



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:56 AM UTC

PDB ID : 8XRF / pdb_00008xrf
Title : The crystal structure of AsfvTopII in complex with G-DNA
Authors : Yang, J.; Gan, J.H.
Deposited on : 2024-01-07
Resolution : 2.94 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

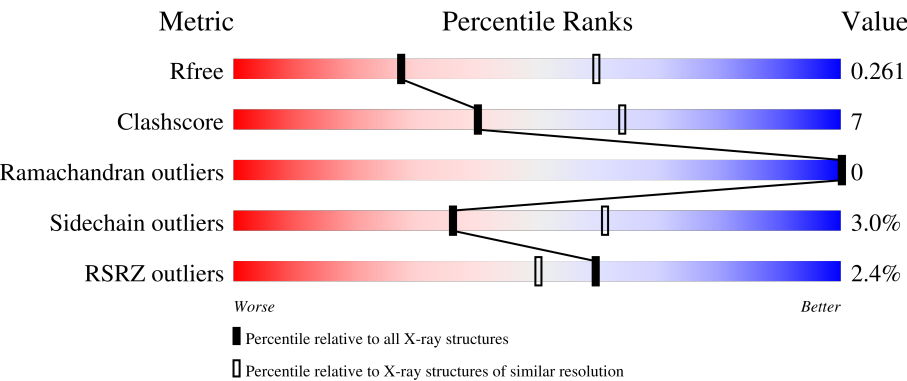
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.94 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	784	
1	B	784	
2	C	52	
2	D	52	
2	E	52	

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Mol	Chain	Length	Quality of chain
2	F	52	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: green (12%), yellow (17%), and grey (71%). The percentages are labeled below the corresponding segments.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13390 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 DNA topoisomerase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	773	Total	C	N	O	S	0	0	0
			6126	3942	1045	1112	27			
1	B	774	Total	C	N	O	S	0	0	0
			6218	3994	1072	1124	28			

- Molecule 2 is a DNA chain called DNA (52-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	P	0	0	0
			205	99	39	58	9			
2	D	15	Total	C	N	O	P	0	0	0
			314	147	63	89	15			
2	E	11	Total	C	N	O	P	0	0	0
			216	105	36	65	10			
2	F	15	Total	C	N	O	P	0	0	0
			303	144	54	90	15			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is water.

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

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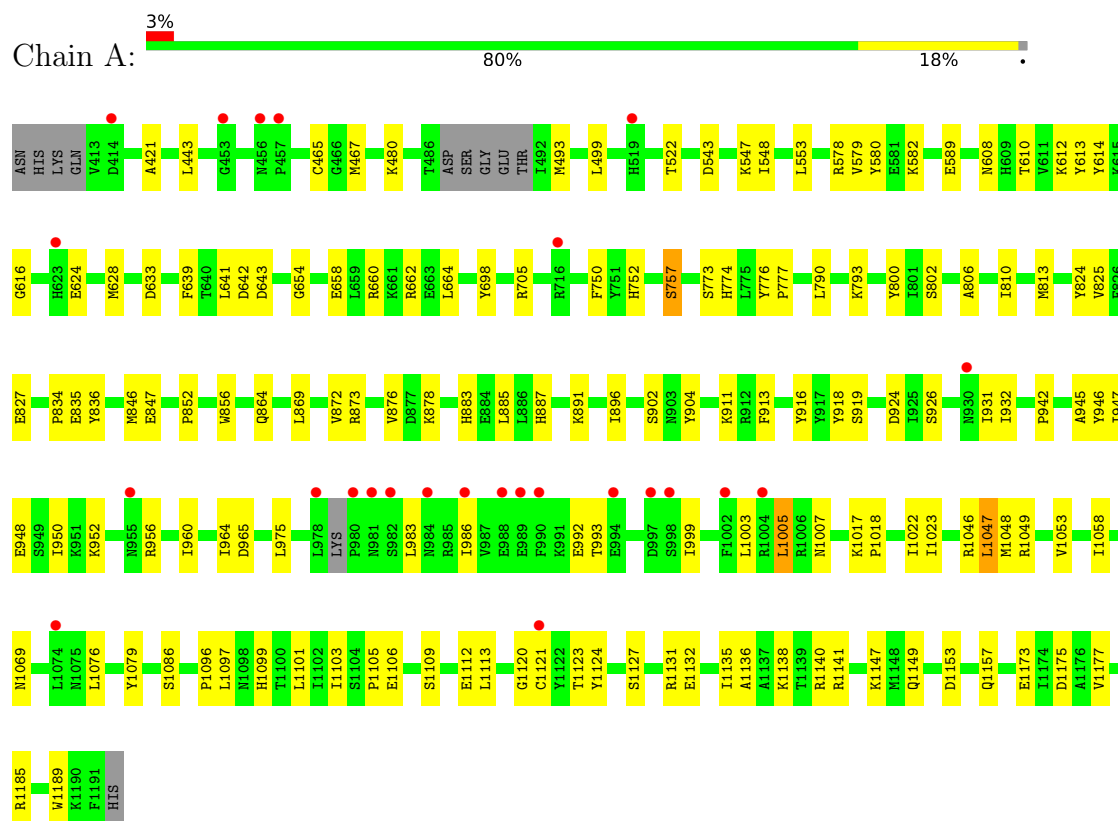
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	O	0	0
			1	1		
4	E	1	Total	O	0	0
			1	1		

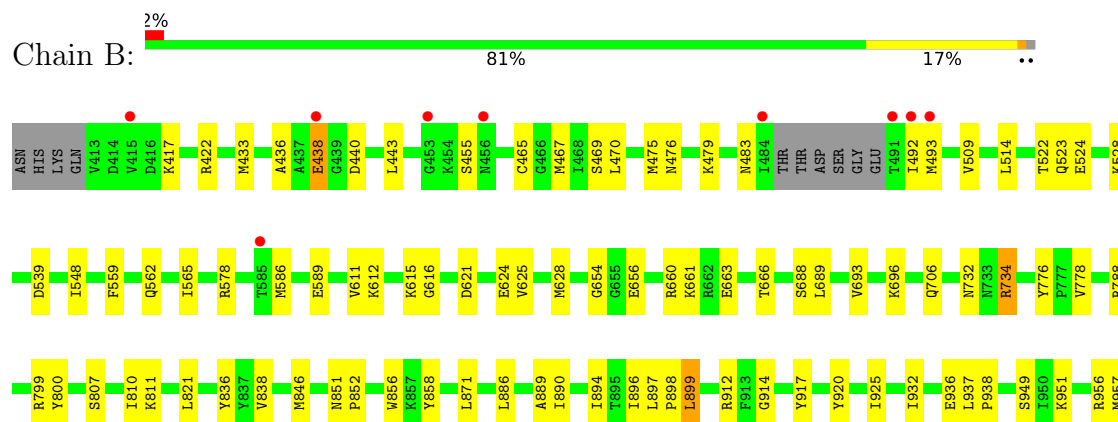
3 Residue-property plots

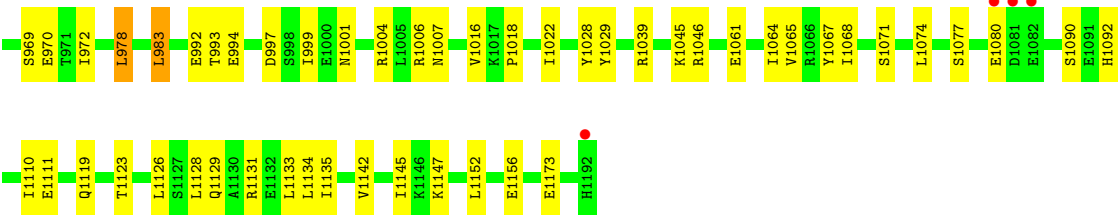
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DNA topoisomerase 2

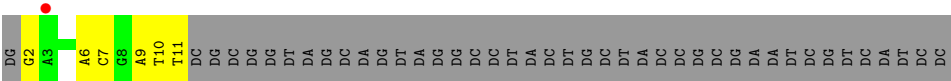


• Molecule 1: DNA topoisomerase 2

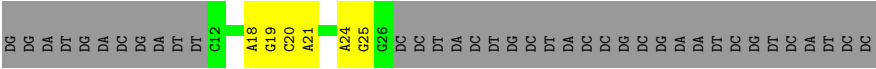




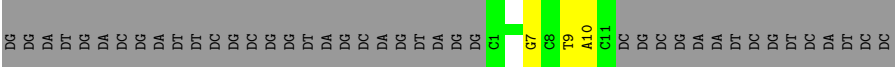
• Molecule 2: DNA (52-MER)



• Molecule 2: DNA (52-MER)



• Molecule 2: DNA (52-MER)



• Molecule 2: DNA (52-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	135.77Å 126.41Å 135.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.86 – 2.94 31.86 – 2.94	Depositor EDS
% Data completeness (in resolution range)	99.9 (31.86-2.94) 99.8 (31.86-2.94)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.95Å)	Xtriage
Refinement program	PHENIX (1.19.1_4122: ???)	Depositor
R, R_{free}	0.218 , 0.263 0.219 , 0.261	Depositor DCC
R_{free} test set	2417 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	68.7	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13390	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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: MG

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	0/6267	0.46	1/8486 (0.0%)
1	B	0.22	0/6363	0.47	7/8601 (0.1%)
2	C	0.31	0/230	0.60	0/354
2	D	0.22	0/353	0.46	0/544
2	E	0.20	0/240	0.43	0/367
2	F	0.24	0/338	0.48	0/518
All	All	0.22	0/13791	0.46	8/18870 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	914	GLY	CA-C-N	-7.30	109.33	123.13
1	B	914	GLY	C-N-CA	-7.30	109.33	123.13
1	B	455	SER	N-CA-C	-5.73	106.14	113.02
1	A	1121	CYS	N-CA-C	-5.03	106.71	114.16
1	B	611	VAL	CA-C-N	-5.03	114.95	122.39
1	B	611	VAL	C-N-CA	-5.03	114.95	122.39
1	B	612	LYS	CA-C-N	5.00	129.24	122.19
1	B	612	LYS	C-N-CA	5.00	129.24	122.19

There are no chirality outliers.

There are no planarity outliers.

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	6126	0	6021	92	0
1	B	6218	0	6169	77	0
2	C	205	0	115	6	0
2	D	314	0	168	5	0
2	E	216	0	126	2	0
2	F	303	0	169	7	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
All	All	13390	0	12768	169	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 7.

All (169) 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:946:TYR:HD2	1:A:947:ILE:HD13	1.45	0.81
1:B:1142:VAL:HA	1:B:1145:ILE:HD12	1.63	0.81
1:A:1132:GLU:HG3	1:A:1141:ARG:HH21	1.49	0.77
2:D:24:DA:H2"	2:D:25:DG:C8	2.24	0.73
1:A:480:LYS:HB2	1:A:499:LEU:HD12	1.76	0.68
1:B:1068:ILE:HD13	1:B:1133:LEU:HD23	1.77	0.65
1:A:904:TYR:CZ	1:A:1185:ARG:HG2	2.32	0.65
1:B:624:GLU:O	1:B:628:MET:HG3	1.98	0.64
1:A:774:HIS:HA	1:A:847:GLU:HG2	1.80	0.64
1:A:1135:ILE:HG12	1:B:1080:GLU:HA	1.80	0.63
1:B:920:TYR:CE2	1:B:1006:ARG:HG3	2.34	0.63
1:A:946:TYR:CD2	1:A:947:ILE:HD13	2.30	0.62
1:A:885:LEU:HD21	1:A:896:ILE:HD13	1.79	0.62
1:B:689:LEU:O	1:B:693:VAL:HG22	2.00	0.62
1:A:1123:THR:HG23	1:B:1131:ARG:HH22	1.65	0.61
1:B:479:LYS:HE2	1:B:654:GLY:O	2.00	0.61
1:A:1076:LEU:HD22	1:B:1134:LEU:HD21	1.81	0.61
1:A:1049:ARG:O	1:A:1053:VAL:HG23	2.01	0.61
1:B:886:LEU:O	1:B:890:ILE:HD12	2.00	0.61
1:A:964:ILE:HG22	1:A:975:LEU:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:21:DT:H2'	2:F:22:DC:C6	2.36	0.61
1:A:612:LYS:HG2	1:A:614:TYR:CZ	2.36	0.60
1:A:1099:HIS:O	1:A:1103:ILE:HD12	2.01	0.59
1:B:578:ARG:HG2	1:B:589:GLU:HG2	1.84	0.59
1:A:1017:LYS:HG2	1:A:1018:PRO:HD2	1.85	0.58
1:B:932:ILE:HG13	1:B:978:LEU:HD21	1.86	0.58
1:B:654:GLY:O	1:B:660:ARG:NH2	2.38	0.57
1:A:654:GLY:O	1:A:660:ARG:NH2	2.38	0.57
1:B:1061:GLU:O	1:B:1065:VAL:HG23	2.05	0.57
1:B:661:LYS:NZ	2:D:21:DA:OP1	2.38	0.56
1:A:443:LEU:HD22	1:A:467:MET:HB3	1.88	0.56
2:C:2:DG:H1	2:F:25:DC:H42	1.53	0.56
1:B:899:LEU:HD13	1:B:1028:TYR:HB2	1.87	0.56
1:B:493:MET:HE3	1:B:559:PHE:HD1	1.71	0.55
1:A:878:LYS:HA	1:A:883:HIS:CG	2.42	0.55
1:A:543:ASP:OD1	1:A:705:ARG:NH2	2.40	0.54
1:A:777:PRO:HG2	1:A:1189:TRP:CD1	2.42	0.54
1:A:948:GLU:HG3	1:A:952:LYS:HE3	1.90	0.54
1:A:641:LEU:HD23	1:A:642:ASP:N	2.23	0.54
1:A:1053:VAL:HG22	1:A:1113:LEU:HD11	1.88	0.54
1:A:965:ASP:O	1:B:422:ARG:NH2	2.41	0.53
1:A:1153:ASP:O	1:A:1157:GLN:HG3	2.08	0.53
1:A:1049:ARG:NH2	1:A:1106:GLU:O	2.41	0.53
1:B:621:ASP:O	1:B:625:VAL:HG23	2.08	0.52
1:A:800:TYR:CE1	1:B:616:GLY:HA3	2.45	0.52
1:B:788:ARG:NH2	1:B:936:GLU:OE1	2.41	0.52
1:A:887:HIS:O	1:A:891:LYS:HG3	2.10	0.52
1:B:443:LEU:HD22	1:B:467:MET:HB3	1.91	0.52
1:B:838:VAL:HG12	1:B:1039:ARG:HD2	1.91	0.52
1:B:949:SER:O	1:B:1004:ARG:NH2	2.43	0.52
1:A:547:LYS:HD2	1:A:698:TYR:CZ	2.45	0.52
1:A:856:TRP:CH2	1:A:1022:ILE:HG21	2.45	0.52
1:B:475:MET:HG3	2:D:18:DA:OP1	2.10	0.52
1:A:1131:ARG:HH12	1:B:1123:THR:HG23	1.75	0.52
2:C:6:DA:N6	2:F:20:DG:C6	2.78	0.51
1:B:851:ASN:OD1	1:B:858:TYR:HD2	1.93	0.51
1:B:889:ALA:HB1	1:B:894:ILE:O	2.10	0.51
1:A:916:TYR:HB2	1:A:918:TYR:CZ	2.46	0.51
1:A:956:ARG:O	1:A:960:ILE:HD12	2.09	0.51
1:B:663:GLU:HG3	1:B:696:LYS:HE2	1.91	0.50
1:B:524:GLU:O	1:B:528:LYS:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:732:ASN:C	1:B:734:ARG:H	2.18	0.50
1:A:913:PHE:HB2	1:A:918:TYR:HE2	1.76	0.50
1:A:1069:ASN:OD1	1:A:1138:LYS:NZ	2.44	0.50
1:B:539:ASP:OD2	1:B:616:GLY:HA2	2.10	0.50
1:A:885:LEU:CD2	1:A:896:ILE:HD13	2.40	0.50
1:A:1136:ALA:O	1:A:1140:ARG:HG3	2.11	0.50
1:A:1058:ILE:HD13	1:A:1149:GLN:HG2	1.92	0.50
1:A:1097:LEU:HD12	1:A:1124:TYR:CZ	2.47	0.50
1:A:836:TYR:CE2	1:A:1018:PRO:HB3	2.47	0.50
1:B:1110:ILE:H	1:B:1110:ILE:HD12	1.77	0.50
2:F:19:DC:H2''	2:F:20:DG:H5'	1.94	0.49
1:B:1119:GLN:HA	1:B:1119:GLN:OE1	2.12	0.49
1:B:856:TRP:CD2	1:B:1022:ILE:HD13	2.48	0.49
1:B:912:ARG:HG3	1:B:917:TYR:CZ	2.48	0.48
1:A:1003:LEU:HB2	1:A:1005:LEU:HD22	1.94	0.48
1:B:436:ALA:HB1	1:B:470:LEU:HD21	1.96	0.48
1:A:624:GLU:O	1:A:628:MET:HG3	2.14	0.48
1:A:806:ALA:O	1:A:810:ILE:HG12	2.14	0.48
1:A:932:ILE:HD13	1:A:999:ILE:HD11	1.96	0.48
1:B:937:LEU:HD13	1:B:972:ILE:HG21	1.95	0.48
1:A:869:LEU:O	1:A:873:ARG:HB2	2.13	0.48
1:A:1097:LEU:C	1:A:1120:GLY:HA2	2.38	0.48
1:B:925:ILE:HD11	1:B:999:ILE:HG13	1.95	0.48
1:B:992:GLU:HG3	1:B:997:ASP:HA	1.96	0.48
1:B:476:ASN:ND2	1:B:479:LYS:HE3	2.29	0.47
1:B:807:SER:O	1:B:811:LYS:HG3	2.15	0.47
1:B:1152:LEU:O	1:B:1156:GLU:HG3	2.13	0.47
1:A:1049:ARG:NH2	1:A:1105:PRO:HB2	2.30	0.47
1:B:417:LYS:NZ	1:B:440:ASP:OD2	2.47	0.47
1:A:757:SER:HB2	2:C:10:DT:C7	2.44	0.47
1:A:582:LYS:NZ	1:A:608:ASN:OD1	2.48	0.47
1:B:483:ASN:CG	1:B:493:MET:H	2.19	0.47
2:C:9:DA:H2''	2:C:10:DT:H5''	1.97	0.47
1:B:1046:ARG:NH2	1:B:1173:GLU:OE2	2.44	0.46
1:B:956:ARG:NH1	1:B:1001:ASN:O	2.49	0.46
1:B:1067:TYR:O	1:B:1071:SER:N	2.49	0.46
1:A:931:ILE:HD12	1:A:931:ILE:O	2.16	0.46
1:A:1046:ARG:NH2	1:A:1173:GLU:OE2	2.36	0.46
1:A:658:GLU:O	1:A:662:ARG:HG3	2.16	0.46
1:A:824:TYR:HA	1:A:834:PRO:HA	1.98	0.46
2:F:12:DC:H2'	2:F:13:DG:O4'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:LEU:HD21	1:A:639:PHE:CD2	2.51	0.46
1:A:983:LEU:HA	1:A:986:ILE:HD12	1.96	0.46
1:B:1065:VAL:HG21	1:B:1145:ILE:HD11	1.96	0.46
1:B:1111:GLU:H	1:B:1111:GLU:CD	2.24	0.46
1:B:852:PRO:HG2	2:D:19:DG:C2	2.51	0.45
1:A:813:MET:HE1	1:A:846:MET:HE1	1.98	0.45
1:A:1022:ILE:HG13	1:A:1023:ILE:N	2.32	0.45
1:A:543:ASP:O	1:A:548:ILE:HG13	2.17	0.45
1:A:926:SER:HB3	1:A:931:ILE:CD1	2.46	0.45
1:B:811:LYS:HB2	1:B:811:LYS:HE2	1.69	0.45
1:A:578:ARG:NH1	1:A:589:GLU:OE2	2.48	0.45
1:B:1064:ILE:HG23	1:B:1128:LEU:HD11	1.98	0.45
1:B:776:TYR:HE2	1:B:846:MET:HB3	1.82	0.45
1:A:421:ALA:HB2	1:A:465:CYS:C	2.41	0.45
1:A:493:MET:HE3	1:A:493:MET:HB2	1.74	0.45
1:A:543:ASP:HB3	2:C:11:DT:H4'	1.97	0.45
1:A:885:LEU:HD23	1:A:885:LEU:C	2.42	0.45
1:A:1047:LEU:HD12	1:A:1047:LEU:HA	1.76	0.45
2:D:19:DG:H2''	2:D:20:DC:H5'	1.98	0.45
1:A:1096:PRO:HB2	1:A:1120:GLY:HA3	1.99	0.45
2:F:15:DG:H2'	2:F:16:DA:C8	2.52	0.45
1:A:1079:TYR:O	1:B:1135:ILE:HD12	2.18	0.44
1:B:706:GLN:O	1:B:851:ASN:ND2	2.50	0.44
1:B:836:TYR:CE2	1:B:1018:PRO:HB3	2.53	0.44
1:B:852:PRO:HD3	2:E:7:DG:C2	2.52	0.44
1:B:951:LYS:HA	1:B:957:MET:SD	2.57	0.44
1:A:911:LYS:HD2	1:A:913:PHE:CZ	2.53	0.44
1:B:433:MET:HE2	1:B:465:CYS:SG	2.58	0.44
1:B:562:GLN:HA	1:B:565:ILE:HD12	2.00	0.44
1:B:615:LYS:HB2	1:B:615:LYS:NZ	2.32	0.43
1:B:438:GLU:CD	1:B:548:ILE:HD12	2.43	0.43
1:B:821:LEU:HB3	1:B:1045:LYS:HD3	2.00	0.43
1:B:983:LEU:HD12	1:B:983:LEU:HA	1.85	0.43
1:A:580:TYR:OH	1:A:624:GLU:OE2	2.35	0.43
1:B:856:TRP:CE3	1:B:1022:ILE:HD13	2.54	0.43
1:A:1173:GLU:O	1:A:1177:VAL:HG23	2.18	0.43
1:A:616:GLY:HA3	1:B:800:TYR:CE1	2.54	0.43
1:A:873:ARG:NH2	1:A:1175:ASP:OD1	2.50	0.43
1:A:613:TYR:CE1	1:A:752:HIS:HB3	2.54	0.43
1:A:1109:SER:OG	1:A:1112:GLU:HG3	2.19	0.43
1:B:509:VAL:HG13	1:B:514:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1147:LYS:HB3	1:B:1147:LYS:HE3	1.82	0.42
1:A:1127:SER:HB3	1:B:1131:ARG:NH1	2.34	0.42
1:A:790:LEU:O	1:A:793:LYS:HG3	2.19	0.42
1:A:750:PHE:HB2	1:A:827:GLU:HB2	2.02	0.42
1:B:938:PRO:HB3	1:B:1007:ASN:HB3	2.02	0.42
1:A:642:ASP:CG	1:A:643:ASP:N	2.79	0.41
1:A:793:LYS:HE2	2:C:7:DC:OP1	2.20	0.41
1:A:1147:LYS:HB2	1:A:1147:LYS:HE2	1.88	0.41
1:B:1074:LEU:HD11	1:B:1092:HIS:CE1	2.55	0.41
1:A:825:VAL:HG23	1:A:835:GLU:HG3	2.02	0.41
1:B:898:PRO:HA	1:B:1029:TYR:OH	2.20	0.41
1:A:942:PRO:HG2	1:A:945:ALA:HB3	2.01	0.41
1:B:778:VAL:HG13	1:B:810:ILE:HD11	2.01	0.41
1:A:1048:MET:HE2	1:A:1048:MET:HB2	1.83	0.41
1:A:1099:HIS:HB3	1:A:1124:TYR:HB3	2.03	0.41
1:B:1110:ILE:HD12	1:B:1110:ILE:N	2.35	0.41
1:A:547:LYS:HD2	1:A:698:TYR:CE2	2.56	0.41
1:A:919:SER:HB2	1:A:1007:ASN:HB3	2.02	0.41
1:A:1131:ARG:HG2	1:B:1126:LEU:HB3	2.03	0.41
1:A:872:VAL:O	1:A:876:VAL:HG23	2.21	0.41
1:A:852:PRO:HB3	2:F:20:DG:N3	2.36	0.40
2:E:9:DT:H2"	2:E:10:DA:H5"	2.03	0.40
1:A:864:GLN:HG3	1:A:902:SER:HA	2.04	0.40
1:A:1005:LEU:HD12	1:A:1005:LEU:HA	1.78	0.40
1:A:776:TYR:HE2	1:A:846:MET:HB3	1.85	0.40
1:B:896:ILE:HD12	1:B:897:LEU:HG	2.02	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	767/784 (98%)	739 (96%)	28 (4%)	0	100	100
1	B	770/784 (98%)	738 (96%)	32 (4%)	0	100	100
All	All	1537/1568 (98%)	1477 (96%)	60 (4%)	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	640/689 (93%)	624 (98%)	16 (2%)	42	66
1	B	660/689 (96%)	637 (96%)	23 (4%)	32	56
All	All	1300/1378 (94%)	1261 (97%)	39 (3%)	36	61

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	522	THR
1	A	579	VAL
1	A	610	THR
1	A	633	ASP
1	A	664	LEU
1	A	757	SER
1	A	773	SER
1	A	802	SER
1	A	924	ASP
1	A	950	ILE
1	A	992	GLU
1	A	993	THR
1	A	1005	LEU
1	A	1047	LEU
1	A	1086	SER
1	A	1101	LEU
1	B	438	GLU
1	B	469	SER

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Mol	Chain	Res	Type
1	B	492	ILE
1	B	522	THR
1	B	523	GLN
1	B	586	MET
1	B	656	GLU
1	B	666	THR
1	B	688	SER
1	B	734	ARG
1	B	799	ARG
1	B	871	LEU
1	B	899	LEU
1	B	969	SER
1	B	970	GLU
1	B	978	LEU
1	B	983	LEU
1	B	993	THR
1	B	994	GLU
1	B	1016	VAL
1	B	1077	SER
1	B	1090	SER
1	B	1129	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	430	GLN
1	A	502	ASN
1	A	510	GLN
1	A	603	GLN
1	A	752	HIS
1	A	1014	ASN
1	A	1098	ASN
1	B	501	ASN
1	B	608	ASN
1	B	675	GLN
1	B	753	HIS
1	B	804	GLN
1	B	864	GLN
1	B	909	HIS

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 5 ligands modelled in this entry, 5 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(Å²)	Q<0.9
1	A	773/784 (98%)	0.25	25 (3%)	50	42	44, 76, 129, 163	0
1	B	774/784 (98%)	0.07	13 (1%)	69	61	38, 63, 105, 158	0
2	C	10/52 (19%)	0.97	1 (10%)	12	11	55, 82, 180, 192	0
2	D	15/52 (28%)	0.25	0	100	100	48, 56, 113, 124	0
2	E	11/52 (21%)	0.29	0	100	100	41, 51, 138, 140	0
2	F	15/52 (28%)	0.11	0	100	100	51, 68, 144, 156	0
All	All	1598/1776 (89%)	0.17	39 (2%)	59	50	38, 70, 121, 192	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	585	THR	4.7
1	A	986	ILE	4.4
1	A	998	SER	4.3
1	A	1002	PHE	3.9
1	A	978	LEU	3.7
1	B	1081	ASP	3.6
1	B	1080	GLU	3.6
1	A	1074	LEU	3.6
1	A	981	ASN	3.4
1	B	484	ILE	3.4
1	A	1121	CYS	3.2
1	A	955	ASN	3.1
1	B	453	GLY	3.0
1	A	930	ASN	3.0
1	A	989	GLU	3.0
1	B	491	THR	3.0
1	A	982	SER	2.9
1	A	456	ASN	2.9
1	B	1082	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	457	PRO	2.8
1	A	990	PHE	2.7
1	A	988	GLU	2.7
1	B	492	ILE	2.6
1	A	980	PRO	2.6
1	A	453	GLY	2.6
1	A	519	HIS	2.6
2	C	3	DA	2.5
1	B	438	GLU	2.4
1	A	994	GLU	2.3
1	A	716	ARG	2.3
1	A	997	ASP	2.2
1	B	493	MET	2.2
1	B	415	VAL	2.2
1	A	984	ASN	2.1
1	A	623	HIS	2.1
1	A	414	ASP	2.1
1	B	1192	HIS	2.0
1	A	1004	ARG	2.0
1	B	456	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	1202	1/1	0.91	0.17	49,49,49,49	0
3	MG	B	1201	1/1	0.93	0.14	56,56,56,56	0
3	MG	A	1201	1/1	0.94	0.15	66,66,66,66	0

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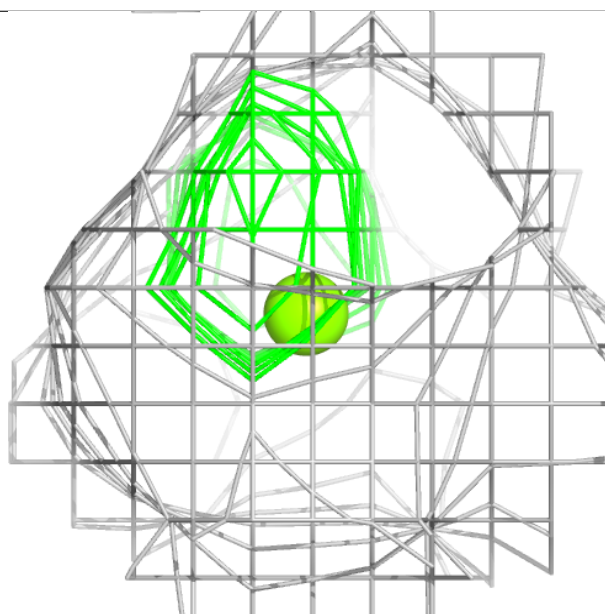
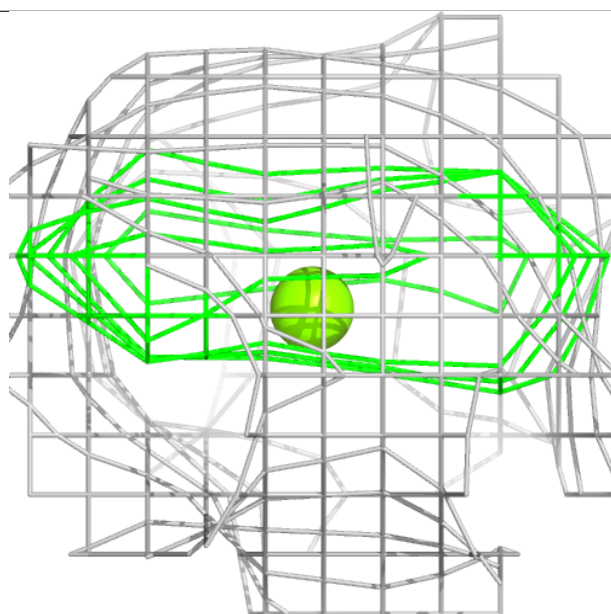
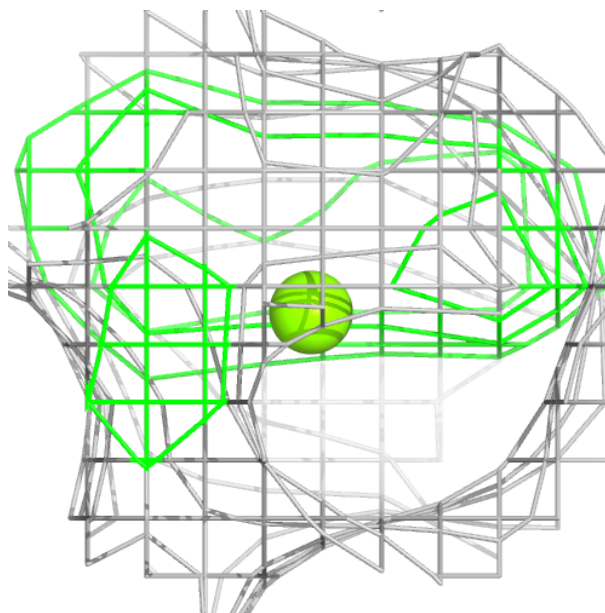
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	1203	1/1	0.98	0.09	77,77,77,77	0
3	MG	B	1202	1/1	0.98	0.13	53,53,53,53	0

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.

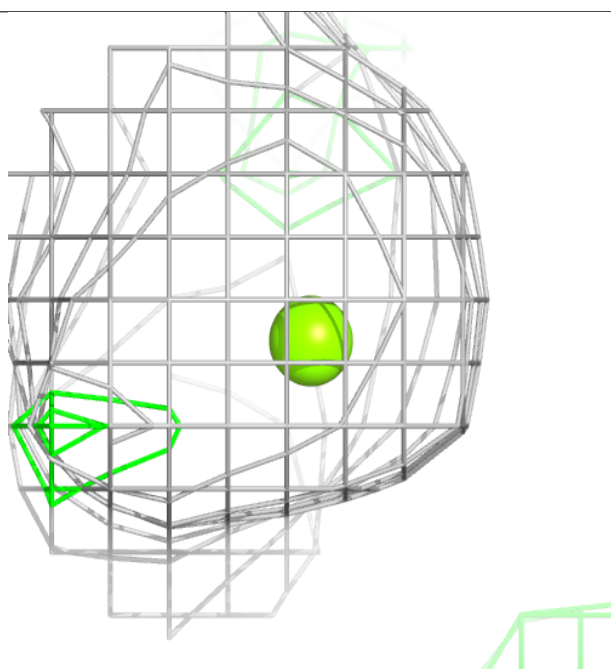
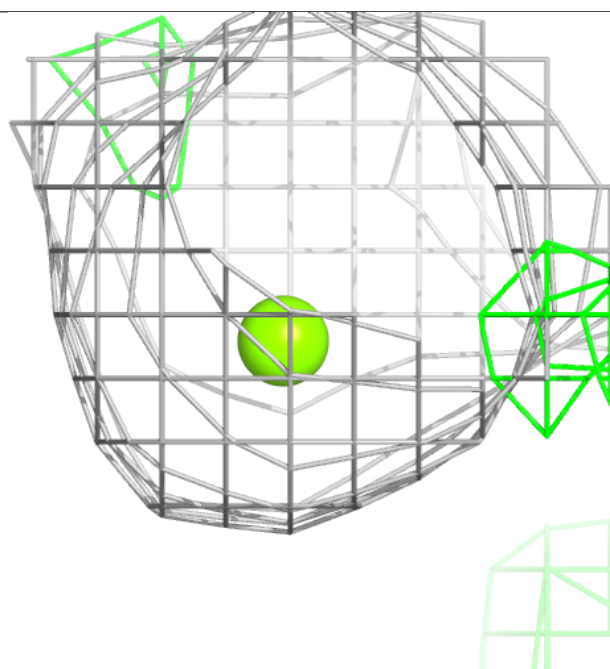
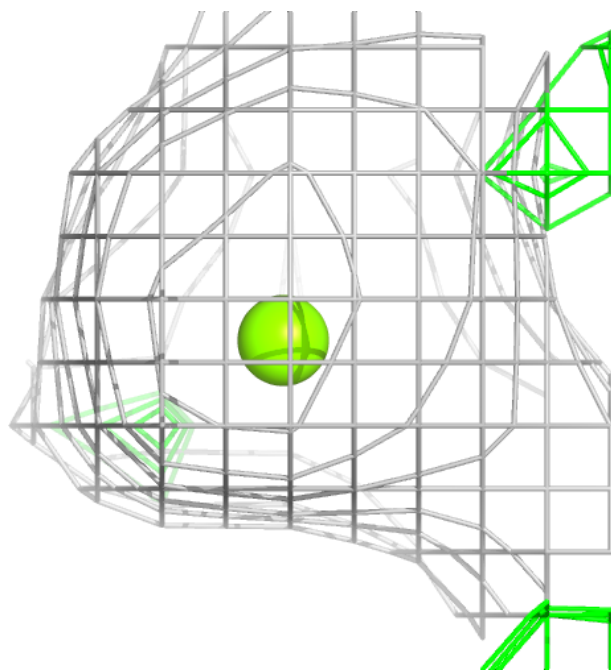
Electron density around MG A 1202:

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



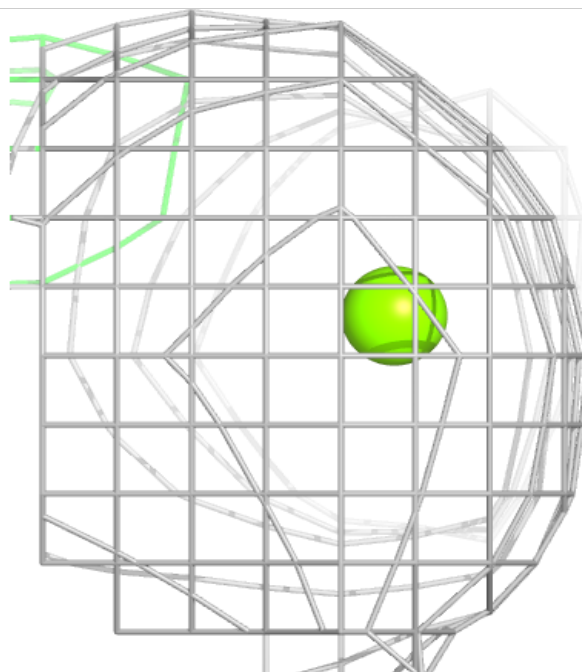
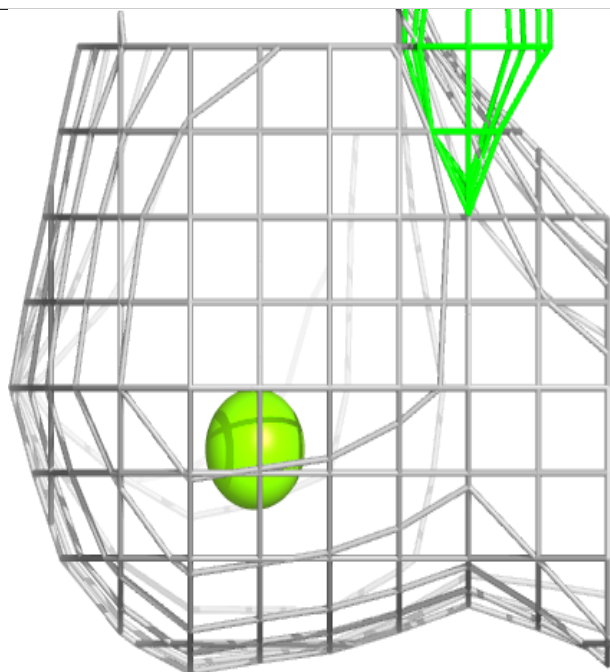
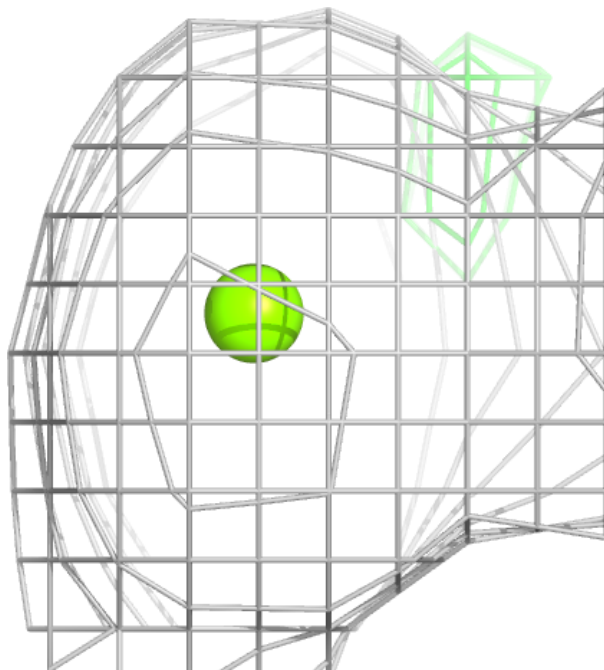
Electron density around MG B 1201:

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



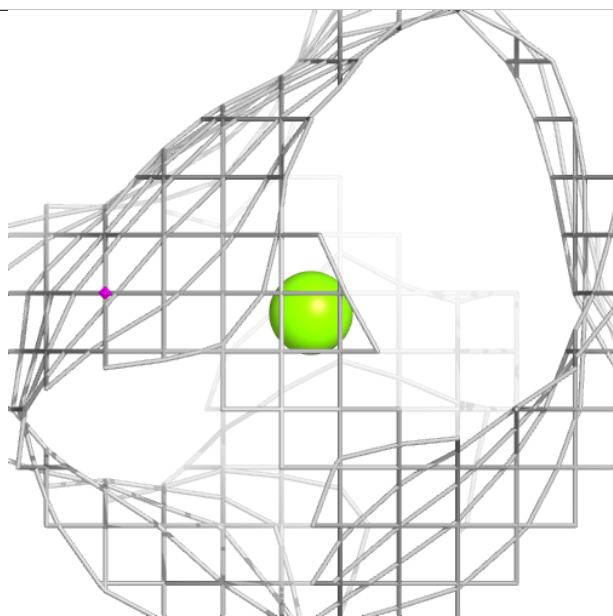
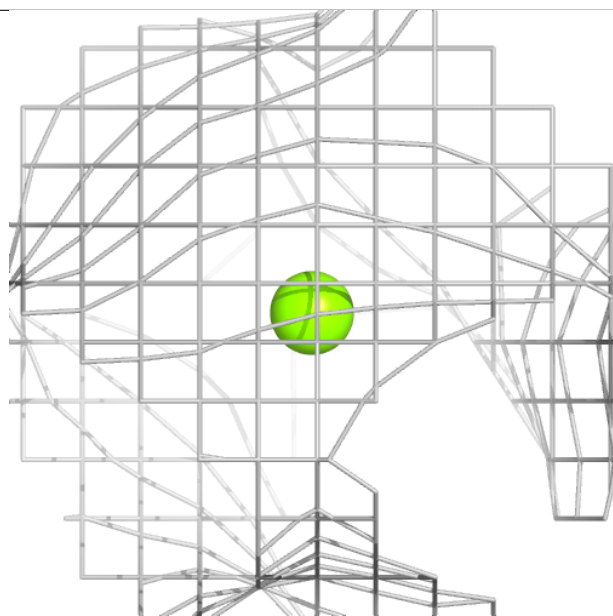
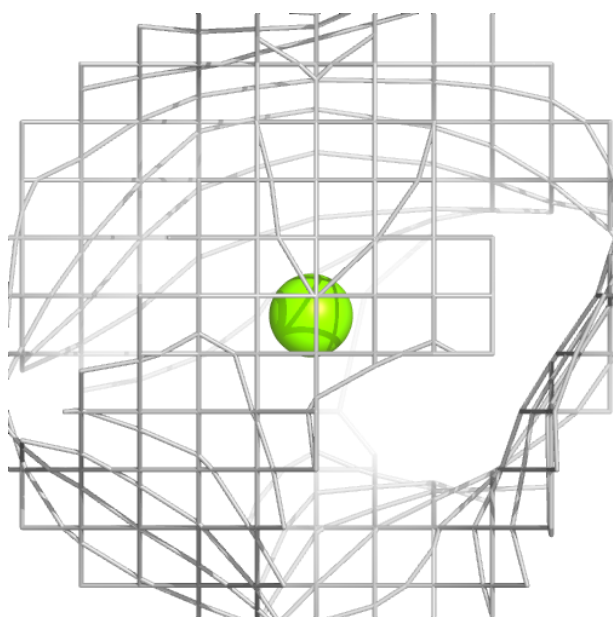
Electron density around MG A 1201:

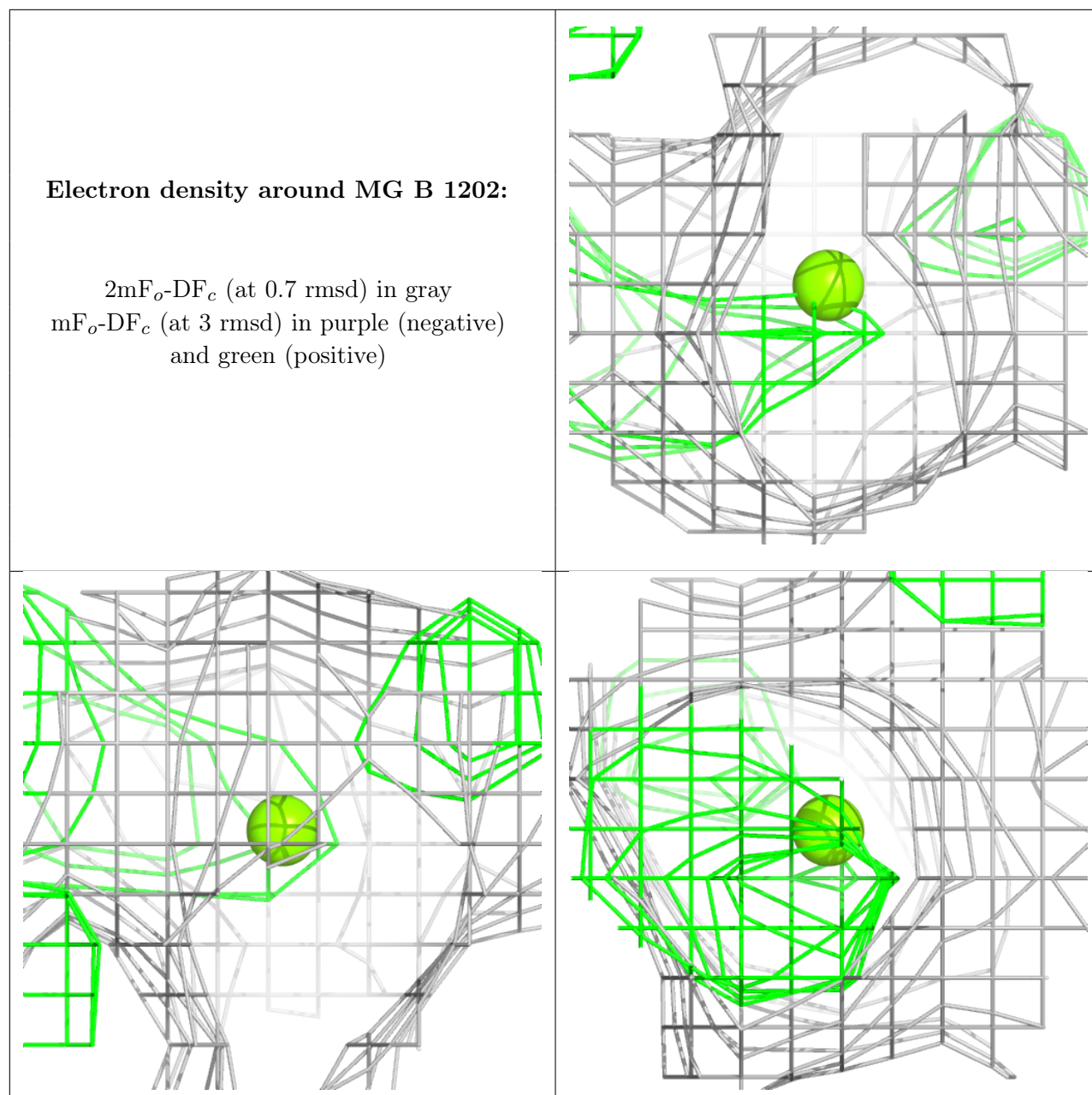
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG A 1203:

$2mF_o-DF_c$ (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.