



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:02 PM UTC

PDB ID : 6K4K / pdb_00006k4k
Title : Crystal structure of SidJ-CaM binary complex at 2.71 Å
Authors : Ouyang, S.Y.
Deposited on : 2019-05-24
Resolution : 2.71 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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

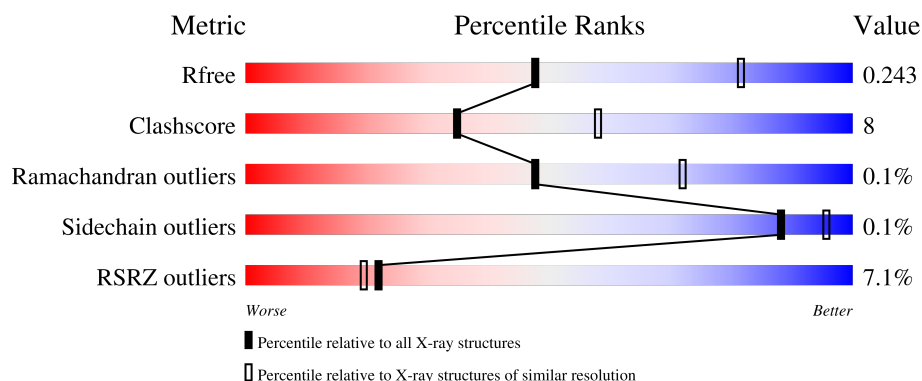
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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}	180053	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	873	3% 72% 12% 16%
1	B	873	2% 72% 12% 16%
2	C	149	25% 54% 26% 19%
2	D	149	23% 42% 20% 36%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13093 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 SidJ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	734	Total	C	N	O	S	0	0	0
			5725	3674	958	1079	14			
1	B	737	Total	C	N	O	S	0	0	0
			5785	3711	968	1091	15			

- Molecule 2 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	120	Total	C	N	O	S	0	0	0
			882	538	142	197	5			
2	D	95	Total	C	N	O	S	0	0	0
			697	426	110	157	4			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		

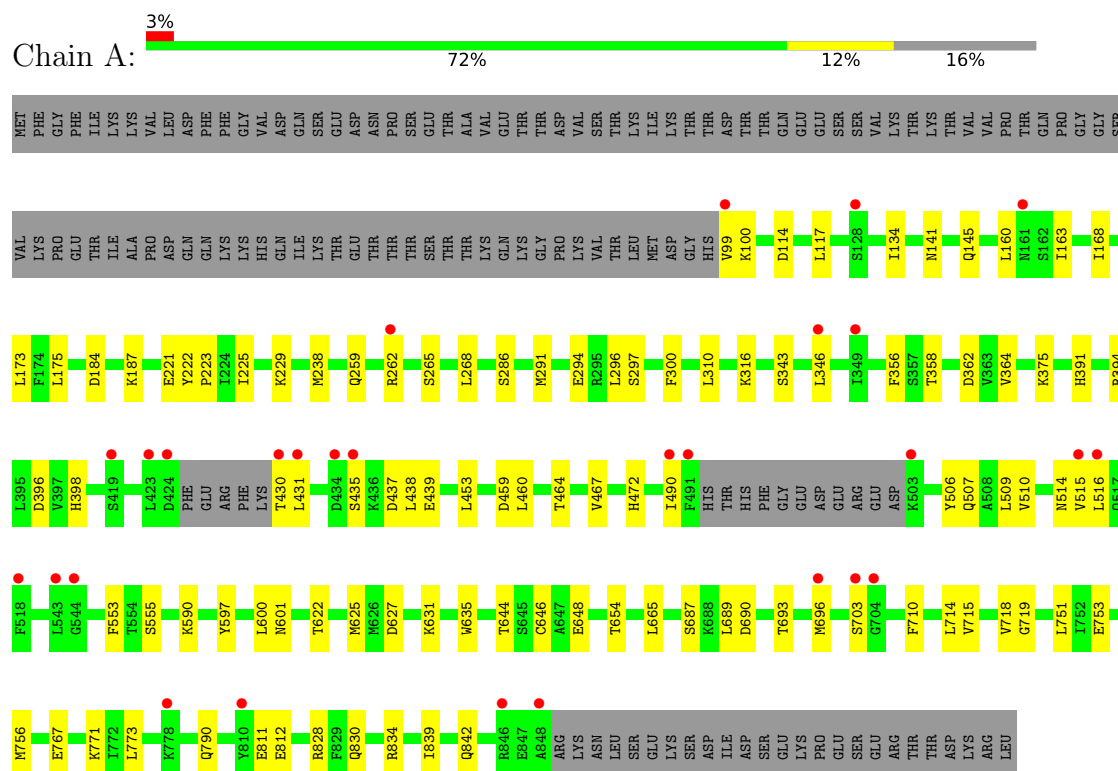
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	O	0	0
			1	1		
4	D	1	Total	O	0	0
			1	1		

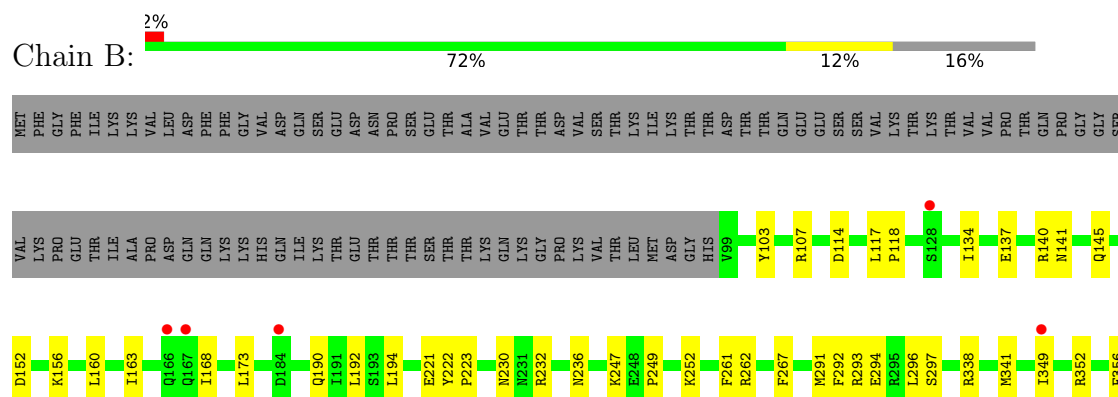
3 Residue-property plots

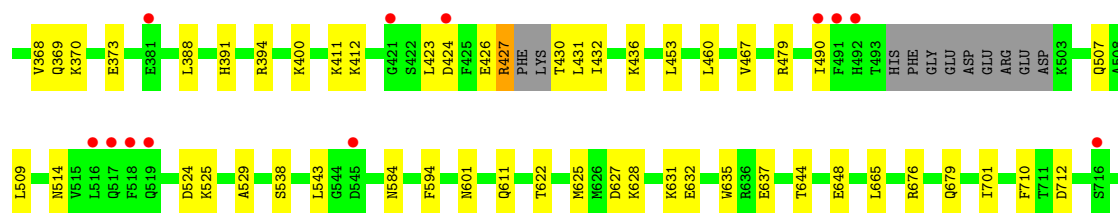
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: SidJ

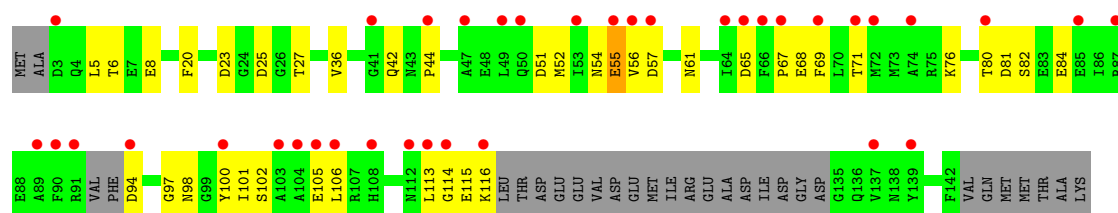


• Molecule 1: SidJ

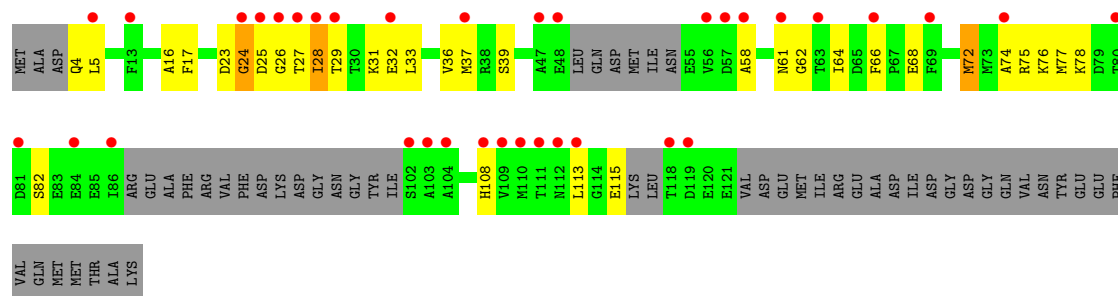




• Molecule 2: Calmodulin-1



• Molecule 2: Calmodulin-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.95Å 159.53Å 135.61Å 90.00° 101.89° 90.00°	Depositor
Resolution (Å)	55.87 – 2.71 55.87 – 2.71	Depositor EDS
% Data completeness (in resolution range)	96.9 (55.87-2.71) 96.9 (55.87-2.71)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.205 , 0.243 0.207 , 0.243	Depositor DCC
R_{free} test set	1995 reflections (2.92%)	wwPDB-VP
Wilson B-factor (Å ²)	61.3	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13093	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	2/5855 (0.0%)	0.52	1/7961 (0.0%)
1	B	0.29	2/5917 (0.0%)	0.49	2/8036 (0.0%)
2	C	0.31	0/888	0.67	2/1197 (0.2%)
2	D	0.30	0/701	0.80	1/941 (0.1%)
All	All	0.29	4/13361 (0.0%)	0.54	6/18135 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	D	0	3
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	134	ILE	CA-C	6.71	1.58	1.53
1	A	719	GLY	C-O	6.22	1.27	1.24
1	A	134	ILE	CA-C	-5.54	1.49	1.53
1	B	719	GLY	C-O	5.20	1.27	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	64	ILE	N-CA-C	-7.21	105.75	112.96
1	B	134	ILE	CA-C-O	-5.34	116.13	119.12
1	B	134	ILE	O-C-N	5.33	125.33	121.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	811	GLU	N-CA-CB	-5.04	102.69	110.20
2	C	55	GLU	CA-C-N	-5.02	112.93	121.97
2	C	55	GLU	C-N-CA	-5.02	112.93	121.97

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	435	SER	Peptide
2	D	24	GLY	Peptide
2	D	28	ILE	Peptide
2	D	72	MET	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5725	0	5510	70	0
1	B	5785	0	5593	78	0
2	C	882	0	775	30	0
2	D	697	0	620	24	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
All	All	13093	0	12498	192	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 8.

All (192) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:78:LYS:HE3	2:D:82:SER:OG	1.61	0.98
1:A:430:THR:HG23	1:A:431:LEU:HD12	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:28:ILE:O	2:D:29:THR:HG23	1.85	0.76
1:B:107:ARG:H	2:D:24:GLY:H	1.33	0.74
1:A:507:GLN:HE22	1:A:514:ASN:HD21	1.34	0.74
2:C:54:ASN:HD22	2:C:56:VAL:H	1.38	0.71
1:A:117:LEU:HD23	1:A:555:SER:HB3	1.73	0.70
1:A:99:VAL:HG22	1:A:100:LYS:H	1.57	0.69
1:B:427:ARG:HA	1:B:430:THR:HB	1.74	0.69
1:B:644:THR:O	1:B:648:GLU:HG3	1.92	0.68
1:A:654:THR:HG22	1:A:756:MET:HE3	1.75	0.68
1:A:396:ASP:OD2	1:A:398:HIS:NE2	2.26	0.67
2:C:42:GLN:HG2	2:C:69:PHE:CD1	2.30	0.67
2:D:25:ASP:O	2:D:27:THR:N	2.28	0.67
1:B:843:ARG:NE	1:B:843:ARG:HA	2.10	0.67
1:B:338:ARG:HH11	1:B:338:ARG:HG3	1.61	0.65
1:B:632:GLU:HG2	1:B:679:GLN:HE22	1.62	0.65
1:B:427:ARG:O	1:B:430:THR:N	2.30	0.65
1:B:103:TYR:HB2	2:D:25:ASP:HB2	1.78	0.65
1:A:644:THR:O	1:A:648:GLU:HG3	1.97	0.64
1:A:703:SER:O	1:B:247:LYS:NZ	2.27	0.63
2:C:54:ASN:OD1	2:C:61:ASN:ND2	2.32	0.63
2:C:52:MET:SD	2:C:55:GLU:HA	2.39	0.63
1:A:173:LEU:HD22	1:A:223:PRO:HB2	1.81	0.62
1:A:238:MET:HE1	1:A:268:LEU:HB2	1.81	0.62
2:C:102:SER:HB3	2:C:106:LEU:O	1.98	0.62
1:A:842:GLN:NE2	2:C:101:ILE:O	2.33	0.61
1:B:804:ARG:NH1	2:D:39:SER:O	2.26	0.61
1:B:490:ILE:HD13	1:B:529:ALA:HB1	1.83	0.60
2:C:51:ASP:OD1	2:C:51:ASP:N	2.35	0.60
1:A:509:LEU:H	1:A:601:ASN:ND2	2.00	0.59
1:A:715:VAL:HB	1:A:718:VAL:CG2	2.33	0.59
2:C:94:ASP:OD1	2:C:97:GLY:N	2.36	0.59
1:B:369:GLN:O	1:B:432:ILE:HG22	2.03	0.58
1:A:163:ILE:HG23	1:A:168:ILE:HD11	1.85	0.58
1:B:411:LYS:HA	1:B:436:LYS:HA	1.85	0.58
1:B:163:ILE:HG23	1:B:168:ILE:HD11	1.86	0.57
1:B:509:LEU:H	1:B:601:ASN:ND2	2.01	0.57
1:A:238:MET:HE2	1:A:265:SER:HB3	1.86	0.57
1:A:507:GLN:HE21	1:A:510:VAL:HG23	1.69	0.57
1:B:391:HIS:HB3	1:B:394:ARG:HH12	1.70	0.56
1:B:423:LEU:H	1:B:423:LEU:HD23	1.69	0.56
2:C:113:LEU:HD12	2:C:114:GLY:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:8:GLU:N	2:C:8:GLU:OE1	2.38	0.56
1:B:391:HIS:CG	1:B:394:ARG:HH12	2.24	0.55
1:A:460:LEU:O	1:A:464:THR:HG23	2.06	0.55
1:A:294:GLU:O	1:A:296:LEU:N	2.39	0.55
1:A:507:GLN:NE2	1:A:510:VAL:HG23	2.22	0.55
2:C:115:GLU:CD	2:C:116:LYS:HB2	2.33	0.54
1:A:622:THR:O	1:A:625:MET:HB3	2.08	0.54
1:A:689:LEU:HB3	1:A:693:THR:HG23	1.90	0.54
1:B:628:LYS:O	1:B:632:GLU:HG3	2.07	0.54
1:B:252:LYS:HE3	1:B:584:ASN:HB2	1.90	0.53
1:B:294:GLU:N	1:B:297:SER:O	2.36	0.53
1:B:137:GLU:OE2	1:B:140:ARG:NH1	2.41	0.53
1:A:238:MET:CE	1:A:268:LEU:HB2	2.38	0.53
1:B:622:THR:HG21	1:B:635:TRP:NE1	2.23	0.53
2:D:17:PHE:HZ	2:D:28:ILE:HG12	1.74	0.53
1:A:262:ARG:NE	1:B:296:LEU:HD23	2.24	0.53
1:B:839:ILE:HD11	2:D:113:LEU:HD13	1.90	0.52
1:B:627:ASP:O	1:B:631:LYS:HG3	2.09	0.52
2:D:78:LYS:O	2:D:78:LYS:HD2	2.09	0.52
1:A:99:VAL:HG22	1:A:100:LYS:N	2.25	0.52
1:B:252:LYS:HE3	1:B:584:ASN:HD22	1.75	0.52
1:A:294:GLU:N	1:A:297:SER:O	2.39	0.51
2:C:67:PRO:O	2:C:71:THR:OG1	2.23	0.51
1:B:460:LEU:HD13	1:B:637:GLU:HG2	1.92	0.51
1:B:665:LEU:HD22	1:B:744:LEU:HD12	1.93	0.50
2:D:23:ASP:N	2:D:23:ASP:OD1	2.43	0.50
1:A:221:GLU:HG2	1:A:828:ARG:HH12	1.74	0.50
1:B:141:ASN:O	1:B:145:GLN:HG2	2.12	0.50
2:D:17:PHE:CZ	2:D:28:ILE:HG12	2.46	0.50
1:A:358:THR:OG1	1:A:362:ASP:OD1	2.21	0.50
1:B:352:ARG:HD2	1:B:368:VAL:O	2.11	0.50
1:A:291:MET:HE2	1:A:300:PHE:HE1	1.76	0.49
2:D:78:LYS:HE3	2:D:82:SER:HG	1.73	0.49
1:A:773:LEU:HD22	1:A:812:GLU:HG2	1.94	0.49
2:C:25:ASP:HB3	2:C:27:THR:H	1.77	0.49
1:B:114:ASP:HA	1:B:117:LEU:HD11	1.94	0.49
2:C:6:THR:HG23	2:C:8:GLU:OE1	2.13	0.49
1:A:830:GLN:O	1:A:834:ARG:HG3	2.13	0.49
2:C:80:THR:O	2:C:84:GLU:HG3	2.12	0.49
1:B:400:LYS:HB2	1:B:538:SER:HB2	1.95	0.49
2:C:20:PHE:CG	2:C:36:VAL:HG22	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:767:GLU:O	1:A:771:LYS:HG3	2.12	0.48
1:B:479:ARG:HG2	1:B:479:ARG:HH11	1.78	0.48
1:B:676:ARG:HB3	1:B:701:ILE:HG22	1.95	0.48
1:B:117:LEU:HD21	1:B:594:PHE:CE2	2.48	0.48
1:B:341:MET:HG2	1:B:356:PHE:CZ	2.47	0.48
2:C:65:ASP:O	2:C:68:GLU:HB2	2.14	0.48
2:D:74:ALA:C	2:D:76:LYS:H	2.21	0.48
1:A:343:SER:O	1:A:346:LEU:HG	2.13	0.48
2:D:37:MET:HE3	2:D:66:PHE:CE1	2.48	0.48
1:A:291:MET:HE2	1:A:300:PHE:CE1	2.49	0.47
1:B:221:GLU:HG2	1:B:828:ARG:HH12	1.79	0.47
1:A:375:LYS:NZ	1:A:439:GLU:OE2	2.48	0.47
1:B:236:ASN:ND2	1:B:262:ARG:O	2.45	0.47
1:B:370:LYS:HA	1:B:431:LEU:O	2.15	0.47
2:D:25:ASP:OD2	2:D:28:ILE:HD12	2.14	0.47
1:A:396:ASP:O	1:A:472:HIS:HE1	1.98	0.47
1:A:316:LYS:HB2	1:A:553:PHE:HE2	1.80	0.47
2:C:54:ASN:HD21	2:C:57:ASP:HA	1.80	0.47
1:B:114:ASP:HA	1:B:117:LEU:CD1	2.45	0.46
1:B:293:ARG:HH22	1:B:296:LEU:HD12	1.80	0.46
1:A:453:LEU:HD21	1:A:467:VAL:HG22	1.97	0.46
1:A:490:ILE:HG13	1:A:506:TYR:HB3	1.97	0.46
1:A:141:ASN:O	1:A:145:GLN:HG2	2.16	0.46
1:B:173:LEU:HD22	1:B:223:PRO:HB2	1.97	0.46
2:D:32:GLU:O	2:D:36:VAL:HG23	2.15	0.46
1:B:767:GLU:O	1:B:771:LYS:HG3	2.15	0.46
2:C:81:ASP:OD1	2:C:82:SER:N	2.48	0.46
1:B:222:TYR:OH	1:B:790:GLN:OE1	2.35	0.45
1:A:221:GLU:HG2	1:A:828:ARG:NH1	2.31	0.45
1:B:190:GLN:OE1	1:B:194:LEU:HG	2.17	0.45
1:B:710:PHE:HA	1:B:734:ARG:HE	1.82	0.45
1:B:760:LYS:HB3	1:B:760:LYS:HE3	1.71	0.45
2:C:105:GLU:C	2:C:106:LEU:HG	2.42	0.45
1:A:710:PHE:CE2	1:A:714:LEU:HD21	2.52	0.44
1:A:430:THR:HG23	1:A:431:LEU:H	1.83	0.44
1:B:352:ARG:NH1	1:B:373:GLU:OE2	2.38	0.44
1:A:346:LEU:HA	1:A:356:PHE:HA	2.00	0.44
1:A:687:SER:OG	1:A:715:VAL:O	2.35	0.44
1:B:292:PHE:C	1:B:292:PHE:CD2	2.96	0.44
1:B:710:PHE:HA	1:B:734:ARG:HH21	1.83	0.44
1:A:696:MET:SD	1:B:249:PRO:HG3	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:MET:HG2	1:B:292:PHE:N	2.31	0.44
1:B:294:GLU:O	1:B:296:LEU:N	2.51	0.43
1:B:391:HIS:CB	1:B:394:ARG:HH12	2.31	0.43
2:C:97:GLY:O	2:C:100:TYR:HB2	2.18	0.43
1:A:600:LEU:HD11	1:A:753:GLU:HB2	2.01	0.43
1:A:259:GLN:O	1:A:262:ARG:NH1	2.51	0.43
1:B:412:LYS:H	1:B:436:LYS:H	1.67	0.43
1:B:622:THR:HG21	1:B:635:TRP:HE1	1.82	0.43
1:B:117:LEU:HB3	1:B:118:PRO:HD2	2.01	0.43
1:B:524:ASP:OD2	1:B:525:LYS:HG3	2.18	0.43
2:C:56:VAL:HG23	2:C:57:ASP:H	1.84	0.43
2:D:58:ALA:O	2:D:62:GLY:N	2.52	0.43
1:B:841:ILE:HD12	1:B:841:ILE:O	2.18	0.43
1:B:349:ILE:HD11	1:B:427:ARG:CD	2.49	0.43
2:D:4:GLN:HG3	2:D:5:LEU:N	2.34	0.43
1:A:175:LEU:HD23	1:A:175:LEU:HA	1.82	0.43
2:C:5:LEU:HG	2:C:67:PRO:HG3	2.00	0.43
1:A:391:HIS:CG	1:A:394:ARG:HH21	2.37	0.42
1:B:261:PHE:HB3	1:B:267:PHE:CD2	2.54	0.42
1:B:424:ASP:O	1:B:426:GLU:N	2.50	0.42
1:B:453:LEU:HD21	1:B:467:VAL:HG22	2.01	0.42
1:B:801:PHE:CZ	2:D:16:ALA:HA	2.55	0.42
1:A:184:ASP:OD2	1:A:187:LYS:HG3	2.20	0.42
2:C:23:ASP:OD1	2:C:23:ASP:N	2.48	0.42
2:C:57:ASP:N	2:C:57:ASP:OD1	2.49	0.42
2:D:31:LYS:C	2:D:33:LEU:N	2.77	0.42
1:A:229:LYS:HD3	1:A:286:SER:HB2	2.02	0.42
1:B:160:LEU:O	1:B:163:ILE:HG22	2.19	0.42
2:D:58:ALA:HB3	2:D:61:ASN:HB2	2.02	0.42
2:D:25:ASP:CG	2:D:28:ILE:HB	2.44	0.42
1:A:590:LYS:HD3	1:A:597:TYR:CZ	2.55	0.42
1:A:790:GLN:HE21	1:A:790:GLN:HB2	1.63	0.42
1:A:437:ASP:C	1:A:438:LEU:HD23	2.44	0.42
1:B:427:ARG:HE	1:B:427:ARG:HB2	1.68	0.42
2:C:113:LEU:HD12	2:C:114:GLY:N	2.33	0.42
1:A:291:MET:SD	1:A:300:PHE:CE1	3.13	0.41
1:B:622:THR:O	1:B:625:MET:HB3	2.20	0.41
2:D:68:GLU:O	2:D:72:MET:HB3	2.19	0.41
1:B:192:LEU:HD23	1:B:192:LEU:HA	1.77	0.41
1:A:114:ASP:HA	1:A:117:LEU:HD11	2.02	0.41
1:A:622:THR:HG21	1:A:635:TRP:NE1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:98:ASN:O	2:C:101:ILE:N	2.45	0.41
1:A:221:GLU:C	1:A:223:PRO:HD3	2.44	0.41
1:A:358:THR:CG2	1:A:364:VAL:HG23	2.51	0.41
1:B:507:GLN:HE22	1:B:514:ASN:HD21	1.68	0.41
1:B:509:LEU:H	1:B:601:ASN:HD22	1.65	0.41
1:B:391:HIS:HB3	1:B:394:ARG:NH1	2.35	0.41
1:B:751:LEU:HA	1:B:751:LEU:HD23	1.86	0.41
2:C:44:PRO:HG3	2:C:69:PHE:CZ	2.55	0.41
1:B:712:ASP:OD1	1:B:712:ASP:N	2.53	0.41
1:A:114:ASP:OD1	1:A:117:LEU:HD12	2.21	0.41
1:B:388:LEU:CD1	1:B:543:LEU:HD22	2.51	0.41
1:A:160:LEU:O	1:A:163:ILE:HG22	2.21	0.41
1:A:459:ASP:OD1	1:A:459:ASP:N	2.51	0.41
1:A:690:ASP:H	1:A:693:THR:CG2	2.33	0.41
1:A:751:LEU:HA	1:A:751:LEU:HD23	1.82	0.41
1:B:152:ASP:OD1	1:B:156:LYS:HE2	2.20	0.41
1:A:839:ILE:HG12	2:C:106:LEU:CD1	2.51	0.41
1:A:310:LEU:HD23	1:A:310:LEU:HA	1.80	0.40
1:A:646:CYS:HB3	1:A:665:LEU:HD21	2.04	0.40
2:C:76:LYS:O	2:C:80:THR:HG23	2.21	0.40
1:A:515:VAL:O	1:A:516:LEU:HB3	2.20	0.40
2:D:75:ARG:C	2:D:77:MET:H	2.29	0.40
1:A:222:TYR:O	1:A:225:ILE:HG12	2.21	0.40
1:A:627:ASP:O	1:A:631:LYS:HG3	2.22	0.40
1:B:230:ASN:HD21	1:B:232:ARG:HH21	1.69	0.40
1:B:611:GLN:HG2	1:B:741:LEU:HD22	2.03	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	728/873 (83%)	696 (96%)	32 (4%)	0	100	100
1	B	731/873 (84%)	694 (95%)	37 (5%)	0	100	100
2	C	114/149 (76%)	98 (86%)	16 (14%)	0	100	100
2	D	87/149 (58%)	60 (69%)	25 (29%)	2 (2%)	5	12
All	All	1660/2044 (81%)	1548 (93%)	110 (7%)	2 (0%)	48	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	26	GLY
2	D	108	HIS

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	604/794 (76%)	604 (100%)	0	100	100
1	B	616/794 (78%)	615 (100%)	1 (0%)	87	95
2	C	87/127 (68%)	87 (100%)	0	100	100
2	D	71/127 (56%)	70 (99%)	1 (1%)	59	80
All	All	1378/1842 (75%)	1376 (100%)	2 (0%)	88	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	427	ARG
2	D	115	GLU

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

Mol	Chain	Res	Type
1	A	145	GLN

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Mol	Chain	Res	Type
1	A	167	GLN
1	A	253	ASN
1	A	289	ASN
1	A	472	HIS
1	A	507	GLN
1	A	601	ASN
1	A	658	GLN
1	A	830	GLN
1	B	145	GLN
1	B	259	GLN
1	B	350	GLN
1	B	369	GLN
1	B	486	GLN
1	B	507	GLN
1	B	527	GLN
1	B	584	ASN
1	B	601	ASN
1	B	679	GLN
2	C	9	GLN
2	C	54	ASN
2	C	61	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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	734/873 (84%)	0.24	28 (3%) 44 40	35, 62, 100, 131	0
1	B	737/873 (84%)	0.12	20 (2%) 56 53	37, 60, 101, 140	0
2	C	120/149 (80%)	1.49	37 (30%) 1 1	45, 98, 143, 172	0
2	D	95/149 (63%)	1.70	35 (36%) 1 1	51, 101, 141, 185	0
All	All	1686/2044 (82%)	0.36	120 (7%) 22 19	35, 63, 117, 185	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	57	ASP	10.7
2	D	113	LEU	6.6
2	C	105	GLU	6.5
2	D	26	GLY	5.2
2	D	63	THR	4.8
2	C	106	LEU	4.6
2	D	27	THR	4.2
1	B	491	PHE	4.2
2	D	56	VAL	4.0
2	D	109	VAL	4.0
2	C	89	ALA	4.0
2	C	66	PHE	4.0
1	A	424	ASP	3.9
2	C	3	ASP	3.9
1	A	491	PHE	3.9
1	A	703	SER	3.9
1	A	430	THR	3.8
2	D	24	GLY	3.8
1	B	518	PHE	3.8
2	C	94	ASP	3.7
2	D	112	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	421	GLY	3.6
2	C	113	LEU	3.6
1	B	716	SER	3.5
2	C	139	TYR	3.5
1	A	518	PHE	3.4
2	C	56	VAL	3.3
2	D	66	PHE	3.3
1	B	167	GLN	3.3
2	D	86	ILE	3.3
1	A	810	TYR	3.2
2	C	104	ALA	3.2
1	A	419	SER	3.2
1	B	841	ILE	3.2
2	D	74	ALA	3.1
2	C	91	ARG	3.1
2	D	28	ILE	3.1
1	A	99	VAL	3.1
2	C	114	GLY	3.0
1	A	431	LEU	3.0
2	C	65	ASP	3.0
2	C	53	ILE	3.0
2	C	41	GLY	3.0
1	B	517	GLN	3.0
2	C	80	THR	2.9
2	D	118	THR	2.9
2	D	29	THR	2.9
2	C	103	ALA	2.9
2	D	58	ALA	2.9
2	C	57	ASP	2.8
1	A	544	GLY	2.8
1	B	845	TRP	2.8
1	B	492	HIS	2.8
2	D	103	ALA	2.8
2	D	84	GLU	2.8
2	D	69	PHE	2.7
1	A	846	ARG	2.7
1	B	184	ASP	2.7
1	A	349	ILE	2.7
1	B	490	ILE	2.7
2	C	90	PHE	2.7
1	A	516	LEU	2.6
2	C	47	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	50	GLN	2.6
1	B	519	GLN	2.6
2	D	61	ASN	2.6
2	D	104	ALA	2.6
2	C	71	THR	2.5
2	C	49	LEU	2.5
1	A	490	ILE	2.5
2	C	55	GLU	2.5
2	C	67	PRO	2.5
2	C	116	LYS	2.5
2	D	102	SER	2.5
2	C	64	ILE	2.4
1	A	128	SER	2.4
2	C	108	HIS	2.4
2	D	81	ASP	2.4
1	A	704	GLY	2.4
1	B	166	GLN	2.4
2	C	100	TYR	2.4
1	A	346	LEU	2.4
2	D	110	MET	2.4
1	A	848	ALA	2.4
1	A	543	LEU	2.3
2	D	37	MET	2.3
2	D	48	GLU	2.3
2	D	25	ASP	2.3
1	B	424	ASP	2.3
2	C	137	VAL	2.3
1	A	696	MET	2.2
2	D	111	THR	2.2
2	C	87	ARG	2.2
2	D	5	LEU	2.2
2	C	69	PHE	2.2
2	D	32	GLU	2.2
1	A	435	SER	2.2
1	A	778	LYS	2.2
1	B	545	ASP	2.2
2	D	47	ALA	2.2
2	C	112	ASN	2.2
1	B	349	ILE	2.2
2	D	80	THR	2.1
2	C	44	PRO	2.1
1	A	161	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	503	LYS	2.1
2	C	72	MET	2.1
2	D	108	HIS	2.1
1	B	128	SER	2.1
2	D	13	PHE	2.1
2	C	74	ALA	2.1
1	B	844	PHE	2.1
1	B	516	LEU	2.1
1	A	262	ARG	2.0
1	A	434	ASP	2.0
1	B	381	GLU	2.0
1	A	515	VAL	2.0
2	C	85	GLU	2.0
2	D	119	ASP	2.0
1	A	423	LEU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

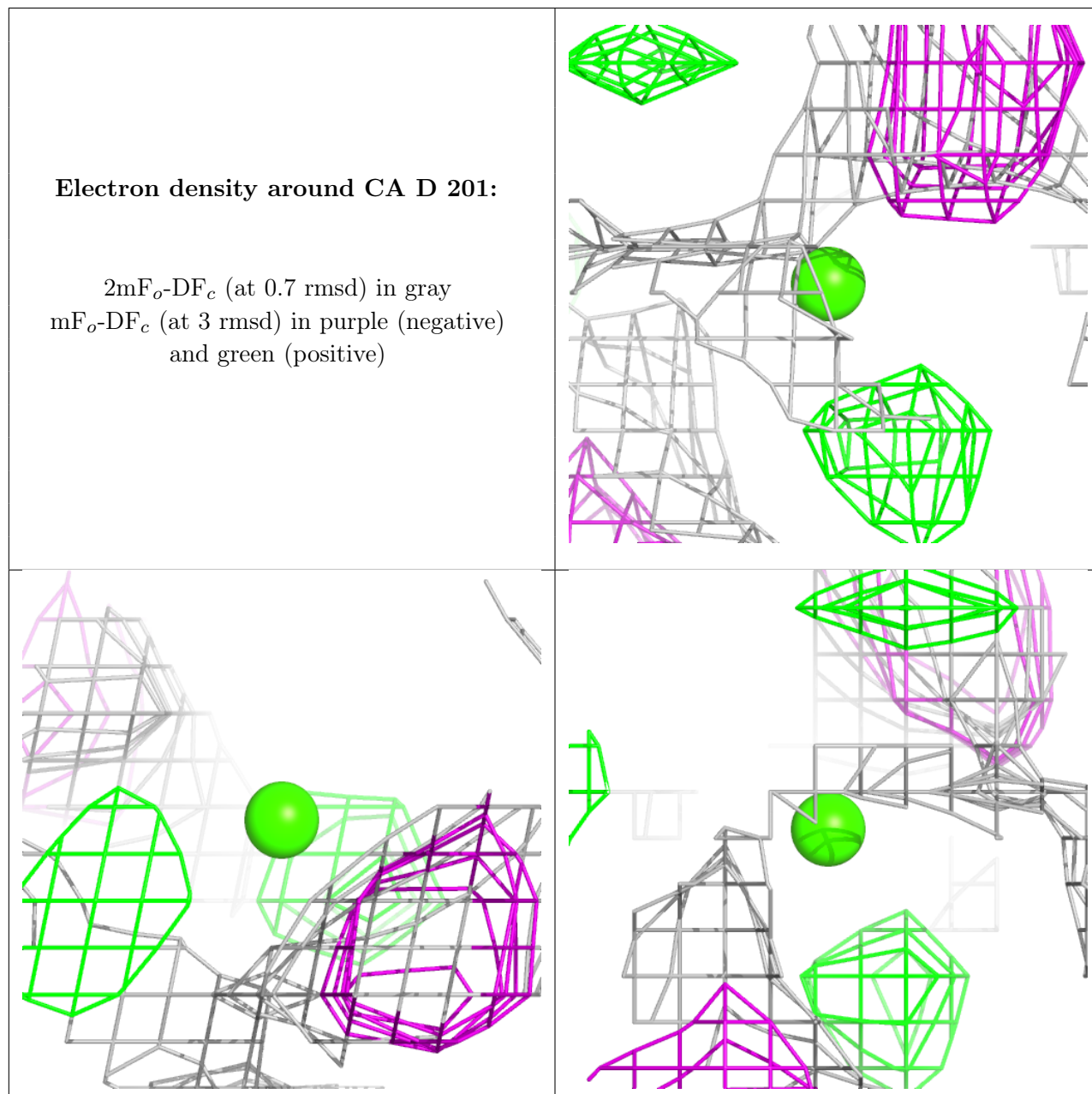
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

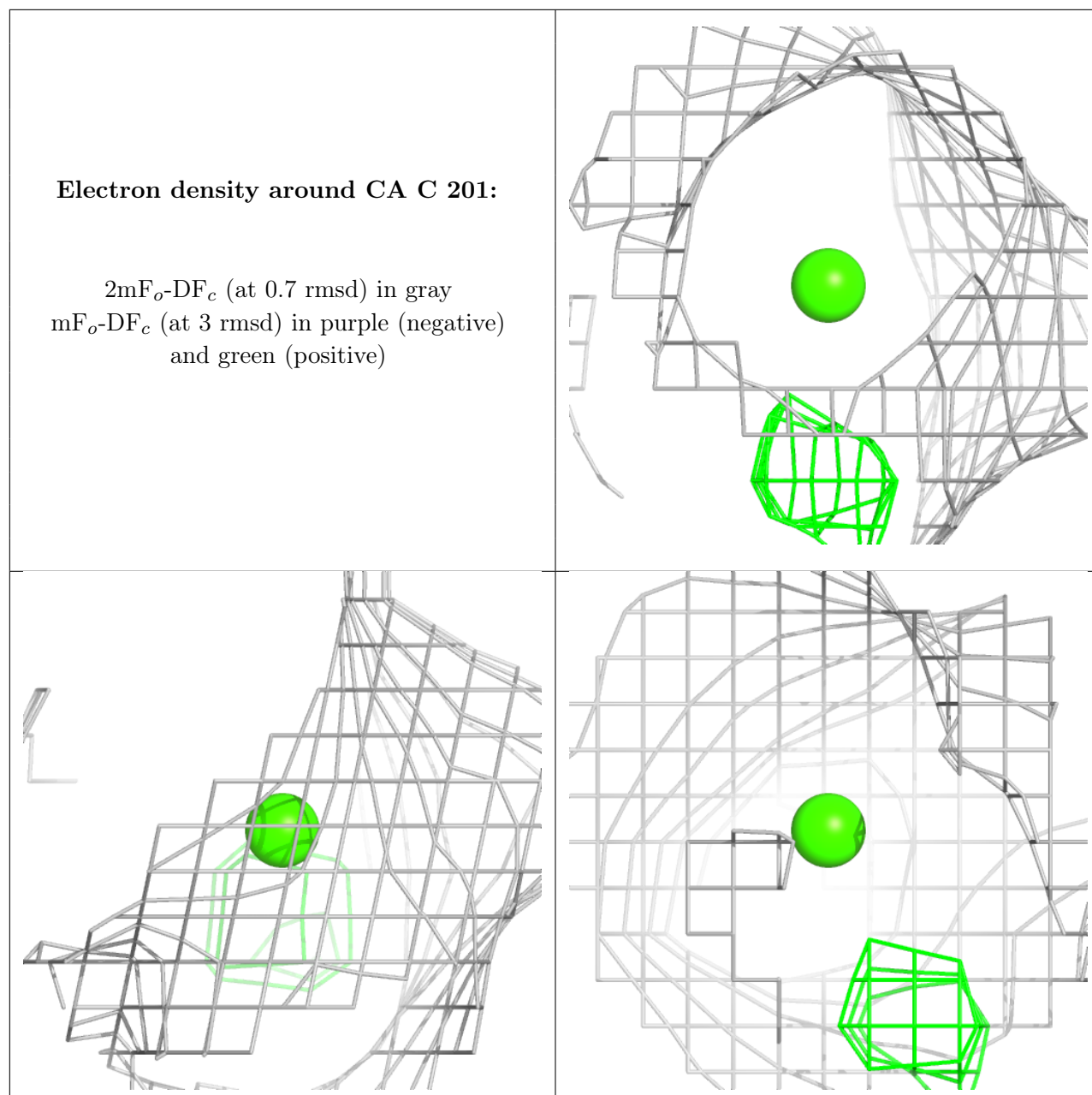
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	D	201	1/1	0.74	0.12	157,157,157,157	0
3	CA	C	201	1/1	0.90	0.08	99,99,99,99	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CA D 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.