



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:40 PM UTC

PDB ID : 6K4L / pdb_00006k4l
Title : Crystal structure of Se-labelled SidJ complex with CaM at 2.95 Å
Authors : Ouyang, S.Y.
Deposited on : 2019-05-24
Resolution : 2.95 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
Mogul : 2022.3.0, CSD as543be (2022)
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

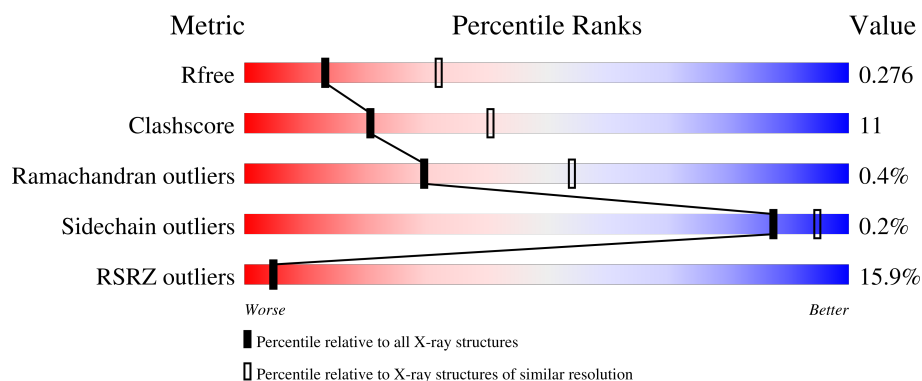
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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	9% 63% 20% 17%
1	B	873	9% 64% 20% 16%
2	C	149	42% 53% 19% 26%
2	D	149	29% 43% 11% 46%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12597 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	728	Total	C	N	O	S	Se	0	0	0
			5637	3613	946	1064	3	11			
1	B	736	Total	C	N	O	S	Se	0	0	0
			5716	3659	961	1082	3	11			

- Molecule 2 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	111	Total	C	N	O	S	0	0	0
			695	430	120	143	2			
2	D	81	Total	C	N	O	S	0	0	0
			527	324	88	114	1			

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		
3	B	2	Total	Cl	0	0
			2	2		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

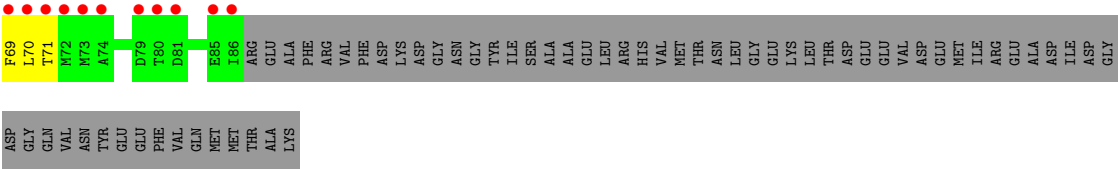
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total 4	O 4	0	0
5	B	5	Total 5	O 5	0	0
5	C	6	Total 6	O 6	0	0
5	D	1	Total 1	O 1	0	0

- Molecule 1: Sid.J





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.06Å 159.25Å 135.81Å 90.00° 101.68° 90.00°	Depositor
Resolution (Å)	68.32 – 2.95 68.32 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (68.32-2.95) 95.4 (68.32-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.243 , 0.269 0.247 , 0.276	Depositor DCC
R_{free} test set	2575 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	58.3	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 62.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12597	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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, CL

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	0.23	0/5753	0.52	2/7808 (0.0%)
1	B	0.19	0/5833	0.48	1/7911 (0.0%)
2	C	0.42	0/701	0.77	2/959 (0.2%)
2	D	0.25	0/531	0.55	0/724
All	All	0.23	0/12818	0.52	5/17402 (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	B	0	1
2	C	0	2
2	D	0	1
All	All	0	4

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	767	GLU	CA-CB-CG	7.36	128.82	114.10
1	B	346	LEU	CA-CB-CG	5.89	136.92	116.30
1	A	830	GLN	CA-CB-CG	5.84	125.78	114.10
2	C	49	LEU	CA-C-N	5.67	132.37	121.54
2	C	49	LEU	C-N-CA	5.67	132.37	121.54

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	625	MSE	Peptide
2	C	50	GLN	Peptide
2	C	53	ILE	Peptide
2	D	66	PHE	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	5637	0	5380	124	1
1	B	5716	0	5482	122	0
2	C	695	0	534	26	1
2	D	527	0	414	12	0
3	A	2	0	0	1	0
3	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	4	0	0	0	0
5	B	5	0	0	0	0
5	C	6	0	0	0	0
5	D	1	0	0	0	0
All	All	12597	0	11810	271	1

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 11.

All (271) 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:C:80:THR:O	2:C:82:SER:N	1.88	1.06
1:B:676:ARG:NH1	1:B:700:SER:O	1.98	0.96
1:A:163:ILE:HG23	1:A:168:ILE:HD11	1.42	0.95
1:A:367:LYS:NZ	1:A:381:GLU:OE1	1.98	0.95
2:C:80:THR:O	2:C:81:ASP:C	2.10	0.92
1:B:341:MSE:HG2	1:B:418:ILE:CD1	1.99	0.92
1:B:349:ILE:HD11	1:B:427:ARG:HD3	1.50	0.90
1:B:768:GLN:O	1:B:772:ILE:HD12	1.76	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:THR:HG22	1:B:360:GLN:H	1.43	0.84
1:A:352:ARG:NH2	1:A:367:LYS:HE3	1.93	0.83
1:A:358:THR:HG23	1:A:360:GLN:H	1.45	0.82
2:C:6:THR:HG22	2:C:9:GLN:OE1	1.80	0.81
1:A:137:GLU:OE2	1:A:140:ARG:NH1	2.13	0.79
2:C:25:ASP:O	2:C:27:THR:HG23	1.84	0.78
1:A:711:THR:HB	1:A:734:ARG:HH22	1.50	0.76
2:C:20:PHE:CG	2:C:36:VAL:HG12	2.22	0.74
1:B:400:LYS:HB2	1:B:538:SER:HB2	1.69	0.74
1:A:155:ILE:HD12	1:A:197:PRO:HB2	1.69	0.74
1:A:392:GLN:HG3	1:A:397:VAL:HG12	1.70	0.73
1:B:341:MSE:HG2	1:B:418:ILE:HD13	1.71	0.71
1:A:173:LEU:HD22	1:A:223:PRO:HB2	1.72	0.70
1:B:173:LEU:HD22	1:B:223:PRO:HB2	1.73	0.70
2:C:52:MET:O	2:C:54:ASN:N	2.26	0.69
1:B:520:LEU:O	1:B:736:SER:N	2.24	0.68
1:A:453:LEU:HD21	1:A:467:VAL:HG22	1.76	0.68
1:B:708:TYR:HE1	1:B:735:GLU:HG2	1.58	0.68
1:A:263:ASP:OD1	1:B:295:ARG:NH2	2.28	0.67
1:A:352:ARG:HH21	1:A:367:LYS:HE3	1.58	0.66
1:B:473:ASP:HA	1:B:476:VAL:HG22	1.79	0.65
2:C:80:THR:C	2:C:82:SER:N	2.55	0.65
1:A:163:ILE:HG23	1:A:168:ILE:CD1	2.24	0.64
1:B:341:MSE:HG2	1:B:418:ILE:HD12	1.78	0.63
1:A:458:GLN:O	1:A:617:TYR:OH	2.15	0.63
2:C:90:PHE:C	2:C:92:VAL:H	2.07	0.63
1:B:622:THR:HG21	1:B:635:TRP:NE1	2.15	0.62
1:B:676:ARG:NH1	1:B:701:ILE:HA	2.14	0.62
1:A:367:LYS:NZ	1:A:381:GLU:CD	2.58	0.61
1:B:631:LYS:HD3	1:B:631:LYS:N	2.14	0.61
1:B:352:ARG:NH1	1:B:373:GLU:OE1	2.30	0.60
1:B:453:LEU:HD21	1:B:467:VAL:HG22	1.82	0.60
1:A:678:THR:HB	1:A:682:MSE:HE2	1.83	0.60
2:D:36:VAL:O	2:D:39:SER:OG	2.15	0.60
1:B:138:ALA:O	1:B:142:GLU:HG3	2.01	0.60
1:B:137:GLU:OE2	1:B:140:ARG:NH1	2.35	0.60
1:B:740:GLU:OE2	1:B:743:LYS:NZ	2.34	0.59
1:A:636:ARG:O	1:A:640:ASN:ND2	2.35	0.59
1:B:341:MSE:SE	1:B:366:VAL:HG11	2.53	0.59
1:A:841:ILE:HD11	2:C:102:SER:OG	2.03	0.59
1:B:635:TRP:CD1	1:B:679:GLN:HG3	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:673:LYS:O	1:B:677:GLN:HG3	2.03	0.58
1:A:143:LEU:HD21	1:A:254:GLN:HB3	1.86	0.58
1:A:400:LYS:HB2	1:A:538:SER:HB2	1.86	0.57
1:B:768:GLN:C	1:B:772:ILE:HD12	2.29	0.57
1:B:375:LYS:O	1:B:379:GLU:HG3	2.04	0.57
1:B:660:ARG:NH2	2:D:15:GLU:OE2	2.37	0.57
1:A:226:HIS:HA	1:A:229:LYS:HD2	1.85	0.57
1:B:550:THR:O	1:B:554:THR:HG23	2.04	0.57
1:B:572:HIS:ND1	1:B:574:THR:OG1	2.34	0.57
2:C:80:THR:O	2:C:83:GLU:N	2.36	0.57
1:A:358:THR:HG21	1:A:362:ASP:OD1	2.04	0.57
1:A:173:LEU:HD21	1:A:213:ILE:HG23	1.86	0.57
1:A:622:THR:HG21	1:A:635:TRP:NE1	2.19	0.57
1:B:632:GLU:O	1:B:636:ARG:HG2	2.04	0.57
1:B:533:VAL:HG22	1:B:535:LEU:HG	1.86	0.57
1:B:251:THR:HG23	1:B:254:GLN:H	1.70	0.56
1:A:384:MSE:HE3	1:A:387:TYR:HB3	1.88	0.56
1:B:168:ILE:HG22	1:B:202:LEU:HD11	1.87	0.56
1:A:533:VAL:HG22	1:A:535:LEU:HG	1.88	0.56
1:A:163:ILE:CG2	1:A:168:ILE:HD11	2.27	0.56
2:C:33:LEU:O	2:C:37:MET:HG3	2.06	0.55
1:A:673:LYS:O	1:A:677:GLN:HG3	2.05	0.55
1:A:792:LEU:HD11	1:A:803:LYS:HD3	1.86	0.55
1:A:415:ILE:O	1:A:419:SER:OG	2.24	0.55
1:B:163:ILE:HG23	1:B:168:ILE:HD11	1.88	0.55
1:A:116:SER:O	1:A:116:SER:OG	2.23	0.55
1:B:654:THR:HG22	1:B:756:MSE:HE3	1.89	0.55
1:A:310:LEU:HD11	1:A:600:LEU:HD12	1.89	0.54
2:C:6:THR:HG22	2:C:9:GLN:HG2	1.89	0.54
1:B:789:ALA:HB1	1:B:828:ARG:HH11	1.72	0.54
1:A:512:LEU:O	1:A:590:LYS:NZ	2.34	0.54
1:A:350:GLN:HE22	1:A:450:PHE:HB3	1.72	0.54
1:A:113:HIS:NE2	1:A:316:LYS:O	2.24	0.54
1:A:141:ASN:O	1:A:145:GLN:HG2	2.08	0.54
1:A:151:ILE:O	1:A:155:ILE:HG12	2.07	0.54
1:B:384:MSE:HE3	1:B:387:TYR:HB3	1.89	0.54
2:D:68:GLU:O	2:D:71:THR:N	2.40	0.54
1:B:352:ARG:HD3	1:B:368:VAL:O	2.07	0.53
1:B:106:ARG:O	2:D:23:ASP:HB2	2.08	0.53
1:A:294:GLU:N	1:A:297:SER:O	2.33	0.53
2:C:30:THR:HA	2:C:33:LEU:HD13	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:LEU:HD21	1:B:254:GLN:HB3	1.90	0.53
1:A:515:VAL:HG21	1:A:575:PHE:CE1	2.44	0.53
1:B:310:LEU:HD11	1:B:600:LEU:HD12	1.91	0.53
1:B:779:THR:HG22	1:B:780:ASP:H	1.73	0.53
1:A:408:TYR:O	1:A:440:VAL:N	2.39	0.52
1:B:165:SER:OG	1:B:209:VAL:HG21	2.10	0.52
1:B:190:GLN:O	1:B:193:SER:HB3	2.09	0.52
1:A:715:VAL:HG21	1:A:724:GLY:HA2	1.92	0.52
1:B:380:GLU:HA	1:B:383:GLU:OE2	2.09	0.52
1:A:632:GLU:O	1:A:636:ARG:HG3	2.09	0.52
1:B:349:ILE:HD11	1:B:427:ARG:CD	2.33	0.52
1:A:556:SER:O	1:A:560:LYS:HG2	2.10	0.51
1:A:773:LEU:HD13	1:A:812:GLU:CD	2.34	0.51
1:A:248:GLU:HG3	1:A:249:PRO:HD2	1.92	0.51
1:A:122:LYS:HG2	1:A:571:TYR:CG	2.44	0.51
1:A:360:GLN:N	1:A:360:GLN:OE1	2.44	0.51
1:B:251:THR:HG22	1:B:254:GLN:CD	2.35	0.51
2:C:66:PHE:O	2:C:69:PHE:N	2.43	0.51
1:A:665:LEU:HD13	1:A:751:LEU:HD12	1.91	0.51
1:B:102:TYR:O	1:B:394:ARG:NH1	2.44	0.51
1:B:117:LEU:HD23	1:B:555:SER:HB2	1.92	0.51
1:B:740:GLU:HA	1:B:743:LYS:HG3	1.93	0.50
1:A:348:ARG:HB3	1:A:355:LEU:HD12	1.92	0.50
1:A:358:THR:HG23	1:A:360:GLN:N	2.21	0.50
1:A:509:LEU:HD11	1:A:749:VAL:HG11	1.94	0.50
1:A:138:ALA:O	1:A:142:GLU:HG3	2.10	0.50
1:B:670:ASN:OD1	1:B:673:LYS:N	2.33	0.50
1:B:264:SER:OG	1:B:266:VAL:HG22	2.12	0.50
1:A:399:SER:OG	1:A:473:ASP:OD2	2.19	0.50
1:A:699:TYR:OH	1:B:247:LYS:HD3	2.12	0.50
1:B:370:LYS:HA	1:B:431:LEU:O	2.11	0.49
1:A:823:ASP:OD1	1:A:823:ASP:N	2.45	0.49
2:C:67:PRO:O	2:C:71:THR:N	2.41	0.49
1:A:103:TYR:HB2	2:C:25:ASP:CB	2.43	0.49
1:A:294:GLU:O	1:A:296:LEU:N	2.45	0.49
1:B:712:ASP:OD1	1:B:712:ASP:N	2.43	0.49
1:B:515:VAL:HG21	1:B:575:PHE:CZ	2.48	0.49
1:B:534:ASN:HB3	1:B:541:ALA:O	2.12	0.49
1:A:213:ILE:O	1:A:217:ILE:HG13	2.13	0.49
1:A:475:PHE:O	1:A:479:ARG:HG3	2.13	0.49
1:B:786:GLU:HG3	1:B:825:TYR:OH	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:ASN:HB3	1:A:541:ALA:O	2.13	0.49
1:A:262:ARG:HE	1:B:296:LEU:HD12	1.78	0.48
1:B:112:THR:HG22	1:B:114:ASP:H	1.78	0.48
1:B:630:LYS:C	1:B:631:LYS:HD3	2.38	0.48
1:B:384:MSE:HG2	1:B:543:LEU:HB3	1.95	0.48
1:A:375:LYS:O	1:A:379:GLU:HG3	2.12	0.48
1:B:779:THR:HG22	1:B:780:ASP:OD1	2.13	0.48
1:A:474:LEU:HG	1:A:540:LEU:HD21	1.95	0.48
1:B:725:VAL:HG23	1:B:726:HIS:ND1	2.29	0.48
1:A:186:ILE:O	1:A:190:GLN:HG2	2.13	0.48
1:B:830:GLN:O	1:B:834:ARG:HG3	2.13	0.48
1:A:409:SER:HA	1:A:439:GLU:HA	1.96	0.48
1:B:509:LEU:HD11	1:B:749:VAL:HG21	1.95	0.48
1:A:338:ARG:HA	1:A:338:ARG:HD3	1.74	0.47
1:B:837:ALA:O	1:B:841:ILE:HG23	2.13	0.47
2:D:64:ILE:O	2:D:67:PRO:HD2	2.13	0.47
1:A:641:VAL:O	1:A:645:SER:OG	2.31	0.47
1:B:348:ARG:HG2	1:B:349:ILE:N	2.29	0.47
1:B:805:LEU:HB2	2:D:39:SER:HB3	1.94	0.47
1:B:838:ALA:O	1:B:841:ILE:HG13	2.14	0.47
2:D:42:GLN:O	2:D:44:PRO:HD3	2.14	0.47
1:A:366:VAL:HG13	1:A:366:VAL:O	2.14	0.47
1:A:509:LEU:O	1:A:513:LEU:HG	2.15	0.47
2:D:37:MET:HB3	2:D:66:PHE:HZ	1.78	0.47
1:A:698:GLN:OE1	1:A:708:TYR:HB3	2.15	0.47
1:A:490:ILE:HG13	1:A:506:TYR:CB	2.43	0.47
1:A:635:TRP:CG	1:A:679:GLN:HB2	2.50	0.47
1:A:781:ALA:HB1	1:A:820:ALA:HB2	1.97	0.47
1:B:132:LYS:HE2	1:B:582:THR:HG21	1.97	0.47
1:B:665:LEU:HD13	1:B:751:LEU:HD12	1.97	0.47
1:B:358:THR:HG22	1:B:360:GLN:N	2.21	0.47
2:C:82:SER:HA	2:C:85:GLU:OE1	2.15	0.47
1:B:766:LEU:O	1:B:769:VAL:HG22	2.15	0.46
2:C:90:PHE:C	2:C:92:VAL:N	2.73	0.46
1:A:190:GLN:O	1:A:193:SER:OG	2.32	0.46
1:A:782:ASN:O	1:A:786:GLU:HG2	2.15	0.46
2:C:6:THR:HG22	2:C:9:GLN:CD	2.40	0.46
1:A:188:LYS:O	1:A:192:LEU:HG	2.15	0.46
1:A:346:LEU:HA	1:A:356:PHE:HA	1.98	0.46
1:B:710:PHE:HA	1:B:734:ARG:HD2	1.97	0.46
1:B:334:ASP:OD1	1:B:336:SER:OG	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:GLN:NE2	3:A:902:CL:CL	2.86	0.46
1:B:474:LEU:HD21	1:B:487:LEU:HD11	1.97	0.46
2:C:90:PHE:O	2:C:92:VAL:N	2.48	0.46
2:C:25:ASP:O	2:C:27:THR:N	2.49	0.46
1:A:468:LYS:HD3	1:A:648:GLU:OE2	2.16	0.46
1:A:600:LEU:HD22	1:A:749:VAL:HG13	1.98	0.45
1:B:511:GLN:OE1	1:B:511:GLN:N	2.40	0.45
1:A:802:GLN:O	1:A:806:VAL:HG13	2.17	0.45
1:A:549:ILE:HD11	1:A:599:TYR:CE1	2.51	0.45
1:B:618:GLY:O	1:B:622:THR:HG23	2.15	0.45
1:B:659:SER:O	1:B:663:THR:HG23	2.17	0.45
1:A:252:LYS:HZ1	1:A:577:ASP:CG	2.24	0.44
1:B:515:VAL:HG12	1:B:565:GLU:OE1	2.17	0.44
1:B:789:ALA:HB1	1:B:828:ARG:NH1	2.31	0.44
1:A:296:LEU:HD11	1:B:258:VAL:HG12	1.98	0.44
1:A:344:ASP:OD1	1:A:344:ASP:N	2.44	0.44
1:A:346:LEU:HD23	1:A:346:LEU:O	2.17	0.44
1:A:712:ASP:OD2	1:A:734:ARG:NH1	2.51	0.44
1:A:766:LEU:O	1:A:769:VAL:HG22	2.17	0.44
1:B:173:LEU:HD23	1:B:173:LEU:HA	1.85	0.44
1:A:549:ILE:HD11	1:A:599:TYR:HE1	1.83	0.44
1:B:520:LEU:O	1:B:735:GLU:HA	2.18	0.44
1:B:708:TYR:CE1	1:B:735:GLU:HG2	2.46	0.44
1:B:509:LEU:O	1:B:513:LEU:HG	2.18	0.44
1:A:290:PRO:HB3	1:A:305:LEU:HD11	2.00	0.44
1:A:690:ASP:OD1	1:A:693:THR:HG22	2.18	0.44
1:B:540:LEU:HD23	1:B:540:LEU:HA	1.81	0.44
1:A:490:ILE:HG13	1:A:506:TYR:HB3	1.99	0.43
1:B:356:PHE:HB2	1:B:364:VAL:HG13	2.00	0.43
1:A:731:GLY:HA3	1:A:734:ARG:HD3	2.00	0.43
1:B:475:PHE:O	1:B:479:ARG:HG3	2.18	0.43
1:B:248:GLU:HG3	1:B:249:PRO:HD2	2.01	0.43
1:B:348:ARG:HD2	1:B:350:GLN:HG3	2.00	0.43
1:B:509:LEU:HB3	1:B:512:LEU:HD12	2.01	0.43
1:A:117:LEU:HD22	1:A:567:LEU:HD23	2.00	0.43
2:C:6:THR:HG22	2:C:9:GLN:CG	2.49	0.43
1:A:343:SER:O	1:A:346:LEU:HD22	2.19	0.43
1:B:233:ALA:O	1:B:264:SER:HB2	2.19	0.43
1:B:752:ILE:O	1:B:756:MSE:HG2	2.19	0.43
1:A:129:ILE:HG23	1:A:581:GLY:O	2.19	0.43
1:A:711:THR:CB	1:A:734:ARG:HH22	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:TRP:HZ3	1:A:682:MSE:HE3	1.84	0.42
1:B:134:ILE:HG23	1:B:253:ASN:HD22	1.83	0.42
1:B:290:PRO:HB3	1:B:305:LEU:HD11	2.01	0.42
1:A:114:ASP:HB2	1:A:591:ARG:C	2.44	0.42
1:B:348:ARG:HG2	1:B:349:ILE:H	1.84	0.42
1:B:388:LEU:HD11	1:B:543:LEU:HG	2.00	0.42
1:B:705:GLU:HB3	1:B:739:ARG:HH21	1.84	0.42
2:C:57:ASP:N	2:C:57:ASP:OD1	2.53	0.42
1:A:217:ILE:HA	1:A:223:PRO:HG3	2.02	0.42
1:A:659:SER:O	1:A:663:THR:HG23	2.20	0.42
1:B:163:ILE:HG13	1:B:164:PRO:HD2	2.01	0.42
1:B:242:ILE:O	1:B:246:HIS:HB3	2.20	0.42
1:B:489:ASP:OD2	1:B:529:ALA:HA	2.20	0.42
1:A:117:LEU:HD23	1:A:555:SER:HB2	2.01	0.42
1:A:345:ARG:O	1:A:357:SER:N	2.30	0.42
1:A:474:LEU:HD21	1:A:487:LEU:HD11	2.02	0.42
1:B:560:LYS:HE3	1:B:560:LYS:HB2	1.82	0.42
1:B:805:LEU:HB2	2:D:39:SER:CB	2.50	0.42
1:A:699:TYR:CD1	1:B:249:PRO:HD3	2.55	0.42
1:B:746:TYR:HA	1:B:749:VAL:HG22	2.02	0.42
2:C:66:PHE:C	2:C:70:LEU:HD12	2.45	0.42
1:B:112:THR:HG22	1:B:114:ASP:N	2.35	0.41
1:B:384:MSE:HE2	1:B:388:LEU:HG	2.01	0.41
1:B:234:HIS:ND1	1:B:301:TYR:OH	2.52	0.41
1:B:617:TYR:CZ	1:B:621:VAL:HG21	2.55	0.41
1:A:371:LYS:HA	1:A:434:ASP:HB3	2.02	0.41
1:A:522:ARG:HD3	1:A:731:GLY:O	2.21	0.41
1:B:216:LEU:HD23	1:B:219:LYS:HD3	2.01	0.41
1:B:807:LEU:O	1:B:811:GLU:HG2	2.20	0.41
2:D:16:ALA:HB1	2:D:36:VAL:HG23	2.02	0.41
1:A:147:TYR:CD1	1:A:238:MSE:HG2	2.56	0.41
1:A:285:ASP:N	1:A:285:ASP:OD1	2.50	0.41
1:A:637:GLU:O	1:A:641:VAL:HG12	2.20	0.41
1:B:122:LYS:HG2	1:B:571:TYR:CG	2.56	0.41
1:B:163:ILE:CG2	1:B:168:ILE:HD11	2.50	0.41
2:D:61:ASN:O	2:D:65:ASP:N	2.52	0.41
1:A:638:LEU:HA	1:A:641:VAL:HG12	2.02	0.41
1:A:685:ASP:N	1:A:685:ASP:OD1	2.53	0.41
1:B:131:LEU:HD13	1:B:569:GLY:O	2.20	0.41
2:C:20:PHE:CD1	2:C:36:VAL:HG12	2.56	0.41
1:A:712:ASP:OD2	1:A:712:ASP:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:807:LEU:HD22	1:A:832:VAL:HG12	2.03	0.41
1:A:804:ARG:HD2	2:C:39:SER:O	2.20	0.41
1:B:192:LEU:HA	1:B:192:LEU:HD23	1.79	0.41
1:A:342:SER:O	1:A:356:PHE:HE1	2.04	0.40
1:A:622:THR:HG21	1:A:635:TRP:HE1	1.84	0.40
1:A:635:TRP:CZ3	1:A:682:MSE:HE3	2.55	0.40
1:B:167:GLN:O	1:B:171:HIS:CD2	2.74	0.40
1:B:229:LYS:HB2	1:B:286:SER:HA	2.03	0.40
1:A:830:GLN:O	1:A:834:ARG:HG3	2.22	0.40
1:B:151:ILE:HG22	1:B:194:LEU:HD22	2.02	0.40
1:B:710:PHE:CE2	1:B:720:LEU:HD21	2.56	0.40
1:A:149:THR:O	1:A:153:LYS:HG3	2.21	0.40
1:A:296:LEU:HB2	1:B:262:ARG:HH21	1.86	0.40
1:A:351:GLY:C	1:A:353:THR:H	2.29	0.40
1:A:622:THR:O	1:A:625:MSE:HB2	2.22	0.40
1:A:628:LYS:N	1:A:629:PRO:HD2	2.37	0.40
2:D:68:GLU:C	2:D:70:LEU:N	2.78	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:SER:CB	2:C:77:MET:CE[2_656]	1.88	0.32

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	720/873 (82%)	685 (95%)	34 (5%)	1 (0%)	48	71
1	B	732/873 (84%)	699 (96%)	33 (4%)	0	100	100
2	C	109/149 (73%)	78 (72%)	26 (24%)	5 (5%)	2	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	77/149 (52%)	50 (65%)	26 (34%)	1 (1%)	9	25
All	All	1638/2044 (80%)	1512 (92%)	119 (7%)	7 (0%)	30	54

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	53	ILE
2	C	81	ASP
2	D	69	PHE
1	A	352	ARG
2	C	80	THR
2	C	89	ALA
2	C	109	VAL

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	588/780 (75%)	587 (100%)	1 (0%)	87	95
1	B	600/780 (77%)	600 (100%)	0	100	100
2	C	46/127 (36%)	45 (98%)	1 (2%)	45	69
2	D	41/127 (32%)	41 (100%)	0	100	100
All	All	1275/1814 (70%)	1273 (100%)	2 (0%)	87	95

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

Mol	Chain	Res	Type
1	A	419	SER
2	C	77	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	ASN
1	A	299	ASN
1	A	407	GLN
1	A	470	ASN
1	A	486	GLN
1	A	514	ASN
1	A	800	HIS
1	B	166	GLN
1	B	253	ASN
1	B	289	ASN
1	B	486	GLN
1	B	561	HIS
2	C	42	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	717/873 (82%)	0.67	77 (10%)	11 10	26, 57, 98, 166	0
1	B	724/873 (82%)	0.68	78 (10%)	11 10	25, 58, 105, 184	0
2	C	111/149 (74%)	2.44	62 (55%)	0 0	41, 92, 152, 177	0
2	D	81/149 (54%)	2.15	43 (53%)	0 0	46, 94, 185, 219	0
All	All	1633/2044 (79%)	0.87	260 (15%)	5 5	25, 60, 119, 219	0

All (260) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	519	GLN	7.9
2	C	104	ALA	7.1
2	D	29	THR	7.0
2	C	105	GLU	6.8
2	C	85	GLU	6.4
1	B	438	LEU	6.0
2	C	53	ILE	5.9
1	A	518	PHE	5.2
2	D	27	THR	5.1
2	C	88	GLU	5.0
1	B	624	ASP	5.0
2	D	57	ASP	5.0
2	D	55	GLU	4.9
1	B	518	PHE	4.9
2	C	4	GLN	4.9
2	C	55	GLU	4.9
2	C	41	GLY	4.8
1	A	435	SER	4.8
2	D	26	GLY	4.7
1	B	491	PHE	4.6
2	C	26	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
2	C	54	ASN	4.6
1	A	691	GLU	4.5
2	C	114	GLY	4.4
2	C	77	MET	4.3
2	C	89	ALA	4.3
1	A	845	TRP	4.3
2	C	93	PHE	4.3
1	A	627	ASP	4.3
2	C	71	THR	4.2
1	B	490	ILE	4.2
2	D	28	ILE	4.2
1	A	491	PHE	4.1
2	D	51	ASP	4.0
2	C	108	HIS	4.0
1	B	342	SER	4.0
1	B	545	ASP	3.9
1	B	167	GLN	3.9
1	A	420	ARG	3.9
2	C	44	PRO	3.9
1	B	372	GLY	3.9
2	C	112	ASN	3.9
1	B	580	SER	3.9
2	C	66	PHE	3.8
2	C	94	ASP	3.8
2	D	49	LEU	3.8
1	A	334	ASP	3.7
1	B	432	ILE	3.7
2	C	52	MET	3.7
1	B	437	ASP	3.7
2	D	74	ALA	3.7
1	B	424	ASP	3.7
1	A	99	VAL	3.7
1	B	168	ILE	3.6
2	C	45	THR	3.6
2	D	4	GLN	3.6
1	B	703	SER	3.6
1	A	517	GLN	3.6
2	C	25	ASP	3.6
2	D	79	ASP	3.6
1	B	839	ILE	3.5
2	D	80	THR	3.5
1	A	826	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
2	C	111	THR	3.5
2	C	74	ALA	3.5
2	D	50	GLN	3.5
1	B	124	LEU	3.5
1	B	423	LEU	3.5
2	D	46	GLU	3.5
1	B	436	LYS	3.4
1	B	347	LEU	3.4
2	C	86	ILE	3.4
2	D	64	ILE	3.4
1	A	166	GLN	3.4
2	C	27	THR	3.4
2	C	65	ASP	3.4
1	A	423	LEU	3.3
1	A	846	ARG	3.3
1	A	708	TYR	3.3
2	C	98	ASN	3.3
2	D	73	MET	3.2
2	C	76	LYS	3.2
2	C	72	MET	3.2
2	C	109	VAL	3.2
2	C	48	GLU	3.2
1	B	841	ILE	3.2
2	C	87	ARG	3.2
1	B	329	GLU	3.1
2	D	25	ASP	3.1
2	C	75	ARG	3.1
2	C	103	ALA	3.1
1	A	844	PHE	3.1
1	A	295	ARG	3.1
1	B	520	LEU	3.1
1	A	695	GLN	3.1
1	B	106	ARG	3.1
1	A	580	SER	3.0
1	B	846	ARG	3.0
2	C	68	GLU	3.0
2	C	47	ALA	3.0
2	C	73	MET	3.0
1	A	688	LYS	3.0
2	C	50	GLN	3.0
2	D	48	GLU	3.0
2	D	30	THR	3.0

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Mol	Chain	Res	Type	RSRZ
2	C	92	VAL	3.0
1	A	436	LYS	3.0
1	B	503	LYS	3.0
2	D	86	ILE	3.0
1	B	128	SER	3.0
1	A	519	GLN	2.9
1	B	434	ASP	2.9
1	B	430	THR	2.9
1	B	431	LEU	2.9
1	A	350	GLN	2.9
1	A	329	GLU	2.9
1	B	489	ASP	2.9
1	A	703	SER	2.9
2	C	106	LEU	2.9
1	A	774	SER	2.9
2	D	69	PHE	2.9
1	B	346	LEU	2.9
2	C	113	LEU	2.9
2	D	52	MET	2.8
1	B	716	SER	2.8
1	A	416	LEU	2.8
2	C	49	LEU	2.8
1	A	830	GLN	2.8
1	B	426	GLU	2.8
2	C	51	ASP	2.8
1	A	545	ASP	2.8
2	D	63	THR	2.7
1	B	517	GLN	2.7
2	D	32	GLU	2.7
1	A	432	ILE	2.7
1	B	349	ILE	2.7
2	C	107	ARG	2.7
1	B	691	GLU	2.7
2	D	45	THR	2.7
1	A	294	GLU	2.7
1	A	516	LEU	2.7
1	B	516	LEU	2.7
2	D	72	MET	2.7
2	D	71	THR	2.7
1	B	579	SER	2.7
2	D	70	LEU	2.7
1	B	627	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	79	ASP	2.6
1	B	359	PRO	2.6
1	A	330	LYS	2.6
1	A	735	GLU	2.6
1	A	624	ASP	2.6
1	A	692	ASP	2.6
2	C	82	SER	2.6
2	C	56	VAL	2.6
1	A	254	GLN	2.6
1	A	570	GLY	2.5
1	A	163	ILE	2.5
1	A	299	ASN	2.5
1	B	782	ASN	2.5
1	B	285	ASP	2.5
1	B	692	ASP	2.5
1	A	503	LYS	2.5
2	D	41	GLY	2.5
2	D	13	PHE	2.5
1	B	345	ARG	2.5
1	B	371	LYS	2.5
1	B	322	SER	2.5
2	D	56	VAL	2.5
2	C	110	MET	2.5
1	A	777	ILE	2.5
1	B	373	GLU	2.5
1	B	844	PHE	2.5
2	C	84	GLU	2.5
1	A	690	ASP	2.4
1	B	386	ASP	2.4
2	C	6	THR	2.4
1	B	815	LEU	2.4
1	A	490	ILE	2.4
2	D	23	ASP	2.4
1	A	520	LEU	2.4
1	A	542	ASP	2.4
1	A	370	LYS	2.4
1	B	323	GLU	2.4
1	B	380	GLU	2.4
1	B	183	THR	2.4
2	C	43	ASN	2.4
1	B	699	TYR	2.4
1	A	418	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	219	LYS	2.3
2	C	58	ALA	2.3
1	A	843	ARG	2.3
1	B	676	ARG	2.3
2	C	90	PHE	2.3
1	A	127	ARG	2.3
1	A	372	GLY	2.3
1	A	704	GLY	2.3
1	B	414	GLU	2.3
2	C	46	GLU	2.3
1	B	330	LYS	2.3
1	B	435	SER	2.3
2	C	67	PRO	2.3
2	D	37	MET	2.3
1	A	543	LEU	2.3
1	A	778	LYS	2.3
2	D	31	LYS	2.3
1	B	421	GLY	2.3
1	B	428	PHE	2.2
2	D	85	GLU	2.2
2	D	59	ASP	2.2
1	A	772	ILE	2.2
1	A	569	GLY	2.2
2	D	47	ALA	2.2
1	A	623	ARG	2.2
1	A	636	ARG	2.2
1	A	622	THR	2.2
1	A	125	SER	2.2
1	B	125	SER	2.2
1	A	775	GLY	2.2
1	B	704	GLY	2.2
1	A	165	SER	2.2
1	B	521	GLY	2.2
1	B	732	TYR	2.2
2	D	20	PHE	2.2
2	C	33	LEU	2.2
1	B	186	ILE	2.2
1	A	375	LYS	2.2
1	A	709	GLU	2.2
1	A	740	GLU	2.2
1	A	489	ASP	2.1
1	B	578	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	80	THR	2.1
1	A	342	SER	2.1
1	B	422	SER	2.1
2	C	91	ARG	2.1
2	D	10	ILE	2.1
1	B	331	GLY	2.1
1	B	581	GLY	2.1
2	D	60	GLY	2.1
1	B	425	PHE	2.1
1	A	422	SER	2.1
1	A	546	SER	2.1
1	A	460	LEU	2.1
2	D	81	ASP	2.1
1	A	579	SER	2.1
2	C	9	GLN	2.1
1	A	161	ASN	2.1
1	A	437	ASP	2.1
1	B	843	ARG	2.1
2	D	21	ASP	2.1
2	C	64	ILE	2.1
1	A	289	ASN	2.0
1	A	720	LEU	2.0
1	A	813	ALA	2.0
1	B	166	GLN	2.0
1	B	687	SER	2.0
1	B	725	VAL	2.0
2	D	5	LEU	2.0
1	A	521	GLY	2.0
1	B	845	TRP	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 oligosaccharides in this entry.

6.4 Ligands

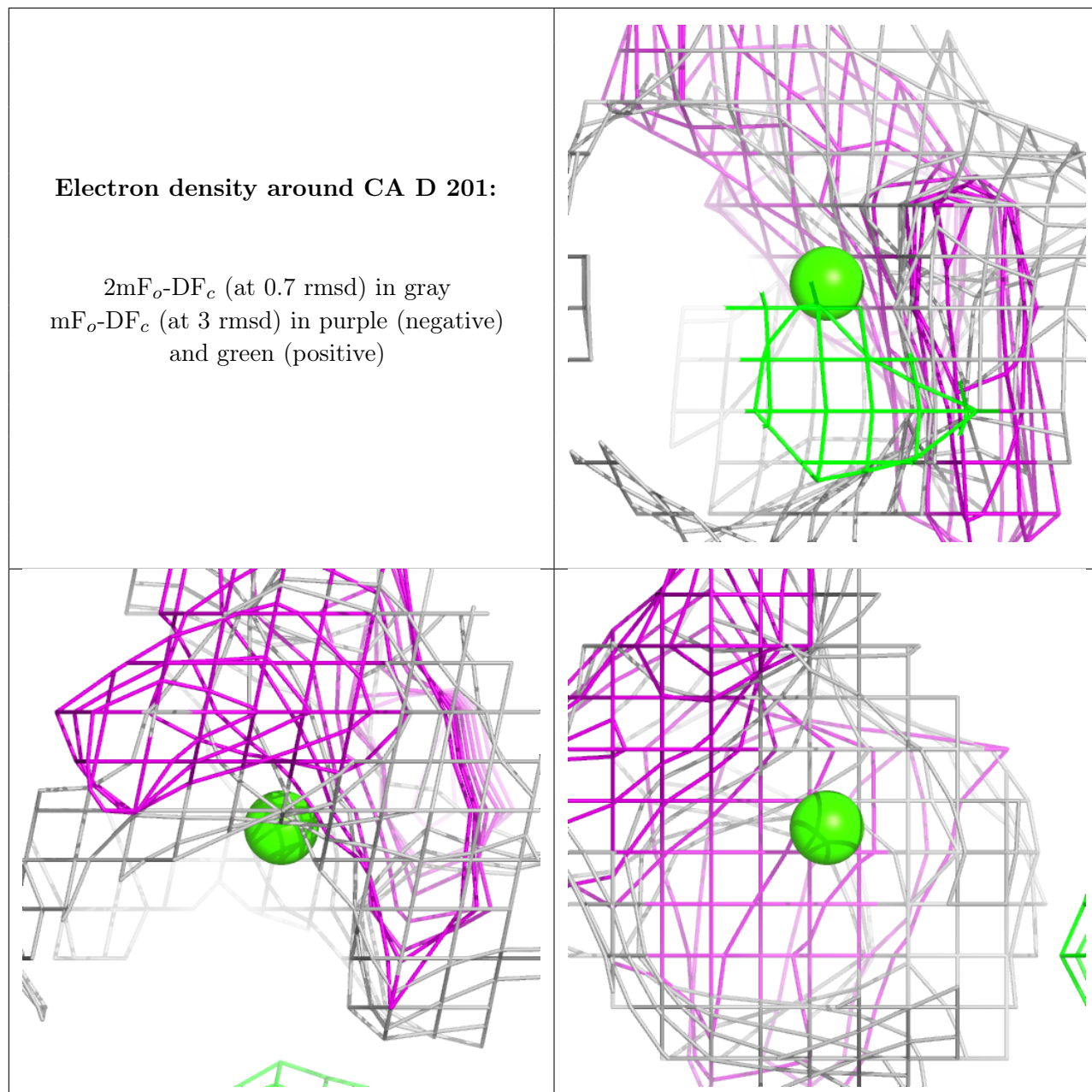
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CA	D	201	1/1	0.56	0.22	134,134,134,134	0
3	CL	A	902	1/1	0.81	0.24	99,99,99,99	0
3	CL	B	902	1/1	0.83	0.14	69,69,69,69	0
4	CA	C	201	1/1	0.90	0.13	113,113,113,113	0
3	CL	B	901	1/1	0.90	0.20	61,61,61,61	0
3	CL	A	901	1/1	0.95	0.13	63,63,63,63	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.

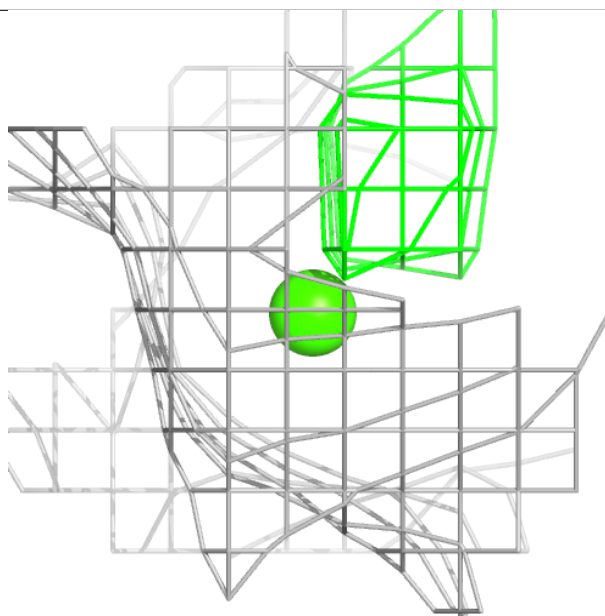
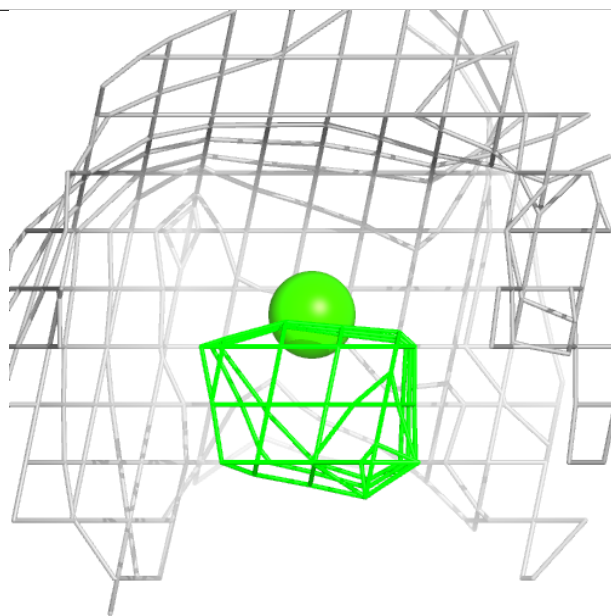
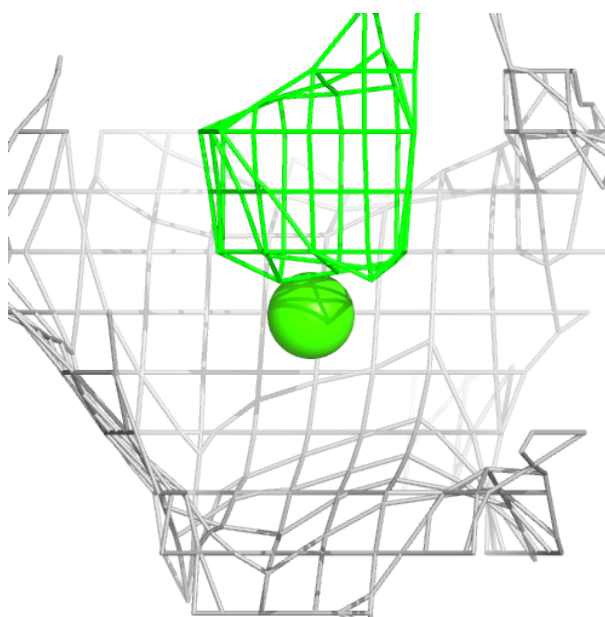
Electron density around CA D 201:

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



Electron density around CA C 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 [i](#)

There are no such residues in this entry.