Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2025 – 05:23 pm BST

PDB ID	:	9HH3 / pdb_00009hh3
Title	:	Structure of the apo ZgCgsA carrageenan-sulfatase (S1_19) from the marine bacterium Zobellia galactanivorans
Authors	:	Chevenier, A.; Czjzek, M.; Michel, G.; Ficko-Blean, E.
Deposited on	:	2024-11-20
Resolution	:	2.26 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:

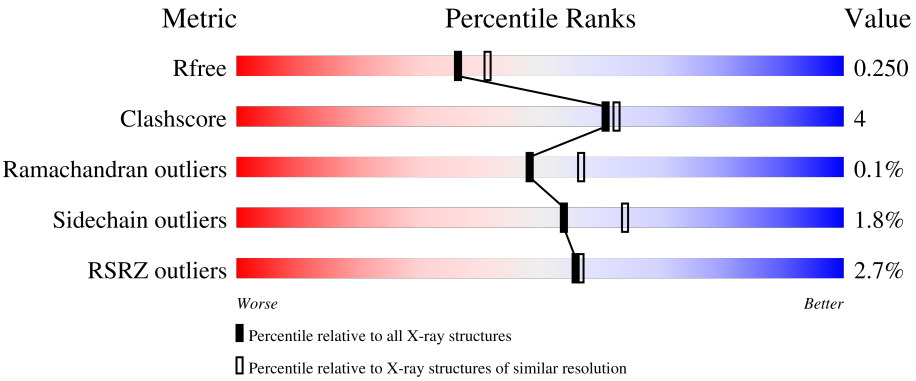
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.26 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}	164625	1763 (2.26-2.26)
Clashscore	180529	1919 (2.26-2.26)
Ramachandran outliers	177936	1884 (2.26-2.26)
Sidechain outliers	177891	1885 (2.26-2.26)
RSRZ outliers	164620	1763 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	481	89% 7%
1	B	481	91% 5%
1	C	481	5% 83% 12%
1	D	481	5% 80% 15%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	A	605	-	-	X	-
3	CL	D	605	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15120 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 Sulfatase, family S1-19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	1	0
			3695	2361	624	697	13			
1	B	464	Total	C	N	O	S	0	1	0
			3679	2350	621	695	13			
1	C	464	Total	C	N	O	S	0	1	0
			3620	2314	608	685	13			
1	D	464	Total	C	N	O	S	0	1	0
			3623	2316	612	682	13			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	MET	-	initiating methionine	UNP G0L000
A	33	GLY	-	expression tag	UNP G0L000
A	34	SER	-	expression tag	UNP G0L000
A	35	SER	-	expression tag	UNP G0L000
A	36	HIS	-	expression tag	UNP G0L000
A	37	HIS	-	expression tag	UNP G0L000
A	38	HIS	-	expression tag	UNP G0L000
A	39	HIS	-	expression tag	UNP G0L000
A	40	HIS	-	expression tag	UNP G0L000
A	41	HIS	-	expression tag	UNP G0L000
A	42	GLY	-	expression tag	UNP G0L000
A	43	SER	-	expression tag	UNP G0L000
B	32	MET	-	initiating methionine	UNP G0L000
B	33	GLY	-	expression tag	UNP G0L000
B	34	SER	-	expression tag	UNP G0L000
B	35	SER	-	expression tag	UNP G0L000
B	36	HIS	-	expression tag	UNP G0L000
B	37	HIS	-	expression tag	UNP G0L000
B	38	HIS	-	expression tag	UNP G0L000
B	39	HIS	-	expression tag	UNP G0L000
B	40	HIS	-	expression tag	UNP G0L000

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Chain	Residue	Modelled	Actual	Comment	Reference
B	41	HIS	-	expression tag	UNP G0L000
B	42	GLY	-	expression tag	UNP G0L000
B	43	SER	-	expression tag	UNP G0L000
C	32	MET	-	initiating methionine	UNP G0L000
C	33	GLY	-	expression tag	UNP G0L000
C	34	SER	-	expression tag	UNP G0L000
C	35	SER	-	expression tag	UNP G0L000
C	36	HIS	-	expression tag	UNP G0L000
C	37	HIS	-	expression tag	UNP G0L000
C	38	HIS	-	expression tag	UNP G0L000
C	39	HIS	-	expression tag	UNP G0L000
C	40	HIS	-	expression tag	UNP G0L000
C	41	HIS	-	expression tag	UNP G0L000
C	42	GLY	-	expression tag	UNP G0L000
C	43	SER	-	expression tag	UNP G0L000
D	32	MET	-	initiating methionine	UNP G0L000
D	33	GLY	-	expression tag	UNP G0L000
D	34	SER	-	expression tag	UNP G0L000
D	35	SER	-	expression tag	UNP G0L000
D	36	HIS	-	expression tag	UNP G0L000
D	37	HIS	-	expression tag	UNP G0L000
D	38	HIS	-	expression tag	UNP G0L000
D	39	HIS	-	expression tag	UNP G0L000
D	40	HIS	-	expression tag	UNP G0L000
D	41	HIS	-	expression tag	UNP G0L000
D	42	GLY	-	expression tag	UNP G0L000
D	43	SER	-	expression tag	UNP G0L000

- Molecule 2 is BROMIDE ION (CCD ID: BR) (formula: Br).

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	9	Total Cl 9 9	0	0
3	B	5	Total Cl 5 5	0	0
3	C	5	Total Cl 5 5	0	0
3	D	6	Total Cl 6 6	0	0

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

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

- Molecule 5 is water.

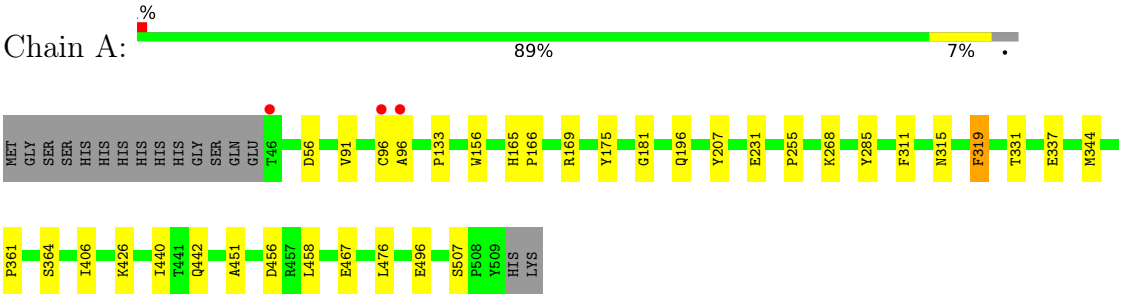
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	194	Total O 196 196	0	2
5	B	187	Total O 192 192	0	5
5	C	40	Total O 40 40	0	0
5	D	35	Total O 36 36	0	1

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.

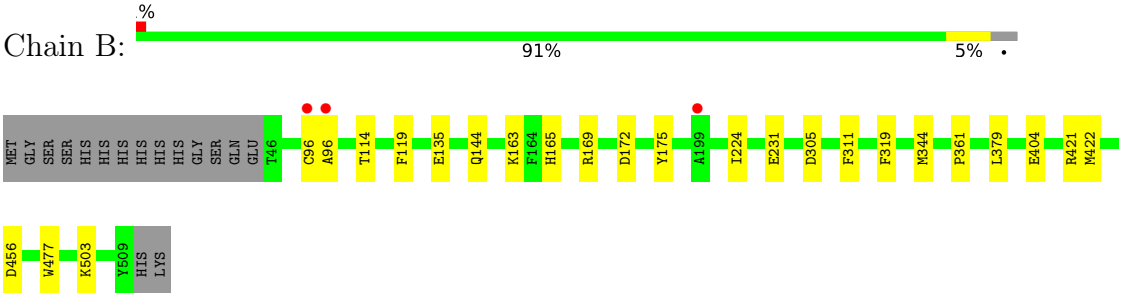
• Molecule 1: Sulfatase, family S1-19

Chain A:



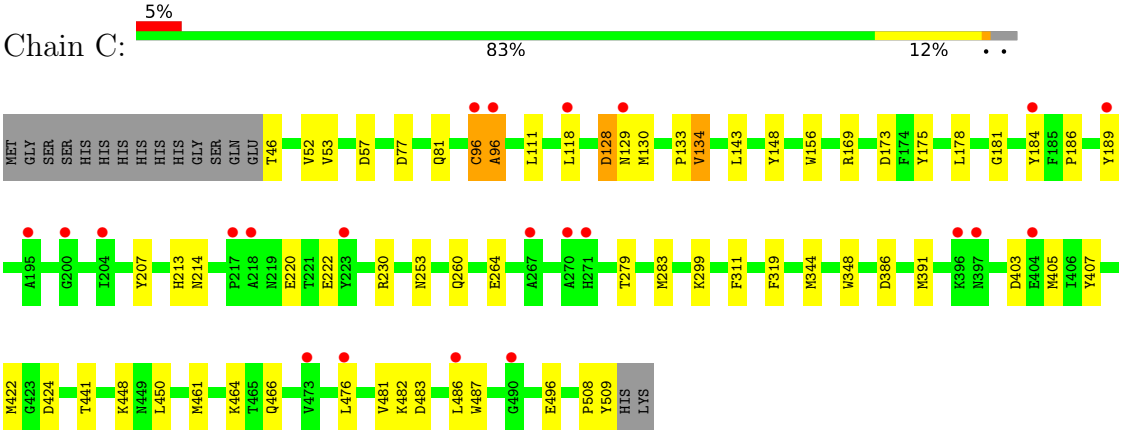
• Molecule 1: Sulfatase, family S1-19

Chain B:



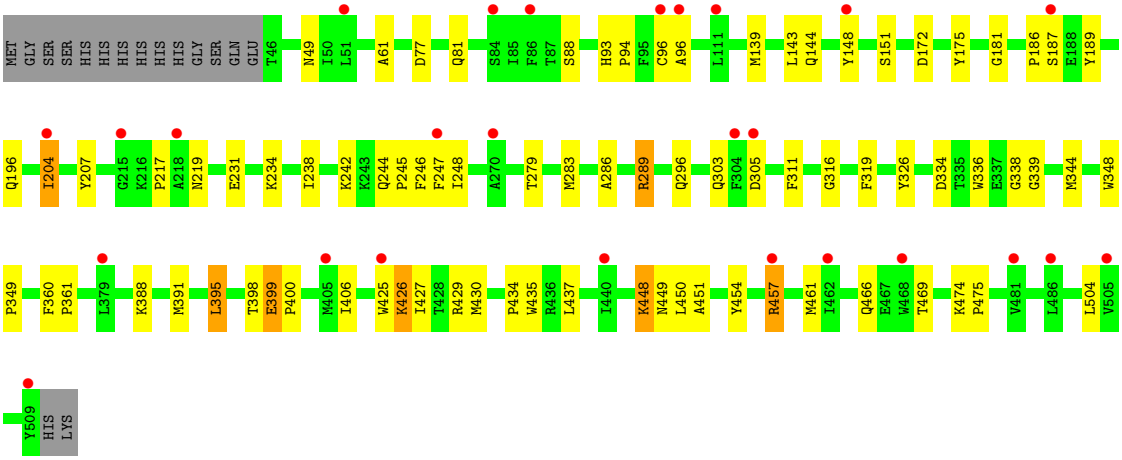
• Molecule 1: Sulfatase, family S1-19

Chain C:



• Molecule 1: Sulfatase, family S1-19

Chain D:


MET GLY SER SER HIS HIS HIS HIS HIS HIS GLY SER GLN GLU T46 N49 I50 L51 A61 D77 Q81 S84 I85 F86 T87 S88 H93 P94 F95 C96 A96 L111 M139 L143 Q144 Y148 S151 D172 Y175 G181 P186 S187 E188 Y189
Q196 I204 Y207 G215 K216 P217 A218 N219 E231 K234 I238 K242 K243 Q244 P245 F246 F247 I248 A270 T279 M283 A286 R289 Q296 Q303 F304 D305 F311 G316 F319 Y326 D334 T335 W336 E337 G338 G339 M344 W348
P349 F360 P361 L379 K388 M391 L395 T398 E399 P400 M405 I406 W425 K426 I427 T428 R429 M430 P434 W435 R436 L437 I440 K448 N449 L450 A451 Y454 R457 M461 I462 Q466 E467 W468 T469 K474 P475 V481 L486 L504 V505
Y509 HIS LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.80Å 199.15Å 75.35Å 90.00° 99.33° 90.00°	Depositor
Resolution (Å)	49.36 – 2.26 49.36 – 2.26	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.36-2.26) 95.6 (49.36-2.26)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.96 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.195 , 0.246 0.201 , 0.250	Depositor DCC
R_{free} test set	5295 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	44.5	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.023 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15120	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DDZ, CA, BR, 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	0.40	0/3793	0.59	0/5148
1	B	0.40	0/3777	0.59	0/5131
1	C	0.28	0/3717	0.48	0/5061
1	D	0.30	0/3720	0.52	0/5063
All	All	0.35	0/15007	0.55	0/20403

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

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	3695	0	3499	18	0
1	B	3679	0	3461	14	0
1	C	3620	0	3348	36	0
1	D	3623	0	3367	47	0
2	A	2	0	0	0	0
2	B	4	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	9	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	2	0
3	C	5	0	0	0	0
3	D	6	0	0	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	196	0	0	2	0
5	B	192	0	0	2	0
5	C	40	0	0	3	0
5	D	36	0	0	1	0
All	All	15120	0	13675	117	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 4.

All (117) 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:D:457:ARG:NH1	3:D:605:CL:CL	2.45	0.86
1:D:448:LYS:HD3	1:D:450:LEU:HD21	1.71	0.72
1:C:128:ASP:O	1:C:130:MET:N	2.23	0.71
1:D:151:SER:HB3	1:D:248:ILE:HD12	1.74	0.68
3:A:608:CL:CL	5:A:732:HOH:O	2.48	0.68
3:A:605:CL:CL	5:A:791:HOH:O	2.49	0.67
3:D:604:CL:CL	5:D:722:HOH:O	2.51	0.64
1:D:391:MET:O	1:D:395:LEU:HD22	1.98	0.64
1:D:425:TRP:HB2	1:D:461:MET:HE1	1.79	0.63
1:D:360:PHE:CE1	1:D:399:GLU:HG2	2.34	0.62
1:B:456:ASP:HB2	3:B:607:CL:CL	2.37	0.62
1:A:456:ASP:HB2	3:A:610:CL:CL	2.39	0.60
1:D:437:LEU:H	1:D:449:ASN:ND2	1.99	0.60
1:D:49:ASN:HD21	1:D:303:GLN:HE21	1.50	0.60
1:A:196:GLN:OE1	3:A:605:CL:CL	2.57	0.59
1:D:144:GLN:NE2	1:D:172:ASP:OD1	2.36	0.59
1:D:217:PRO:O	1:D:219:ASN:N	2.34	0.58
1:D:49:ASN:ND2	1:D:303:GLN:HG3	2.19	0.58
1:A:165:HIS:O	1:A:169:ARG:HG2	2.05	0.57
1:B:503:LYS:HG2	3:B:605:CL:CL	2.42	0.56
1:D:246:PHE:CD1	1:D:248:ILE:HG12	2.40	0.56
1:C:407:TYR:OH	1:C:464:LYS:HG2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:466:GLN:O	1:D:469:THR:HG22	2.06	0.56
1:C:403:ASP:HA	1:C:422:MET:HE3	1.87	0.56
1:C:222:GLU:OE2	1:C:230:ARG:NH1	2.39	0.55
1:D:361:PRO:HB2	1:D:406:ILE:HD12	1.89	0.55
1:C:466:GLN:NE2	1:C:496:GLU:OE1	2.40	0.54
1:C:405:MET:SD	1:C:422:MET:HG3	2.48	0.54
1:D:181:GLY:HA3	1:D:207:TYR:CZ	2.42	0.54
1:B:175:TYR:CD1	1:B:231:GLU:HG3	2.42	0.53
1:C:422:MET:HB2	1:C:461:MET:HE3	1.90	0.53
1:B:144:GLN:NE2	1:B:172:ASP:OD1	2.39	0.52
1:C:299:LYS:NZ	5:C:701:HOH:O	2.30	0.52
1:A:156:TRP:CD2	1:A:166:PRO:HG3	2.45	0.51
1:D:449:ASN:ND2	1:D:451:ALA:H	2.09	0.51
1:A:361:PRO:HB2	1:A:406:ILE:HD12	1.93	0.51
1:D:311:PHE:O	1:D:344:MET:HA	2.11	0.51
1:C:348:TRP:CZ3	1:C:391:MET:HE3	2.47	0.50
1:C:184:TYR:H	1:C:260:GLN:NE2	2.09	0.50
1:C:57:ASP:HB3	5:C:720:HOH:O	2.12	0.50
1:A:56:ASP:O	1:A:255:PRO:HD2	2.11	0.50
1:A:311:PHE:O	1:A:344:MET:HA	2.11	0.50
1:D:457:ARG:HD3	3:D:605:CL:CL	2.49	0.49
1:A:451:ALA:HB1	1:A:458:LEU:HD22	1.93	0.49
1:C:184:TYR:H	1:C:260:GLN:HE22	1.60	0.49
1:C:96[A]:CYS:SG	5:C:722:HOH:O	2.60	0.49
1:C:173:ASP:OD1	1:C:214:ASN:ND2	2.40	0.48
1:D:139:MET:O	1:D:143:LEU:HD13	2.13	0.48
1:C:181:GLY:HA3	1:C:207:TYR:CZ	2.48	0.48
1:C:133:PRO:HG3	1:C:476:LEU:HD11	1.94	0.48
1:B:165:HIS:O	1:B:169:ARG:HG2	2.13	0.48
1:C:508:PRO:HG2	1:C:509:TYR:CE2	2.49	0.47
1:C:311:PHE:O	1:C:344:MET:HA	2.14	0.47
1:C:186:PRO:HA	1:C:189:TYR:CE2	2.50	0.47
1:D:336:TRP:CE2	1:D:430:MET:HG3	2.49	0.47
1:D:434:PRO:HA	1:D:504:LEU:HD13	1.97	0.47
1:D:437:LEU:HD23	1:D:450:LEU:HB2	1.97	0.47
1:D:454:TYR:HB3	3:D:605:CL:CL	2.51	0.47
1:D:348:TRP:CE3	1:D:391:MET:HE2	2.50	0.47
1:C:220:GLU:OE2	1:C:222:GLU:HG2	2.15	0.46
1:D:61:ALA:HB2	1:D:326:TYR:O	2.15	0.46
1:D:175:TYR:CD1	1:D:231:GLU:HG3	2.50	0.46
1:C:483:ASP:O	1:C:487:TRP:HD1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:508:PRO:HG2	1:C:509:TYR:CZ	2.51	0.46
1:A:181:GLY:HA3	1:A:207:TYR:CZ	2.51	0.46
1:A:337:GLU:OE2	1:A:426:LYS:NZ	2.45	0.46
1:C:184:TYR:CZ	1:C:253:ASN:ND2	2.84	0.46
1:D:425:TRP:CB	1:D:461:MET:HE1	2.46	0.46
1:D:426:LYS:HD2	1:D:427:ILE:O	2.15	0.46
1:C:482:LYS:O	1:C:486:LEU:HG	2.16	0.45
1:C:143:LEU:O	1:C:148:TYR:HB2	2.16	0.45
1:D:286:ALA:HA	1:D:289:ARG:HG3	1.98	0.45
1:A:496:GLU:H	1:A:496:GLU:CD	2.23	0.45
1:D:334:ASP:O	1:D:339:GLY:HA3	2.17	0.45
1:B:361:PRO:HG3	1:B:421:ARG:CZ	2.47	0.45
1:D:279:THR:O	1:D:283:MET:HG3	2.16	0.45
1:D:316:GLY:HA3	1:D:338:GLY:O	2.16	0.45
1:D:348:TRP:CZ3	1:D:391:MET:HE2	2.52	0.44
1:A:175:TYR:CD1	1:A:231:GLU:HG3	2.53	0.44
1:A:268:LYS:HD2	1:A:285:TYR:CE2	2.53	0.44
1:D:242:LYS:NZ	1:D:244:GLN:HE22	2.15	0.44
1:C:175:TYR:OH	1:C:220:GLU:OE1	2.28	0.44
1:D:196:GLN:HE21	1:D:204:ILE:HG23	1.82	0.44
1:C:424:ASP:OD1	1:C:441:THR:OG1	2.33	0.44
1:C:77:ASP:O	1:C:81:GLN:HG3	2.18	0.44
1:C:111:LEU:HD12	1:C:386:ASP:OD2	2.18	0.44
1:D:234:LYS:O	1:D:238:ILE:HG12	2.18	0.44
1:B:114:THR:HG22	1:B:477:TRP:CH2	2.53	0.43
1:B:305:ASP:OD2	5:B:701:HOH:O	2.21	0.43
1:C:279:THR:O	1:C:283:MET:HG3	2.17	0.43
1:D:77:ASP:O	1:D:81:GLN:HG3	2.19	0.43
1:C:448:LYS:HE3	1:C:450:LEU:HD21	1.99	0.43
1:D:388:LYS:HE3	1:D:400:PRO:O	2.19	0.43
1:C:264:GLU:OE1	1:C:264:GLU:N	2.34	0.43
1:D:427:ILE:HD13	1:D:461:MET:HB3	2.00	0.43
1:B:379:LEU:HD23	1:B:379:LEU:HA	1.83	0.42
1:A:319:PHE:CE2	1:A:331:THR:HB	2.54	0.42
1:C:173:ASP:OD1	1:C:213:HIS:HE1	2.03	0.42
1:B:311:PHE:O	1:B:344:MET:HA	2.19	0.42
1:D:429:ARG:HD2	1:D:435:TRP:NE1	2.34	0.42
1:A:507:SER:HB2	1:B:119:PHE:CD1	2.54	0.42
1:C:134:VAL:HA	1:C:169:ARG:NH2	2.34	0.42
1:D:88:SER:O	1:D:361:PRO:HA	2.20	0.41
1:B:135:GLU:H	1:B:135:GLU:CD	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:GLU:H	1:C:264:GLU:CD	2.25	0.41
1:A:91:VAL:HA	1:A:364:SER:OG	2.21	0.41
1:A:133:PRO:HG3	1:A:476:LEU:HD11	2.01	0.41
1:C:156:TRP:HB3	1:C:178:LEU:HA	2.03	0.41
1:A:196:GLN:NE2	3:A:605:CL:CL	2.91	0.41
1:B:224:ILE:HD13	1:B:224:ILE:HG21	1.87	0.41
1:D:93:HIS:HA	1:D:94:PRO:HD3	1.94	0.41
1:D:148:TYR:CE2	1:D:245:PRO:HB2	2.56	0.41
1:D:474:LYS:HG2	1:D:475:PRO:HD2	2.03	0.41
1:D:247:PHE:C	1:D:248:ILE:HD13	2.46	0.40
1:B:422:MET:HE1	5:B:722:HOH:O	2.21	0.40
1:D:186:PRO:HA	1:D:189:TYR:CE2	2.56	0.40
1:D:305:ASP:OD2	1:D:349:PRO: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	461/481 (96%)	450 (98%)	11 (2%)	0	100 100
1	B	461/481 (96%)	450 (98%)	11 (2%)	0	100 100
1	C	461/481 (96%)	451 (98%)	9 (2%)	1 (0%)	44 51
1	D	461/481 (96%)	446 (97%)	15 (3%)	0	100 100
All	All	1844/1924 (96%)	1797 (98%)	46 (2%)	1 (0%)	48 57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	129	ASN

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	382/407 (94%)	377 (99%)	5 (1%)	65	74
1	B	378/407 (93%)	375 (99%)	3 (1%)	79	86
1	C	363/407 (89%)	355 (98%)	8 (2%)	47	56
1	D	364/407 (89%)	353 (97%)	11 (3%)	36	44
All	All	1487/1628 (91%)	1460 (98%)	27 (2%)	54	64

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	315	ASN
1	A	319	PHE
1	A	440	ILE
1	A	442	GLN
1	A	467	GLU
1	B	163	LYS
1	B	319	PHE
1	B	404	GLU
1	C	46	THR
1	C	52	VAL
1	C	53	VAL
1	C	118	LEU
1	C	128	ASP
1	C	134	VAL
1	C	319	PHE
1	C	481	VAL
1	D	187	SER
1	D	204	ILE
1	D	289	ARG
1	D	296	GLN
1	D	319	PHE
1	D	395	LEU
1	D	398	THR
1	D	399	GLU

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Mol	Chain	Res	Type
1	D	426	LYS
1	D	448	LYS
1	D	457	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	356	GLN
1	B	271	HIS
1	B	356	GLN
1	C	78	ASN
1	C	120	HIS
1	C	213	HIS
1	C	260	GLN
1	C	296	GLN
1	C	491	GLN
1	D	196	GLN
1	D	203	ASN
1	D	219	ASN
1	D	244	GLN
1	D	303	GLN
1	D	320	ASN
1	D	449	ASN
1	D	466	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)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	DDZ	C	96[B]	4,1	4,6,7	1.05	0	3,7,9	1.56	1 (33%)
1	DDZ	B	96[B]	4,1	4,6,7	1.10	0	3,7,9	1.39	1 (33%)
1	DDZ	D	96[B]	4,1	4,6,7	1.08	0	3,7,9	1.49	1 (33%)
1	DDZ	A	96[B]	4,1	4,6,7	1.06	0	3,7,9	1.50	1 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	DDZ	C	96[B]	4,1	-	0/2/6/8	-
1	DDZ	B	96[B]	4,1	-	0/2/6/8	-
1	DDZ	D	96[B]	4,1	-	0/2/6/8	-
1	DDZ	A	96[B]	4,1	-	0/2/6/8	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	96[B]	DDZ	O-C-CA	-2.67	117.78	124.78
1	D	96[B]	DDZ	O-C-CA	-2.53	118.15	124.78
1	A	96[B]	DDZ	O-C-CA	-2.40	118.49	124.78
1	B	96[B]	DDZ	O-C-CA	-2.36	118.60	124.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 39 ligands modelled in this entry, 39 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	463/481 (96%)	-0.28	1 (0%)	92	93	33, 45, 60, 67	0
1	B	463/481 (96%)	-0.27	1 (0%)	92	93	32, 44, 61, 83	0
1	C	463/481 (96%)	0.72	20 (4%)	40	40	53, 68, 82, 93	0
1	D	463/481 (96%)	0.78	24 (5%)	34	34	54, 67, 82, 89	0
All	All	1852/1924 (96%)	0.24	46 (2%)	56	59	32, 57, 79, 93	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	187	SER	3.1
1	D	270	ALA	2.9
1	C	129	ASN	2.7
1	C	204	ILE	2.7
1	D	425	TRP	2.6
1	C	195	ALA	2.6
1	C	404	GLU	2.6
1	D	457	ARG	2.6
1	C	473	VAL	2.6
1	C	200	GLY	2.5
1	C	490	GLY	2.5
1	D	468	TRP	2.5
1	C	218	ALA	2.5
1	D	204	ILE	2.5
1	D	111	LEU	2.5
1	B	199	ALA	2.4
1	D	509	TYR	2.4
1	C	270	ALA	2.4
1	C	189	TYR	2.4
1	D	486	LEU	2.4
1	D	305	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	271	HIS	2.3
1	D	218	ALA	2.3
1	D	405	MET	2.3
1	C	267	ALA	2.2
1	C	486	LEU	2.2
1	C	118	LEU	2.2
1	D	379	LEU	2.2
1	D	304	PHE	2.2
1	D	462	ILE	2.1
1	C	223	TYR	2.1
1	C	397	ASN	2.1
1	D	51	LEU	2.1
1	C	217	PRO	2.1
1	D	84	SER	2.1
1	A	46	THR	2.1
1	C	184	TYR	2.1
1	D	505	VAL	2.1
1	D	481	VAL	2.0
1	D	86	PHE	2.0
1	D	215	GLY	2.0
1	D	148	TYR	2.0
1	D	247	PHE	2.0
1	C	396	LYS	2.0
1	D	440	ILE	2.0
1	C	476	LEU	2.0

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

MODRES-RSR INFOmissingINFO

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

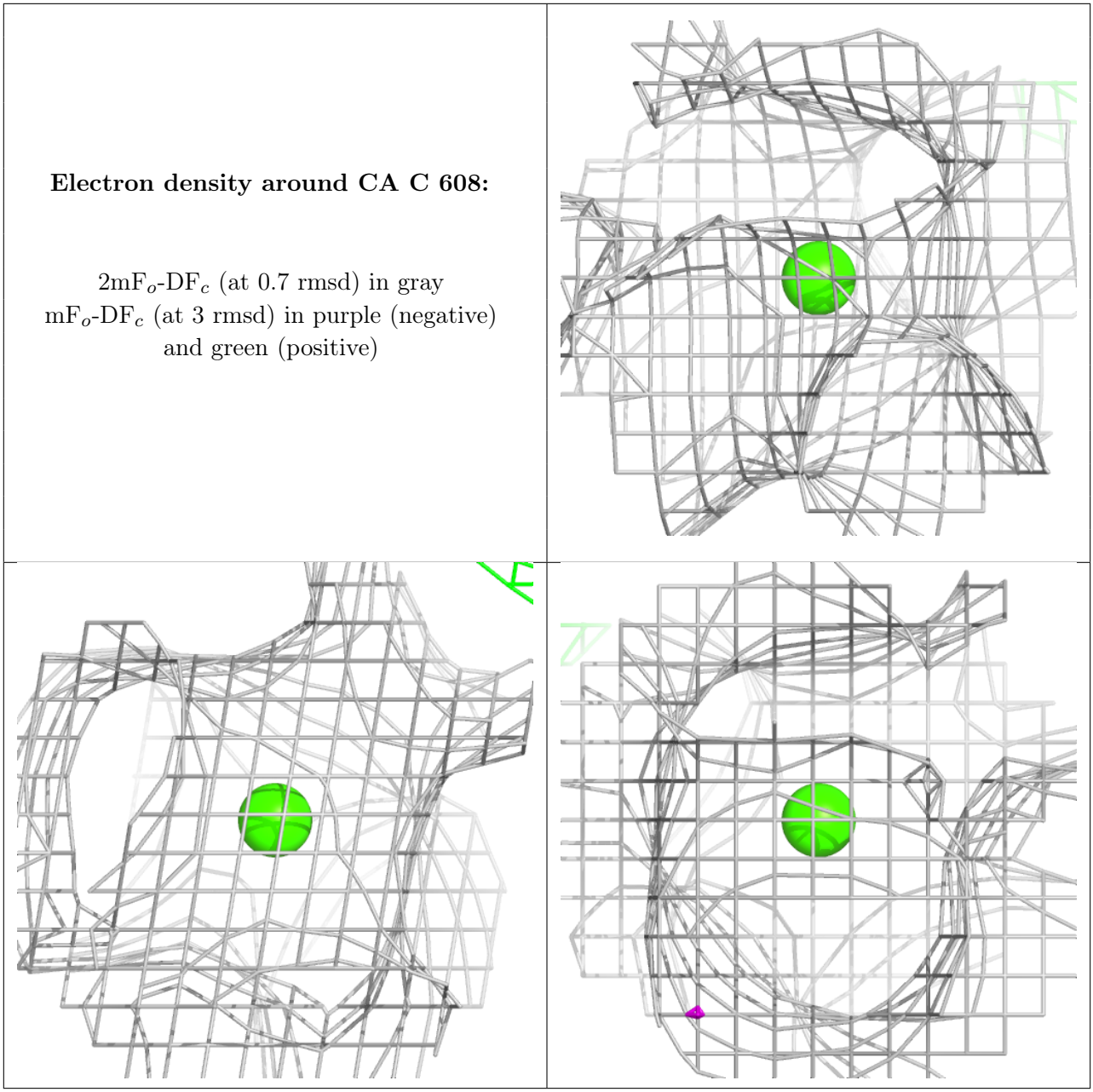
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CL	B	607	1/1	0.83	0.17	63,63,63,63	0
3	CL	B	608	1/1	0.88	0.18	84,84,84,84	0
3	CL	D	605	1/1	0.88	0.11	84,84,84,84	0
3	CL	D	607	1/1	0.88	0.12	68,68,68,68	0
3	CL	D	608	1/1	0.90	0.11	85,85,85,85	0
3	CL	C	606	1/1	0.91	0.13	80,80,80,80	0
3	CL	A	610	1/1	0.91	0.11	71,71,71,71	0
3	CL	B	609	1/1	0.92	0.12	85,85,85,85	0
3	CL	C	603	1/1	0.92	0.13	62,62,62,62	0
3	CL	A	611	1/1	0.92	0.13	77,77,77,77	0
2	BR	C	602	1/1	0.93	0.09	71,71,71,71	1
3	CL	C	604	1/1	0.93	0.10	70,70,70,70	0
3	CL	C	607	1/1	0.94	0.11	83,83,83,83	0
3	CL	C	605	1/1	0.94	0.12	79,79,79,79	0
3	CL	B	606	1/1	0.95	0.10	61,61,61,61	0
3	CL	A	609	1/1	0.96	0.07	53,53,53,53	0
3	CL	D	606	1/1	0.96	0.08	65,65,65,65	0
2	BR	C	601	1/1	0.96	0.07	73,73,73,73	1
2	BR	D	602	1/1	0.96	0.08	70,70,70,70	1
3	CL	A	607	1/1	0.97	0.10	50,50,50,50	0
3	CL	D	603	1/1	0.97	0.05	65,65,65,65	0
3	CL	D	604	1/1	0.97	0.06	72,72,72,72	0
3	CL	B	605	1/1	0.97	0.07	41,41,41,41	0
3	CL	A	608	1/1	0.97	0.06	43,43,43,43	0
3	CL	A	603	1/1	0.97	0.08	40,40,40,40	0
3	CL	A	605	1/1	0.97	0.05	49,49,49,49	0
2	BR	B	604	1/1	0.98	0.07	96,96,96,96	0
2	BR	D	601	1/1	0.98	0.05	72,72,72,72	0
4	CA	C	608	1/1	0.98	0.08	70,70,70,70	0
4	CA	D	609	1/1	0.98	0.10	67,67,67,67	0
3	CL	A	606	1/1	0.99	0.03	42,42,42,42	0
2	BR	B	603	1/1	0.99	0.04	60,60,60,60	1
2	BR	A	601	1/1	0.99	0.03	44,44,44,44	1
2	BR	B	601	1/1	0.99	0.05	51,51,51,51	1
4	CA	A	612	1/1	0.99	0.07	52,52,52,52	0
4	CA	B	610	1/1	0.99	0.07	51,51,51,51	0
3	CL	A	604	1/1	0.99	0.03	39,39,39,39	0
2	BR	B	602	1/1	0.99	0.03	49,49,49,49	1
2	BR	A	602	1/1	1.00	0.03	48,48,48,48	1

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.

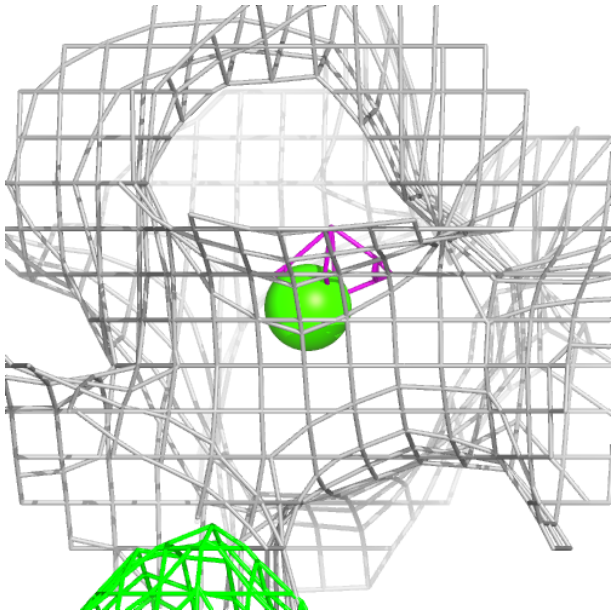
Electron density around CA C 608:

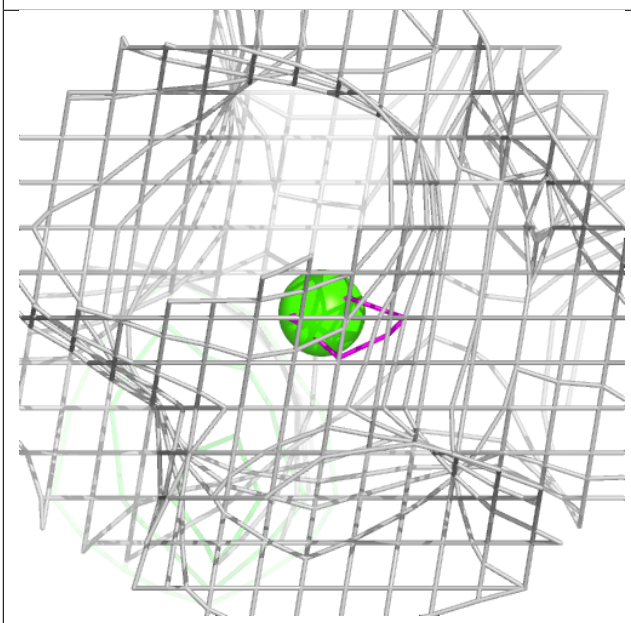
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

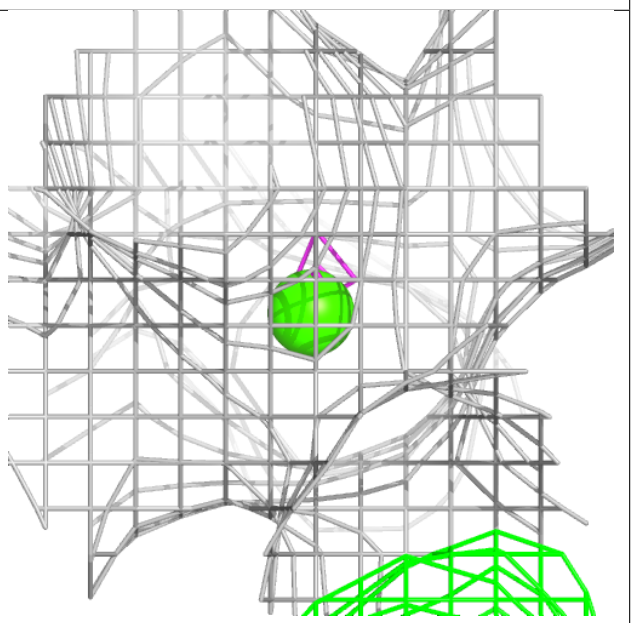


Electron density around CA D 609:

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

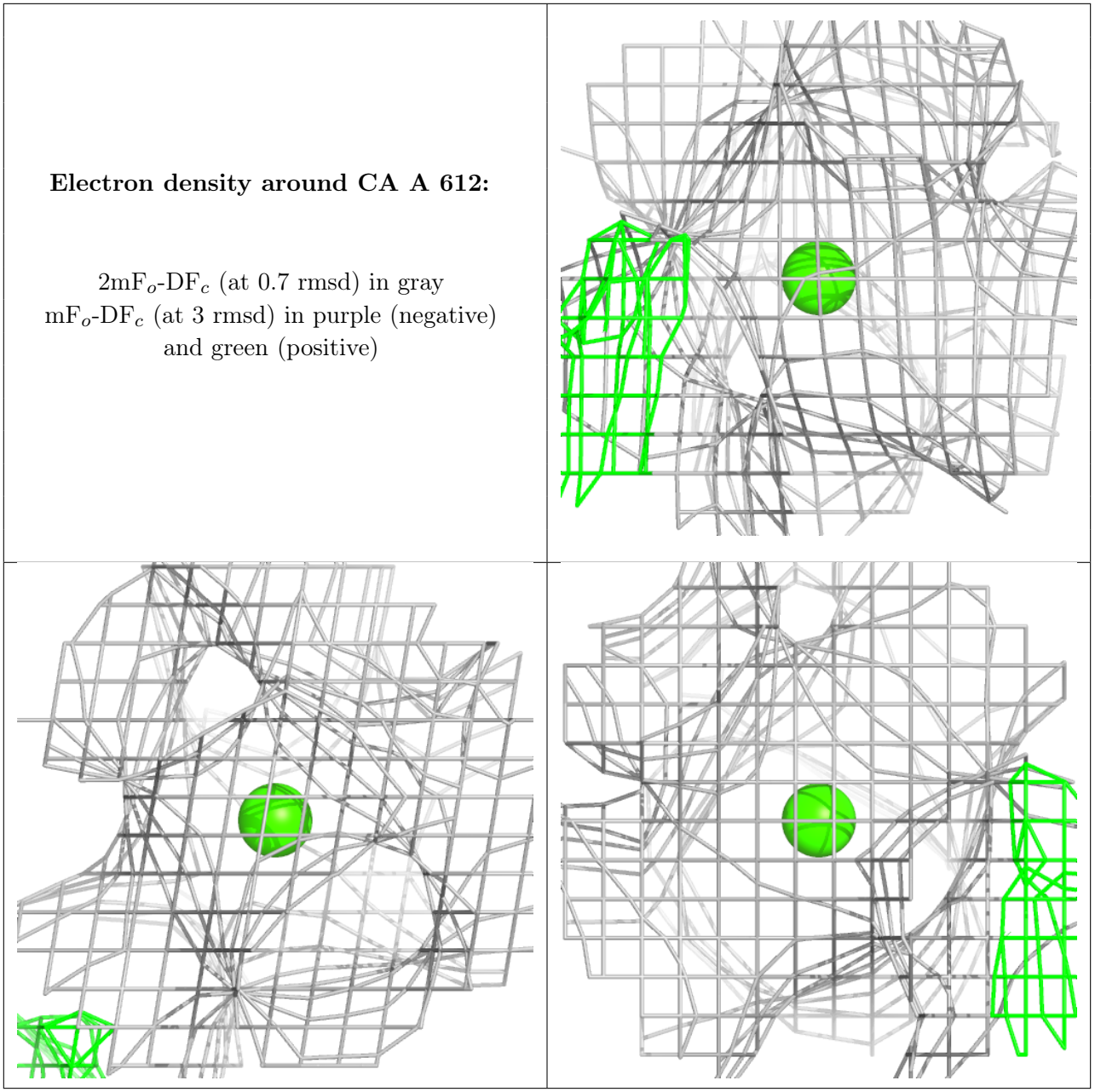






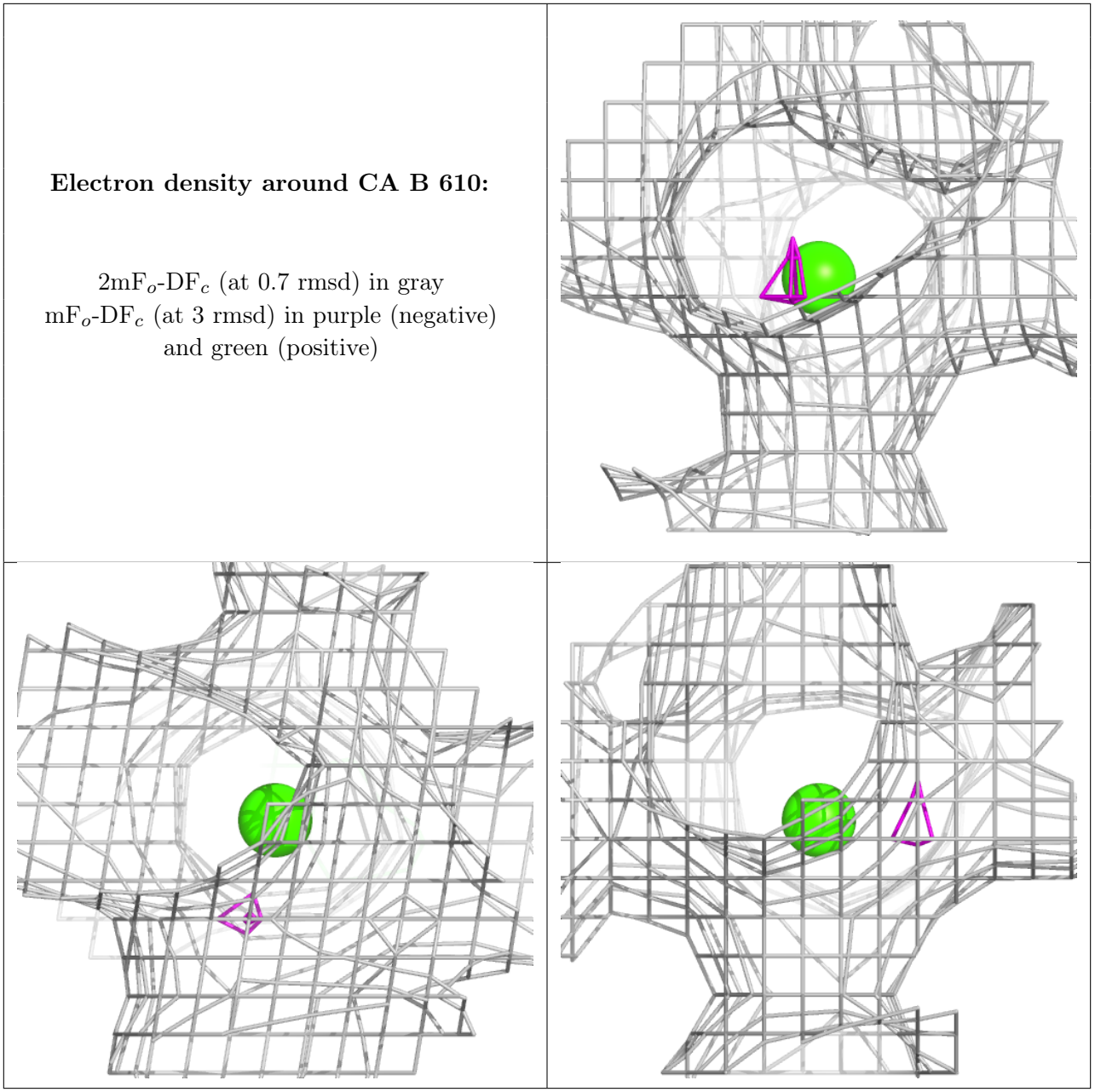
Electron density around CA A 612:

$2mF_o$-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 B 610:

$2mF_o$-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.