Full wwPDB X-ray Structure Validation Report ⓘ

Jul 31, 2024 – 02:19 PM JST

PDB ID	:	8XRF
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:

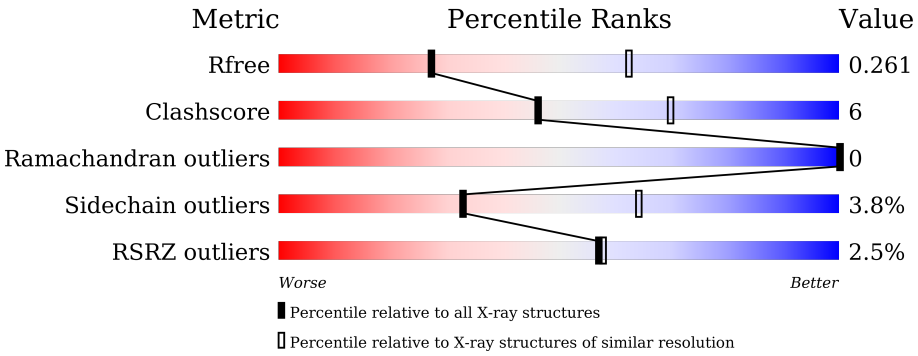
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.94 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}	130704	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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	784	2% 80% 18%
1	B	784	2% 82% 17%
2	C	52	6% 6% 13% 81%
2	D	52	4% 15% 13% 71%
2	E	52	8% 15% 6% 79%
2	F	52	12% 15% 71%

2 Entry composition (i)

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 (three-letter code: 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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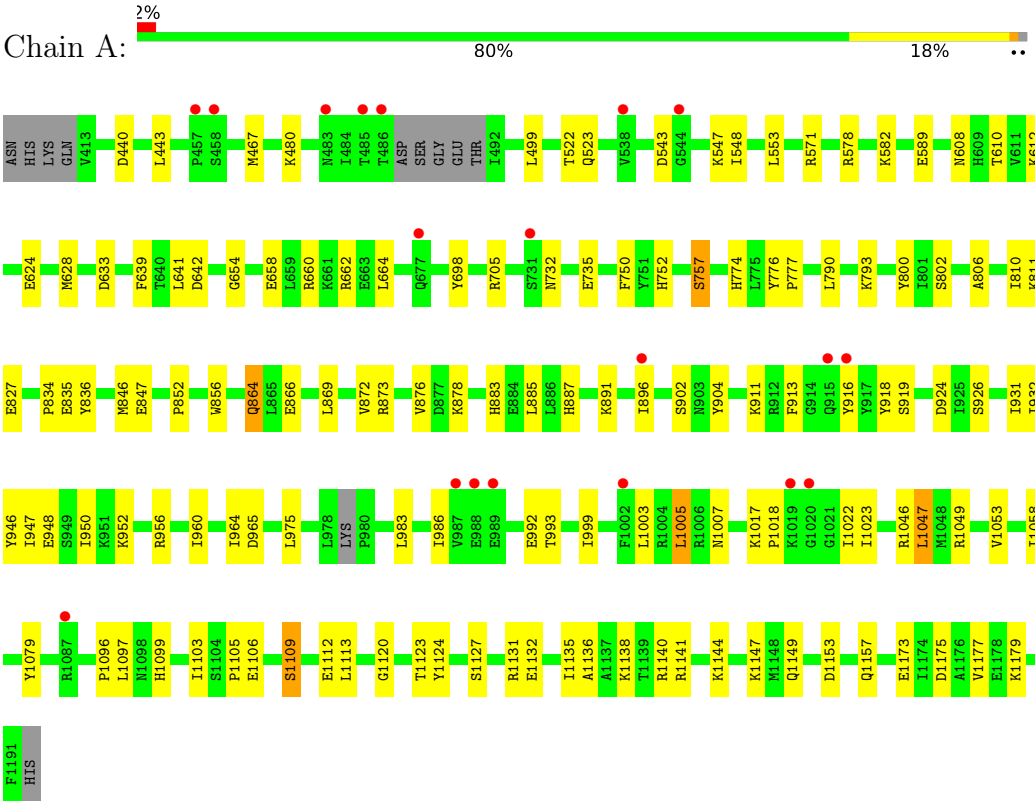
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total O 1 1	0	0
4	E	1	Total O 1 1	0	0

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.

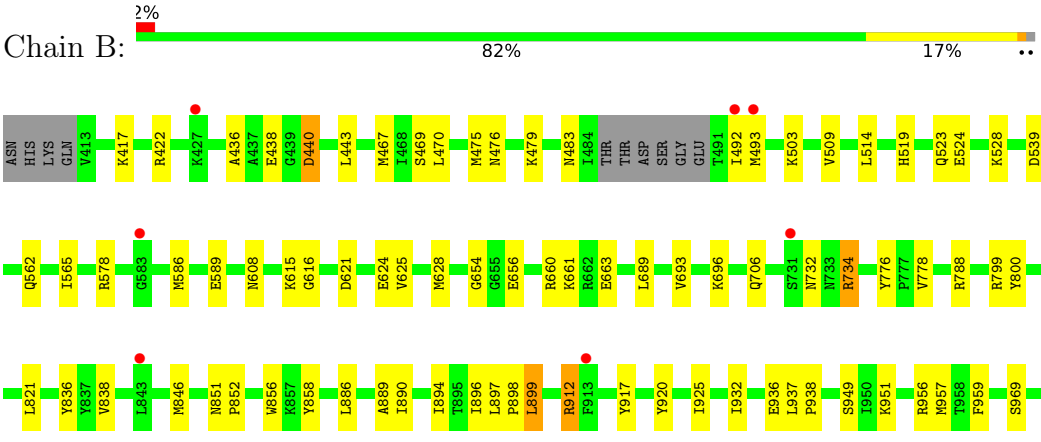
• Molecule 1: DNA topoisomerase 2

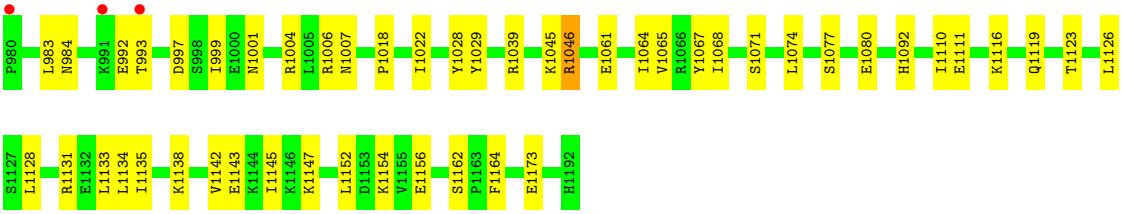
Chain A:



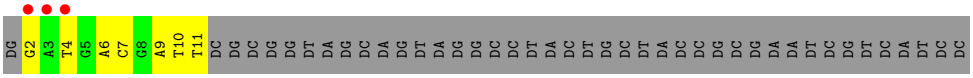
• Molecule 1: DNA topoisomerase 2

Chain B:

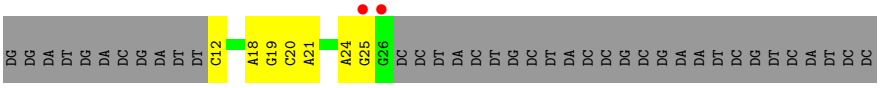




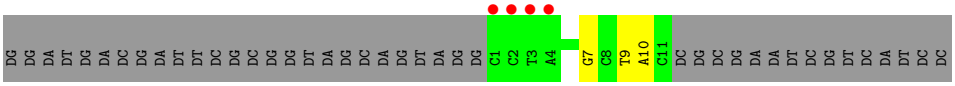
• Molecule 2: DNA (52-MER)



• Molecule 2: DNA (52-MER)



• Molecule 2: DNA (52-MER)



• Molecule 2: DNA (52-MER)

4 Data and refinement statistics (i)

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) 99.9 (31.86-2.94)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 2.95Å)	Xtriage
Refinement program	PHENIX (1.19.1_4122: ???)	Depositor
R, R_{free}	0.218 , 0.263 0.218 , 0.261	Depositor DCC
R_{free} test set	2416 reflections (4.81%)	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 , 47.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[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: 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	0.28	0/6267	0.53	0/8486
1	B	0.28	0/6363	0.53	0/8601
2	C	0.60	0/230	1.09	1/354 (0.3%)
2	D	0.57	0/353	0.95	1/544 (0.2%)
2	E	0.54	0/240	0.94	0/367
2	F	0.59	0/338	1.00	1/518 (0.2%)
All	All	0.32	0/13791	0.59	3/18870 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	12	DC	O4'-C4'-C3'	-7.97	101.22	106.00
2	D	12	DC	O4'-C4'-C3'	-5.83	102.17	104.50
2	C	4	DT	OP2-P-O3'	5.42	117.12	105.20

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	6126	0	6021	86	0
1	B	6218	0	6169	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	160	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 6.

All (160) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:443:LEU:HD22	1:A:467:MET:HB3	1.88	0.56
1:B:661:LYS:NZ	2:D:21:DA:OP1	2.38	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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:732:ASN:C	1:B:734:ARG:H	2.18	0.46
1:B:1065:VAL:HG21	1:B:1145:ILE:HD11	1.96	0.46
1:B:852:PRO:HG2	2:D:19:DG:C2	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:543:ASP:HB3	2:C:11:DT:H4'	1.97	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:A:1097:LEU:C	1:A:1120:GLY:HA2	2.38	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: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: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
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:B:483:ASN:CG	1:B:493:MET:H	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: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:1099:HIS:HB3	1:A:1124:TYR:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1111:GLU:H	1:B:1111:GLU:CD	2.24	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:885:LEU:C	1:A:885:LEU:HD23	2.42	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 (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	640/689 (93%)	616 (96%)	24 (4%)	33	64
1	B	660/689 (96%)	634 (96%)	26 (4%)	32	63
All	All	1300/1378 (94%)	1250 (96%)	50 (4%)	33	64

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	440	ASP
1	A	522	THR
1	A	523	GLN
1	A	571	ARG
1	A	610	THR
1	A	633	ASP
1	A	664	LEU
1	A	732	ASN
1	A	735	GLU
1	A	757	SER
1	A	802	SER
1	A	811	LYS
1	A	864	GLN
1	A	866	GLU
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	1109	SER
1	A	1144	LYS
1	A	1179	LYS
1	A	1189	TRP
1	B	438	GLU
1	B	440	ASP
1	B	469	SER
1	B	492	ILE
1	B	503	LYS
1	B	519	HIS
1	B	523	GLN
1	B	586	MET
1	B	608	ASN

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Mol	Chain	Res	Type
1	B	656	GLU
1	B	734	ARG
1	B	799	ARG
1	B	899	LEU
1	B	912	ARG
1	B	959	PHE
1	B	969	SER
1	B	984	ASN
1	B	993	THR
1	B	1046	ARG
1	B	1077	SER
1	B	1116	LYS
1	B	1138	LYS
1	B	1143	GLU
1	B	1154	LYS
1	B	1162	SER
1	B	1164	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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, 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	773/784 (98%)	-0.11	19 (2%) 57 58	44, 76, 129, 163	0
1	B	774/784 (98%)	-0.14	12 (1%) 72 73	38, 63, 105, 158	0
2	C	10/52 (19%)	1.43	3 (30%) 0 0	55, 82, 180, 192	0
2	D	15/52 (28%)	0.34	2 (13%) 3 2	48, 56, 113, 124	0
2	E	11/52 (21%)	0.89	4 (36%) 0 0	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%)	-0.10	40 (2%) 57 58	38, 70, 121, 192	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	3	DA	6.4
2	C	2	DG	4.5
1	A	457	PRO	3.9
2	E	2	DC	3.8
1	B	427	LYS	3.5
1	B	493	MET	3.2
1	B	583	GLY	3.1
1	A	988	GLU	2.9
1	B	492	ILE	2.9
1	A	987	VAL	2.8
1	A	731	SER	2.8
1	A	1002	PHE	2.8
2	E	1	DC	2.7
2	D	25	DG	2.7
2	E	4	DA	2.5
1	A	1087	ARG	2.5
1	A	989	GLU	2.5
1	A	915	GLN	2.4
2	C	4	DT	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	486	THR	2.4
1	B	731	SER	2.4
1	A	485	THR	2.3
2	D	26	DG	2.3
1	B	913	PHE	2.3
1	A	1019	LYS	2.3
1	A	916	TYR	2.3
1	A	458	SER	2.3
1	A	538	VAL	2.2
1	A	483	ASN	2.2
1	B	991	LYS	2.2
1	A	896	ILE	2.2
1	B	545	CYS	2.2
1	B	993	THR	2.1
1	A	544	GLY	2.1
1	B	550	GLY	2.1
1	B	843	LEU	2.1
2	E	3	DT	2.1
1	B	980	PRO	2.1
1	A	1020	GLY	2.0
1	A	677	GLN	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
3	MG	A	1203	1/1	0.88	0.25	77,77,77,77	0
3	MG	B	1202	1/1	0.91	0.34	53,53,53,53	0

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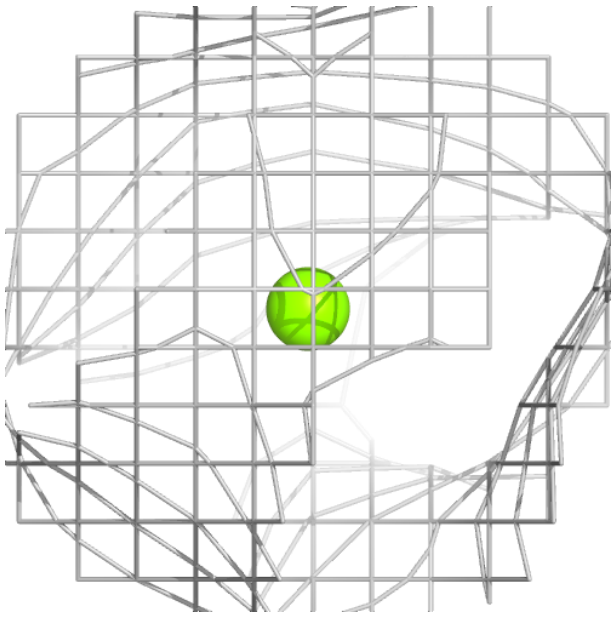
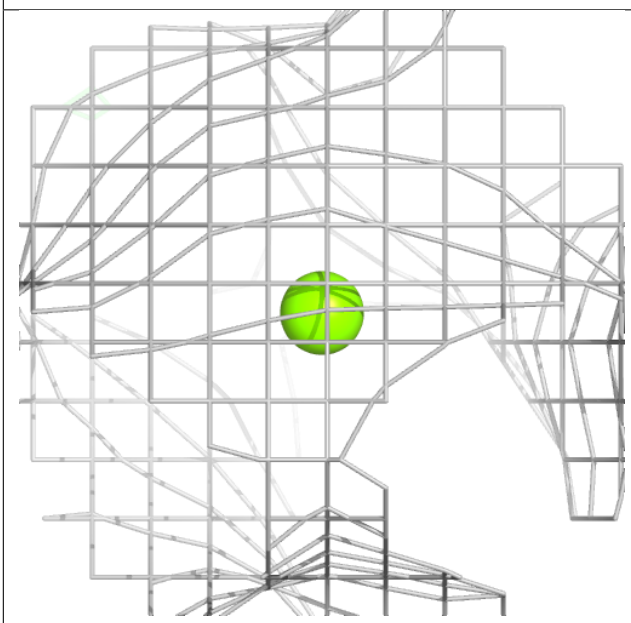
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	B	1201	1/1	0.92	0.24	56,56,56,56	0
3	MG	A	1202	1/1	0.92	0.40	49,49,49,49	0
3	MG	A	1201	1/1	0.94	0.22	66,66,66,66	0

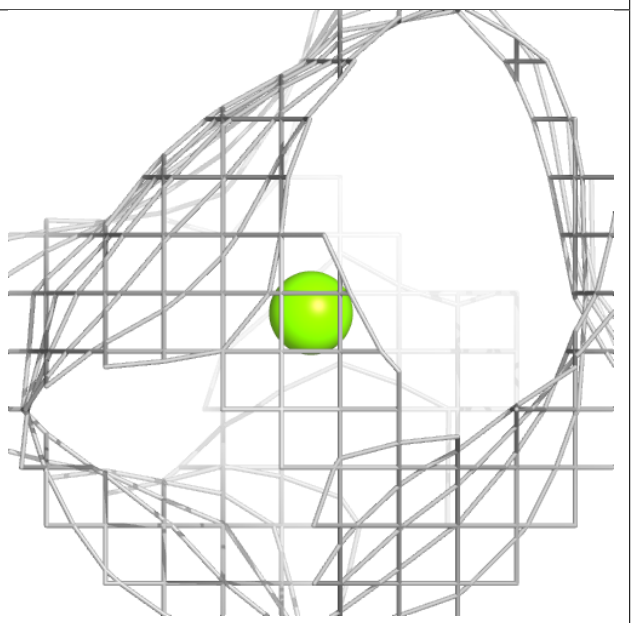
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MG A 1203:

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

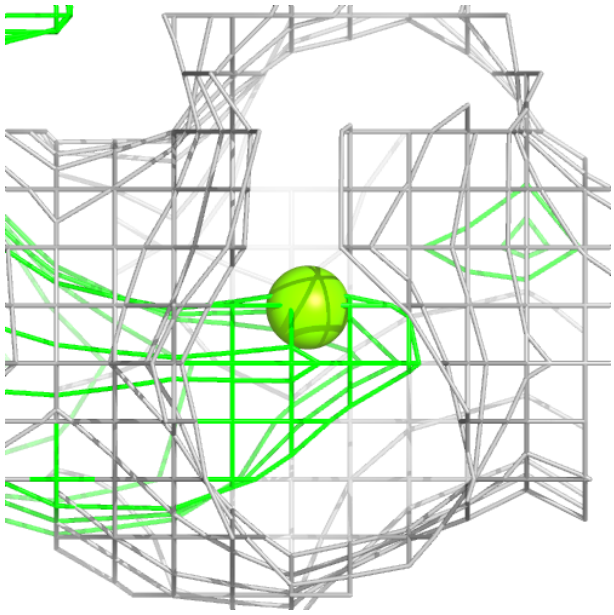


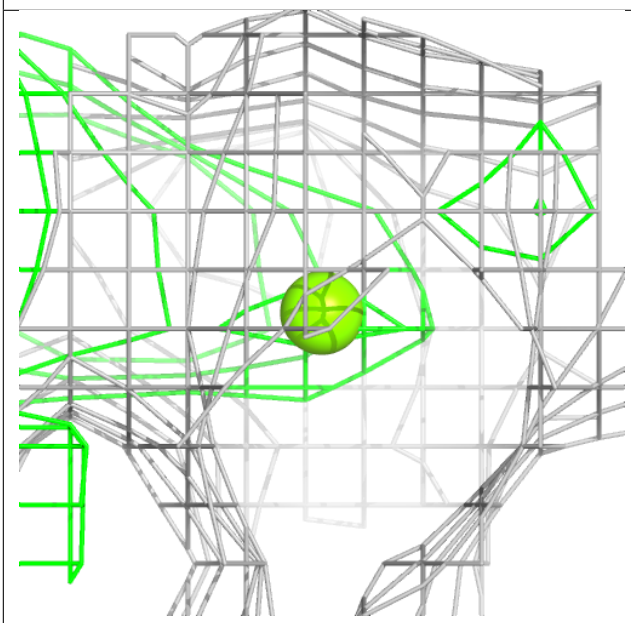


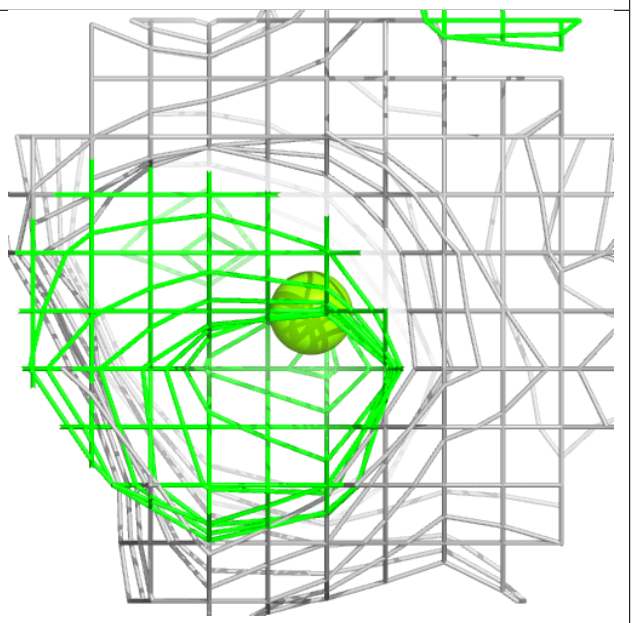


Electron density around MG B 1202:

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

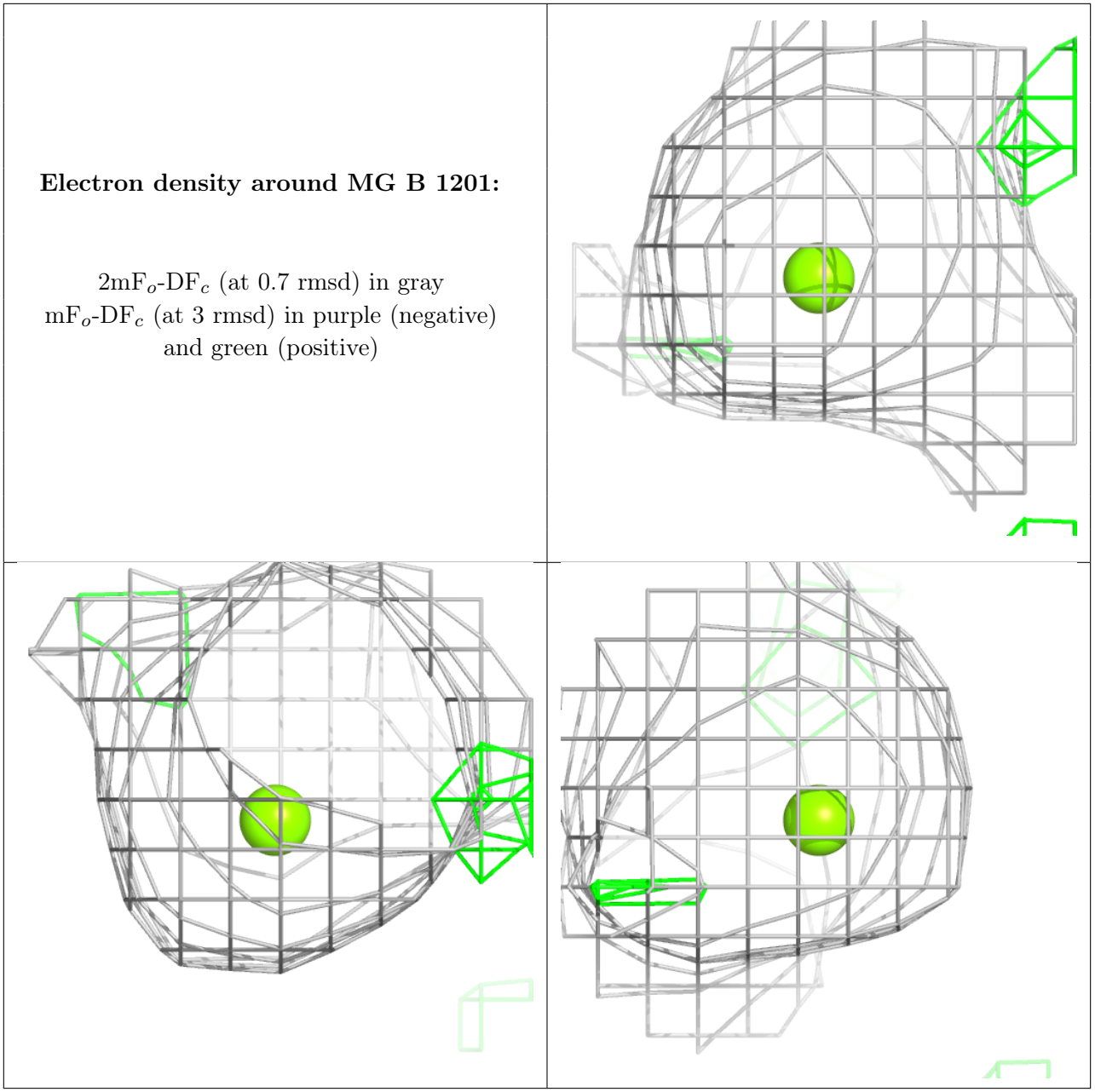






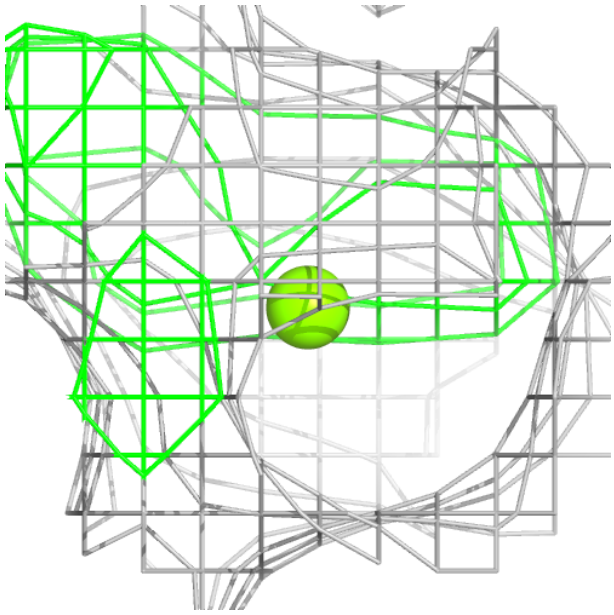
Electron density around MG B 1201:

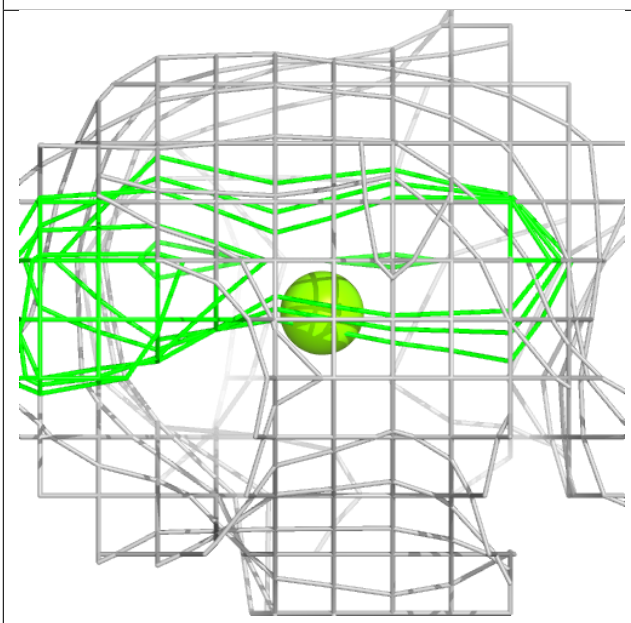
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

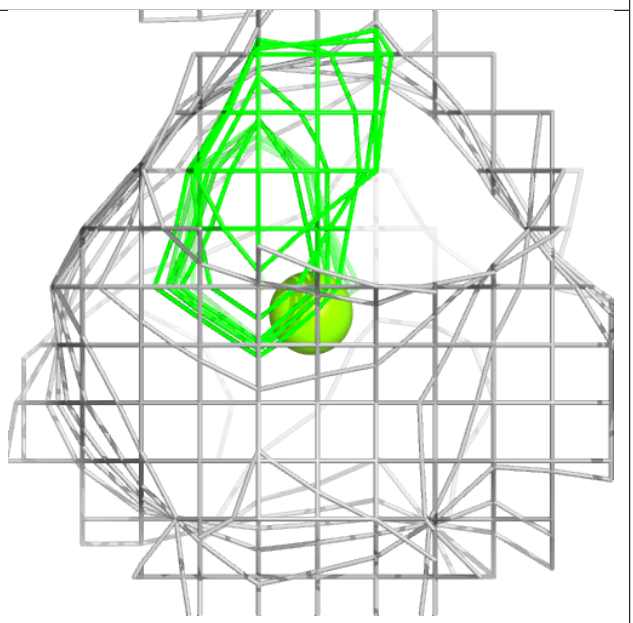


Electron density around MG A 1202:

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

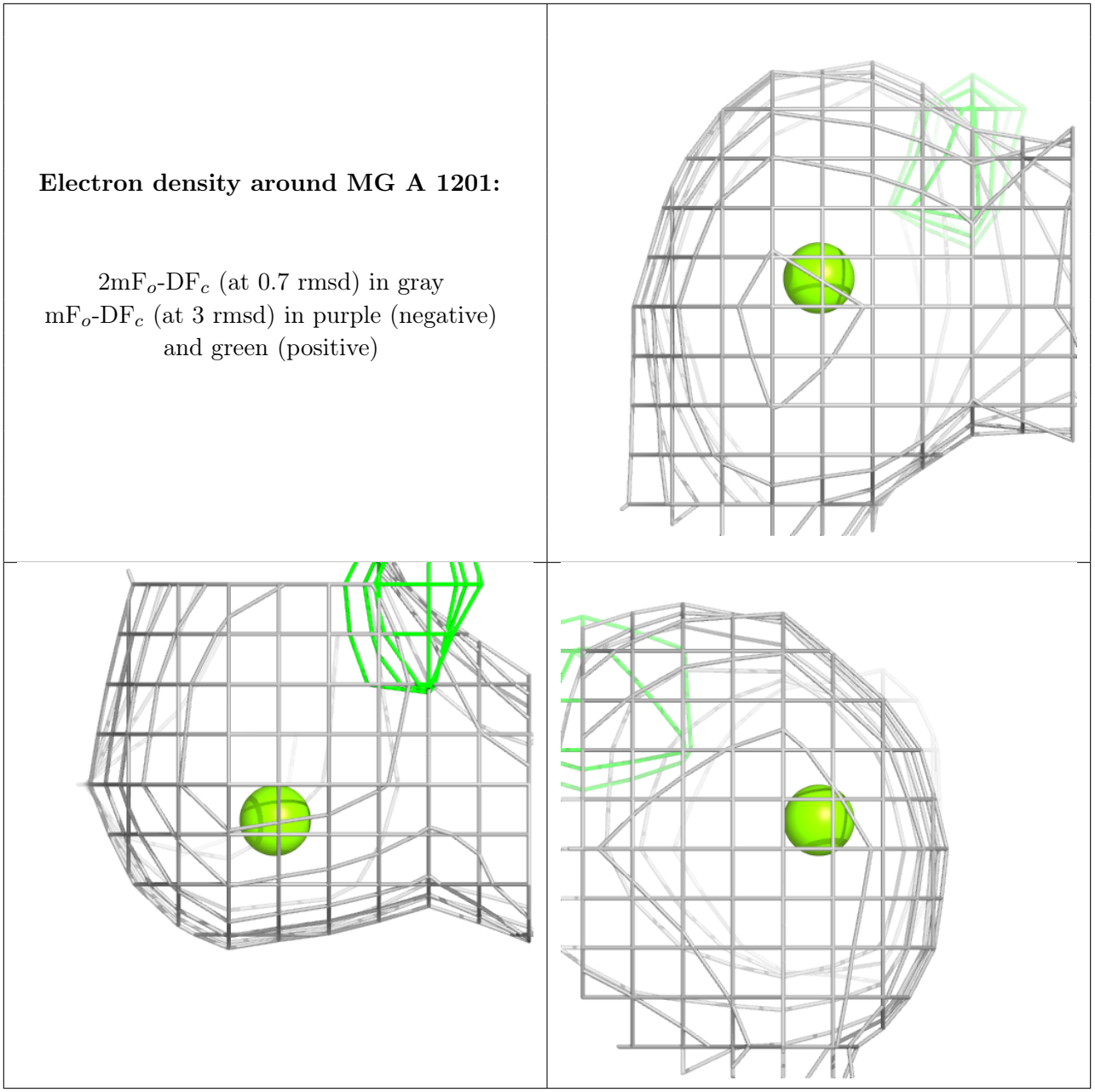






Electron density around MG A 1201:

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



6.5 Other polymers

There are no such residues in this entry.