



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 02:39 am BST

PDB ID : 3G43
Title : Crystal structure of the calmodulin-bound Cav1.2 C-terminal regulatory domain dimer
Authors : Fallon, J.L.; Quiococho, F.A.
Deposited on : 2009-02-03
Resolution : 2.10 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

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
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

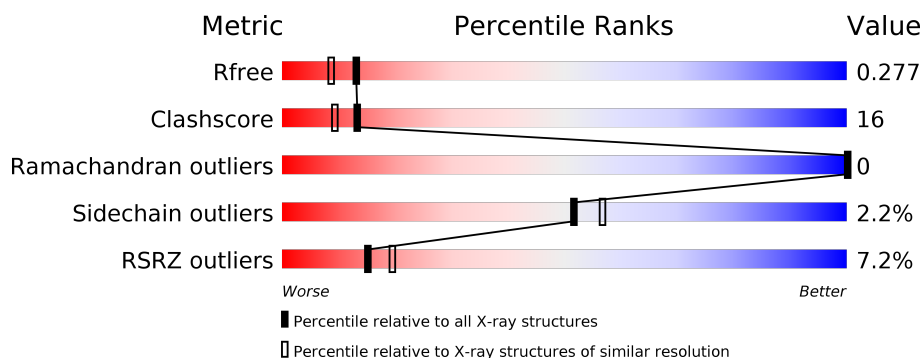
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	148	<div> <div>5%</div> <div> <div></div> <div>34%</div> <div>16%</div> <div>•</div> <div>49%</div> </div> </div>
1	B	148	<div> <div>7%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div>• •</div> </div> </div>
1	C	148	<div> <div>6%</div> <div> <div></div> <div>72%</div> <div>28%</div> <div>•</div> </div> </div>
1	D	148	<div> <div>5%</div> <div> <div></div> <div>71%</div> <div>28%</div> <div>•</div> </div> </div>
2	E	81	<div> <div>11%</div> <div> <div></div> <div>58%</div> <div>26%</div> <div>16%</div> </div> </div>
2	F	81	<div> <div>4%</div> <div> <div></div> <div>44%</div> <div>11%</div> <div>44%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5526 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	75	Total	C	N	O	S	0	0	0
			584	362	93	124	5			
1	B	147	Total	C	N	O	S	0	0	0
			1161	711	187	254	9			
1	C	148	Total	C	N	O	S	0	0	0
			1166	714	188	255	9			
1	D	146	Total	C	N	O	S	0	0	0
			1153	707	186	251	9			

- Molecule 2 is a protein called Voltage-dependent L-type calcium channel subunit alpha-1C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	68	Total	C	N	O	S	0	0	0
			567	370	101	95	1			
2	F	45	Total	C	N	O	S	0	0	0
			363	230	67	65	1			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1604	GLY	-	EXPRESSION TAG	UNP Q13936
E	1605	PRO	-	EXPRESSION TAG	UNP Q13936
E	1606	LEU	-	EXPRESSION TAG	UNP Q13936
E	1607	GLY	-	EXPRESSION TAG	UNP Q13936
E	1608	SER	-	EXPRESSION TAG	UNP Q13936
E	1683	GLU	-	EXPRESSION TAG	UNP Q13936
E	1684	GLN	-	EXPRESSION TAG	UNP Q13936
F	1604	GLY	-	EXPRESSION TAG	UNP Q13936
F	1605	PRO	-	EXPRESSION TAG	UNP Q13936
F	1606	LEU	-	EXPRESSION TAG	UNP Q13936
F	1607	GLY	-	EXPRESSION TAG	UNP Q13936
F	1608	SER	-	EXPRESSION TAG	UNP Q13936

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1683	GLU	-	EXPRESSION TAG	UNP Q13936
F	1684	GLN	-	EXPRESSION TAG	UNP Q13936

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

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

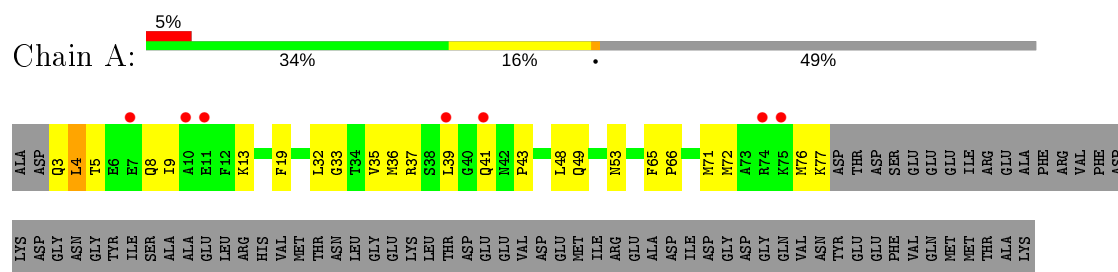
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	56	Total O 56 56	0	0
4	B	145	Total O 145 145	0	0
4	C	134	Total O 134 134	0	0
4	D	97	Total O 97 97	0	0
4	E	54	Total O 54 54	0	0
4	F	32	Total O 32 32	0	0

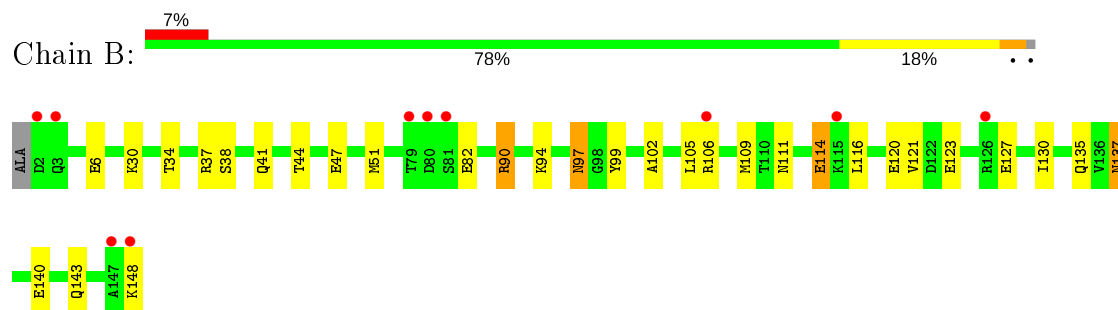
3 Residue-property plots [i](#)

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.

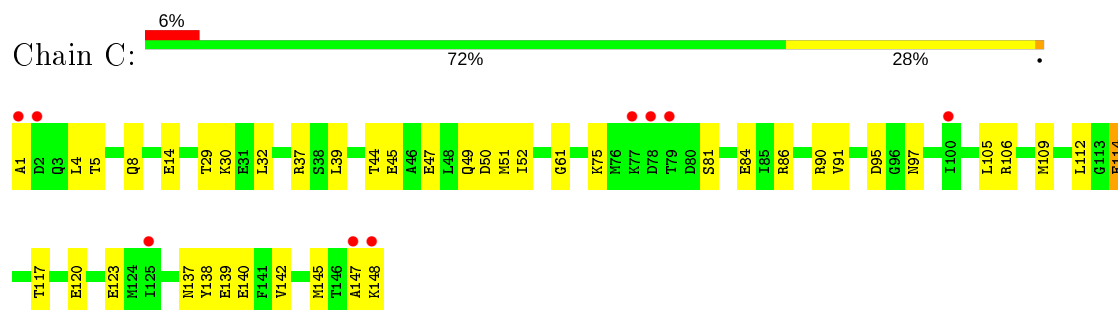
• Molecule 1: Calmodulin



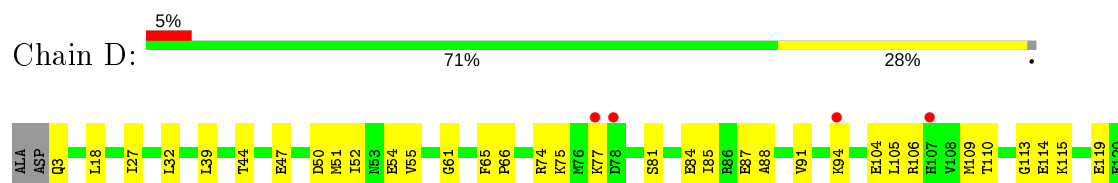
• Molecule 1: Calmodulin

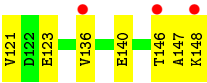


• Molecule 1: Calmodulin

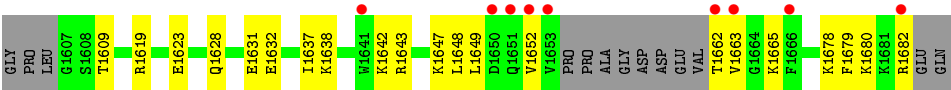


• Molecule 1: Calmodulin

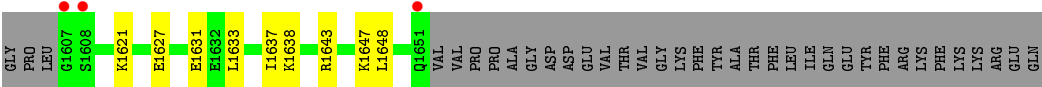




● Molecule 2: Voltage-dependent L-type calcium channel subunit alpha-1C



● Molecule 2: Voltage-dependent L-type calcium channel subunit alpha-1C



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	39.79Å 113.98Å 182.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.93 – 2.10 25.03 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.3 (19.93-2.10) 97.3 (25.03-2.10)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.12 (at 2.10Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.220 , 0.269 0.229 , 0.277	Depositor DCC
R_{free} test set	3476 reflections (7.08%)	wwPDB-VP
Wilson B-factor (Å ²)	35.0	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5526	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.29	0/590	0.49	0/791
1	B	0.31	0/1173	0.53	0/1573
1	C	0.32	0/1178	0.53	0/1580
1	D	0.30	0/1165	0.51	0/1562
2	E	0.34	0/574	0.45	0/764
2	F	0.31	0/365	0.50	0/487
All	All	0.31	0/5045	0.51	0/6757

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	584	0	563	26	0
1	B	1161	0	1088	38	0
1	C	1166	0	1096	47	0
1	D	1153	0	1084	35	0
2	E	567	0	610	33	0
2	F	363	0	394	13	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	A	56	0	0	0	0
4	B	145	0	0	4	0
4	C	134	0	0	8	0
4	D	97	0	0	4	0
4	E	54	0	0	1	0
4	F	32	0	0	1	0
All	All	5526	0	4835	159	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 16.

All (159) 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:147:ALA:HB3	2:E:1638:LYS:NZ	1.80	0.95
1:C:86:ARG:HD2	1:C:90:ARG:HH22	1.35	0.91
1:C:147:ALA:CB	2:E:1638:LYS:NZ	2.34	0.90
1:B:123:GLU:O	1:B:127:GLU:HG2	1.69	0.89
1:C:148:LYS:H	1:C:148:LYS:HD2	1.41	0.84
1:C:147:ALA:CB	2:E:1638:LYS:HZ1	1.90	0.84
1:C:112:LEU:HD11	2:E:1648:LEU:HD13	1.61	0.80
1:B:137:ASN:ND2	1:B:140:GLU:H	1.79	0.80
1:C:44:THR:HG22	1:C:47:GLU:HG3	1.63	0.79
2:E:1679:PHE:O	2:E:1682:ARG:HG3	1.85	0.77
1:D:50:ASP:O	1:D:54:GLU:HG3	1.84	0.76
1:B:109:MET:HG3	1:B:114:GLU:HB3	1.69	0.74
1:C:147:ALA:HB3	2:E:1638:LYS:HZ3	1.53	0.73
1:C:86:ARG:CD	1:C:90:ARG:HH22	2.01	0.73
2:E:1649:LEU:O	2:E:1652:VAL:HG12	1.90	0.71
1:A:5:THR:HG22	1:A:8:GLN:HG3	1.72	0.71
1:B:44:THR:HG23	1:B:47:GLU:H	1.56	0.70
1:D:51:MET:HG2	2:E:1609:THR:CG2	2.22	0.70
1:B:148:LYS:O	2:E:1678:LYS:HB3	1.93	0.69
2:F:1627:GLU:O	2:F:1631:GLU:HG3	1.93	0.69
1:A:37:ARG:HA	1:A:41:GLN:O	1.94	0.68
1:A:32:LEU:O	1:A:36:MET:HB2	1.94	0.67
1:D:119:GLU:HG3	4:D:267:HOH:O	1.95	0.67
1:D:91:VAL:HG21	2:F:1648:LEU:HD11	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1682:ARG:O	2:E:1682:ARG:HD2	1.95	0.67
1:C:14:GLU:HG2	2:F:1621:LYS:NZ	2.10	0.67
1:B:41:GLN:OE1	2:E:1665:LYS:HE3	1.94	0.66
1:D:44:THR:OG1	1:D:47:GLU:HG3	1.96	0.66
1:D:74:ARG:HA	1:D:77:LYS:HE3	1.76	0.66
1:B:137:ASN:C	1:B:137:ASN:HD22	1.97	0.66
1:C:29:THR:HG21	1:C:49:GLN:NE2	2.11	0.65
4:C:281:HOH:O	2:E:1647:LYS:HE3	1.96	0.65
1:A:5:THR:HG23	1:A:8:GLN:H	1.63	0.64
1:C:109:MET:HE1	1:C:114:GLU:HG2	1.78	0.63
1:C:14:GLU:HG2	2:F:1621:LYS:HZ3	1.64	0.63
1:C:44:THR:HG23	1:C:47:GLU:H	1.64	0.63
1:D:148:LYS:HE2	4:F:202:HOH:O	1.99	0.62
1:A:71:MET:SD	1:A:72:MET:HE2	2.40	0.62
1:C:147:ALA:HB1	2:E:1638:LYS:NZ	2.13	0.62
1:D:51:MET:HG2	2:E:1609:THR:HG23	1.81	0.62
1:C:81:SER:HB3	1:C:84:GLU:HG3	1.82	0.62
1:B:116:LEU:HD21	2:E:1680:LYS:HE2	1.82	0.61
1:C:147:ALA:CB	2:E:1638:LYS:HZ3	2.07	0.60
1:B:38:SER:HB2	1:B:111:ASN:HD22	1.66	0.59
1:C:123:GLU:HG2	2:E:1637:ILE:HD11	1.83	0.59
1:A:4:LEU:HD12	1:A:4:LEU:O	2.03	0.59
1:B:30:LYS:O	1:B:34:THR:HG23	2.03	0.59
1:C:147:ALA:HB1	2:E:1638:LYS:HZ1	1.66	0.58
1:C:147:ALA:HB3	2:E:1638:LYS:CE	2.34	0.58
1:C:44:THR:CG2	1:C:47:GLU:HG3	2.34	0.57
1:D:74:ARG:O	1:D:77:LYS:HG3	2.05	0.57
1:A:19:PHE:HA	1:A:35:VAL:HG21	1.86	0.57
1:C:30:LYS:HG3	4:C:159:HOH:O	2.05	0.57
1:B:6:GLU:HG3	4:B:427:HOH:O	2.04	0.57
1:B:137:ASN:HD21	1:B:140:GLU:H	1.53	0.56
1:C:109:MET:CE	1:C:114:GLU:HG2	2.35	0.56
1:A:49:GLN:NE2	1:A:53:ASN:HD21	2.04	0.56
1:C:145:MET:O	2:E:1642:LYS:HE2	2.06	0.55
1:C:86:ARG:HD2	1:C:90:ARG:NH2	2.14	0.55
1:A:4:LEU:HA	1:A:8:GLN:OE1	2.06	0.55
2:E:1678:LYS:HD2	4:E:330:HOH:O	2.07	0.55
1:A:36:MET:HG2	1:A:43:PRO:HG3	1.89	0.55
2:E:1628:GLN:O	2:E:1631:GLU:HG2	2.07	0.55
1:D:55:VAL:O	1:D:55:VAL:HG22	2.07	0.55
1:D:114:GLU:HG3	2:E:1619:ARG:CZ	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:MET:SD	2:E:1663:VAL:HG23	2.47	0.55
1:B:148:LYS:HA	2:E:1678:LYS:HD3	1.89	0.54
1:D:27:ILE:CG2	1:D:32:LEU:HD13	2.38	0.54
1:D:65:PHE:HB3	1:D:66:PRO:HD3	1.89	0.54
1:A:49:GLN:HE21	1:A:53:ASN:ND2	2.06	0.53
1:B:123:GLU:HG2	2:E:1682:ARG:NH1	2.23	0.53
1:C:44:THR:HG22	1:C:47:GLU:CG	2.37	0.53
1:C:37:ARG:NH1	4:C:339:HOH:O	2.40	0.53
1:B:97:ASN:ND2	1:B:99:TYR:H	2.07	0.52
1:C:147:ALA:O	1:C:148:LYS:OXT	2.27	0.52
1:A:4:LEU:HD13	1:A:9:ILE:HD11	1.91	0.52
1:B:94:LYS:HG3	4:B:203:HOH:O	2.10	0.52
1:D:81:SER:OG	1:D:84:GLU:HG3	2.11	0.51
1:B:90:ARG:HH21	1:B:90:ARG:HG2	1.76	0.50
1:D:91:VAL:CG1	2:F:1648:LEU:HD21	2.41	0.50
1:A:3:GLN:N	1:A:77:LYS:HZ1	2.10	0.50
1:C:5:THR:OG1	1:C:8:GLN:HG3	2.12	0.50
1:D:27:ILE:HG21	1:D:32:LEU:HD13	1.93	0.49
4:B:400:HOH:O	2:E:1662:THR:HA	2.11	0.49
1:B:137:ASN:HD22	1:B:140:GLU:H	1.58	0.49
1:B:109:MET:CG	1:B:114:GLU:HB3	2.39	0.49
1:B:94:LYS:HB2	4:C:409:HOH:O	2.12	0.49
1:A:33:GLY:HA3	1:A:48:LEU:HD21	1.95	0.48
1:C:95:ASP:OD2	1:C:97:ASN:HB3	2.14	0.48
1:D:91:VAL:HG13	2:F:1648:LEU:HD21	1.95	0.48
1:A:33:GLY:CA	1:A:48:LEU:HD21	2.43	0.48
1:B:105:LEU:HD23	1:B:105:LEU:C	2.34	0.48
1:B:109:MET:SD	1:B:116:LEU:HB2	2.53	0.47
2:F:1643:ARG:O	2:F:1647:LYS:HG3	2.14	0.47
1:B:99:TYR:HB3	1:B:135:GLN:NE2	2.30	0.47
1:D:147:ALA:HB3	2:F:1638:LYS:NZ	2.30	0.47
1:B:99:TYR:HB3	1:B:135:GLN:HE21	1.79	0.47
1:C:1:ALA:O	1:C:4:LEU:HB3	2.15	0.47
1:D:87:GLU:O	1:D:91:VAL:HG12	2.15	0.47
1:C:91:VAL:HG11	2:E:1648:LEU:HG	1.96	0.47
1:C:138:TYR:O	1:C:142:VAL:HG23	2.16	0.46
1:D:88:ALA:O	1:D:91:VAL:HG13	2.15	0.46
1:A:5:THR:CG2	1:A:8:GLN:HG3	2.43	0.46
1:C:86:ARG:O	1:C:90:ARG:HD3	2.16	0.46
1:C:75:LYS:HD2	4:C:234:HOH:O	2.16	0.46
1:D:18:LEU:HD13	1:D:18:LEU:C	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:192:HOH:O	2:E:1609:THR:HG21	2.15	0.46
1:D:52:ILE:HG21	1:D:61:GLY:O	2.16	0.45
1:C:81:SER:HB3	1:C:84:GLU:CG	2.45	0.45
1:A:35:VAL:O	1:A:39:LEU:HG	2.17	0.45
1:D:110:THR:HG21	4:D:373:HOH:O	2.17	0.45
1:D:3:GLN:HA	1:D:3:GLN:HE21	1.82	0.45
1:A:76:MET:HG2	1:A:76:MET:O	2.17	0.45
1:B:105:LEU:HD22	1:B:121:VAL:HG13	1.99	0.45
1:D:123:GLU:OE2	2:F:1633:LEU:HD21	2.17	0.45
1:D:3:GLN:HA	1:D:3:GLN:NE2	2.32	0.45
1:A:49:GLN:NE2	1:A:53:ASN:ND2	2.64	0.45
1:D:105:LEU:O	1:D:109:MET:HG2	2.17	0.45
1:B:90:ARG:HG2	1:B:90:ARG:NH2	2.32	0.44
1:B:41:GLN:HG3	4:B:182:HOH:O	2.16	0.44
1:D:136:VAL:HA	1:D:140:GLU:OE1	2.18	0.44
1:C:14:GLU:HG3	4:C:154:HOH:O	2.17	0.44
1:C:117:THR:OG1	1:C:120:GLU:HG3	2.18	0.44
1:A:36:MET:HA	1:A:36:MET:CE	2.47	0.44
1:D:85:ILE:HD11	1:D:146:THR:HG23	2.00	0.43
1:A:19:PHE:HD2	1:A:32:LEU:HD12	1.82	0.43
1:B:82:GLU:O	1:B:82:GLU:HG2	2.19	0.43
1:C:137:ASN:OD1	1:C:140:GLU:HG3	2.18	0.43
1:C:1:ALA:HB1	4:C:149:HOH:O	2.19	0.43
1:D:106:ARG:HB2	1:D:121:VAL:HG11	1.99	0.43
2:E:1619:ARG:O	2:E:1623:GLU:HG3	2.18	0.43
1:A:65:PHE:HB3	1:A:66:PRO:HD3	2.00	0.43
1:B:37:ARG:HA	1:B:41:GLN:O	2.19	0.43
1:C:105:LEU:O	1:C:109:MET:HG2	2.19	0.42
1:D:75:LYS:HD2	4:D:157:HOH:O	2.19	0.42
1:D:123:GLU:HG2	2:F:1637:ILE:HD11	2.02	0.42
2:E:1662:THR:HG23	2:E:1662:THR:O	2.20	0.41
1:C:32:LEU:HD21	1:C:51:MET:SD	2.61	0.41
1:D:94:LYS:HB3	1:D:104:GLU:HG2	2.01	0.41
1:D:113:GLY:C	1:D:115:LYS:H	2.22	0.41
1:B:105:LEU:HD23	1:B:105:LEU:O	2.19	0.41
1:B:102:ALA:O	1:B:106:ARG:HG3	2.20	0.41
1:A:13:LYS:HA	1:A:65:PHE:CE2	2.56	0.41
1:B:109:MET:HG2	1:B:114:GLU:O	2.20	0.41
1:B:120:GLU:O	1:B:123:GLU:HB3	2.20	0.41
1:B:137:ASN:C	1:B:137:ASN:ND2	2.68	0.41
1:B:137:ASN:HD21	1:B:140:GLU:HG3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:GLU:CD	2:F:1621:LYS:HZ1	2.23	0.41
1:A:5:THR:HG22	1:A:8:GLN:CG	2.45	0.41
1:C:50:ASP:HB2	4:C:165:HOH:O	2.21	0.41
1:B:130:ILE:CD1	1:B:143:GLN:NE2	2.84	0.41
1:C:52:ILE:HG21	1:C:61:GLY:O	2.21	0.41
1:A:19:PHE:CD2	1:A:32:LEU:HD12	2.56	0.40
1:C:147:ALA:C	1:C:148:LYS:OXT	2.57	0.40
1:D:147:ALA:HB3	2:F:1638:LYS:HZ2	1.85	0.40
2:E:1643:ARG:HH21	2:E:1643:ARG:HG3	1.86	0.40
1:A:48:LEU:HA	1:A:48:LEU:HD12	1.92	0.40
1:C:14:GLU:CG	2:F:1621:LYS:NZ	2.84	0.40
1:B:123:GLU:HG2	2:E:1682:ARG:HH12	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	73/148 (49%)	68 (93%)	5 (7%)	0	100	100
1	B	145/148 (98%)	138 (95%)	7 (5%)	0	100	100
1	C	146/148 (99%)	142 (97%)	4 (3%)	0	100	100
1	D	144/148 (97%)	138 (96%)	6 (4%)	0	100	100
2	E	64/81 (79%)	62 (97%)	2 (3%)	0	100	100
2	F	43/81 (53%)	43 (100%)	0	0	100	100
All	All	615/754 (82%)	591 (96%)	24 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	64/126 (51%)	63 (98%)	1 (2%)	62	69
1	B	126/126 (100%)	122 (97%)	4 (3%)	39	41
1	C	126/126 (100%)	121 (96%)	5 (4%)	31	32
1	D	125/126 (99%)	124 (99%)	1 (1%)	81	86
2	E	60/70 (86%)	59 (98%)	1 (2%)	60	67
2	F	39/70 (56%)	39 (100%)	0	100	100
All	All	540/644 (84%)	528 (98%)	12 (2%)	52	57

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	B	90	ARG
1	B	97	ASN
1	B	114	GLU
1	B	137	ASN
1	C	39	LEU
1	C	45	GLU
1	C	106	ARG
1	C	114	GLU
1	C	139	GLU
1	D	39	LEU
2	E	1632	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	49	GLN
1	A	53	ASN
1	B	3	GLN
1	B	49	GLN

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Mol	Chain	Res	Type
1	B	53	ASN
1	B	97	ASN
1	B	111	ASN
1	B	135	GLN
1	B	137	ASN
1	B	143	GLN
1	C	3	GLN
1	C	49	GLN
1	C	135	GLN
1	D	3	GLN
1	D	49	GLN
1	D	53	ASN
1	D	135	GLN
2	E	1625	ASN
2	E	1651	GLN
2	F	1625	ASN
2	F	1651	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](#)

Of 14 ligands modelled in this entry, 14 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, 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	75/148 (50%)	0.80	7 (9%) 8 11	35, 51, 86, 88	0
1	B	147/148 (99%)	0.50	10 (6%) 17 21	21, 41, 81, 88	0
1	C	148/148 (100%)	0.59	9 (6%) 21 26	23, 43, 80, 92	0
1	D	146/148 (98%)	0.40	7 (4%) 30 36	32, 43, 69, 76	0
2	E	68/81 (83%)	0.74	9 (13%) 3 4	28, 38, 73, 90	0
2	F	45/81 (55%)	0.59	3 (6%) 17 22	27, 34, 69, 87	0
All	All	629/754 (83%)	0.57	45 (7%) 15 19	21, 43, 79, 92	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	ALA	7.9
1	B	80	ASP	7.4
1	C	148	LYS	7.2
2	F	1607	GLY	7.1
2	E	1662	THR	6.5
2	E	1651	GLN	5.4
1	C	2	ASP	4.9
1	B	81	SER	4.3
1	D	148	LYS	4.3
1	B	148	LYS	4.2
1	A	74	ARG	4.1
1	D	77	LYS	3.8
2	E	1652	VAL	3.7
1	B	147	ALA	3.6
1	D	146	THR	3.6
1	C	147	ALA	3.6
2	E	1653	VAL	3.5
1	C	77	LYS	3.4
1	B	115	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	7	GLU	3.3
1	D	107	HIS	3.3
1	A	39	LEU	3.3
1	B	79	THR	3.2
1	C	78	ASP	3.1
1	A	75	LYS	3.0
1	A	41	GLN	2.9
1	D	136	VAL	2.8
2	F	1651	GLN	2.8
1	B	126	ARG	2.8
1	A	10	ALA	2.7
1	C	100	ILE	2.7
1	B	106	ARG	2.5
2	E	1666	PHE	2.5
2	E	1682	ARG	2.4
2	E	1641	TRP	2.3
1	D	94	LYS	2.3
2	E	1650	ASP	2.3
1	C	79	THR	2.2
1	B	3	GLN	2.2
1	C	125	ILE	2.2
2	E	1663	VAL	2.2
1	B	2	ASP	2.1
2	F	1608	SER	2.1
1	D	78	ASP	2.1
1	A	11	GLU	2.1

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 [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
3	CA	D	714	1/1	0.96	0.05	44,44,44,44	0
3	CA	B	703	1/1	0.97	0.09	38,38,38,38	0
3	CA	D	713	1/1	0.97	0.06	43,43,43,43	0
3	CA	C	710	1/1	0.98	0.06	34,34,34,34	0
3	CA	D	711	1/1	0.98	0.04	39,39,39,39	0
3	CA	C	707	1/1	0.98	0.04	38,38,38,38	0
3	CA	A	701	1/1	0.99	0.06	40,40,40,40	0
3	CA	B	706	1/1	0.99	0.09	28,28,28,28	0
3	CA	C	708	1/1	0.99	0.13	40,40,40,40	0
3	CA	C	709	1/1	0.99	0.08	30,30,30,30	0
3	CA	D	712	1/1	0.99	0.11	38,38,38,38	0
3	CA	A	702	1/1	0.99	0.08	37,37,37,37	0
3	CA	B	704	1/1	0.99	0.04	43,43,43,43	0
3	CA	B	705	1/1	1.00	0.12	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.