



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:37 PM UTC

PDB ID : 9F38 / pdb_00009f38
Title : BsmI (wild-type) crystallized with Ca²⁺ and cognate dsDNA
Authors : Sieskind, R.; Missouri, 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 ⓘ 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:

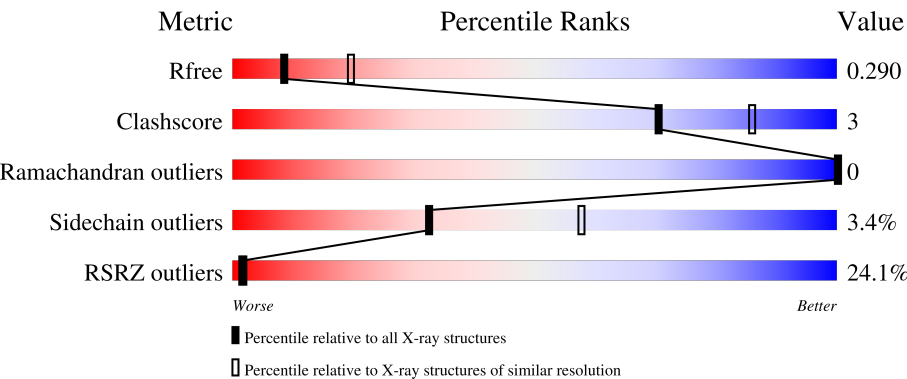
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance 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}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (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 $\leq 5\%$. 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	676	26% 89% 11%
1	Z	676	23% 88% 11%
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	8% 62% 38%

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			

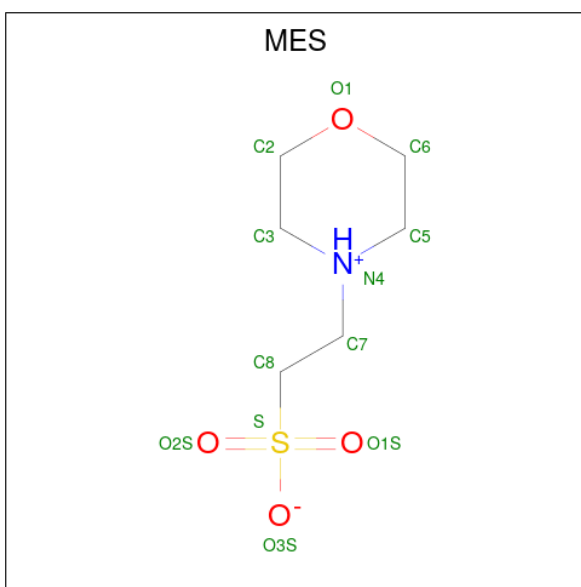
- Molecule 3 is a DNA chain called DNA (Top strand).

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 (CCD ID: 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 (CCD ID: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 7 is water.

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

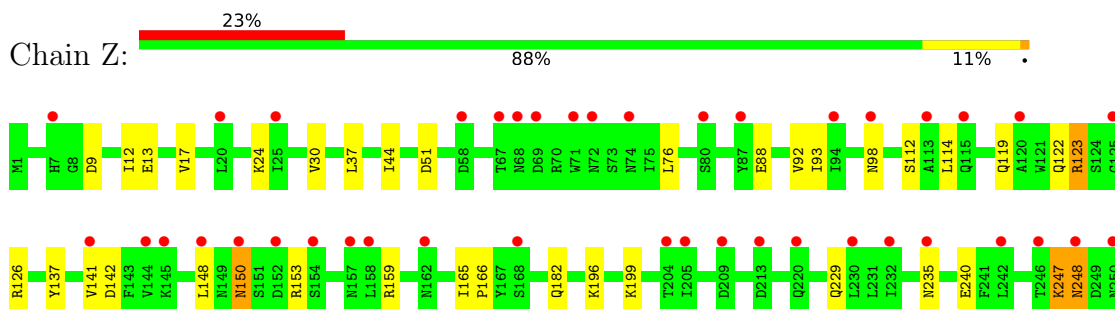
3 Residue-property plots

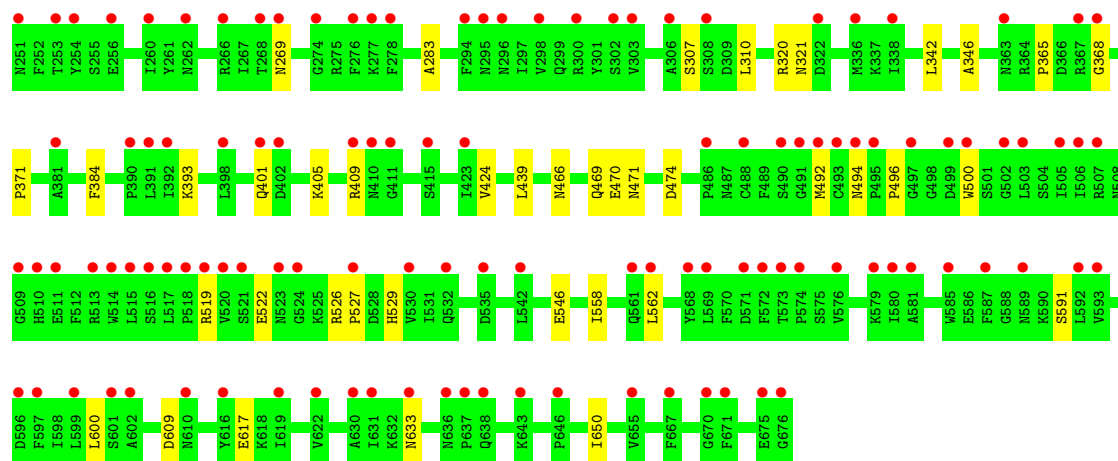
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: BsmI

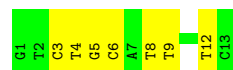




• Molecule 2: DNA (Bottom strand)



• Molecule 2: DNA (Bottom strand)



• Molecule 3: DNA (Top strand)



• Molecule 3: DNA (Top strand)



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	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.*

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: 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	0.55	0/5650	0.94	2/7631 (0.0%)
1	Z	0.56	0/5650	0.95	4/7631 (0.1%)
2	E	0.31	0/285	0.56	0/437
2	V	0.31	0/285	0.56	0/437
3	F	0.28	0/305	0.44	0/470
3	U	0.27	0/305	0.43	0/470
All	All	0.54	0/12480	0.91	6/17076 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	609	ASP	CA-CB-CG	8.83	121.43	112.60
1	Z	98	ASN	CA-CB-CG	6.29	118.89	112.60
1	Z	269	ASN	CA-CB-CG	5.56	118.16	112.60
1	A	269	ASN	CA-CB-CG	5.53	118.13	112.60
1	Z	248	ASN	CA-CB-CG	5.38	117.98	112.60
1	Z	150	ASN	CA-CB-CG	5.34	117.94	112.60

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	34	0
1	Z	5521	0	5507	40	0
2	E	257	0	150	5	0
2	V	257	0	150	9	0
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	81	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 (81) 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:A:401:GLN:NE2	1:A:405:LYS:HZ2	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:GLN:HE22	1:A:405:LYS:HZ2	1.48	0.60
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: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: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: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:Z:368:GLY:C	1:Z:371:PRO:HD2	2.43	0.44
1:A:384:PHE:CZ	1:A:424:VAL:HG21	2.53	0.43
1:A:368:GLY:C	1:A:371:PRO:HD2	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:401:GLN:NE2	1:A:405:LYS:HZ1	2.14	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 ⓘ

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%)	593 (97%)	20 (3%)	33	58
1	Z	613/613 (100%)	591 (96%)	22 (4%)	31	56
All	All	1226/1226 (100%)	1184 (97%)	42 (3%)	32	58

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ILE
1	A	24	LYS
1	A	51	ASP
1	A	98	ASN
1	A	123	ARG
1	A	141	VAL
1	A	142	ASP
1	A	150	ASN
1	A	229	GLN
1	A	240	GLU
1	A	247	LYS
1	A	321	ASN
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	591	SER
1	A	609	ASP
1	Z	12	ILE
1	Z	24	LYS
1	Z	51	ASP
1	Z	112	SER
1	Z	123	ARG

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Mol	Chain	Res	Type
1	Z	141	VAL
1	Z	142	ASP
1	Z	229	GLN
1	Z	240	GLU
1	Z	247	LYS
1	Z	248	ASN
1	Z	321	ASN
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	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 (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	50	HIS
1	A	119	GLN
1	A	220	GLN
1	A	235	ASN
1	A	296	ASN
1	A	380	ASN
1	A	401	GLN
1	A	404	ASN
1	A	444	ASN
1	A	445	ASN
1	A	466	ASN
1	A	561	GLN
1	A	589	ASN
1	A	595	ASN
1	A	661	ASN
1	A	665	ASN
1	Z	10	ASN
1	Z	50	HIS
1	Z	99	ASN
1	Z	119	GLN

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Mol	Chain	Res	Type
1	Z	220	GLN
1	Z	235	ASN
1	Z	248	ASN
1	Z	251	ASN
1	Z	296	ASN
1	Z	380	ASN
1	Z	401	GLN
1	Z	404	ASN
1	Z	442	ASN
1	Z	444	ASN
1	Z	445	ASN
1	Z	466	ASN
1	Z	561	GLN
1	Z	589	ASN
1	Z	595	ASN
1	Z	661	ASN
1	Z	665	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 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	0.92	0	15,16,16	0.67	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, 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	676/676 (100%)	1.47	179 (26%)  	24, 43, 79, 88	0
1	Z	676/676 (100%)	1.42	156 (23%)  	24, 42, 76, 87	0
2	E	13/13 (100%)	0.67	0  	35, 43, 59, 63	0
2	V	13/13 (100%)	0.68	0  	38, 44, 57, 63	0
3	F	13/13 (100%)	1.09	2 (15%)  	36, 48, 72, 73	0
3	U	13/13 (100%)	0.68	1 (7%)  	36, 41, 60, 60	0
All	All	1404/1404 (100%)	1.42	338 (24%)  	24, 43, 77, 88	0

All (338) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Z	520	VAL	6.3
1	A	67	THR	5.8
1	A	521	SER	5.7
1	A	491	GLY	5.5
1	Z	523	ASN	5.5
1	A	676	GLY	5.3
1	A	520	VAL	5.3
1	Z	67	THR	5.2
1	Z	676	GLY	5.0
1	Z	517	LEU	4.9
1	Z	491	GLY	4.9
1	Z	250	ASN	4.8
1	Z	308	SER	4.7
1	Z	253	THR	4.7
1	A	596	ASP	4.5
1	A	518	PRO	4.5
1	A	671	PHE	4.5
1	A	547	SER	4.5
1	A	515	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	Z	602	ALA	4.2
1	Z	643	LYS	4.2
1	Z	596	ASP	4.2
1	A	633	ASN	4.1
1	Z	497	GLY	4.1
1	Z	601	SER	4.1
1	A	576	VAL	4.0
1	A	592	LEU	4.0
1	Z	503	LEU	4.0
3	F	13	DC	4.0
1	A	68	ASN	3.9
1	A	575	SER	3.9
1	Z	516	SER	3.9
1	Z	589	ASN	3.8
1	A	517	LEU	3.8
1	A	514	TRP	3.8
1	A	622	VAL	3.8
1	A	572	PHE	3.8
1	A	490	SER	3.7
1	A	455	LYS	3.7
1	A	20	LEU	3.7
1	A	120	ALA	3.7
1	A	368	GLY	3.6
1	Z	220	GLN	3.6
1	Z	120	ALA	3.6
1	Z	490	SER	3.6
1	Z	571	ASP	3.6
1	A	532	GLN	3.6
1	Z	530	VAL	3.5
1	A	499	ASP	3.5
1	Z	581	ALA	3.5
1	A	278	PHE	3.5
1	Z	363	ASN	3.5
1	A	630	ALA	3.5
1	Z	367	ARG	3.4
1	A	69	ASP	3.4
1	A	456	GLN	3.4
1	Z	518	PRO	3.4
1	A	570	PHE	3.4
1	A	595	ASN	3.4
1	Z	98	ASN	3.4
1	Z	580	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	585	TRP	3.4
1	A	649	THR	3.4
1	Z	574	PRO	3.3
1	A	489	PHE	3.3
1	Z	573	THR	3.3
1	A	535	ASP	3.3
1	Z	368	GLY	3.3
1	Z	515	LEU	3.3
1	A	675	GLU	3.3
1	A	616	TYR	3.3
1	Z	398	LEU	3.3
1	A	302	SER	3.3
1	A	367	ARG	3.2
1	A	571	ASP	3.2
1	A	150	ASN	3.2
1	Z	494	ASN	3.2
1	Z	519	ARG	3.2
1	Z	509	GLY	3.2
1	Z	670	GLY	3.2
1	A	516	SER	3.2
1	A	243	SER	3.2
1	A	412	LEU	3.2
1	Z	144	VAL	3.2
1	Z	499	ASP	3.1
1	A	519	ARG	3.1
1	Z	514	TRP	3.1
1	Z	569	LEU	3.1
1	A	533	ILE	3.1
1	A	657	TYR	3.1
1	Z	521	SER	3.1
1	Z	150	ASN	3.1
1	Z	638	GLN	3.1
1	A	253	THR	3.1
1	Z	246	THR	3.1
1	A	604	ALA	3.1
1	A	269	ASN	3.0
1	Z	671	PHE	3.0
1	A	308	SER	3.0
1	A	165	ILE	3.0
1	A	564	LYS	3.0
1	A	251	ASN	3.0
1	Z	585	TRP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	619	ILE	3.0
1	Z	506	ILE	3.0
1	Z	306	ALA	3.0
1	A	568	TYR	2.9
1	Z	568	TYR	2.9
1	Z	535	ASP	2.9
1	A	453	THR	2.9
1	Z	507	ARG	2.9
1	Z	500	TRP	2.9
1	A	401	GLN	2.9
1	A	74	ASN	2.9
1	A	544	SER	2.9
1	A	601	SER	2.9
1	Z	587	PHE	2.9
1	A	15	GLU	2.9
1	A	248	ASN	2.9
1	A	643	LYS	2.8
1	Z	72	ASN	2.8
3	F	12	DA	2.8
1	A	154	SER	2.8
1	Z	336	MET	2.8
1	A	634	GLN	2.8
1	A	593	VAL	2.8
1	A	542	LEU	2.8
1	Z	402	ASP	2.8
1	Z	168	SER	2.8
1	Z	493	CYS	2.8
1	Z	303	VAL	2.8
1	Z	338	ILE	2.8
1	A	607	ASP	2.8
1	Z	213	ASP	2.8
1	A	504	SER	2.8
1	A	530	VAL	2.8
1	A	127	ALA	2.8
1	Z	113	ALA	2.8
1	A	605	PHE	2.7
1	A	227	ILE	2.7
1	Z	242	LEU	2.7
1	Z	269	ASN	2.7
1	Z	502	GLY	2.7
1	A	602	ALA	2.7
1	A	606	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	525	LYS	2.7
1	Z	248	ASN	2.7
1	A	314	VAL	2.7
1	A	452	LYS	2.7
1	A	573	THR	2.7
1	Z	513	ARG	2.7
1	Z	145	LYS	2.7
1	Z	576	VAL	2.7
1	Z	20	LEU	2.7
1	Z	148	LEU	2.7
1	Z	266	ARG	2.6
1	Z	74	ASN	2.6
1	Z	262	ASN	2.6
1	A	577	GLN	2.6
1	Z	511	GLU	2.6
1	Z	572	PHE	2.6
1	A	637	PRO	2.6
1	A	636	ASN	2.6
1	Z	579	LYS	2.6
1	Z	381	ALA	2.6
1	Z	7	HIS	2.6
1	Z	527	PRO	2.6
1	A	327	VAL	2.6
1	A	19	ASP	2.6
1	Z	322	ASP	2.6
1	Z	277	LYS	2.6
1	Z	158	LEU	2.6
1	Z	622	VAL	2.6
1	A	548	LYS	2.5
1	A	495	PRO	2.5
1	A	148	LEU	2.5
1	Z	87	TYR	2.5
1	Z	593	VAL	2.5
1	A	635	ASN	2.5
1	Z	68	ASN	2.5
1	A	611	LEU	2.5
1	Z	631	ILE	2.5
1	Z	278	PHE	2.5
1	A	562	LEU	2.5
1	Z	492	MET	2.5
1	Z	495	PRO	2.5
1	A	505	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	Z	675	GLU	2.5
1	Z	204	THR	2.5
1	A	168	SER	2.5
1	Z	409	ARG	2.5
1	A	250	ASN	2.5
1	Z	599	LEU	2.4
1	Z	302	SER	2.4
1	A	581	ALA	2.4
1	Z	561	GLN	2.4
1	Z	390	PRO	2.4
1	Z	637	PRO	2.4
1	A	524	GLY	2.4
1	A	279	ARG	2.4
1	A	539	LYS	2.4
1	A	672	PHE	2.4
1	A	87	TYR	2.4
1	A	146	TYR	2.4
1	Z	401	GLN	2.4
1	A	336	MET	2.4
1	Z	162	ASN	2.4
1	Z	505	ILE	2.4
1	A	645	LYS	2.4
1	A	459	ILE	2.4
1	Z	392	ILE	2.4
1	Z	619	ILE	2.4
1	A	162	ASN	2.4
1	A	303	VAL	2.4
1	Z	655	VAL	2.4
1	A	488	CYS	2.4
1	A	553	ASP	2.4
1	Z	597	PHE	2.4
1	A	307	SER	2.4
1	A	448	SER	2.4
1	A	501	SER	2.4
1	A	569	LEU	2.4
1	Z	562	LEU	2.4
1	Z	411	GLY	2.3
1	Z	232	ILE	2.3
1	A	199	LYS	2.3
1	A	494	ASN	2.3
1	A	587	PHE	2.3
1	A	536	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	Z	542	LEU	2.3
1	A	608	TYR	2.3
1	A	174	LYS	2.3
1	A	155	ARG	2.3
1	Z	296	ASN	2.3
1	A	537	PHE	2.3
1	Z	115	GLN	2.3
1	A	50	HIS	2.3
1	A	674	ILE	2.3
1	Z	80	SER	2.3
1	Z	260	ILE	2.3
1	Z	254	TYR	2.3
1	A	498	GLY	2.3
1	A	603	GLY	2.3
1	Z	610	ASN	2.3
1	A	91	ASP	2.3
1	Z	205	ILE	2.3
1	A	300	ARG	2.3
1	A	500	TRP	2.3
1	Z	141	VAL	2.3
1	Z	298	VAL	2.3
1	Z	94	ILE	2.2
1	A	507	ARG	2.2
1	A	167	TYR	2.2
1	A	567	GLU	2.2
1	A	149	ASN	2.2
1	Z	157	ASN	2.2
1	Z	25	ILE	2.2
1	A	322	ASP	2.2
1	A	615	ASP	2.2
1	A	540	PRO	2.2
1	A	509	GLY	2.2
1	Z	274	GLY	2.2
1	A	522	GLU	2.2
1	A	584	ASN	2.2
1	A	298	VAL	2.2
1	Z	486	PRO	2.2
1	Z	154	SER	2.2
1	A	632	LYS	2.2
1	Z	667	PHE	2.2
1	A	534	LEU	2.2
1	A	566	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	578	ARG	2.2
1	A	220	GLN	2.2
1	Z	235	ASN	2.2
1	Z	532	GLN	2.2
1	A	276	PHE	2.2
1	Z	616	TYR	2.2
1	Z	630	ALA	2.2
1	A	383	ILE	2.1
1	Z	636	ASN	2.1
1	Z	58	ASP	2.1
1	Z	209	ASP	2.1
1	A	100	GLY	2.1
1	A	670	GLY	2.1
1	Z	276	PHE	2.1
1	A	363	ASN	2.1
1	A	95	THR	2.1
1	A	541	LEU	2.1
1	Z	391	LEU	2.1
1	Z	592	LEU	2.1
1	A	306	ALA	2.1
1	A	454	SER	2.1
1	A	673	HIS	2.1
1	Z	295	ASN	2.1
1	A	609	ASP	2.1
1	Z	69	ASP	2.1
1	Z	125	GLY	2.1
1	Z	152	ASP	2.1
1	Z	268	THR	2.1
1	Z	71	TRP	2.1
1	A	418	SER	2.1
1	A	664	SER	2.1
1	A	496	PRO	2.1
1	Z	646	PRO	2.1
1	A	26	ASN	2.1
1	Z	410	ASN	2.1
1	A	419	LEU	2.1
1	Z	300	ARG	2.1
1	A	638	GLN	2.0
1	Z	488	CYS	2.0
1	Z	510	HIS	2.0
1	A	410	ASN	2.0
1	A	460	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	523	ASN	2.0
1	A	552	ASN	2.0
1	A	628	LEU	2.0
1	Z	251	ASN	2.0
1	Z	294	PHE	2.0
1	Z	524	GLY	2.0
3	U	13	DC	2.0
1	A	612	THR	2.0
1	A	623	THR	2.0
1	A	579	LYS	2.0
1	A	151	SER	2.0
1	A	350	VAL	2.0
1	A	591	SER	2.0
1	A	655	VAL	2.0
1	Z	415	SER	2.0
1	A	556	PRO	2.0
1	Z	230	LEU	2.0
1	A	233	ASN	2.0
1	A	589	ASN	2.0
1	Z	633	ASN	2.0
1	A	260	ILE	2.0
1	Z	423	ILE	2.0
1	A	511	GLU	2.0
1	Z	256	GLU	2.0
1	A	169	TYR	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 ⓘ

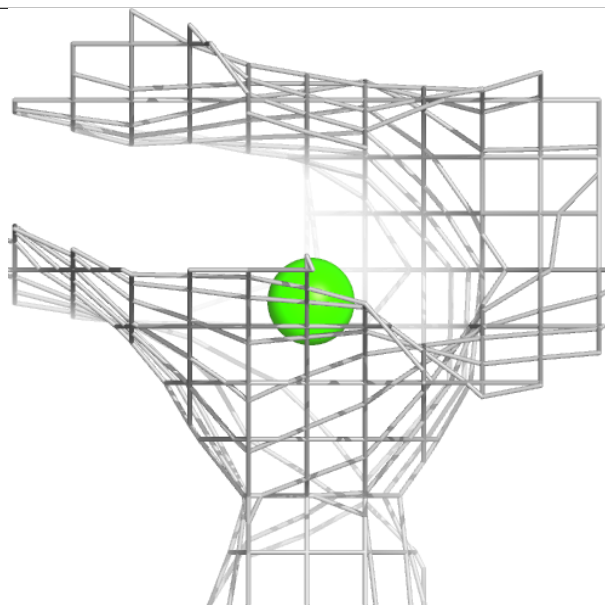
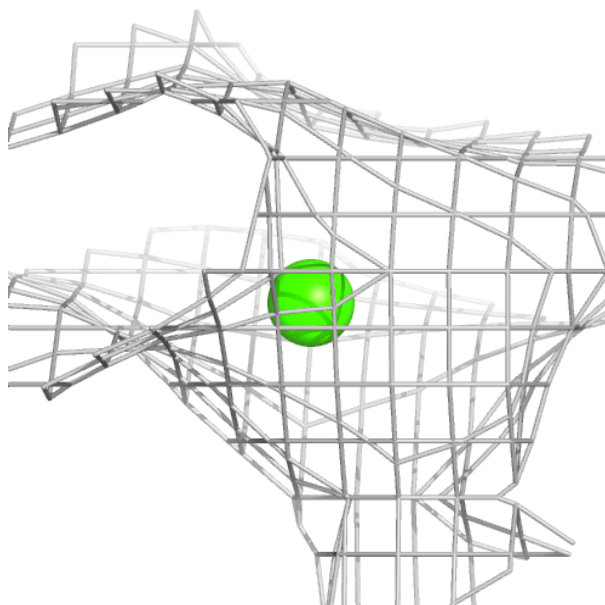
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	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.

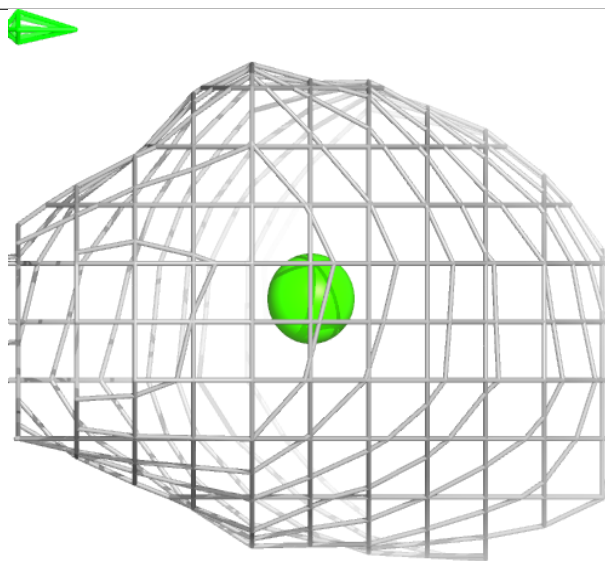
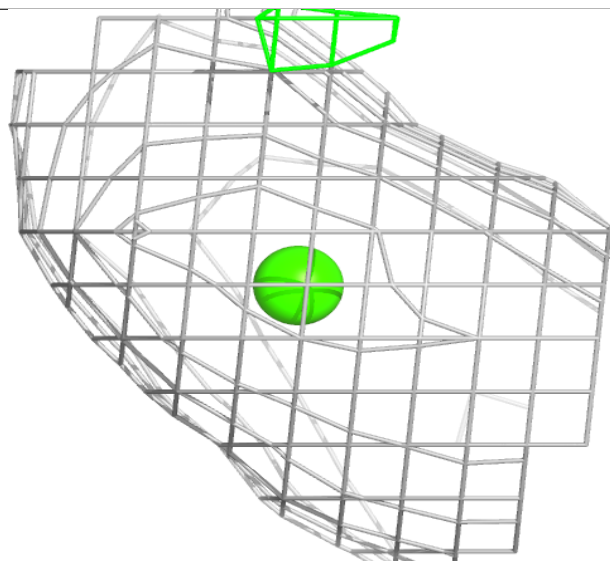
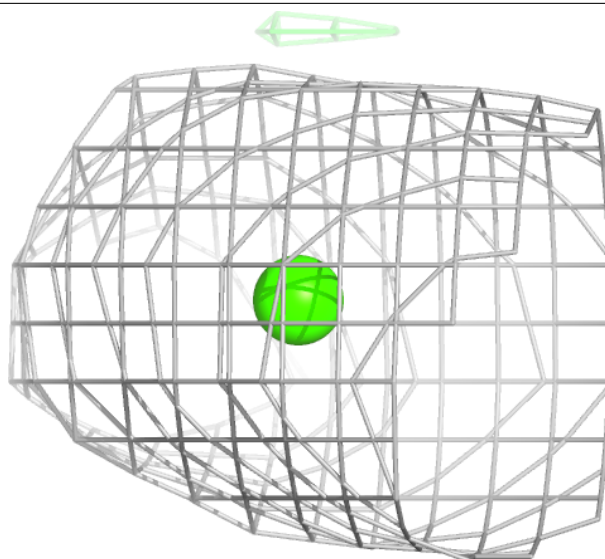
Electron density around CA Z 703:

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



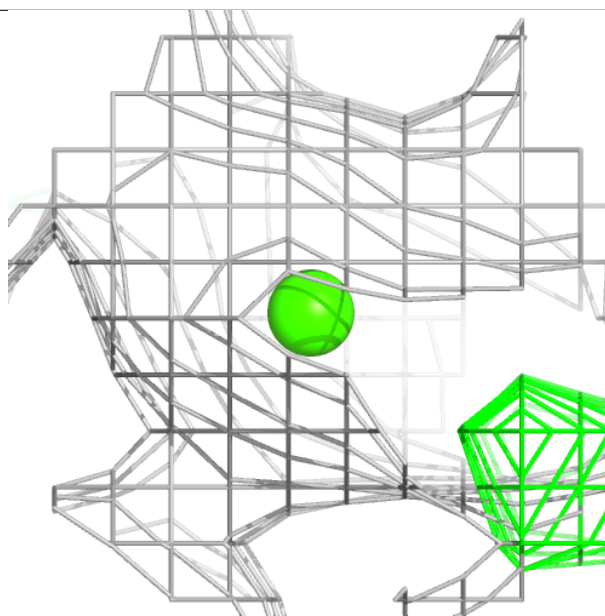
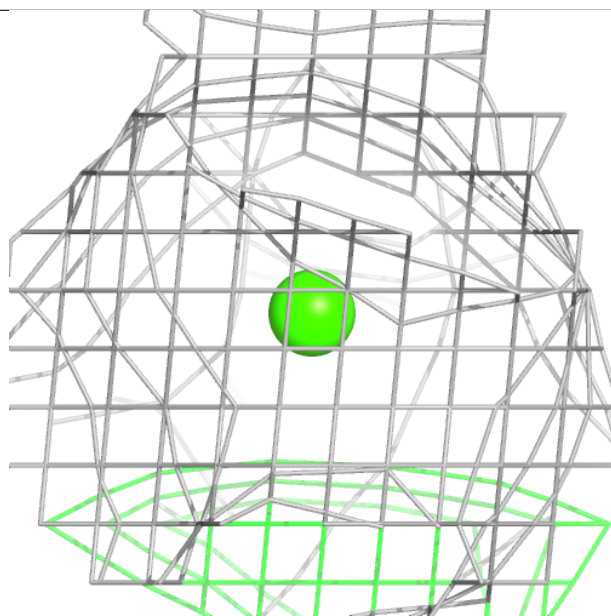
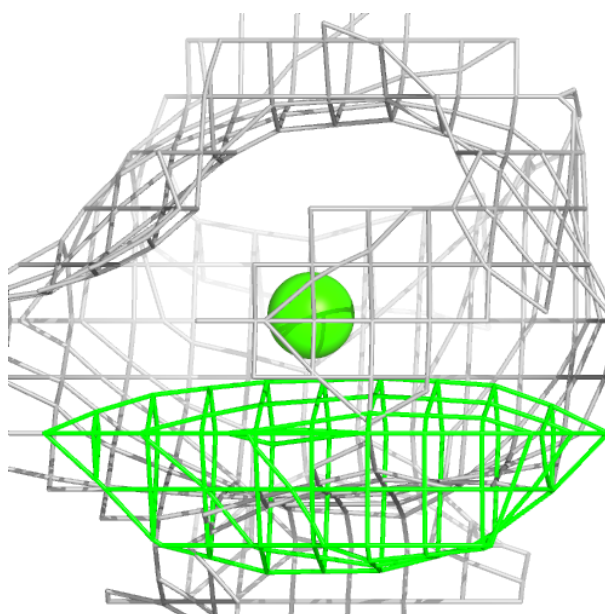
Electron density around CA A 703:

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



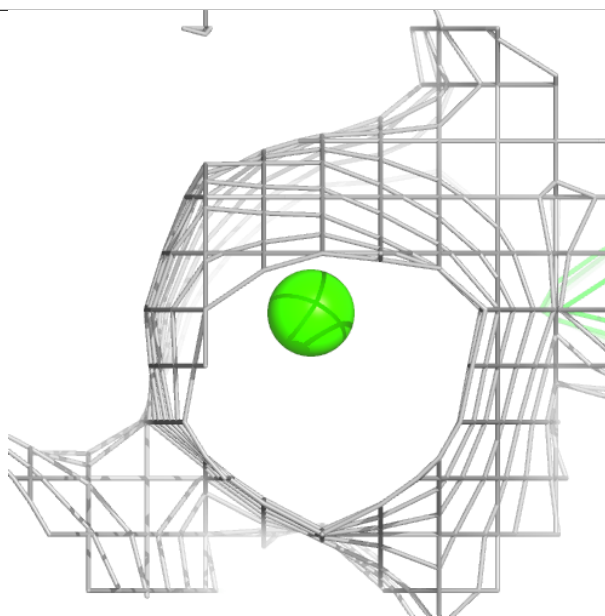
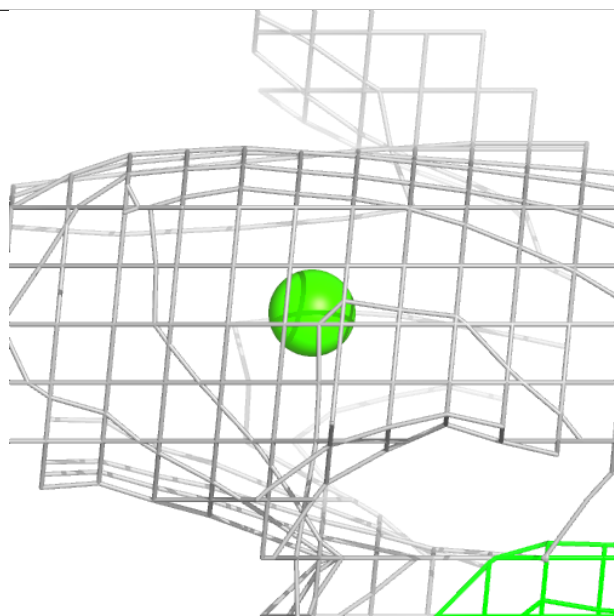
Electron density around CA Z 702:

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



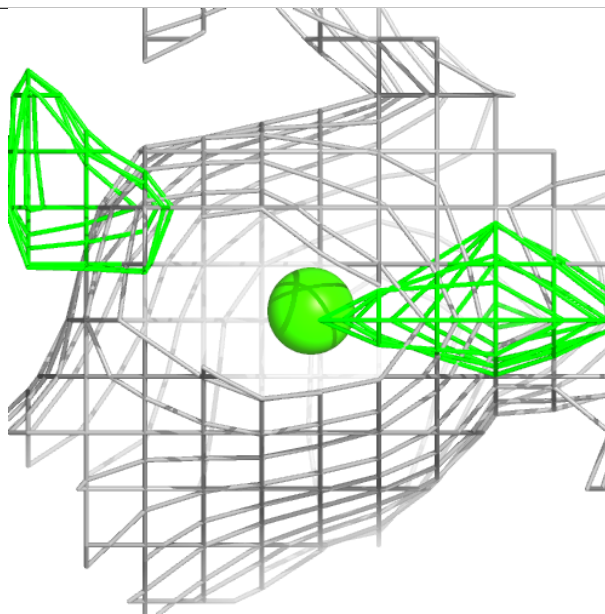
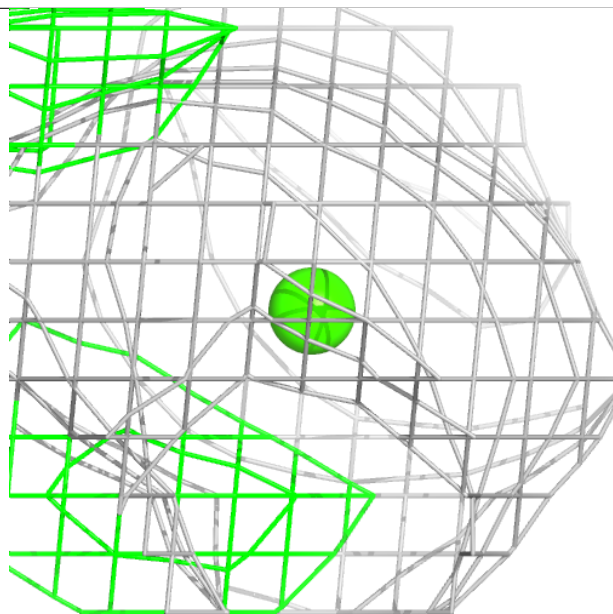
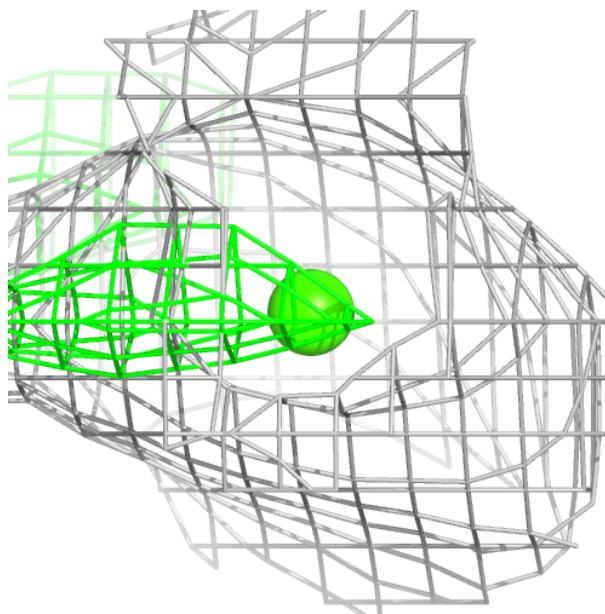
Electron density around CA A 702:

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



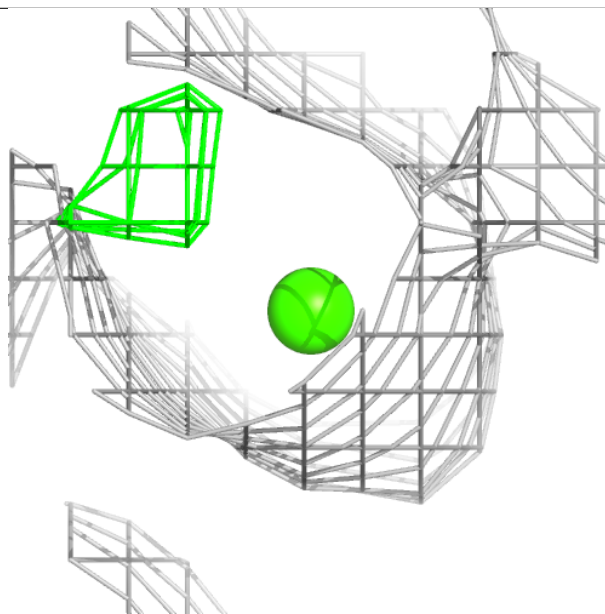
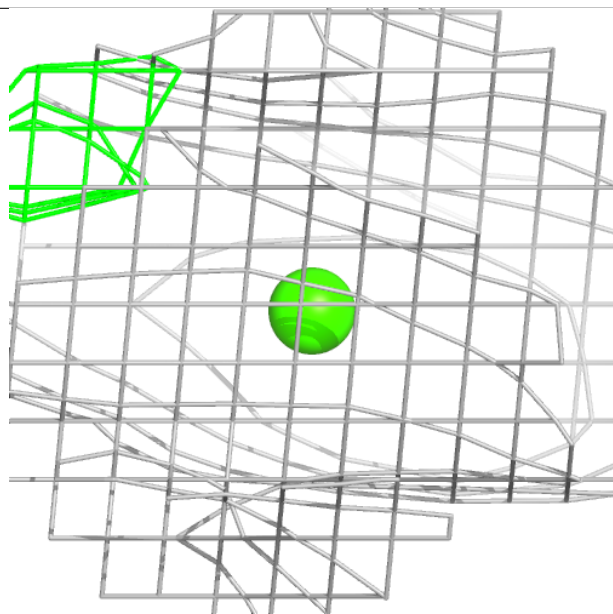
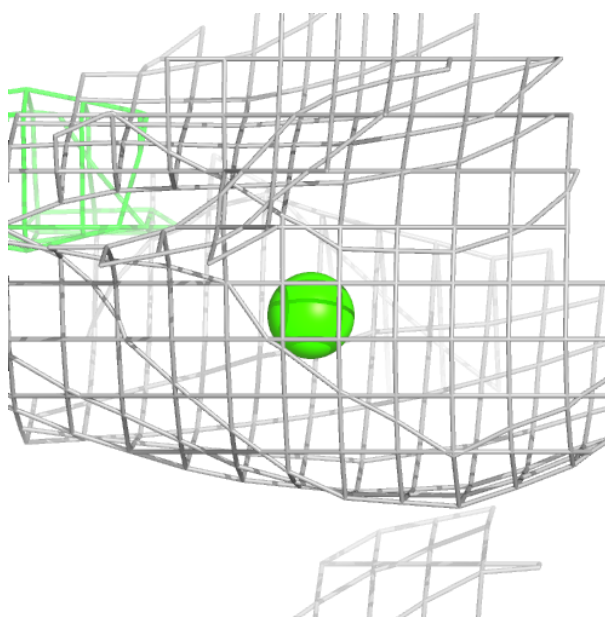
Electron density around CA A 701:

$2mF_o-DF_c$ (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 ⓘ

There are no such residues in this entry.