Full wwPDB X-ray Structure Validation Report (i)

Mar 24, 2025 – 03:12 pm GMT

PDB ID	:	9F38
Title	:	BsmI (wild-type) crystallized with Ca2+ and cognate dsDNA
Authors	:	Sieskind, R.; Missoury, S.; Madru, C.; Commenge, I.; Niogret, G.; Hollenstein, M.; Rondelez, Y.; Haouz, A.; Sauguet, L.; Legrand, P.; Delarue, M.
Deposited on	:	2024-04-25
Resolution	:	2.85 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 (i) 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 (i)) were used in the production of this report:

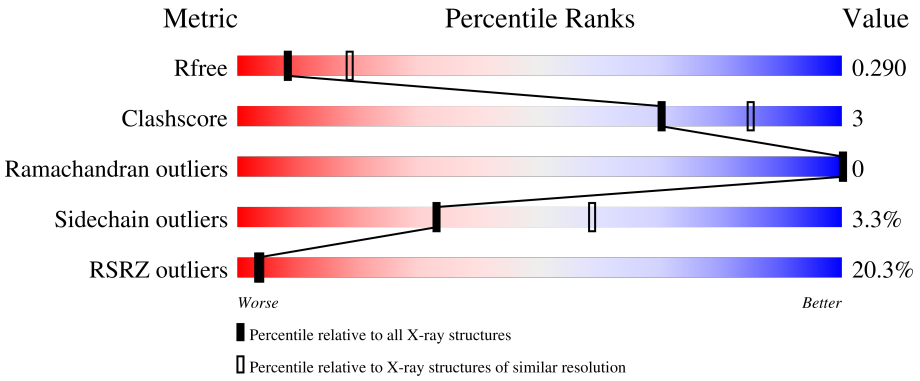
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.5

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 2.85 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	1268 (2.88-2.84)
Clashscore	180529	1351 (2.88-2.84)
Ramachandran outliers	177936	1318 (2.88-2.84)
Sidechain outliers	177891	1319 (2.88-2.84)
RSRZ outliers	164620	1269 (2.88-2.84)

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	676	22% 90% 10%
1	Z	676	20% 89% 10%
2	E	13	69% 31%
2	V	13	46% 54%
3	F	13	15% 69% 31%

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Mol	Chain	Length	Quality of chain
3	U	13	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12302 atoms, of which 13 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 BsmI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	676	Total	C	N	O	S	0	0	0
			5521	3557	932	1015	17			
1	Z	676	Total	C	N	O	S	0	0	0
			5521	3557	932	1015	17			

- Molecule 2 is a DNA chain called DNA (Bottom strand).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	13	Total	C	N	O	P	0	0	0
			257	125	40	80	12			
2	V	13	Total	C	N	O	P	0	0	0
			257	125	40	80	12			

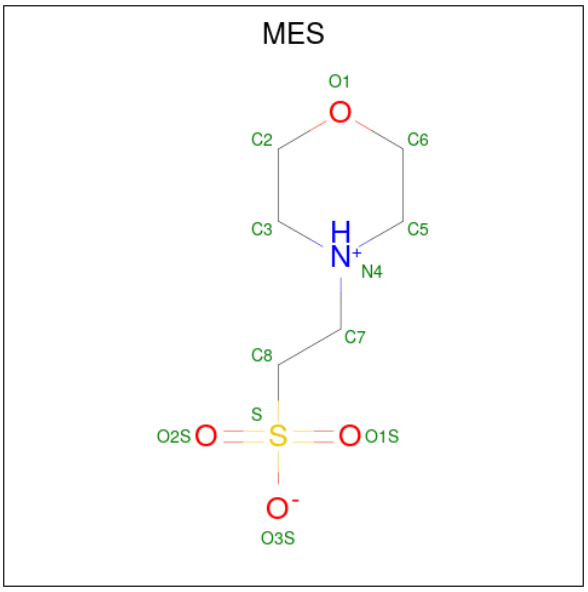
- Molecule 3 is a DNA chain called DNA (Top strand).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	13	Total	C	N	O	P	0	0	0
			270	128	58	72	12			
3	U	13	Total	C	N	O	P	0	0	0
			270	128	58	72	12			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Ca	0	0
			3	3		
4	Z	3	Total	Ca	0	0
			3	3		

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	Z	1	Total	C	H	N	O	S	13	0
			25	6	13	1	4	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	Z	1	Total	Cl	0	0
			1	1		

- Molecule 7 is water.

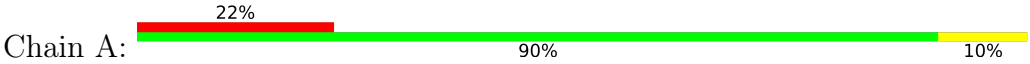
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	71	Total	O	0	0
			71	71		
7	E	2	Total	O	0	0
			2	2		
7	F	6	Total	O	0	0
			6	6		
7	U	8	Total	O	0	0
			8	8		
7	V	7	Total	O	0	0
			7	7		
7	Z	80	Total	O	0	0
			80	80		

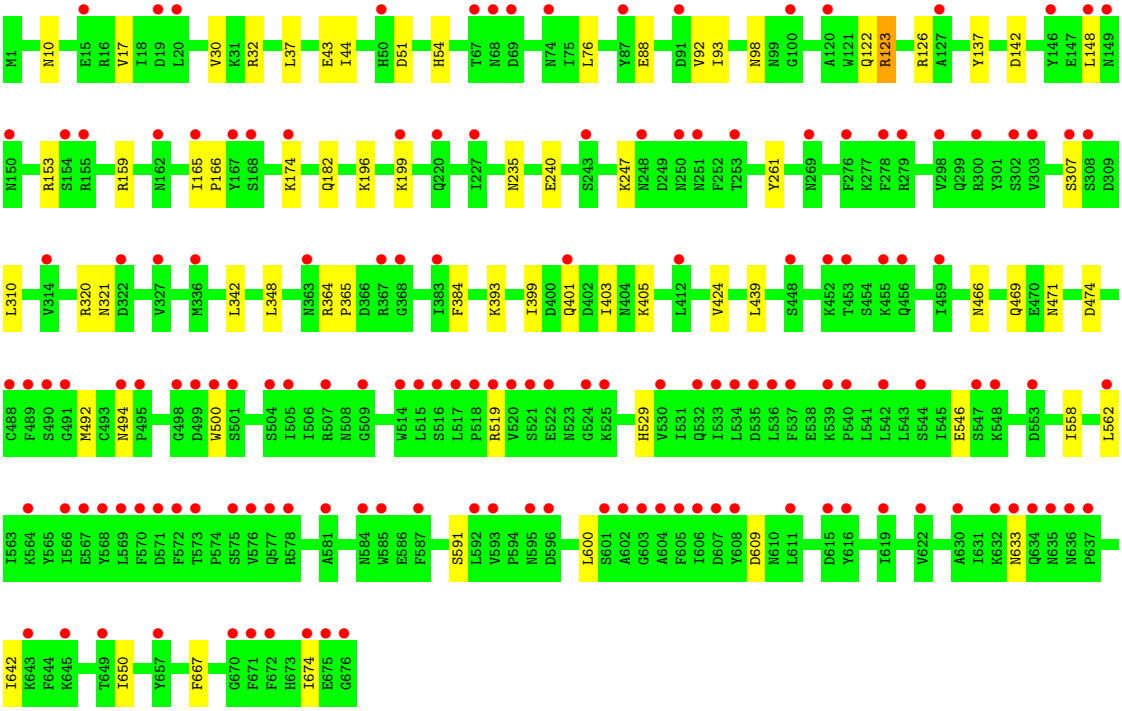
3 Residue-property plots (i)

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: BsmI

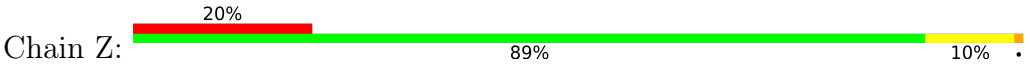
Chain A:

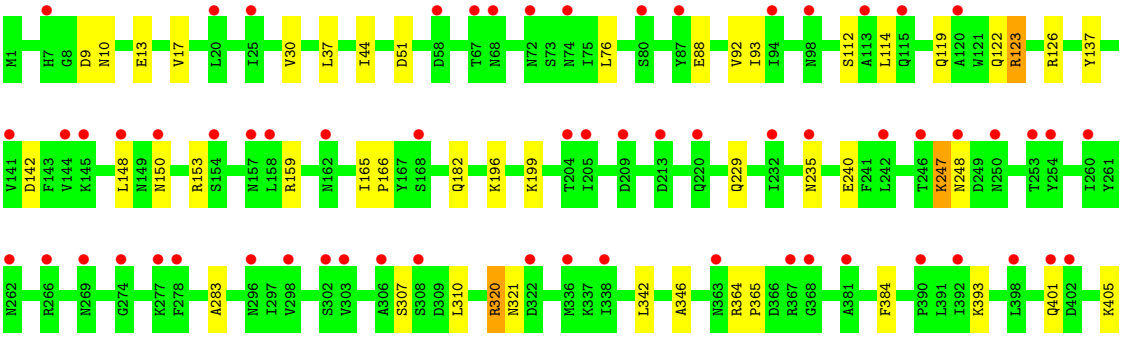


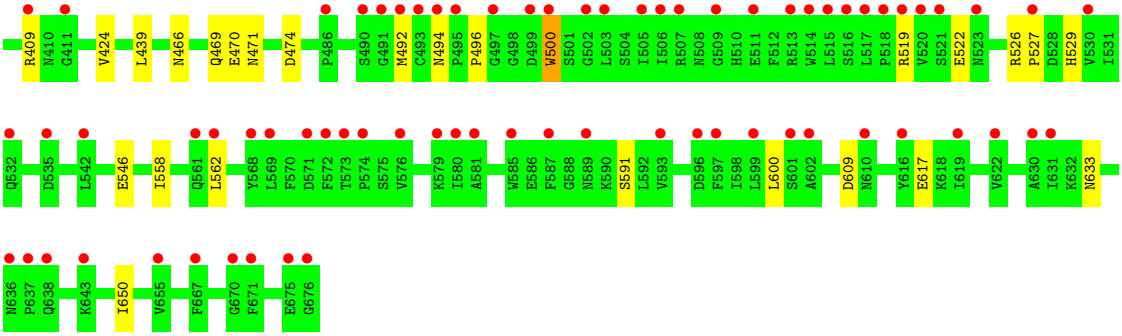


• Molecule 1: BsmI

Chain Z:

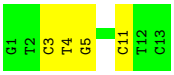






• Molecule 2: DNA (Bottom strand)

Chain E:

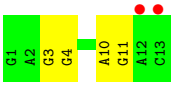


• Molecule 2: DNA (Bottom strand)

Chain V:

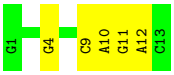
• Molecule 3: DNA (Top strand)

Chain F:



• Molecule 3: DNA (Top strand)

Chain U:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.73Å 129.88Å 100.73Å 90.00° 95.50° 90.00°	Depositor
Resolution (Å)	48.70 – 2.85 48.70 – 2.85	Depositor EDS
% Data completeness (in resolution range)	61.8 (48.70-2.85) 61.8 (48.70-2.85)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 2.86Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.274 , 0.293 0.266 , 0.290	Depositor DCC
R_{free} test set	1187 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	37.2	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 55.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	12302	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.34% 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: MES, CL, 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	0.27	0/5650	0.50	1/7631 (0.0%)
1	Z	0.27	0/5650	0.50	0/7631
2	E	0.67	0/285	0.86	0/437
2	V	0.66	0/285	0.85	0/437
3	F	0.64	0/305	0.84	0/470
3	U	0.62	0/305	0.83	0/470
All	All	0.33	0/12480	0.55	1/17076 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	123	ARG	CD-NE-CZ	5.09	130.73	123.60

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	5521	0	5507	33	0
1	Z	5521	0	5507	39	0
2	E	257	0	150	5	0
2	V	257	0	150	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	270	0	146	5	0
3	U	270	0	146	8	0
4	A	3	0	0	0	0
4	Z	3	0	0	0	0
5	Z	12	13	13	0	0
6	Z	1	0	0	0	0
7	A	71	0	0	0	0
7	E	2	0	0	0	0
7	F	6	0	0	0	0
7	U	8	0	0	0	0
7	V	7	0	0	0	0
7	Z	80	0	0	0	0
All	All	12289	13	11619	79	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 3.

All (79) 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:A:174:LYS:NZ	1:A:261:TYR:HA	1.80	0.96
3:U:4:DG:N7	1:Z:159:ARG:NH2	2.23	0.86
1:A:174:LYS:HZ1	1:A:261:TYR:HA	1.44	0.77
3:U:9:DC:H4'	1:Z:519:ARG:NE	2.01	0.74
1:Z:401:GLN:NE2	1:Z:405:LYS:NZ	2.40	0.69
1:A:401:GLN:NE2	1:A:405:LYS:NZ	2.41	0.68
3:U:10:DA:OP1	1:Z:519:ARG:NH1	2.27	0.68
1:Z:474:ASP:OD1	1:Z:529:HIS:NE2	2.28	0.66
1:Z:401:GLN:HE22	1:Z:405:LYS:NZ	1.94	0.65
1:A:401:GLN:HE22	1:A:405:LYS:NZ	1.95	0.65
1:A:474:ASP:OD1	1:A:529:HIS:NE2	2.29	0.65
3:U:11:DG:H1	2:V:3:DC:H42	1.46	0.64
1:Z:320:ARG:NH1	1:Z:346:ALA:O	2.30	0.64
1:A:159:ARG:NH2	3:F:4:DG:N7	2.47	0.62
1:Z:17:VAL:HG21	1:Z:92:VAL:HG11	1.82	0.62
1:A:17:VAL:HG21	1:A:92:VAL:HG11	1.82	0.61
3:U:11:DG:H4'	1:Z:496:PRO:HB3	1.81	0.61
2:V:5:DG:OP1	1:Z:88:GLU:HA	2.01	0.60
1:A:174:LYS:HZ3	1:A:261:TYR:HA	1.65	0.58
1:Z:401:GLN:NE2	1:Z:405:LYS:HZ2	2.00	0.58
1:A:401:GLN:NE2	1:A:405:LYS:HZ1	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:148:LEU:HD13	1:Z:153:ARG:HG2	1.87	0.56
1:Z:401:GLN:HE22	1:Z:405:LYS:HZ2	1.51	0.56
1:A:401:GLN:HE22	1:A:405:LYS:HZ2	1.54	0.56
1:A:76:LEU:HD23	1:A:93:ILE:HD11	1.88	0.55
2:E:3:DC:H42	3:F:11:DG:H1	1.55	0.54
1:Z:76:LEU:HD23	1:Z:93:ILE:HD11	1.89	0.54
1:Z:342:LEU:HD11	1:Z:439:LEU:HD21	1.90	0.53
1:A:342:LEU:HD11	1:A:439:LEU:HD21	1.91	0.53
1:Z:401:GLN:NE2	1:Z:405:LYS:HZ1	2.06	0.53
1:A:148:LEU:HD13	1:A:153:ARG:HG2	1.89	0.52
1:Z:165:ILE:HB	1:Z:166:PRO:HD3	1.92	0.52
1:A:401:GLN:NE2	1:A:405:LYS:HZ2	2.04	0.51
1:Z:307:SER:HB2	1:Z:310:LEU:HG	1.91	0.51
1:A:165:ILE:HB	1:A:166:PRO:HD3	1.92	0.51
2:E:11:DC:H42	3:F:3:DG:H1	1.58	0.50
1:A:600:LEU:HD11	1:A:650:ILE:HG22	1.93	0.50
1:A:307:SER:HB2	1:A:310:LEU:HG	1.92	0.50
2:V:3:DC:H5”	1:Z:409:ARG:O	2.11	0.50
2:V:9:DT:OP1	1:Z:150:ASN:HB3	2.11	0.49
1:A:126:ARG:HG3	1:A:137:TYR:OH	2.12	0.49
1:Z:600:LEU:HD11	1:Z:650:ILE:HG22	1.94	0.49
3:U:12:DA:OP1	1:Z:470:GLU:HB3	2.13	0.48
1:A:88:GLU:HA	2:E:5:DG:OP1	2.14	0.48
1:Z:126:ARG:HG3	1:Z:137:TYR:OH	2.13	0.47
1:A:43:GLU:OE2	1:A:54:HIS:NE2	2.42	0.47
3:U:9:DC:H4’	1:Z:519:ARG:HE	1.76	0.47
1:Z:196:LYS:HD2	1:Z:199:LYS:NZ	2.29	0.47
1:Z:37:LEU:HD13	1:Z:633:ASN:HB2	1.98	0.46
3:U:11:DG:H1	2:V:3:DC:N4	2.10	0.46
1:A:37:LEU:HD13	1:A:633:ASN:HB2	1.99	0.45
1:A:196:LYS:HD2	1:A:199:LYS:NZ	2.32	0.44
1:Z:30:VAL:HG22	1:Z:44:ILE:HG22	1.99	0.44
1:A:30:VAL:HG22	1:A:44:ILE:HG22	1.99	0.44
1:A:384:PHE:CZ	1:A:424:VAL:HG21	2.53	0.43
2:V:6:DC:H2”	1:Z:500:TRP:CZ3	2.54	0.43
1:Z:384:PHE:CZ	1:Z:424:VAL:HG21	2.54	0.43
2:V:8:DT:H73	1:Z:114:LEU:HB2	2.01	0.42
1:A:558:ILE:O	1:A:562:LEU:HG	2.20	0.42
1:A:182:GLN:H	1:A:235:ASN:ND2	2.17	0.42
2:V:4:DT:H2”	2:V:5:DG:C8	2.55	0.42
2:V:12:DT:C5’	1:Z:283:ALA:HA	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4:DT:H2"	2:E:5:DG:C8	2.55	0.42
1:A:320:ARG:NE	1:A:348:LEU:HB2	2.35	0.42
1:Z:122:GLN:HA	1:Z:365:PRO:HA	2.02	0.42
1:Z:546:GLU:HB2	1:Z:562:LEU:HD11	2.02	0.41
2:E:3:DC:N4	3:F:11:DG:H1	2.16	0.41
1:Z:9:ASP:HB2	1:Z:13:GLU:HG3	2.02	0.41
1:A:32:ARG:HB3	1:A:667:PHE:CD1	2.56	0.41
1:Z:119:GLN:HE22	1:Z:123:ARG:HH11	1.67	0.41
1:Z:247:LYS:HE2	1:Z:247:LYS:HB2	1.84	0.41
1:A:519:ARG:NH1	3:F:10:DA:OP1	2.54	0.41
1:Z:558:ILE:O	1:Z:562:LEU:HG	2.20	0.41
1:A:399:ILE:HG12	1:A:403:ILE:HD13	2.04	0.41
1:A:546:GLU:HB2	1:A:562:LEU:HD11	2.03	0.41
1:A:642:ILE:HB	1:A:674:ILE:HG22	2.03	0.40
1:Z:182:GLN:H	1:Z:235:ASN:ND2	2.18	0.40
1:A:122:GLN:HA	1:A:365:PRO:HA	2.03	0.40
1:Z:526:ARG:HA	1:Z:527:PRO:HD3	1.97	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	674/676 (100%)	660 (98%)	14 (2%)	0	100	100
1	Z	674/676 (100%)	658 (98%)	16 (2%)	0	100	100
All	All	1348/1352 (100%)	1318 (98%)	30 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	613/613 (100%)	595 (97%)	18 (3%)	37	63
1	Z	613/613 (100%)	590 (96%)	23 (4%)	28	54
All	All	1226/1226 (100%)	1185 (97%)	41 (3%)	33	59

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	51	ASP
1	A	98	ASN
1	A	123	ARG
1	A	142	ASP
1	A	240	GLU
1	A	247	LYS
1	A	321	ASN
1	A	364	ARG
1	A	393	LYS
1	A	466	ASN
1	A	469	GLN
1	A	471	ASN
1	A	492	MET
1	A	494	ASN
1	A	500	TRP
1	A	591	SER
1	A	609	ASP
1	Z	10	ASN
1	Z	51	ASP
1	Z	112	SER
1	Z	123	ARG
1	Z	142	ASP
1	Z	229	GLN
1	Z	240	GLU
1	Z	247	LYS
1	Z	248	ASN

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Mol	Chain	Res	Type
1	Z	320	ARG
1	Z	321	ASN
1	Z	364	ARG
1	Z	393	LYS
1	Z	466	ASN
1	Z	469	GLN
1	Z	471	ASN
1	Z	492	MET
1	Z	494	ASN
1	Z	500	TRP
1	Z	522	GLU
1	Z	591	SER
1	Z	609	ASP
1	Z	617	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	50	HIS
1	A	68	ASN
1	A	220	GLN
1	A	235	ASN
1	A	248	ASN
1	A	251	ASN
1	A	296	ASN
1	A	321	ASN
1	A	401	GLN
1	A	444	ASN
1	Z	10	ASN
1	Z	50	HIS
1	Z	98	ASN
1	Z	220	GLN
1	Z	235	ASN
1	Z	251	ASN
1	Z	296	ASN
1	Z	380	ASN
1	Z	401	GLN
1	Z	444	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 7 are monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\| > 2$
5	MES	Z	704	-	12,12,12	0.91	0	14,16,16	0.73	0

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
5	MES	Z	704	-	-	1/6/14/14	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Z	704	MES	N4-C7-C8-S

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, 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	676/676 (100%)	1.35	149 (22%) 3 3	24, 43, 79, 88	0
1	Z	676/676 (100%)	1.29	134 (19%) 3 4	24, 42, 76, 87	0
2	E	13/13 (100%)	0.51	0 100 100	35, 43, 59, 63	0
2	V	13/13 (100%)	0.52	0 100 100	38, 44, 57, 63	0
3	F	13/13 (100%)	0.91	2 (15%) 6 6	36, 48, 72, 73	0
3	U	13/13 (100%)	0.50	0 100 100	36, 41, 60, 60	0
All	All	1404/1404 (100%)	1.29	285 (20%) 3 4	24, 43, 77, 88	0

All (285) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Z	520	VAL	6.2
1	A	67	THR	5.8
1	A	521	SER	5.6
1	Z	523	ASN	5.5
1	A	491	GLY	5.4
1	A	676	GLY	5.3
1	A	520	VAL	5.2
1	Z	67	THR	5.1
1	Z	676	GLY	4.9
1	Z	517	LEU	4.8
1	Z	491	GLY	4.8
1	Z	250	ASN	4.8
1	Z	308	SER	4.7
1	Z	253	THR	4.6
1	A	596	ASP	4.4
1	A	547	SER	4.4
1	A	518	PRO	4.4
1	A	671	PHE	4.3
1	Z	643	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	515	LEU	4.2
1	Z	602	ALA	4.2
1	Z	596	ASP	4.1
1	A	633	ASN	4.1
1	Z	497	GLY	4.0
1	Z	601	SER	4.0
1	A	576	VAL	4.0
1	A	592	LEU	3.9
1	Z	503	LEU	3.9
1	A	68	ASN	3.9
1	A	575	SER	3.9
3	F	13	DC	3.9
1	Z	516	SER	3.8
1	Z	589	ASN	3.8
1	A	517	LEU	3.7
1	A	622	VAL	3.7
1	A	455	LYS	3.7
1	A	490	SER	3.7
1	A	514	TRP	3.7
1	A	572	PHE	3.6
1	A	120	ALA	3.6
1	Z	220	GLN	3.6
1	A	20	LEU	3.6
1	Z	490	SER	3.5
1	A	532	GLN	3.5
1	Z	120	ALA	3.5
1	Z	571	ASP	3.5
1	A	368	GLY	3.5
1	A	499	ASP	3.4
1	Z	530	VAL	3.4
1	Z	581	ALA	3.4
1	Z	363	ASN	3.4
1	Z	367	ARG	3.4
1	A	630	ALA	3.4
1	A	456	GLN	3.4
1	A	69	ASP	3.3
1	A	278	PHE	3.3
1	A	595	ASN	3.3
1	Z	98	ASN	3.3
1	Z	580	ILE	3.3
1	Z	518	PRO	3.3
1	A	649	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	675	GLU	3.3
1	A	570	PHE	3.2
1	A	535	ASP	3.2
1	Z	573	THR	3.2
1	A	585	TRP	3.2
1	Z	574	PRO	3.2
1	Z	368	GLY	3.2
1	A	367	ARG	3.2
1	Z	515	LEU	3.2
1	A	489	PHE	3.2
1	Z	519	ARG	3.2
1	A	302	SER	3.2
1	A	616	TYR	3.1
1	A	150	ASN	3.1
1	Z	494	ASN	3.1
1	Z	398	LEU	3.1
1	A	571	ASP	3.1
1	A	516	SER	3.1
1	Z	509	GLY	3.1
1	Z	670	GLY	3.1
1	A	243	SER	3.1
1	A	519	ARG	3.1
1	Z	144	VAL	3.1
1	Z	499	ASP	3.1
1	A	412	LEU	3.0
1	Z	638	GLN	3.0
1	Z	150	ASN	3.0
1	A	533	ILE	3.0
1	Z	521	SER	3.0
1	Z	569	LEU	3.0
1	A	253	THR	3.0
1	Z	246	THR	3.0
1	A	604	ALA	3.0
1	Z	514	TRP	3.0
1	A	657	TYR	3.0
1	A	269	ASN	3.0
1	A	564	LYS	2.9
1	A	308	SER	2.9
1	A	251	ASN	2.9
1	A	165	ILE	2.9
1	Z	671	PHE	2.9
1	A	619	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	Z	506	ILE	2.9
1	Z	306	ALA	2.9
1	Z	507	ARG	2.9
1	Z	535	ASP	2.8
1	Z	585	TRP	2.8
1	A	401	GLN	2.8
1	A	568	TYR	2.8
1	Z	568	TYR	2.8
1	A	15	GLU	2.8
1	A	453	THR	2.8
1	A	74	ASN	2.8
1	A	544	SER	2.8
1	A	601	SER	2.8
1	A	643	LYS	2.8
1	A	248	ASN	2.8
1	Z	72	ASN	2.7
1	Z	500	TRP	2.7
1	A	634	GLN	2.7
1	A	154	SER	2.7
1	Z	587	PHE	2.7
1	A	593	VAL	2.7
1	Z	168	SER	2.7
1	Z	402	ASP	2.7
1	Z	336	MET	2.7
1	Z	303	VAL	2.7
1	A	542	LEU	2.7
1	A	504	SER	2.7
1	Z	338	ILE	2.7
1	A	607	ASP	2.7
1	Z	213	ASP	2.7
3	F	12	DA	2.7
1	A	127	ALA	2.7
1	A	530	VAL	2.7
1	Z	113	ALA	2.7
1	Z	493	CYS	2.6
1	A	525	LYS	2.6
1	Z	269	ASN	2.6
1	A	227	ILE	2.6
1	Z	513	ARG	2.6
1	A	452	LYS	2.6
1	A	602	ALA	2.6
1	Z	242	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	Z	248	ASN	2.6
1	A	606	ILE	2.6
1	Z	502	GLY	2.6
1	Z	145	LYS	2.6
1	A	314	VAL	2.6
1	A	605	PHE	2.6
1	Z	266	ARG	2.6
1	A	573	THR	2.6
1	Z	511	GLU	2.6
1	Z	576	VAL	2.6
1	A	577	GLN	2.5
1	Z	74	ASN	2.5
1	Z	262	ASN	2.5
1	Z	579	LYS	2.5
1	Z	20	LEU	2.5
1	Z	148	LEU	2.5
1	A	636	ASN	2.5
1	Z	381	ALA	2.5
1	Z	277	LYS	2.5
1	A	637	PRO	2.5
1	Z	7	HIS	2.5
1	A	327	VAL	2.5
1	Z	572	PHE	2.5
1	A	19	ASP	2.5
1	A	548	LYS	2.5
1	Z	322	ASP	2.5
1	Z	527	PRO	2.5
1	Z	622	VAL	2.5
1	Z	158	LEU	2.4
1	Z	593	VAL	2.4
1	A	635	ASN	2.4
1	Z	68	ASN	2.4
1	A	495	PRO	2.4
1	A	148	LEU	2.4
1	Z	675	GLU	2.4
1	Z	631	ILE	2.4
1	Z	87	TYR	2.4
1	Z	409	ARG	2.4
1	A	611	LEU	2.4
1	A	505	ILE	2.4
1	Z	204	THR	2.4
1	Z	495	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	562	LEU	2.4
1	Z	492	MET	2.4
1	A	168	SER	2.4
1	Z	278	PHE	2.4
1	A	250	ASN	2.4
1	A	279	ARG	2.4
1	Z	561	GLN	2.3
1	A	539	LYS	2.3
1	Z	302	SER	2.3
1	A	581	ALA	2.3
1	Z	599	LEU	2.3
1	Z	401	GLN	2.3
1	A	645	LYS	2.3
1	Z	162	ASN	2.3
1	Z	390	PRO	2.3
1	Z	637	PRO	2.3
1	A	524	GLY	2.3
1	Z	505	ILE	2.3
1	A	336	MET	2.3
1	A	162	ASN	2.3
1	A	87	TYR	2.3
1	A	146	TYR	2.3
1	A	303	VAL	2.3
1	A	459	ILE	2.3
1	Z	392	ILE	2.3
1	Z	619	ILE	2.3
1	Z	655	VAL	2.3
1	A	672	PHE	2.3
1	A	307	SER	2.3
1	A	448	SER	2.3
1	A	501	SER	2.3
1	A	553	ASP	2.3
1	A	199	LYS	2.3
1	A	155	ARG	2.2
1	A	569	LEU	2.2
1	Z	562	LEU	2.2
1	A	174	LYS	2.2
1	A	494	ASN	2.2
1	Z	232	ILE	2.2
1	Z	411	GLY	2.2
1	A	488	CYS	2.2
1	Z	597	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	Z	115	GLN	2.2
1	Z	296	ASN	2.2
1	A	300	ARG	2.2
1	A	536	LEU	2.2
1	Z	542	LEU	2.2
1	Z	80	SER	2.2
1	A	674	ILE	2.2
1	Z	260	ILE	2.2
1	A	50	HIS	2.2
1	A	507	ARG	2.2
1	A	587	PHE	2.2
1	A	608	TYR	2.2
1	Z	610	ASN	2.2
1	A	91	ASP	2.2
1	Z	205	ILE	2.2
1	Z	141	VAL	2.2
1	Z	298	VAL	2.2
1	A	498	GLY	2.1
1	A	603	GLY	2.1
1	A	537	PHE	2.1
1	Z	254	TYR	2.1
1	A	567	GLU	2.1
1	Z	94	ILE	2.1
1	A	149	ASN	2.1
1	Z	157	ASN	2.1
1	A	522	GLU	2.1
1	A	500	TRP	2.1
1	Z	25	ILE	2.1
1	A	322	ASP	2.1
1	A	578	ARG	2.1
1	A	615	ASP	2.1
1	A	632	LYS	2.1
1	A	167	TYR	2.1
1	A	584	ASN	2.1
1	A	540	PRO	2.1
1	A	298	VAL	2.1
1	A	509	GLY	2.1
1	Z	274	GLY	2.1
1	A	220	GLN	2.1
1	Z	154	SER	2.1
1	Z	532	GLN	2.1
1	Z	235	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	Z	486	PRO	2.1
1	A	566	ILE	2.1
1	A	534	LEU	2.0
1	Z	630	ALA	2.0
1	A	383	ILE	2.0
1	Z	636	ASN	2.0
1	Z	667	PHE	2.0
1	Z	58	ASP	2.0
1	Z	209	ASP	2.0
1	Z	616	TYR	2.0
1	A	363	ASN	2.0
1	A	100	GLY	2.0
1	A	276	PHE	2.0
1	A	670	GLY	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 monosaccharides in this entry.

6.4 Ligands (i)

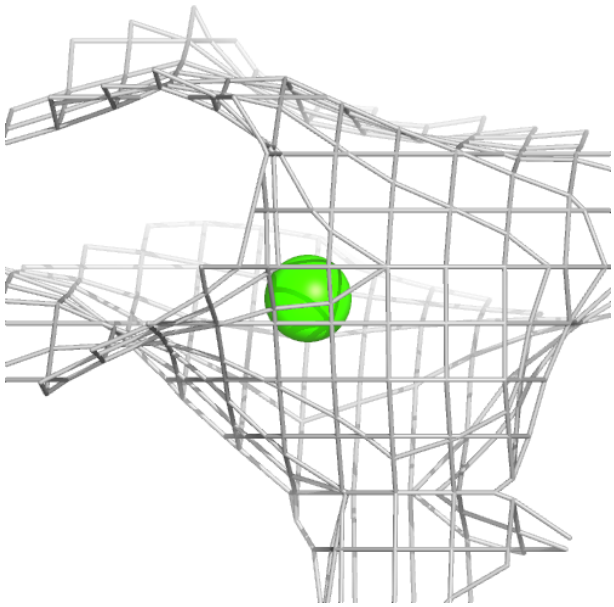
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

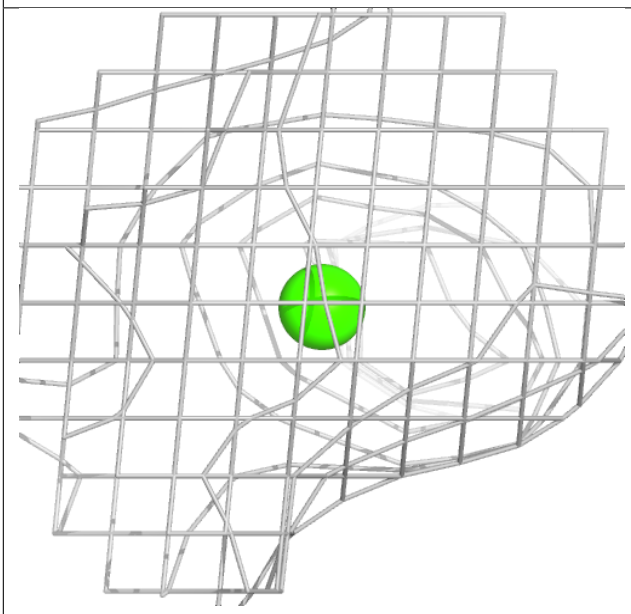
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	CL	Z	705	1/1	0.73	0.24	63,63,63,63	0
5	MES	Z	704	12/12	0.86	0.16	62,62,64,64	13
4	CA	Z	703	1/1	0.86	0.09	68,68,68,68	0
4	CA	A	703	1/1	0.95	0.08	50,50,50,50	0
4	CA	Z	702	1/1	0.96	0.07	31,31,31,31	0
4	CA	A	702	1/1	0.96	0.04	35,35,35,35	0
4	CA	A	701	1/1	0.98	0.07	24,24,24,24	0
4	CA	Z	701	1/1	0.98	0.03	20,20,20,20	0

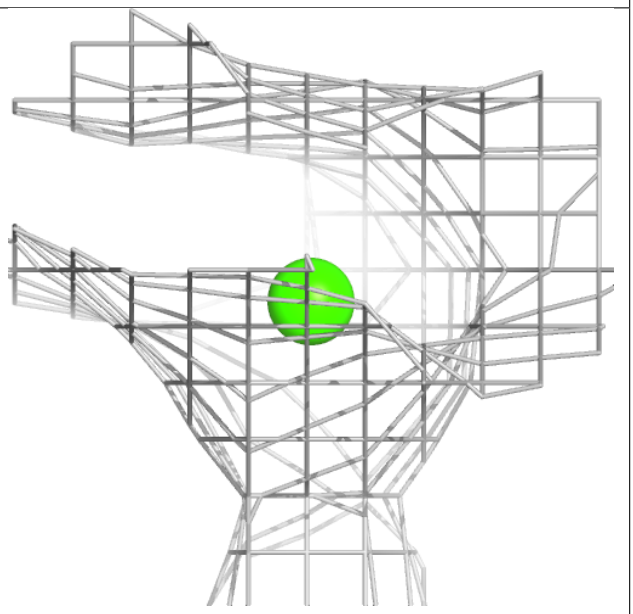
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CA Z 703:

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

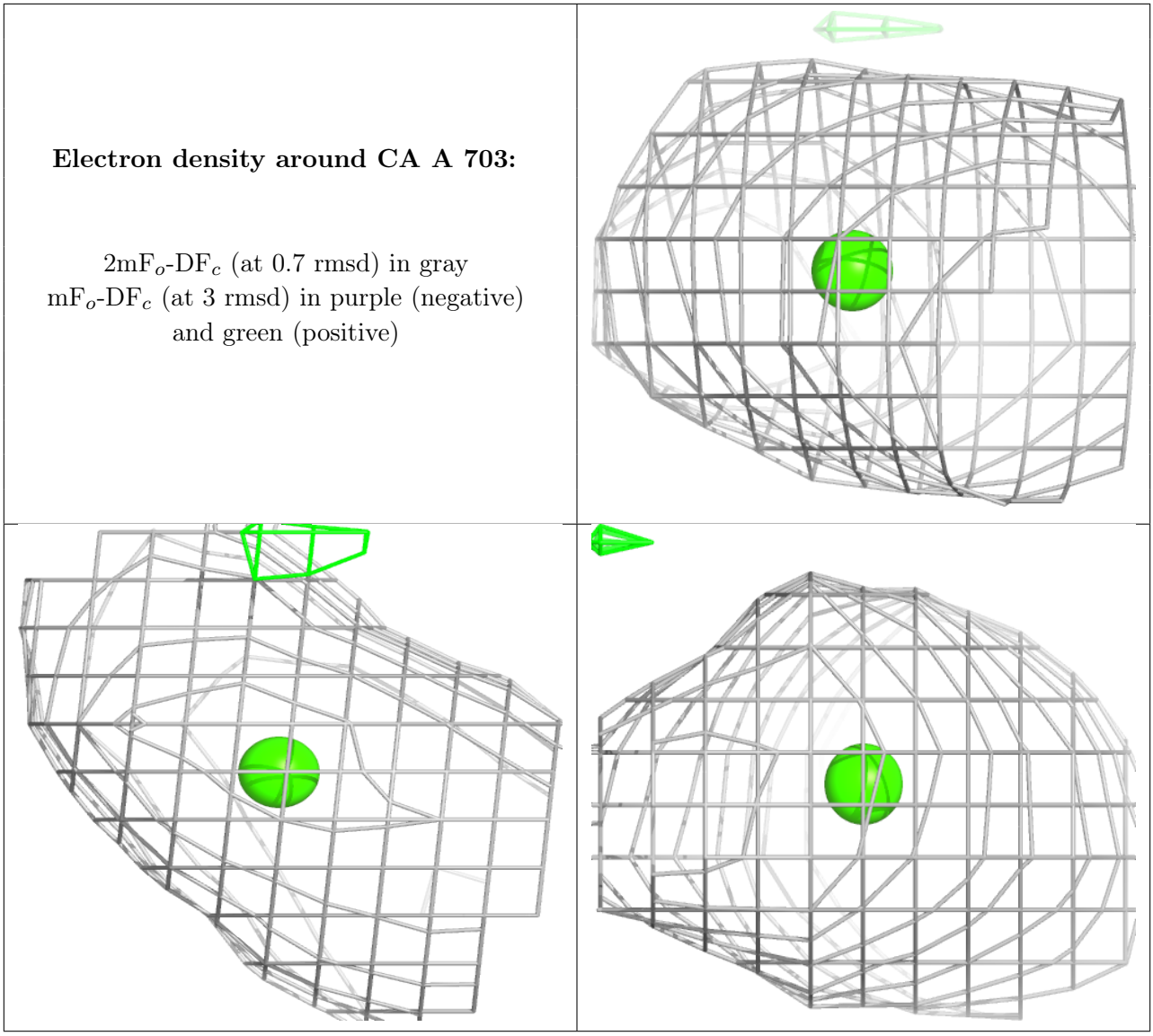






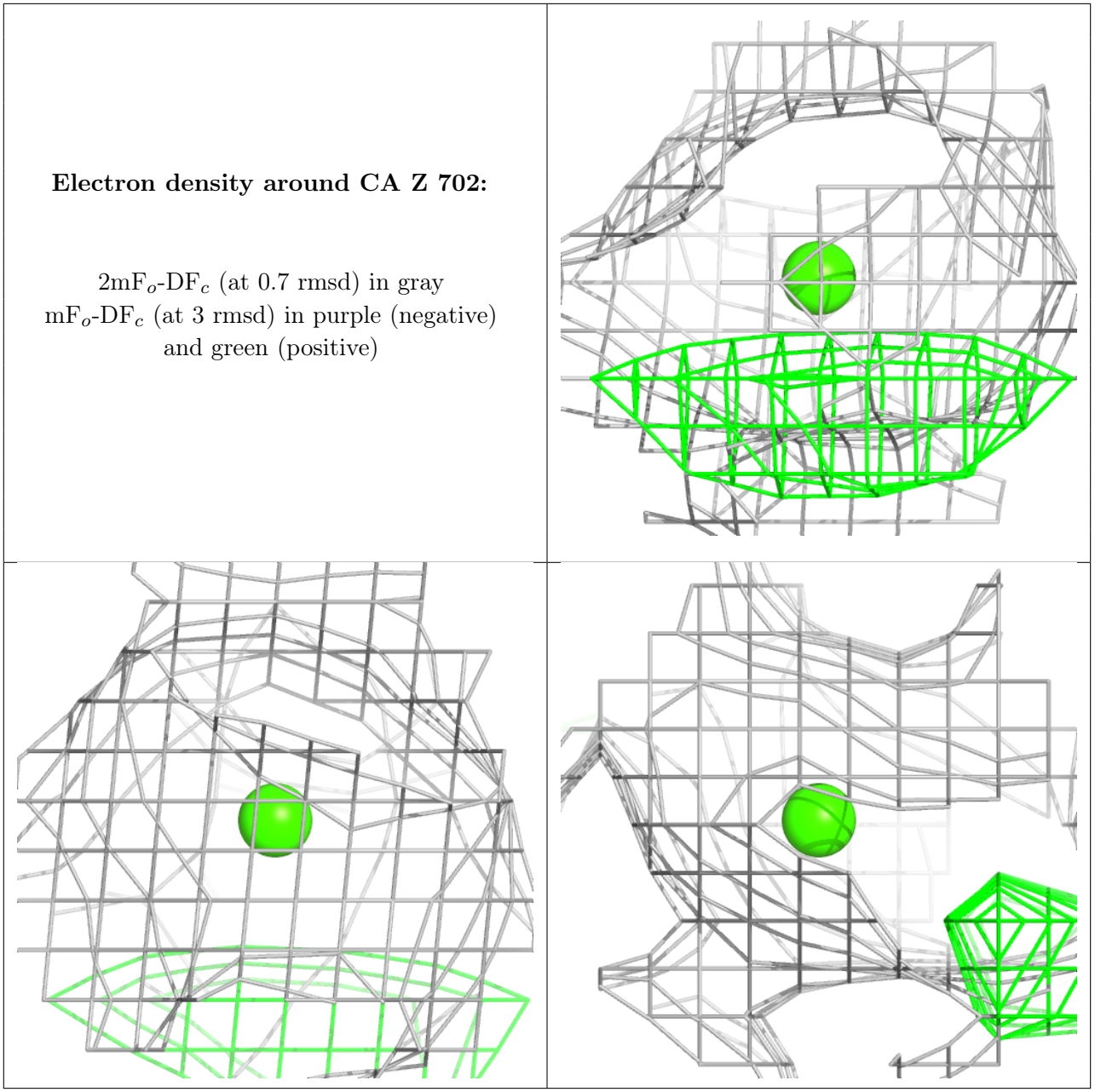
Electron density around CA A 703:

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



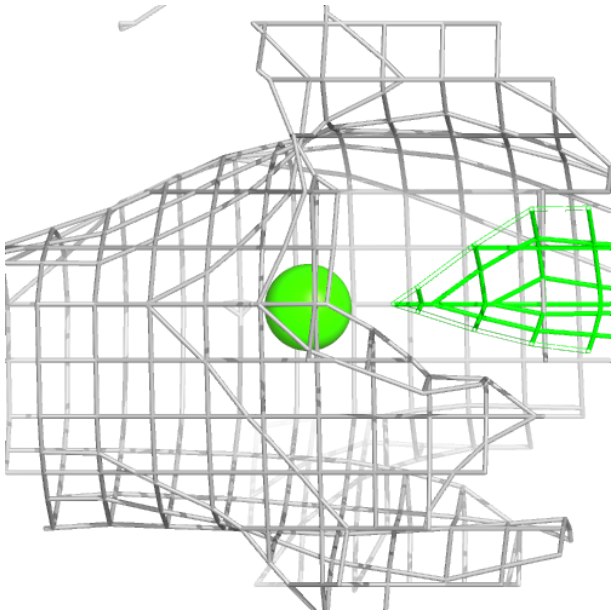
Electron density around CA Z 702:

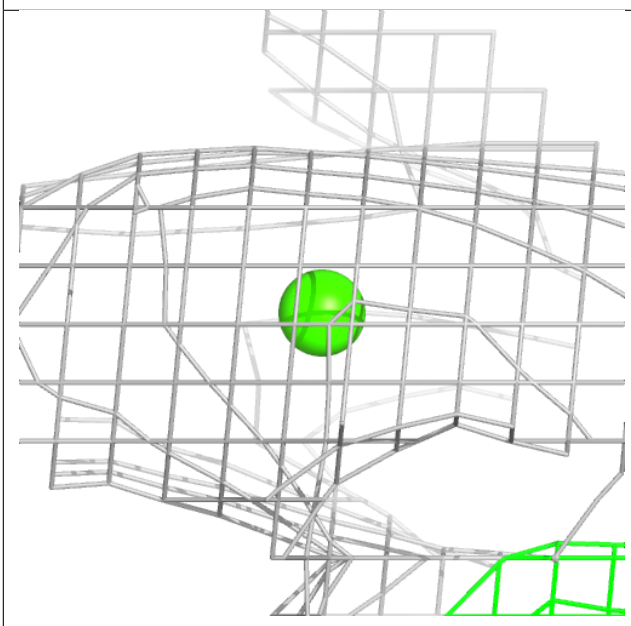
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

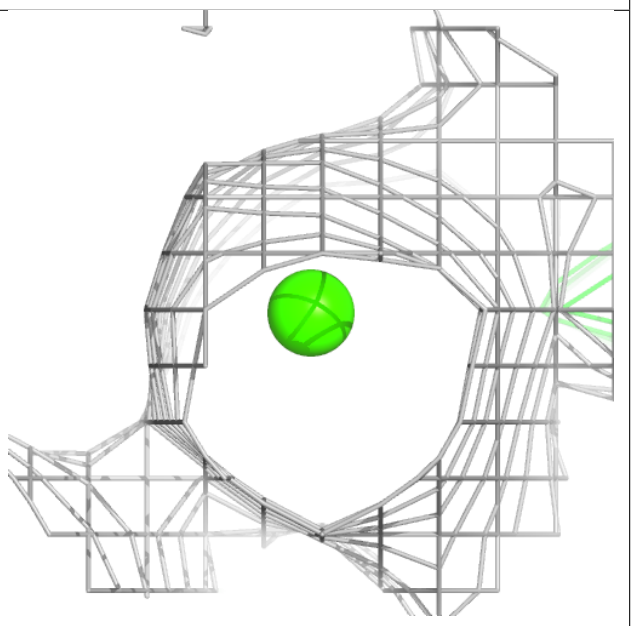


Electron density around CA A 702:

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

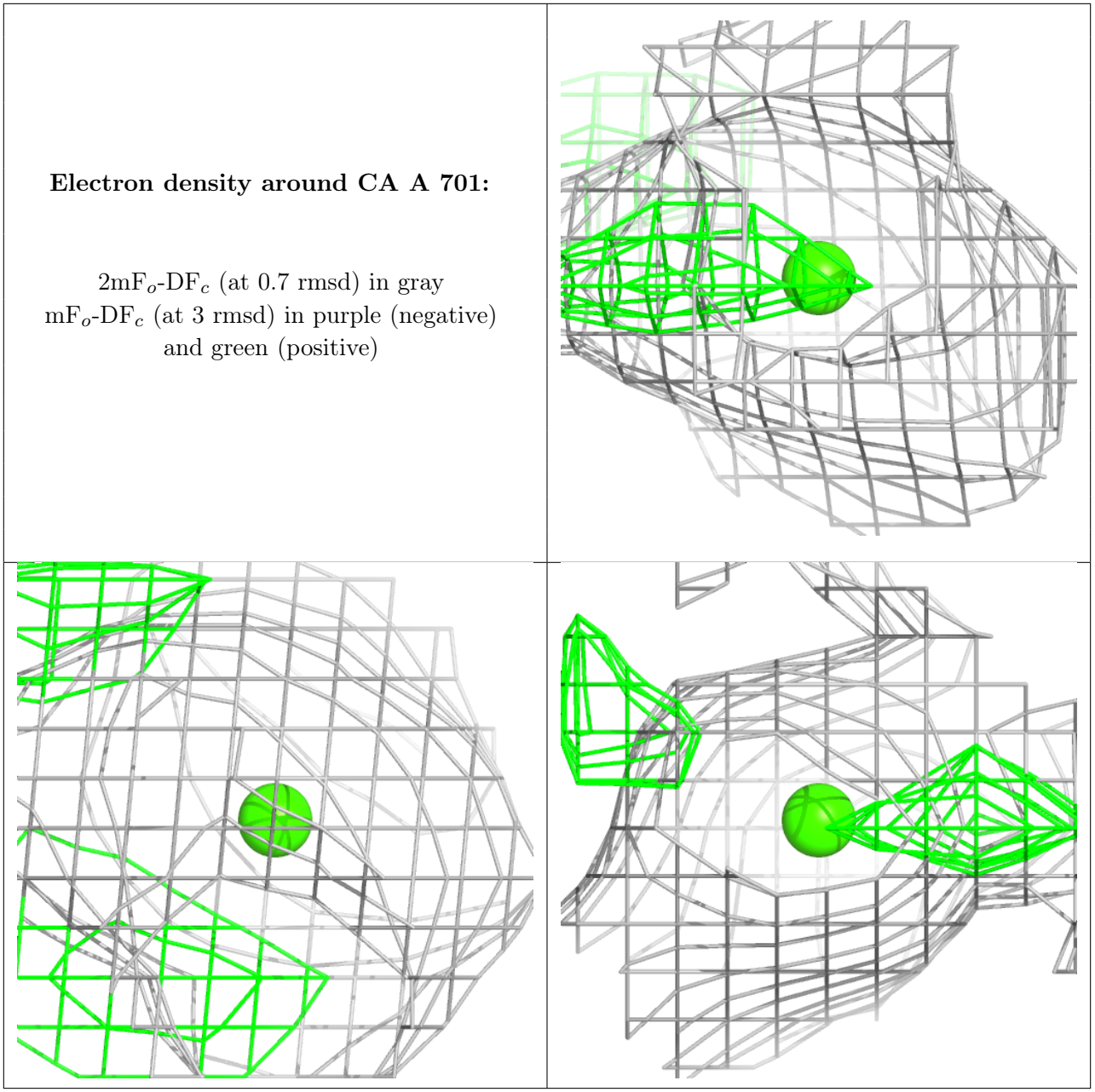






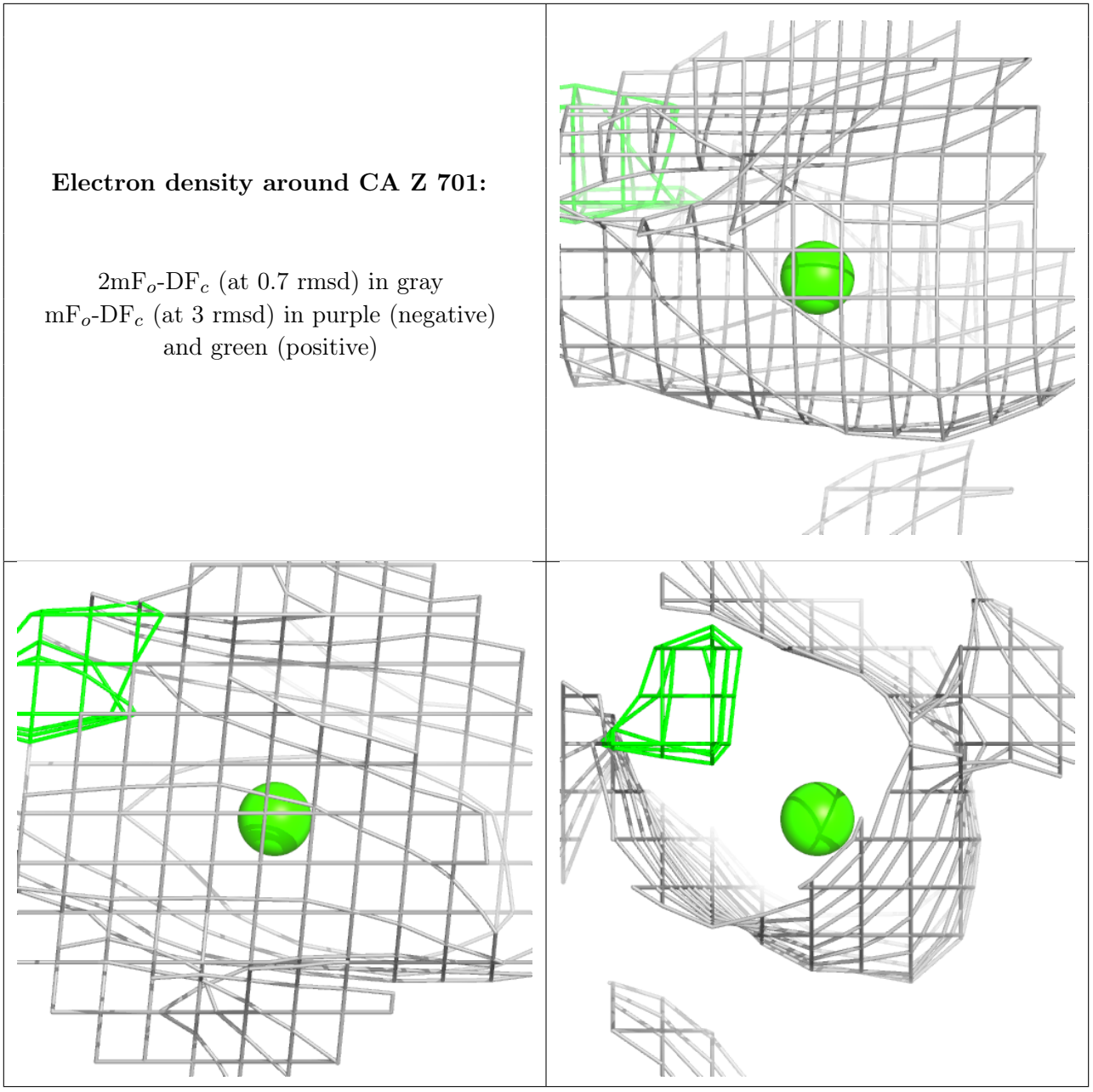
Electron density around CA A 701:

$2mF_o$-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 Z 701:

$2mF_o$-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.