin subunit B type 1, Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	529	Total	C	N	O	S	0	0	0
			4280	2737	718	796	29			
1	B	528	Total	C	N	O	S	0	0	0
			4277	2734	720	795	28			
1	C	529	Total	C	N	O	S	0	0	0
			4281	2739	718	796	28			
1	D	528	Total	C	N	O	S	0	0	0
			4277	2734	720	795	28			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	150	GLY	-	LINKER	UNP P62161
A	151	GLY	-	LINKER	UNP P62161
A	152	GLY	-	LINKER	UNP P62161
A	153	GLY	-	LINKER	UNP P62161
A	154	GLY	-	LINKER	UNP P62161
A	155	GLY	-	LINKER	UNP P62161
A	156	GLY	-	LINKER	UNP P62161
A	157	GLY	-	LINKER	UNP P62161
A	158	GLY	-	LINKER	UNP P62161
A	328	GLY	-	LINKER	UNP P63100
A	329	GLY	-	LINKER	UNP P63100
A	330	GLY	-	LINKER	UNP P63100
A	331	GLY	-	LINKER	UNP P63100
A	332	GLY	-	LINKER	UNP P63100
A	333	GLY	-	LINKER	UNP P63100
A	816	LEU	-	EXPRESSION TAG	UNP P63329
A	817	GLU	-	EXPRESSION TAG	UNP P63329
A	818	HIS	-	EXPRESSION TAG	UNP P63329
A	819	HIS	-	EXPRESSION TAG	UNP P63329
A	820	HIS	-	EXPRESSION TAG	UNP P63329

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Chain	Residue	Modelled	Actual	Comment	Reference
A	821	HIS	-	EXPRESSION TAG	UNP P63329
A	822	HIS	-	EXPRESSION TAG	UNP P63329
A	823	HIS	-	EXPRESSION TAG	UNP P63329
B	150	GLY	-	LINKER	UNP P62161
B	151	GLY	-	LINKER	UNP P62161
B	152	GLY	-	LINKER	UNP P62161
B	153	GLY	-	LINKER	UNP P62161
B	154	GLY	-	LINKER	UNP P62161
B	155	GLY	-	LINKER	UNP P62161
B	156	GLY	-	LINKER	UNP P62161
B	157	GLY	-	LINKER	UNP P62161
B	158	GLY	-	LINKER	UNP P62161
B	328	GLY	-	LINKER	UNP P63100
B	329	GLY	-	LINKER	UNP P63100
B	330	GLY	-	LINKER	UNP P63100
B	331	GLY	-	LINKER	UNP P63100
B	332	GLY	-	LINKER	UNP P63100
B	333	GLY	-	LINKER	UNP P63100
B	816	LEU	-	EXPRESSION TAG	UNP P63329
B	817	GLU	-	EXPRESSION TAG	UNP P63329
B	818	HIS	-	EXPRESSION TAG	UNP P63329
B	819	HIS	-	EXPRESSION TAG	UNP P63329
B	820	HIS	-	EXPRESSION TAG	UNP P63329
B	821	HIS	-	EXPRESSION TAG	UNP P63329
B	822	HIS	-	EXPRESSION TAG	UNP P63329
B	823	HIS	-	EXPRESSION TAG	UNP P63329
C	150	GLY	-	LINKER	UNP P62161
C	151	GLY	-	LINKER	UNP P62161
C	152	GLY	-	LINKER	UNP P62161
C	153	GLY	-	LINKER	UNP P62161
C	154	GLY	-	LINKER	UNP P62161
C	155	GLY	-	LINKER	UNP P62161
C	156	GLY	-	LINKER	UNP P62161
C	157	GLY	-	LINKER	UNP P62161
C	158	GLY	-	LINKER	UNP P62161
C	328	GLY	-	LINKER	UNP P63100
C	329	GLY	-	LINKER	UNP P63100
C	330	GLY	-	LINKER	UNP P63100
C	331	GLY	-	LINKER	UNP P63100
C	332	GLY	-	LINKER	UNP P63100
C	333	GLY	-	LINKER	UNP P63100
C	816	LEU	-	EXPRESSION TAG	UNP P63329

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Chain	Residue	Modelled	Actual	Comment	Reference
C	817	GLU	-	EXPRESSION TAG	UNP P63329
C	818	HIS	-	EXPRESSION TAG	UNP P63329
C	819	HIS	-	EXPRESSION TAG	UNP P63329
C	820	HIS	-	EXPRESSION TAG	UNP P63329
C	821	HIS	-	EXPRESSION TAG	UNP P63329
C	822	HIS	-	EXPRESSION TAG	UNP P63329
C	823	HIS	-	EXPRESSION TAG	UNP P63329
D	150	GLY	-	LINKER	UNP P62161
D	151	GLY	-	LINKER	UNP P62161
D	152	GLY	-	LINKER	UNP P62161
D	153	GLY	-	LINKER	UNP P62161
D	154	GLY	-	LINKER	UNP P62161
D	155	GLY	-	LINKER	UNP P62161
D	156	GLY	-	LINKER	UNP P62161
D	157	GLY	-	LINKER	UNP P62161
D	158	GLY	-	LINKER	UNP P62161
D	328	GLY	-	LINKER	UNP P63100
D	329	GLY	-	LINKER	UNP P63100
D	330	GLY	-	LINKER	UNP P63100
D	331	GLY	-	LINKER	UNP P63100
D	332	GLY	-	LINKER	UNP P63100
D	333	GLY	-	LINKER	UNP P63100
D	816	LEU	-	EXPRESSION TAG	UNP P63329
D	817	GLU	-	EXPRESSION TAG	UNP P63329
D	818	HIS	-	EXPRESSION TAG	UNP P63329
D	819	HIS	-	EXPRESSION TAG	UNP P63329
D	820	HIS	-	EXPRESSION TAG	UNP P63329
D	821	HIS	-	EXPRESSION TAG	UNP P63329
D	822	HIS	-	EXPRESSION TAG	UNP P63329
D	823	HIS	-	EXPRESSION TAG	UNP P63329

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	4	Total Ca 4 4	0	0
2	A	4	Total Ca 4 4	0	0
2	D	4	Total Ca 4 4	0	0
2	C	4	Total Ca 4 4	0	0

- Molecule 3 is water.

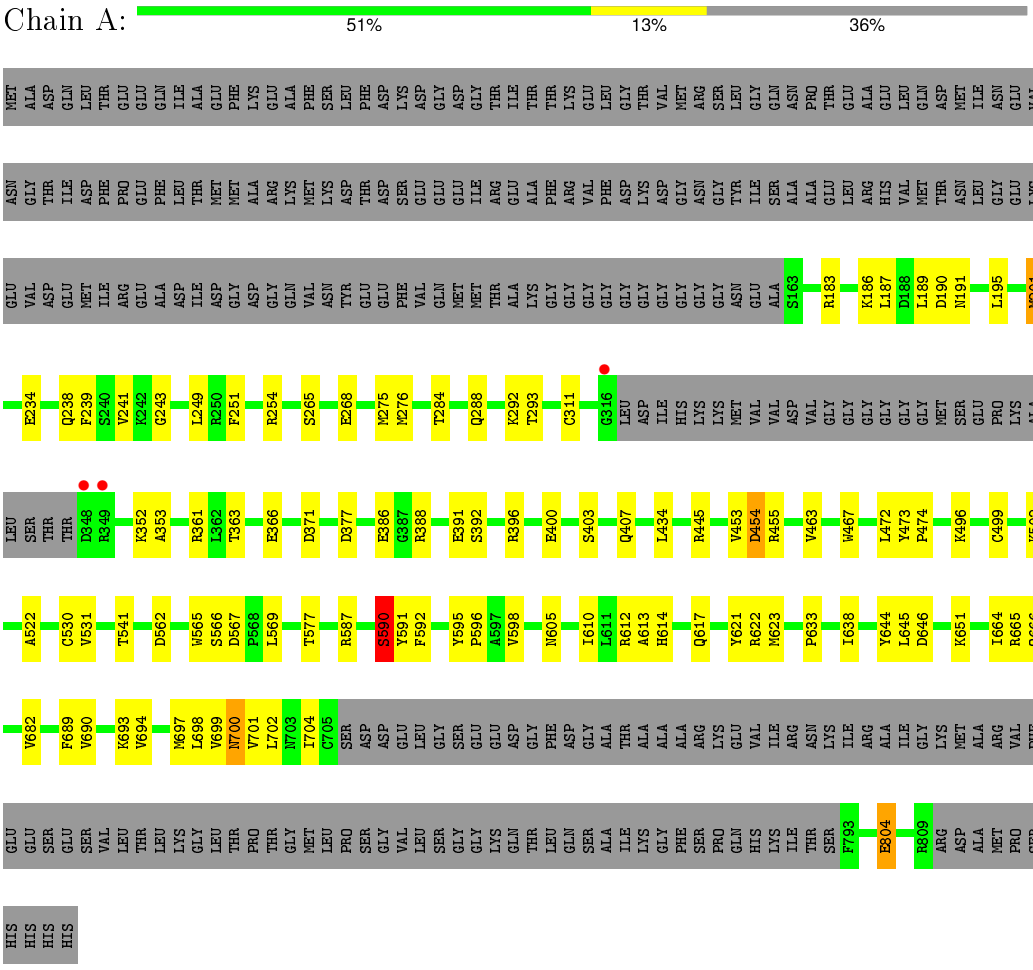
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	29	Total O 29 29	0	0
3	B	26	Total O 26 26	0	0
3	C	34	Total O 34 34	0	0
3	D	35	Total O 35 35	0	0

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 errors 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.

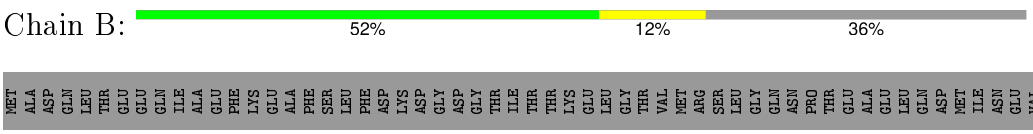
• Molecule 1: Calmodulin, Calcineurin subunit B type 1, Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform

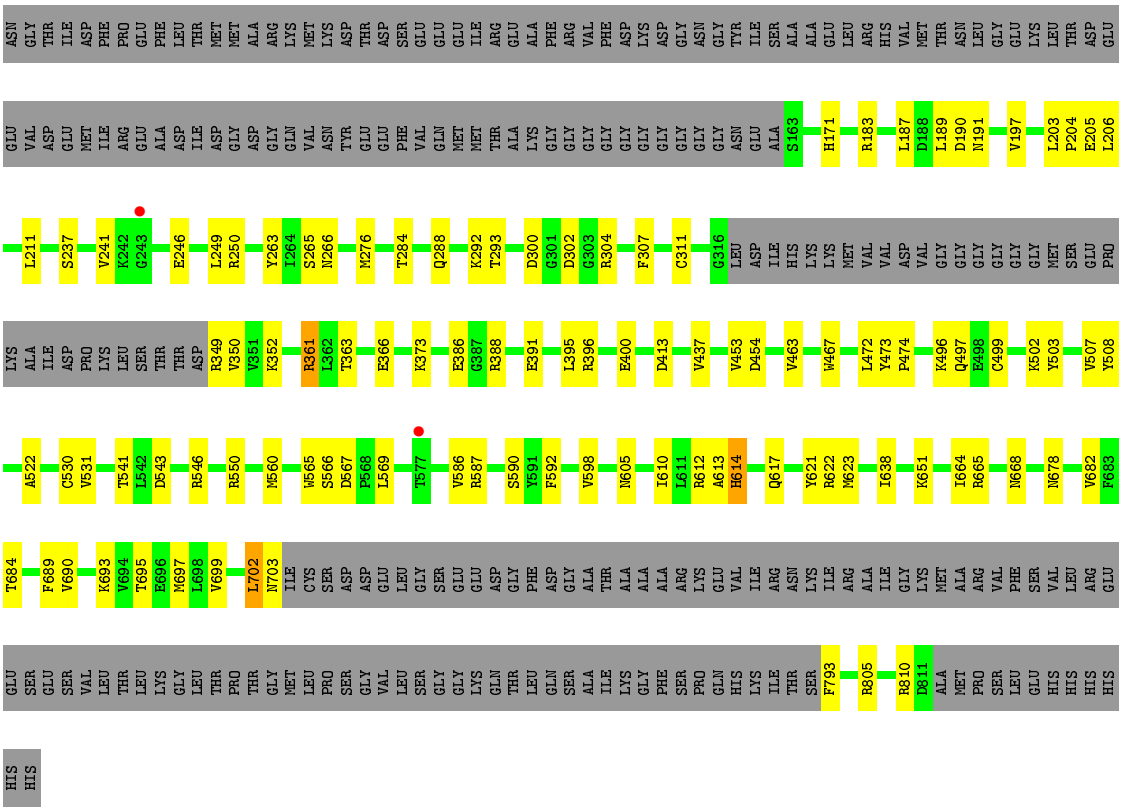
Chain A:



• Molecule 1: Calmodulin, Calcineurin subunit B type 1, Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform

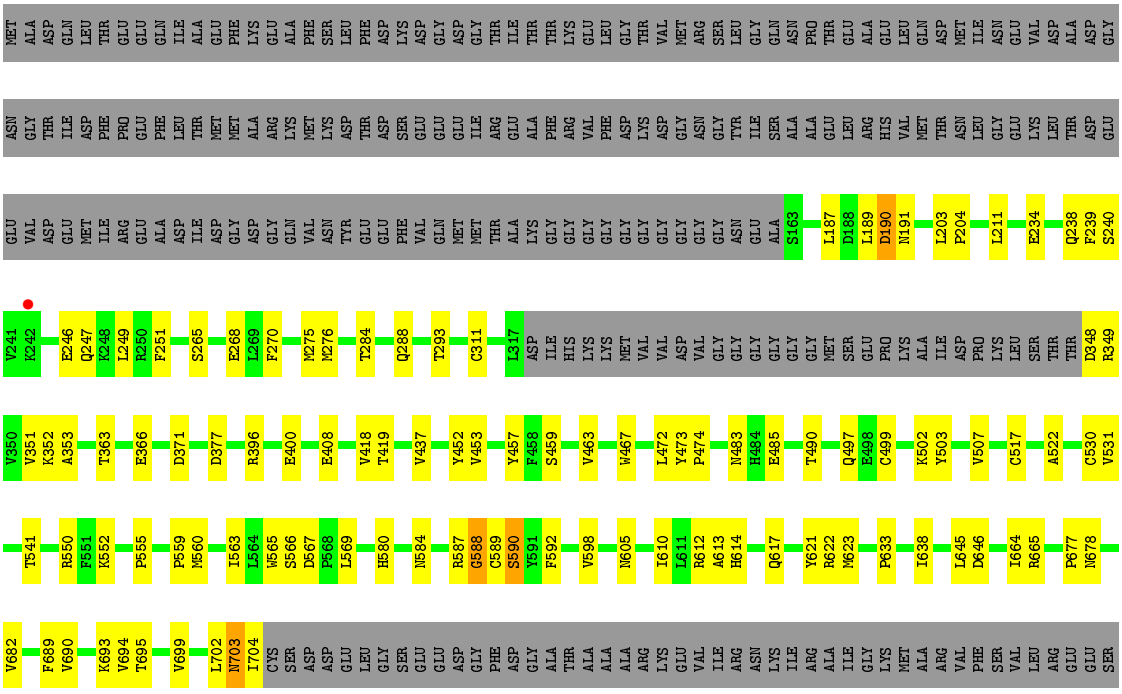
Chain B:

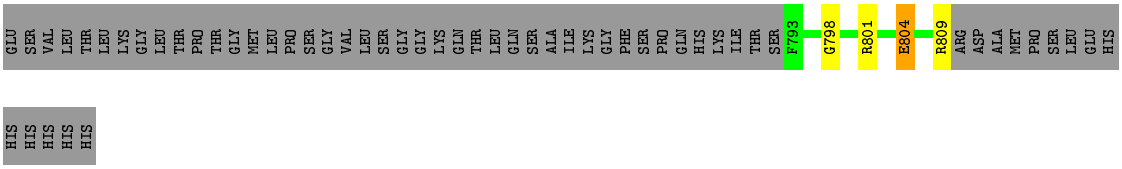




• Molecule 1: Calmodulin, Calcineurin subunit B type 1, Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform

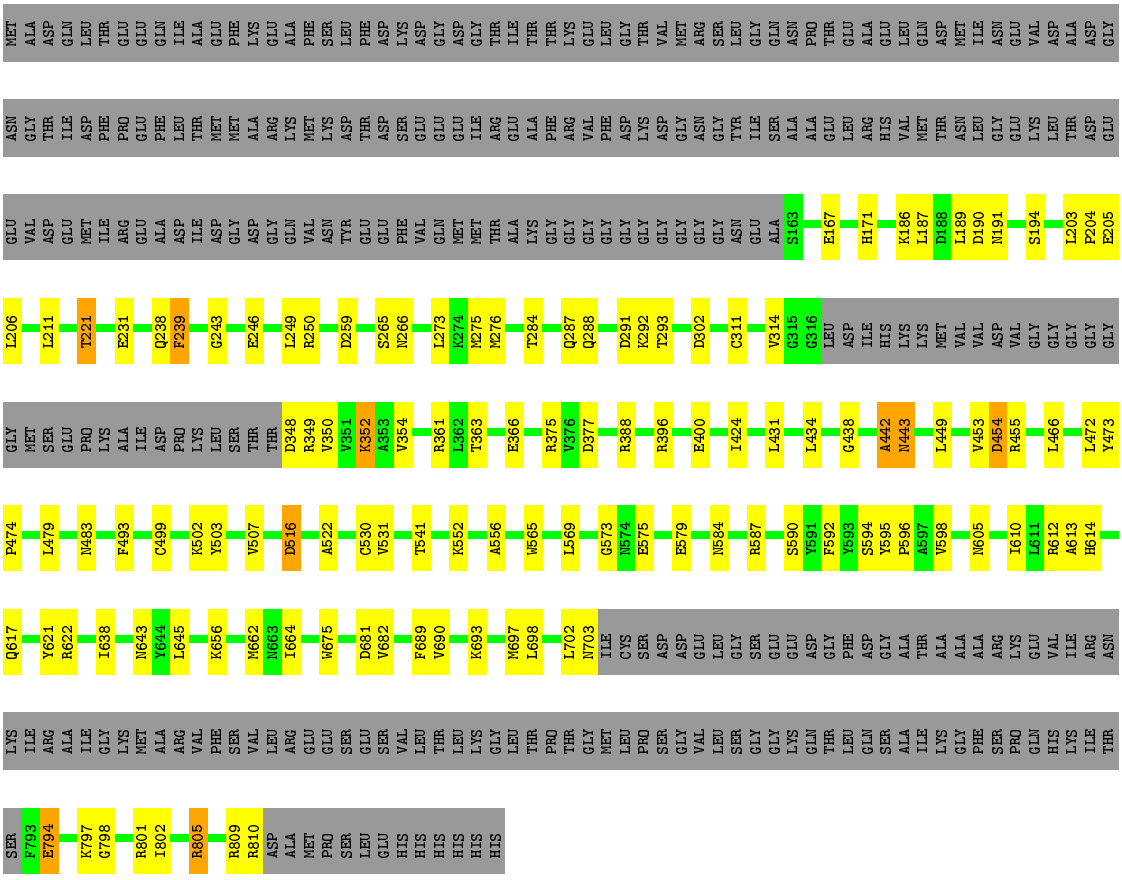
Chain C:





• Molecule 1: Calmodulin, Calcineurin subunit B type 1, Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	99.30Å 193.85Å 107.82Å 90.00° 90.09° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00 19.79 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (10.00-3.00) 99.5 (19.79-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.241 , 0.273 0.243 , 0.275	Depositor DCC
R_{free} test set	1977 reflections (2.56%)	DCC
Wilson B-factor (Å^2)	61.5	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 18.5	EDS
Estimated twinning fraction	0.447 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Outliers	0 of 81046 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17255	wwPDB-VP
Average B, all atoms (Å^2)	63.0	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 37.56 % 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 4.2090e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.61	0/4379	0.78	2/5914 (0.0%)
1	B	0.61	0/4376	0.79	4/5909 (0.1%)
1	C	0.61	0/4380	0.78	5/5916 (0.1%)
1	D	0.62	0/4376	0.80	6/5909 (0.1%)
All	All	0.61	0/17511	0.79	17/23648 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	190	ASP	CB-CG-OD2	9.37	126.73	118.30
1	D	259	ASP	CB-CG-OD2	8.55	126.00	118.30
1	B	302	ASP	CB-CG-OD2	8.05	125.54	118.30
1	B	361	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	C	190	ASP	CB-CG-OD1	-6.53	112.43	118.30
1	D	275	MET	CG-SD-CE	6.50	110.60	100.20
1	A	190	ASP	CB-CG-OD1	-6.14	112.78	118.30
1	D	302	ASP	CB-CG-OD1	6.05	123.75	118.30
1	D	190	ASP	CB-CG-OD2	5.75	123.47	118.30
1	B	190	ASP	CB-CG-OD1	-5.59	113.27	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	442	ALA	N-CA-C	-5.57	95.95	111.00
1	C	275	MET	CG-SD-CE	-5.54	91.34	100.20
1	C	268	GLU	OE1-CD-OE2	-5.42	116.79	123.30
1	B	190	ASP	CB-CG-OD2	5.40	123.16	118.30
1	C	588	GLY	N-CA-C	-5.10	100.35	113.10
1	D	275	MET	CA-CB-CG	5.09	121.95	113.30
1	A	190	ASP	CB-CG-OD2	5.06	122.85	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	452	TYR	Peptide
1	D	449	LEU	Peptide

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	4280	0	4186	90	0
1	B	4277	0	4183	62	0
1	C	4281	0	4187	73	0
1	D	4277	0	4182	87	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
3	A	29	0	0	2	0
3	B	26	0	0	1	0
3	C	34	0	0	1	0
3	D	35	0	0	1	0
All	All	17255	0	16738	310	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 (310) 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:C:453:VAL:O	1:C:459:SER:OG	1.62	1.15
1:A:187:LEU:HD23	1:A:195:LEU:HD21	1.26	1.08
1:A:455:ARG:HD3	1:A:644:TYR:OH	1.61	1.00
1:C:517:CYS:O	1:C:550:ARG:NH1	1.96	0.98
1:D:579:GLU:O	1:D:594:SER:OG	1.81	0.98
1:C:352:LYS:HB3	1:C:353:ALA:HA	1.48	0.96
1:C:239:PHE:CZ	1:C:694:VAL:HG21	2.02	0.94
1:A:187:LEU:CD2	1:A:195:LEU:HD21	1.99	0.93
1:D:273:LEU:HD11	1:D:682:VAL:HG11	1.50	0.93
1:C:239:PHE:HZ	1:C:694:VAL:HG21	1.34	0.91
1:C:555:PRO:HD2	1:C:560:MET:HG2	1.56	0.88
1:A:352:LYS:CG	1:A:353:ALA:HA	2.02	0.87
1:D:442:ALA:O	1:D:443:ASN:HB3	1.73	0.86
1:A:239:PHE:CZ	1:A:251:PHE:CZ	2.63	0.86
1:B:203:LEU:HD11	1:B:206:LEU:HB2	1.58	0.85
1:C:352:LYS:HB3	1:C:353:ALA:CA	2.07	0.83
1:A:212:VAL:HA	1:A:697:MET:HE1	1.61	0.82
1:C:203:LEU:HD12	1:C:204:PRO:HD2	1.63	0.81
1:A:352:LYS:HG3	1:A:353:ALA:HA	1.63	0.81
1:D:249:LEU:HD23	1:D:311:CYS:SG	2.23	0.79
1:A:249:LEU:HD23	1:A:311:CYS:SG	2.24	0.78
1:A:403:SER:O	1:A:407:GLN:NE2	2.16	0.78
1:C:249:LEU:HD23	1:C:311:CYS:SG	2.24	0.77
1:C:408:GLU:O	1:C:550:ARG:NH2	2.18	0.77
1:B:249:LEU:HD23	1:B:311:CYS:SG	2.24	0.77
1:B:437:VAL:HG13	1:B:665:ARG:HE	1.51	0.75
1:B:203:LEU:CD1	1:B:206:LEU:HB2	2.17	0.74
1:D:794:GLU:N	1:D:794:GLU:OE1	2.20	0.74
1:D:424:ILE:HD13	1:D:431:LEU:HD13	1.70	0.74
1:D:809:ARG:HG2	1:D:810:ARG:H	1.52	0.74
1:A:665:ARG:NH1	1:A:666:GLN:O	2.21	0.73
1:C:437:VAL:HG13	1:C:665:ARG:HE	1.52	0.73
1:A:698:LEU:O	1:A:701:VAL:HB	1.88	0.73
1:A:187:LEU:HD23	1:A:195:LEU:CD2	2.15	0.72
1:C:239:PHE:CZ	1:C:694:VAL:CG2	2.72	0.72
1:B:350:VAL:HG11	1:B:352:LYS:HD2	1.71	0.72
1:A:239:PHE:HZ	1:A:251:PHE:CZ	2.05	0.72
1:C:453:VAL:O	1:C:459:SER:CB	2.38	0.72
1:D:584:ASN:HB3	1:D:590:SER:O	1.90	0.71
1:A:187:LEU:CD2	1:A:195:LEU:CD2	2.69	0.71
1:D:350:VAL:HG11	1:D:352:LYS:NZ	2.06	0.70
1:C:499:CYS:O	1:C:502:LYS:O	2.11	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:CYS:O	1:A:502:LYS:O	2.11	0.69
1:C:623:MET:CE	1:C:633:PRO:HG2	2.22	0.69
1:D:499:CYS:O	1:D:502:LYS:O	2.11	0.68
1:B:499:CYS:O	1:B:502:LYS:O	2.11	0.68
1:A:623:MET:CE	1:A:633:PRO:HG2	2.24	0.68
1:B:437:VAL:HG13	1:B:665:ARG:NE	2.09	0.68
1:C:453:VAL:HG23	1:C:485:GLU:OE2	1.94	0.68
1:C:352:LYS:CB	1:C:353:ALA:HA	2.22	0.68
1:C:239:PHE:HE1	1:C:251:PHE:CE1	2.11	0.68
1:B:171:HIS:CG	1:B:241:VAL:CG1	2.77	0.67
1:C:798:GLY:O	1:C:801:ARG:NH1	2.27	0.67
1:D:798:GLY:O	1:D:801:ARG:NE	2.24	0.66
1:C:437:VAL:HG13	1:C:665:ARG:NE	2.09	0.66
1:C:584:ASN:HB3	1:C:590:SER:O	1.96	0.66
1:A:352:LYS:HG2	1:A:353:ALA:HA	1.78	0.65
1:A:352:LYS:HG2	1:A:353:ALA:CA	2.25	0.65
1:C:265:SER:HB3	1:C:349:ARG:HH11	1.61	0.65
1:B:171:HIS:CG	1:B:241:VAL:HG11	2.31	0.65
1:C:623:MET:HE3	1:C:633:PRO:HG2	1.79	0.64
1:D:442:ALA:O	1:D:443:ASN:CB	2.43	0.64
1:D:575:GLU:HG3	1:D:594:SER:HB2	1.78	0.64
1:A:455:ARG:CD	1:A:644:TYR:OH	2.41	0.63
1:D:556:ALA:HB2	1:D:809:ARG:HH11	1.62	0.63
1:A:292:LYS:HE2	1:A:386:GLU:OE2	1.99	0.62
1:D:702:LEU:O	1:D:703:ASN:O	2.17	0.62
1:B:266:ASN:HB3	1:B:350:VAL:HG22	1.82	0.62
1:D:211:LEU:HD12	1:D:693:LYS:HB2	1.82	0.62
1:A:698:LEU:O	1:A:701:VAL:N	2.32	0.61
1:A:201:MET:HE2	1:A:201:MET:HA	1.80	0.61
1:B:246:GLU:O	1:B:250:ARG:HG2	1.99	0.61
1:A:183:ARG:HG2	1:A:704:ILE:HG12	1.81	0.61
1:A:211:LEU:HD12	1:A:693:LYS:HB2	1.83	0.60
1:B:665:ARG:NH1	1:D:171:HIS:O	2.34	0.60
1:C:211:LEU:HD12	1:C:693:LYS:HB2	1.84	0.60
1:C:552:LYS:NZ	3:C:1004:HOH:O	2.30	0.60
1:B:211:LEU:HD12	1:B:693:LYS:HB2	1.83	0.60
1:A:623:MET:HE3	1:A:633:PRO:HG2	1.84	0.59
1:B:702:LEU:O	1:B:703:ASN:OD1	2.21	0.58
1:B:531:VAL:O	1:B:612:ARG:HA	2.04	0.58
1:A:241:VAL:C	1:A:243:GLY:H	2.06	0.58
1:D:352:LYS:HD2	1:D:354:VAL:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:THR:HG21	1:C:682:VAL:HG22	1.86	0.58
1:D:584:ASN:CB	1:D:590:SER:O	2.51	0.58
1:A:211:LEU:HD11	1:A:690:VAL:HA	1.86	0.57
1:A:453:VAL:O	1:A:454:ASP:HB2	2.03	0.57
1:C:276:MET:HB2	1:C:689:PHE:CE2	2.39	0.57
1:A:702:LEU:HD11	3:A:1006:HOH:O	2.04	0.57
1:A:212:VAL:HA	1:A:697:MET:CE	2.32	0.57
1:A:455:ARG:HH11	1:A:455:ARG:HG2	1.69	0.56
1:B:361:ARG:NH2	1:B:388:ARG:NH2	2.53	0.56
1:A:293:THR:HG21	1:A:682:VAL:HG22	1.85	0.56
1:B:293:THR:HG21	1:B:682:VAL:HG22	1.86	0.56
1:D:809:ARG:HG2	1:D:810:ARG:N	2.20	0.56
1:D:352:LYS:CD	1:D:354:VAL:O	2.54	0.56
1:A:531:VAL:O	1:A:612:ARG:HA	2.05	0.56
1:B:171:HIS:ND1	1:B:237:SER:OG	2.39	0.56
1:C:531:VAL:O	1:C:612:ARG:HA	2.06	0.56
1:B:211:LEU:HD11	1:B:690:VAL:HA	1.88	0.56
1:D:587:ARG:HH21	1:D:614:HIS:CD2	2.24	0.56
1:D:556:ALA:HB2	1:D:809:ARG:NH1	2.20	0.56
1:A:183:ARG:HG2	1:A:704:ILE:CG1	2.36	0.56
1:B:453:VAL:O	1:B:454:ASP:HB2	2.05	0.56
1:D:238:GLN:O	1:D:239:PHE:CB	2.54	0.55
1:D:284:THR:O	1:D:288:GLN:HG3	2.06	0.55
1:A:213:GLN:HG2	1:A:275:MET:CE	2.36	0.55
1:D:453:VAL:O	1:D:454:ASP:HB2	2.05	0.55
1:C:238:GLN:OE1	1:C:247:GLN:NE2	2.40	0.55
1:B:543:ASP:HA	1:B:546:ARG:HG3	1.88	0.55
1:C:555:PRO:CD	1:C:560:MET:HG2	2.34	0.55
1:D:266:ASN:HB3	1:D:350:VAL:HG22	1.89	0.55
1:A:292:LYS:NZ	1:A:674:TYR:O	2.39	0.55
1:D:273:LEU:HD11	1:D:682:VAL:CG1	2.32	0.54
1:C:584:ASN:CB	1:C:590:SER:O	2.55	0.54
1:A:700:ASN:OD1	1:A:700:ASN:C	2.45	0.54
1:D:531:VAL:O	1:D:612:ARG:HA	2.07	0.54
1:B:284:THR:O	1:B:288:GLN:HG3	2.07	0.54
1:D:794:GLU:O	1:D:797:LYS:HB3	2.08	0.54
1:A:213:GLN:HG2	1:A:275:MET:HE1	1.88	0.54
1:C:587:ARG:NH1	1:C:804:GLU:HG3	2.23	0.54
1:A:690:VAL:O	1:A:694:VAL:HG23	2.07	0.54
1:D:238:GLN:O	1:D:239:PHE:HB2	2.08	0.54
1:A:239:PHE:CZ	1:A:251:PHE:CE1	2.95	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:THR:OG1	1:D:231:GLU:HG2	2.08	0.54
1:C:284:THR:O	1:C:288:GLN:HG3	2.08	0.53
1:C:234:GLU:O	1:C:238:GLN:HG3	2.08	0.53
1:C:265:SER:HB3	1:C:349:ARG:NH1	2.23	0.53
1:D:211:LEU:HD11	1:D:690:VAL:HA	1.91	0.53
1:D:291:ASP:OD2	1:D:352:LYS:HE2	2.09	0.53
1:C:702:LEU:O	1:C:703:ASN:HB3	2.09	0.53
1:D:350:VAL:HG11	1:D:352:LYS:HZ2	1.75	0.52
1:A:352:LYS:HG2	1:A:353:ALA:HB2	1.91	0.52
1:D:287:GLN:NE2	1:D:291:ASP:OD1	2.37	0.52
1:B:391:GLU:O	1:B:395:LEU:HD13	2.09	0.52
1:D:573:GLY:H	1:D:575:GLU:CD	2.13	0.52
1:A:623:MET:HE2	1:A:633:PRO:HG2	1.91	0.52
1:C:211:LEU:HD11	1:C:690:VAL:HA	1.92	0.52
1:B:292:LYS:HE3	1:B:386:GLU:OE2	2.10	0.52
1:C:437:VAL:HG13	1:C:665:ARG:CD	2.40	0.51
1:B:206:LEU:HD11	1:B:697:MET:HG3	1.93	0.51
1:C:623:MET:HE2	1:C:633:PRO:HG2	1.93	0.51
1:A:361:ARG:HH12	1:A:388:ARG:CZ	2.23	0.51
1:D:556:ALA:N	1:D:809:ARG:HH12	2.08	0.51
1:A:284:THR:O	1:A:288:GLN:HG3	2.09	0.51
1:C:541:THR:HA	1:C:605:ASN:OD1	2.11	0.51
1:C:703:ASN:O	1:C:704:ILE:HB	2.10	0.51
1:C:270:PHE:CD1	1:C:351:VAL:HG11	2.46	0.51
1:C:239:PHE:CE1	1:C:251:PHE:CE1	2.96	0.50
1:B:550:ARG:HA	1:B:560:MET:HE1	1.93	0.50
1:B:437:VAL:HG13	1:B:665:ARG:CD	2.41	0.50
1:A:702:LEU:CD1	3:A:1006:HOH:O	2.58	0.50
1:D:396:ARG:O	1:D:400:GLU:HB2	2.11	0.50
1:A:276:MET:HB2	1:A:689:PHE:CE2	2.46	0.50
1:B:522:ALA:HB3	1:B:530:CYS:HB2	1.93	0.50
1:A:352:LYS:HG2	1:A:353:ALA:CB	2.40	0.50
1:D:293:THR:HG23	1:D:681:ASP:OD1	2.12	0.50
1:A:699:VAL:C	1:A:701:VAL:H	2.14	0.50
1:A:239:PHE:CZ	1:A:694:VAL:HG11	2.47	0.50
1:D:265:SER:HB2	1:D:349:ARG:HG3	1.94	0.49
1:D:363:THR:HG23	1:D:366:GLU:OE1	2.12	0.49
1:A:213:GLN:CG	1:A:275:MET:HE1	2.40	0.49
1:B:396:ARG:O	1:B:400:GLU:HB2	2.12	0.49
1:C:565:TRP:O	1:C:566:SER:C	2.49	0.49
1:C:363:THR:HG23	1:C:366:GLU:OE1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:567:ASP:OD2	1:C:587:ARG:NE	2.39	0.49
1:D:438:GLY:HA2	1:D:656:LYS:HE3	1.95	0.49
1:A:567:ASP:OD2	1:A:587:ARG:NE	2.42	0.49
1:C:396:ARG:O	1:C:400:GLU:HB2	2.13	0.49
1:D:556:ALA:N	1:D:809:ARG:NH1	2.60	0.49
1:A:396:ARG:O	1:A:400:GLU:HB2	2.13	0.49
1:C:555:PRO:HD2	1:C:560:MET:CG	2.37	0.49
1:D:311:CYS:HA	1:D:314:VAL:HG22	1.95	0.48
1:A:587:ARG:NH1	1:A:804:GLU:HG3	2.29	0.48
1:A:234:GLU:O	1:A:238:GLN:HG3	2.14	0.48
1:A:352:LYS:CG	1:A:353:ALA:CA	2.79	0.48
1:D:203:LEU:HD12	1:D:206:LEU:HD12	1.96	0.48
1:C:522:ALA:HB3	1:C:530:CYS:HB2	1.95	0.48
1:C:473:TYR:N	1:C:474:PRO:HD3	2.29	0.48
1:B:541:THR:HA	1:B:605:ASN:OD1	2.14	0.47
1:B:567:ASP:OD2	1:B:587:ARG:NE	2.40	0.47
1:A:363:THR:HG23	1:A:366:GLU:OE1	2.13	0.47
1:C:621:TYR:CD2	1:C:664:ILE:HD13	2.49	0.47
1:D:643:ASN:HB3	3:D:1027:HOH:O	2.14	0.47
1:A:212:VAL:HG22	1:A:697:MET:HE2	1.97	0.47
1:A:186:LYS:HD2	1:A:704:ILE:CD1	2.45	0.47
1:D:239:PHE:CD2	1:D:698:LEU:HD11	2.50	0.47
1:B:586:VAL:O	1:B:805:ARG:HG2	2.15	0.47
1:A:541:THR:HA	1:A:605:ASN:OD1	2.14	0.47
1:B:363:THR:HG23	1:B:366:GLU:OE1	2.15	0.47
1:A:612:ARG:NH2	1:A:614:HIS:HB3	2.30	0.47
1:B:598:VAL:HG13	1:B:610:ILE:HD12	1.97	0.47
1:B:350:VAL:CG1	1:B:352:LYS:HD2	2.42	0.46
1:D:239:PHE:HD2	1:D:698:LEU:HD11	1.80	0.46
1:C:418:VAL:HG12	1:C:419:THR:N	2.30	0.46
1:B:810:ARG:NE	1:B:810:ARG:HA	2.30	0.46
1:D:598:VAL:HG13	1:D:610:ILE:HD12	1.97	0.46
1:B:569:LEU:HD23	1:B:592:PHE:HB3	1.98	0.46
1:C:483:ASN:ND2	1:C:614:HIS:HE1	2.13	0.46
1:A:522:ALA:HB3	1:A:530:CYS:HB2	1.96	0.46
1:C:559:PRO:O	1:C:563:ILE:HG13	2.15	0.46
1:D:473:TYR:N	1:D:474:PRO:HD3	2.30	0.46
1:A:455:ARG:NH1	1:A:455:ARG:HG2	2.31	0.46
1:D:239:PHE:CD2	1:D:698:LEU:CD1	2.98	0.46
1:A:562:ASP:OD1	1:A:590:SER:HB2	2.16	0.46
1:D:569:LEU:HD23	1:D:592:PHE:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:698:LEU:O	1:A:701:VAL:CB	2.61	0.46
1:A:621:TYR:CD2	1:A:664:ILE:HD13	2.51	0.46
1:B:473:TYR:N	1:B:474:PRO:HD3	2.31	0.46
1:C:472:LEU:C	1:C:474:PRO:HD3	2.36	0.45
1:B:503:TYR:HB3	1:B:507:VAL:HG21	1.98	0.45
1:D:204:PRO:HG2	1:D:205:GLU:OE2	2.16	0.45
1:B:621:TYR:CD2	1:B:664:ILE:HD13	2.51	0.45
1:A:700:ASN:OD1	1:A:701:VAL:N	2.49	0.45
1:D:503:TYR:HB3	1:D:507:VAL:HG21	1.98	0.45
1:B:651:LYS:HD3	1:B:668:ASN:OD1	2.15	0.45
1:D:239:PHE:CE2	1:D:698:LEU:HD12	2.52	0.45
1:B:587:ARG:CZ	1:B:614:HIS:CE1	2.99	0.45
1:D:455:ARG:HH21	1:D:645:LEU:HD11	1.82	0.45
1:A:251:PHE:HA	1:A:254:ARG:HD2	1.99	0.45
1:B:263:TYR:CD2	1:B:304:ARG:NH1	2.85	0.45
1:A:569:LEU:HD23	1:A:592:PHE:HB3	1.97	0.45
1:D:579:GLU:O	1:D:594:SER:CB	2.62	0.45
1:C:503:TYR:HB3	1:C:507:VAL:HG21	1.98	0.45
1:C:453:VAL:HG11	1:C:490:THR:HG22	1.97	0.45
1:D:565:TRP:HB2	1:D:590:SER:HB2	1.99	0.45
1:B:204:PRO:HG2	1:B:205:GLU:OE2	2.16	0.45
1:D:621:TYR:CD2	1:D:664:ILE:HD13	2.52	0.45
1:A:503:TYR:HB3	1:A:507:VAL:HG21	1.99	0.45
1:B:565:TRP:O	1:B:566:SER:C	2.56	0.44
1:B:276:MET:HB2	1:B:689:PHE:CE2	2.52	0.44
1:D:522:ALA:HB3	1:D:530:CYS:HB2	1.98	0.44
1:D:239:PHE:CG	1:D:239:PHE:O	2.70	0.44
1:D:348:ASP:HB3	1:D:349:ARG:H	1.66	0.44
1:A:613:ALA:CB	1:A:638:ILE:O	2.66	0.44
1:D:702:LEU:O	1:D:703:ASN:C	2.56	0.44
1:C:613:ALA:CB	1:C:638:ILE:O	2.65	0.44
1:D:613:ALA:CB	1:D:638:ILE:O	2.66	0.44
1:D:466:LEU:HB3	1:D:479:LEU:HD21	1.99	0.44
1:A:201:MET:HE1	1:A:212:VAL:HG11	1.99	0.44
1:C:569:LEU:HD23	1:C:592:PHE:HB3	1.99	0.44
1:A:201:MET:HA	1:A:201:MET:CE	2.44	0.44
1:D:350:VAL:HG11	1:D:352:LYS:CE	2.48	0.44
1:C:348:ASP:O	1:C:348:ASP:OD1	2.36	0.44
1:B:171:HIS:CD2	1:B:241:VAL:HG11	2.53	0.43
1:C:265:SER:CB	1:C:349:ARG:HD3	2.47	0.43
1:D:541:THR:HA	1:D:605:ASN:OD1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:LYS:NZ	1:D:703:ASN:O	2.38	0.43
1:A:617:GLN:OE1	1:A:622:ARG:HB2	2.18	0.43
1:B:617:GLN:OE1	1:B:622:ARG:HB2	2.18	0.43
1:C:589:CYS:SG	1:C:590:SER:N	2.91	0.43
1:B:187:LEU:O	1:B:189:LEU:HD22	2.18	0.43
1:C:617:GLN:OE1	1:C:622:ARG:HB2	2.19	0.43
1:B:496:LYS:HA	1:B:508:TYR:CD1	2.54	0.43
1:D:516:ASP:OD2	1:D:552:LYS:C	2.56	0.43
1:B:613:ALA:CB	1:B:638:ILE:O	2.67	0.43
1:D:472:LEU:C	1:D:474:PRO:HD3	2.38	0.43
1:C:598:VAL:HG13	1:C:610:ILE:HD12	1.99	0.43
1:A:463:VAL:O	1:A:467:TRP:HB2	2.19	0.43
1:B:197:VAL:HG23	3:B:1006:HOH:O	2.19	0.43
1:D:276:MET:HB2	1:D:689:PHE:CE2	2.54	0.43
1:A:187:LEU:HD21	1:A:195:LEU:CD2	2.49	0.43
1:A:239:PHE:HZ	1:A:251:PHE:CE1	2.33	0.43
1:A:565:TRP:O	1:A:566:SER:C	2.57	0.43
1:D:802:ILE:O	1:D:805:ARG:HB2	2.17	0.43
1:A:651:LYS:HE2	1:A:668:ASN:OD1	2.18	0.43
1:B:623:MET:HE1	1:D:167:GLU:OE2	2.19	0.43
1:C:587:ARG:HB2	1:C:588:GLY:O	2.18	0.42
1:A:699:VAL:C	1:A:701:VAL:N	2.72	0.42
1:C:703:ASN:O	1:C:704:ILE:CB	2.67	0.42
1:B:497:GLN:HG2	1:B:678:ASN:OD1	2.20	0.42
1:A:598:VAL:HG13	1:A:610:ILE:HD12	2.00	0.42
1:B:472:LEU:C	1:B:474:PRO:HD3	2.39	0.42
1:C:187:LEU:O	1:C:189:LEU:HD22	2.20	0.42
1:D:617:GLN:OE1	1:D:622:ARG:HB2	2.19	0.42
1:D:292:LYS:HD2	1:D:675:TRP:CZ2	2.55	0.42
1:A:265:SER:HB3	1:A:268:GLU:HB2	2.02	0.42
1:D:794:GLU:N	1:D:794:GLU:CD	2.72	0.42
1:C:457:TYR:OH	1:C:677:PRO:HA	2.20	0.42
1:C:645:LEU:O	1:C:646:ASP:HB2	2.20	0.42
1:D:595:TYR:HB3	1:D:596:PRO:HD3	2.02	0.42
1:A:239:PHE:CD2	1:A:698:LEU:HD11	2.55	0.42
1:D:187:LEU:O	1:D:189:LEU:HD22	2.20	0.42
1:D:434:LEU:HD23	1:D:434:LEU:C	2.40	0.41
1:B:307:PHE:CZ	1:B:311:CYS:SG	3.13	0.41
1:D:361:ARG:HH11	1:D:388:ARG:NE	2.18	0.41
1:A:472:LEU:C	1:A:474:PRO:HD3	2.40	0.41
1:D:273:LEU:CD1	1:D:682:VAL:HG11	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:695:THR:O	1:B:699:VAL:HG23	2.20	0.41
1:C:695:THR:O	1:C:699:VAL:HG23	2.21	0.41
1:D:206:LEU:HD21	1:D:697:MET:HA	2.02	0.41
1:B:373:LYS:HD3	1:B:472:LEU:HD12	2.02	0.41
1:C:463:VAL:O	1:C:467:TRP:HB2	2.21	0.41
1:A:595:TYR:HB3	1:A:596:PRO:HD3	2.02	0.41
1:C:190:ASP:OD1	1:C:190:ASP:N	2.54	0.41
1:A:434:LEU:HD23	1:A:434:LEU:C	2.41	0.41
1:D:455:ARG:NH1	1:D:493:PHE:CE1	2.87	0.41
1:A:473:TYR:N	1:A:474:PRO:HD3	2.35	0.41
1:D:246:GLU:O	1:D:250:ARG:HB2	2.21	0.41
1:A:187:LEU:O	1:A:189:LEU:HD22	2.20	0.41
1:A:645:LEU:O	1:A:646:ASP:HB2	2.21	0.41
1:A:496:LYS:HA	1:A:508:TYR:CD1	2.56	0.41
1:B:265:SER:HB2	1:B:349:ARG:HD2	2.03	0.40
1:A:590:SER:OG	1:A:591:TYR:N	2.50	0.40
1:B:203:LEU:C	1:B:203:LEU:HD12	2.42	0.40
1:B:203:LEU:HD11	1:B:206:LEU:CB	2.42	0.40
1:C:497:GLN:HG2	1:C:678:ASN:OD1	2.22	0.40
1:D:483:ASN:ND2	1:D:614:HIS:CE1	2.90	0.40
1:D:424:ILE:CD1	1:D:431:LEU:HD13	2.47	0.40
1:B:463:VAL:O	1:B:467:TRP:HB2	2.21	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	523/823 (64%)	494 (94%)	24 (5%)	5 (1%)	19	61
1	B	522/823 (63%)	499 (96%)	21 (4%)	2 (0%)	39	80
1	C	523/823 (64%)	496 (95%)	23 (4%)	4 (1%)	24	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	522/823 (63%)	492 (94%)	25 (5%)	5 (1%)	19 61
All	All	2090/3292 (64%)	1981 (95%)	93 (4%)	16 (1%)	24 66

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	454	ASP
1	A	590	SER
1	C	703	ASN
1	D	239	PHE
1	D	454	ASP
1	C	191	ASN
1	A	191	ASN
1	A	700	ASN
1	B	191	ASN
1	D	191	ASN
1	A	201	MET
1	B	614	HIS
1	C	590	SER
1	D	443	ASN
1	C	246	GLU
1	D	243	GLY

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	472/708 (67%)	464 (98%)	8 (2%)	68 91
1	B	471/708 (66%)	464 (98%)	7 (2%)	72 92
1	C	471/708 (66%)	465 (99%)	6 (1%)	76 93
1	D	471/708 (66%)	462 (98%)	9 (2%)	65 90
All	All	1885/2832 (67%)	1855 (98%)	30 (2%)	70 92

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	371	ASP
1	A	377	ASP
1	A	391	GLU
1	A	392	SER
1	A	445	ARG
1	A	577	THR
1	A	590	SER
1	A	804	GLU
1	B	183	ARG
1	B	300	ASP
1	B	413	ASP
1	B	590	SER
1	B	684	THR
1	B	702	LEU
1	B	793	PHE
1	C	240	SER
1	C	371	ASP
1	C	377	ASP
1	C	580	HIS
1	C	804	GLU
1	C	809	ARG
1	D	194	SER
1	D	221	THR
1	D	352	LYS
1	D	375	ARG
1	D	377	ASP
1	D	516	ASP
1	D	662	MET
1	D	794	GLU
1	D	805	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	407	GLN
1	A	443	ASN
1	A	483	ASN
1	A	614	HIS
1	B	614	HIS
1	C	238	GLN
1	C	247	GLN
1	C	614	HIS
1	D	483	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 16 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	529/823 (64%)	-0.53	3 (0%) 90 73	32, 59, 96, 154	0
1	B	528/823 (64%)	-0.51	2 (0%) 93 80	33, 61, 100, 149	0
1	C	529/823 (64%)	-0.51	1 (0%) 95 87	34, 58, 99, 144	0
1	D	528/823 (64%)	-0.51	0 100 100	35, 61, 95, 134	0
All	All	2114/3292 (64%)	-0.52	6 (0%) 94 84	32, 60, 98, 154	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	316	GLY	4.4
1	B	577	THR	3.8
1	A	349	ARG	2.3
1	C	242	LYS	2.3
1	A	348	ASP	2.1
1	B	243	GLY	2.0

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, 95^{th} 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
2	CA	B	903	1/1	0.99	0.16	0.57	67,67,67,67	0
2	CA	C	903	1/1	0.99	0.16	-0.04	65,65,65,65	0
2	CA	D	901	1/1	0.94	0.12	-0.12	91,91,91,91	0
2	CA	A	903	1/1	0.99	0.13	-0.34	59,59,59,59	0
2	CA	A	902	1/1	0.99	0.12	-0.49	65,65,65,65	0
2	CA	A	904	1/1	0.97	0.12	-0.67	72,72,72,72	0
2	CA	C	904	1/1	0.99	0.11	-0.82	70,70,70,70	0
2	CA	C	901	1/1	0.86	0.12	-1.01	102,102,102,102	0
2	CA	D	904	1/1	0.97	0.12	-1.24	76,76,76,76	0
2	CA	C	902	1/1	0.98	0.09	-1.44	70,70,70,70	0
2	CA	B	901	1/1	0.92	0.08	-1.63	85,85,85,85	0
2	CA	B	902	1/1	0.89	0.09	-1.73	66,66,66,66	0
2	CA	D	903	1/1	0.96	0.09	-1.75	69,69,69,69	0
2	CA	B	904	1/1	0.98	0.07	-2.09	80,80,80,80	0
2	CA	D	902	1/1	0.93	0.08	-2.46	69,69,69,69	0
2	CA	A	901	1/1	0.93	0.06	-2.57	109,109,109,109	0

6.5 Other polymers (i)

There are no such residues in this entry.