



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:34 PM UTC

PDB ID : 9HPB / pdb\_00009hpb  
Title : Mouse phosphomannomutase 2 in apo state from crystals with PEG 8000  
Authors : Ramon-Maiques, S.; Del Cano-Ochoa, F.; Company, R.  
Deposited on : 2024-12-12  
Resolution : 2.43 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](mailto: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>.

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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

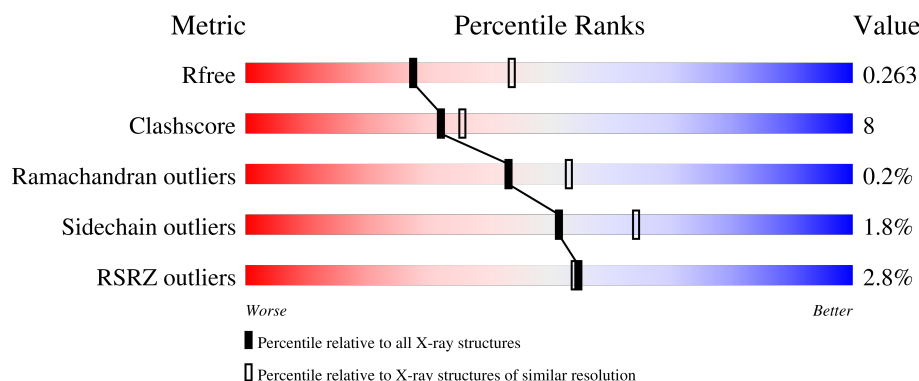
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.43 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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  $\geq 3$ , 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	244	
1	B	244	
1	C	244	
1	D	244	
1	E	244	

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Mol	Chain	Length	Quality of chain
1	F	244	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NA	C	304	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22856 atoms, of which 11091 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 Phosphomannomutase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	242	Total	C	H	N	O	S	0	0	0
			3830	1231	1897	327	365	10			
1	B	242	Total	C	H	N	O	S	0	0	0
			3774	1219	1863	325	358	9			
1	D	241	Total	C	H	N	O	S	0	1	0
			3809	1224	1888	328	359	10			
1	F	240	Total	C	H	N	O	S	0	0	0
			3578	1167	1738	315	348	10			
1	C	243	Total	C	H	N	O	S	0	0	0
			3870	1240	1925	332	362	11			
1	E	242	Total	C	H	N	O	S	0	0	0
			3659	1195	1780	316	358	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q9Z2M7
A	0	PRO	-	expression tag	UNP Q9Z2M7
B	-1	GLY	-	expression tag	UNP Q9Z2M7
B	0	PRO	-	expression tag	UNP Q9Z2M7
D	-1	GLY	-	expression tag	UNP Q9Z2M7
D	0	PRO	-	expression tag	UNP Q9Z2M7
F	-1	GLY	-	expression tag	UNP Q9Z2M7
F	0	PRO	-	expression tag	UNP Q9Z2M7
C	-1	GLY	-	expression tag	UNP Q9Z2M7
C	0	PRO	-	expression tag	UNP Q9Z2M7
E	-1	GLY	-	expression tag	UNP Q9Z2M7
E	0	PRO	-	expression tag	UNP Q9Z2M7

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Mg 2	0	0
2	B	2	Total 2	Mg 2	0	0
2	D	2	Total 2	Mg 2	0	0
2	F	2	Total 2	Mg 2	0	0
2	C	1	Total 1	Mg 1	0	0
2	E	2	Total 2	Mg 2	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Cl 1	0	0
3	D	1	Total 1	Cl 1	0	0
3	C	1	Total 1	Cl 1	0	0
3	E	1	Total 1	Cl 1	0	0

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Na 1	0	0
4	D	1	Total 1	Na 1	0	0
4	C	2	Total 2	Na 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	96	Total 96	O 96	0	0
5	B	48	Total 48	O 48	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	57	Total 57	O 57	0	0
5	F	16	Total 16	O 16	0	0
5	C	70	Total 70	O 70	0	0
5	E	30	Total 30	O 30	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.

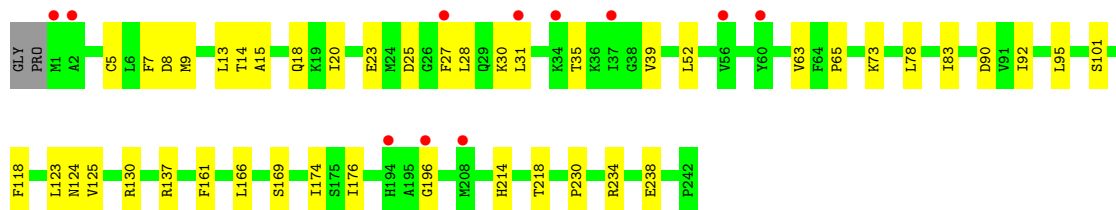
#### • Molecule 1: Phosphomannomutase 2

Chain A:  89% 10% .




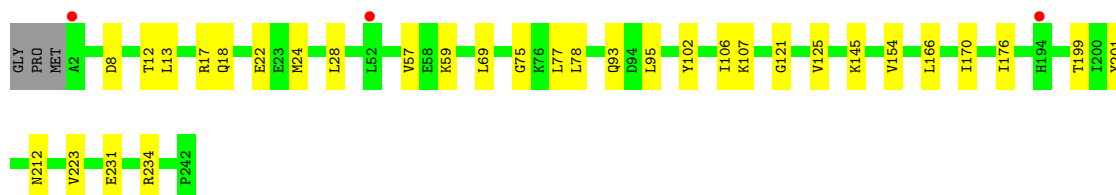
#### • Molecule 1: Phosphomannomutase 2

Chain B:  5% 81% 18% .



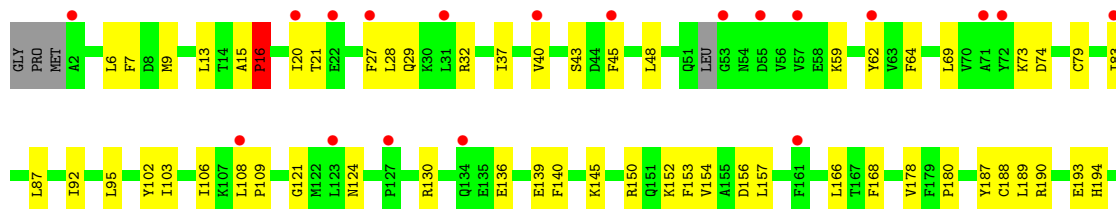
#### • Molecule 1: Phosphomannomutase 2

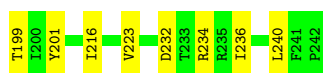
Chain D:  86% 13% .



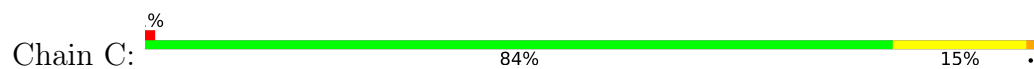
#### • Molecule 1: Phosphomannomutase 2

Chain F:  8% 72% 26% .

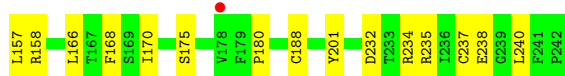
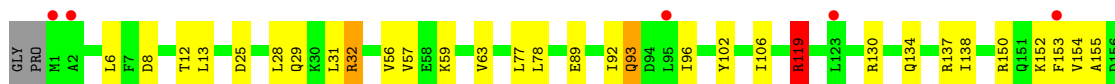
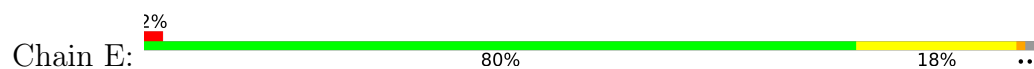




• Molecule 1: Phosphomannomutase 2



• Molecule 1: Phosphomannomutase 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.66Å 98.61Å 212.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.21 – 2.43 53.21 – 2.43	Depositor EDS
% Data completeness (in resolution range)	99.8 (53.21-2.43) 99.8 (53.21-2.43)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.20.1-4487	Depositor
R, $R_{free}$	0.234 , 0.271 (Not available) , 0.263	Depositor DCC
$R_{free}$ test set	3148 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.1	Xtriage
Anisotropy	0.509	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	22856	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CL, MG, NA

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	0.18	0/1973	0.31	0/2654
1	B	0.23	1/1951 (0.1%)	0.34	0/2628
1	C	0.21	0/1986	0.37	0/2669
1	D	0.19	0/1963	0.34	0/2641
1	E	0.18	0/1918	0.36	0/2593
1	F	0.20	0/1877	0.34	0/2534
All	All	0.20	1/11668 (0.0%)	0.34	0/15719

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2
1	E	0	3
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	230	PRO	N-CD	5.04	1.54	1.47

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	119	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	137	ARG	Sidechain
1	E	119	ARG	Sidechain
1	E	130	ARG	Sidechain
1	E	32	ARG	Sidechain

## 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	1933	1897	1899	17	0
1	B	1911	1863	1865	31	0
1	C	1945	1925	1927	24	0
1	D	1921	1888	1888	27	0
1	E	1879	1780	1782	30	0
1	F	1840	1738	1729	54	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	1	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
5	A	96	0	0	2	0
5	B	48	0	0	0	0
5	C	70	0	0	0	0
5	D	57	0	0	3	0
5	E	30	0	0	0	0
5	F	16	0	0	0	0
All	All	11765	11091	11090	181	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 8.

All (181) 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:F:83:ILE:HG12	1:F:92:ILE:HD11	1.52	0.91
1:B:31:LEU:HD11	1:B:35:THR:HG22	1.55	0.88
1:B:83:ILE:HG12	1:B:92:ILE:HD11	1.59	0.84
1:B:214:HIS:O	1:B:218:THR:HG23	1.77	0.84
1:F:32:ARG:HD2	1:F:37:ILE:HG12	1.60	0.83
1:D:145:LYS:NZ	5:D:402:HOH:O	2.14	0.80
1:D:13:LEU:HD22	1:D:28:LEU:HD11	1.63	0.80
1:A:46:GLU:OE1	5:A:401:HOH:O	2.00	0.79
1:B:31:LEU:HD12	1:B:31:LEU:O	1.83	0.78
1:B:63:VAL:HG12	1:B:65:PRO:HD3	1.67	0.77
1:D:107:LYS:NZ	5:D:403:HOH:O	2.18	0.76
1:B:27:PHE:CZ	1:B:238:GLU:HG3	2.21	0.76
1:F:193:GLU:OE1	1:F:194:HIS:CE1	2.39	0.75
1:E:232:ASP:OD1	1:E:235:ARG:NH2	2.21	0.73
1:B:137:ARG:HG3	1:B:174:ILE:HG21	1.71	0.73
1:F:199:THR:HG21	1:F:201:TYR:CE2	2.24	0.72
1:E:77:LEU:HD23	1:E:78:LEU:N	2.06	0.71
1:B:31:LEU:CD1	1:B:35:THR:HG22	2.22	0.70
1:A:47:LYS:NZ	1:A:50:GLU:OE1	2.26	0.68
1:A:208:MET:HG3	1:A:209:PRO:HD2	1.77	0.67
1:C:208:MET:HB3	1:C:209:PRO:HD3	1.76	0.67
1:B:15:ALA:HB3	1:B:18:GLN:HG3	1.75	0.67
1:D:212:ASN:OD1	5:D:401:HOH:O	2.13	0.65
1:F:7:PHE:HB3	1:F:13:LEU:HD13	1.78	0.64
1:E:13:LEU:HD22	1:E:28:LEU:HD11	1.79	0.64
1:E:119:ARG:HH11	1:E:119:ARG:HG2	1.63	0.63
1:B:27:PHE:CD1	1:B:234:ARG:NH2	2.67	0.63
1:D:59:LYS:HA	1:D:59:LYS:HE2	1.80	0.63
1:D:95:LEU:HD11	1:D:166:LEU:HD11	1.81	0.62
1:B:13:LEU:HD22	1:B:28:LEU:HD11	1.81	0.62
1:F:32:ARG:HD2	1:F:37:ILE:CG1	2.28	0.61
1:C:73:LYS:HB3	1:C:78:LEU:HD11	1.82	0.61
1:F:189:LEU:HD11	1:F:216:ILE:HD11	1.83	0.60
1:F:83:ILE:HD12	1:F:180:PRO:HD3	1.84	0.59
1:B:5:CYS:SG	1:B:35:THR:HG21	2.42	0.59
1:D:57:VAL:HG22	1:D:75:GLY:HA2	1.85	0.58
1:B:31:LEU:HD11	1:B:35:THR:CG2	2.31	0.58
1:F:87:LEU:HD11	1:F:166:LEU:HD21	1.85	0.57
1:F:199:THR:HG21	1:F:201:TYR:CZ	2.38	0.57
1:F:232:ASP:OD2	1:F:236:ILE:HD11	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:193:GLU:OE1	1:F:194:HIS:NE2	2.37	0.57
1:B:7:PHE:HB2	1:B:13:LEU:HD11	1.87	0.56
1:A:77:LEU:HD21	1:A:80:LYS:HD2	1.87	0.56
1:C:107:LYS:HE2	1:C:107:LYS:HA	1.87	0.56
1:F:95:LEU:HD21	1:F:178:VAL:HG11	1.87	0.56
1:A:69:LEU:HD11	1:A:183:TRP:CE3	2.41	0.56
1:C:185:LYS:NZ	1:C:212:ASN:OD1	2.39	0.56
1:F:103:ILE:HA	1:F:106:ILE:HG12	1.87	0.55
1:C:69:LEU:HD11	1:C:183:TRP:CE3	2.40	0.55
1:F:83:ILE:HG12	1:F:92:ILE:CD1	2.29	0.55
1:F:9:MET:SD	1:F:48:LEU:HD23	2.47	0.55
1:F:201:TYR:HD2	1:F:223:VAL:HB	1.72	0.55
1:D:154:VAL:HG21	1:D:170:ILE:HG13	1.88	0.54
1:F:232:ASP:OD2	1:F:236:ILE:CD1	2.55	0.54
1:A:234:ARG:O	1:A:238:GLU:HG3	2.08	0.54
1:C:209:PRO:HA	1:C:214:HIS:ND1	2.23	0.53
1:F:28:LEU:HD22	1:F:37:ILE:HG21	1.90	0.53
1:A:117:GLU:OE2	1:A:130:ARG:NH1	2.42	0.53
1:C:157:LEU:HD22	1:C:168:PHE:CE1	2.44	0.53
1:D:77:LEU:C	1:D:78:LEU:HD12	2.34	0.53
1:D:102:TYR:CD1	1:D:106:ILE:HD11	2.44	0.53
1:F:62:TYR:CE2	1:F:73:LYS:HG3	2.45	0.52
1:D:199:THR:HG23	1:D:223:VAL:HG21	1.92	0.52
1:F:102:TYR:CE1	1:F:153:PHE:CG	2.98	0.52
1:C:154:VAL:HG12	1:C:158:ARG:HD2	1.91	0.51
1:E:89:GLU:O	1:E:93:GLN:HG3	2.11	0.51
1:E:152:LYS:O	1:E:155:ALA:N	2.43	0.51
1:D:22:GLU:H	1:D:22:GLU:CD	2.19	0.51
1:F:106:ILE:N	1:F:106:ILE:HD13	2.25	0.51
1:D:13:LEU:HD23	1:D:24:MET:HE2	1.93	0.51
1:F:69:LEU:HD13	1:F:187:TYR:CZ	2.46	0.50
1:E:25:ASP:O	1:E:29:GLN:HG2	2.11	0.50
1:C:69:LEU:HD13	1:C:121:GLY:HA2	1.93	0.50
1:F:9:MET:HE1	1:F:48:LEU:HG	1.93	0.50
1:F:102:TYR:CE1	1:F:106:ILE:HD11	2.47	0.50
1:D:234:ARG:HH11	1:D:234:ARG:HG2	1.77	0.50
1:D:93:GLN:NE2	1:C:107:LYS:HE2	2.27	0.49
1:F:108:LEU:HD22	1:F:109:PRO:HD2	1.94	0.49
1:A:63:VAL:HG12	1:A:65:PRO:HD3	1.94	0.49
1:B:15:ALA:CB	1:B:18:GLN:HG3	2.42	0.49
1:D:95:LEU:HD11	1:D:166:LEU:CD1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:ASP:O	1:E:12:THR:HB	2.12	0.49
1:D:102:TYR:O	1:D:106:ILE:HG13	2.13	0.49
1:F:187:TYR:CZ	1:F:190:ARG:HD2	2.48	0.49
1:C:73:LYS:HE3	1:C:78:LEU:HD21	1.95	0.49
1:C:95:LEU:HD11	1:C:166:LEU:HD11	1.95	0.48
1:C:208:MET:HB3	1:C:209:PRO:CD	2.41	0.48
1:F:69:LEU:HD13	1:F:187:TYR:CE2	2.49	0.48
1:C:187:TYR:HA	1:C:190:ARG:NH1	2.29	0.48
1:B:137:ARG:HG3	1:B:174:ILE:CG2	2.43	0.48
1:A:234:ARG:NH2	5:A:403:HOH:O	2.32	0.48
1:D:17:ARG:HB3	1:D:18:GLN:OE1	2.14	0.48
1:E:29:GLN:OE1	1:E:32:ARG:NH2	2.46	0.48
1:C:150:ARG:O	1:C:154:VAL:HG23	2.14	0.48
1:D:199:THR:HG21	1:D:201:TYR:CZ	2.49	0.48
1:C:141:TYR:CD1	1:C:173:GLN:HB3	2.49	0.48
1:E:166:LEU:HD23	1:E:180:PRO:HA	1.95	0.47
1:F:62:TYR:HE2	1:F:73:LYS:HG3	1.78	0.47
1:F:136:GLU:O	1:F:139:GLU:HG2	2.14	0.47
1:B:95:LEU:HD11	1:B:166:LEU:HD13	1.95	0.47
1:F:73:LYS:O	1:F:74:ASP:HB2	2.13	0.47
1:E:56:VAL:HG13	1:E:57:VAL:N	2.29	0.47
1:C:69:LEU:HD13	1:C:121:GLY:CA	2.44	0.47
1:A:227:VAL:HG12	1:A:236:ILE:HD12	1.96	0.47
1:B:14:THR:HG22	1:B:20:ILE:HB	1.97	0.47
1:D:69:LEU:HD13	1:D:121:GLY:HA3	1.97	0.47
1:B:27:PHE:CZ	1:B:238:GLU:CG	2.96	0.47
1:E:77:LEU:HD23	1:E:77:LEU:C	2.40	0.46
1:E:153:PHE:CE1	1:E:157:LEU:HD11	2.50	0.46
1:B:95:LEU:HD23	1:B:161:PHE:CE2	2.50	0.46
1:D:93:GLN:HE22	1:C:107:LYS:HE2	1.81	0.46
1:E:102:TYR:CE1	1:E:106:ILE:HD11	2.51	0.46
1:B:31:LEU:HD12	1:B:31:LEU:C	2.40	0.46
1:C:161:PHE:HA	1:C:164:LYS:HG3	1.96	0.46
1:B:27:PHE:HZ	1:B:238:GLU:HG3	1.76	0.46
1:B:73:LYS:HB3	1:B:78:LEU:HD13	1.98	0.46
1:B:27:PHE:HA	1:B:30:LYS:HG3	1.97	0.46
1:F:150:ARG:O	1:F:154:VAL:HG23	2.16	0.46
1:E:6:LEU:HD21	1:E:188:CYS:SG	2.55	0.46
1:E:57:VAL:HA	1:E:63:VAL:HG21	1.98	0.46
1:E:138:ILE:HD12	1:E:138:ILE:N	2.31	0.46
1:A:168:PHE:CE1	1:A:178:VAL:HG13	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:124:ASN:HB3	1:F:130:ARG:HE	1.80	0.45
1:E:92:ILE:HG22	1:E:96:ILE:HD12	1.98	0.45
1:D:231:GLU:OE1	1:D:234:ARG:HD3	2.17	0.45
1:E:134:GLN:O	1:E:138:ILE:HD13	2.17	0.45
1:C:154:VAL:HG21	1:C:170:ILE:HG13	1.98	0.45
1:F:45:PHE:HD1	1:F:45:PHE:O	2.00	0.45
1:F:236:ILE:O	1:F:240:LEU:HD23	2.17	0.45
1:B:39:VAL:HG11	1:B:52:LEU:HD11	1.99	0.44
1:E:32:ARG:HH22	1:E:59:LYS:HA	1.81	0.44
1:F:152:LYS:O	1:F:156:ASP:OD1	2.35	0.44
1:E:201:TYR:CE1	1:E:240:LEU:HD22	2.52	0.44
1:F:15:ALA:O	1:F:16:PRO:C	2.60	0.44
1:E:234:ARG:O	1:E:238:GLU:HG3	2.17	0.44
1:B:118:PHE:HA	1:B:123:LEU:HD23	1.99	0.44
1:E:150:ARG:O	1:E:154:VAL:HG23	2.18	0.44
1:A:83:ILE:HG12	1:A:87:LEU:HD12	1.99	0.44
1:A:117:GLU:OE1	1:A:119:ARG:NE	2.51	0.44
1:F:157:LEU:HB3	1:F:168:PHE:CD2	2.53	0.44
1:E:166:LEU:HD23	1:E:166:LEU:HA	1.92	0.43
1:F:20:ILE:CG1	1:F:21:THR:N	2.81	0.43
1:A:47:LYS:HA	1:A:47:LYS:HD3	1.81	0.43
1:F:27:PHE:CB	1:F:234:ARG:NE	2.81	0.43
1:F:187:TYR:CE1	1:F:190:ARG:NE	2.87	0.43
1:C:7:PHE:CG	1:C:13:LEU:HD21	2.53	0.43
1:B:125:VAL:O	1:B:176:ILE:N	2.49	0.43
1:C:42:GLY:O	1:C:119:ARG:NH2	2.48	0.42
1:B:8:ASP:OD2	1:B:9:MET:N	2.53	0.42
1:E:102:TYR:O	1:E:106:ILE:HD13	2.19	0.42
1:E:32:ARG:O	1:E:32:ARG:HG3	2.18	0.42
1:A:19:LYS:HD3	1:A:50:GLU:O	2.20	0.42
1:E:152:LYS:O	1:E:153:PHE:C	2.62	0.42
1:B:214:HIS:CE1	1:B:218:THR:HG21	2.54	0.42
1:C:148:HIS:O	1:C:152:LYS:HG3	2.20	0.42
1:F:168:PHE:CD1	1:F:168:PHE:N	2.88	0.41
1:F:188:CYS:SG	1:F:189:LEU:CD1	3.08	0.41
1:C:95:LEU:HD11	1:C:166:LEU:CD1	2.50	0.41
1:D:8:ASP:O	1:D:12:THR:HB	2.20	0.41
1:F:87:LEU:CD1	1:F:166:LEU:HD21	2.48	0.41
1:D:125:VAL:O	1:D:176:ILE:N	2.48	0.41
1:F:37:ILE:HD11	1:F:59:LYS:O	2.20	0.41
1:A:208:MET:HG3	1:A:209:PRO:CD	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:VAL:HG11	1:A:233:THR:HA	2.02	0.41
1:D:24:MET:SD	1:D:234:ARG:HG3	2.60	0.41
1:F:102:TYR:O	1:F:106:ILE:HG12	2.20	0.41
1:F:124:ASN:HB3	1:F:130:ARG:NE	2.35	0.41
1:E:134:GLN:O	1:E:137:ARG:N	2.53	0.41
1:D:78:LEU:HD12	1:D:78:LEU:N	2.35	0.41
1:F:28:LEU:HD23	1:F:28:LEU:HA	1.94	0.41
1:B:28:LEU:N	1:B:28:LEU:HD23	2.35	0.41
1:F:108:LEU:HD11	1:F:140:PHE:CE1	2.56	0.41
1:E:158:ARG:NH2	1:E:168:PHE:O	2.54	0.41
1:F:108:LEU:HD22	1:F:109:PRO:CD	2.51	0.41
1:D:69:LEU:HD13	1:D:121:GLY:CA	2.51	0.40
1:E:31:LEU:HD11	1:E:237:CYS:HB3	2.02	0.40
1:F:29:GLN:H	1:F:29:GLN:HG2	1.73	0.40
1:F:40:VAL:HG23	1:F:64:PHE:CB	2.51	0.40
1:B:124:ASN:HB3	1:B:130:ARG:HH11	1.86	0.40
1:F:62:TYR:HE2	1:F:73:LYS:CG	2.35	0.40
1:F:157:LEU:HB3	1:F:168:PHE:CE2	2.56	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	240/244 (98%)	232 (97%)	8 (3%)	0	100	100
1	B	240/244 (98%)	229 (95%)	10 (4%)	1 (0%)	30	36
1	C	241/244 (99%)	229 (95%)	12 (5%)	0	100	100
1	D	240/244 (98%)	228 (95%)	12 (5%)	0	100	100
1	E	240/244 (98%)	224 (93%)	16 (7%)	0	100	100
1	F	236/244 (97%)	218 (92%)	16 (7%)	2 (1%)	16	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1437/1464 (98%)	1360 (95%)	74 (5%)	3 (0%)	43	53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	196	GLY
1	F	16	PRO
1	F	121	GLY

### 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	207/211 (98%)	207 (100%)	0	100	100
1	B	201/211 (95%)	196 (98%)	5 (2%)	42	54
1	C	209/211 (99%)	202 (97%)	7 (3%)	33	45
1	D	204/211 (97%)	204 (100%)	0	100	100
1	E	193/211 (92%)	189 (98%)	4 (2%)	47	60
1	F	185/211 (88%)	180 (97%)	5 (3%)	39	52
All	All	1199/1266 (95%)	1178 (98%)	21 (2%)	51	64

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	23	GLU
1	B	25	ASP
1	B	90	ASP
1	B	101	SER
1	B	169	SER
1	F	6	LEU
1	F	16	PRO
1	F	43	SER
1	F	79	CYS

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Mol	Chain	Res	Type
1	F	145	LYS
1	C	58	GLU
1	C	92	ILE
1	C	145	LYS
1	C	147	GLU
1	C	169	SER
1	C	173	GLN
1	C	175	SER
1	E	93	GLN
1	E	119	ARG
1	E	170	ILE
1	E	175	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	HIS
1	B	18	GLN
1	B	124	ASN
1	B	148	HIS
1	B	191	HIS
1	D	93	GLN
1	D	191	HIS
1	D	214	HIS
1	F	151	GLN
1	F	191	HIS
1	E	81	GLN
1	E	86	HIS

### 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 19 ligands modelled in this entry, 19 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	242/244 (99%)	0.01	0 100 100	50, 65, 81, 97	0
1	B	242/244 (99%)	0.47	11 (4%) 38 35	50, 74, 95, 104	0
1	C	243/244 (99%)	0.17	2 (0%) 82 83	44, 68, 93, 109	0
1	D	241/244 (98%)	0.27	3 (1%) 76 78	49, 73, 97, 116	1 (0%)
1	E	242/244 (99%)	0.40	6 (2%) 58 59	61, 89, 106, 116	0
1	F	240/244 (98%)	0.84	19 (7%) 18 16	73, 98, 117, 127	0
All	All	1450/1464 (99%)	0.36	41 (2%) 55 54	44, 77, 107, 127	1 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	4.5
1	F	72	TYR	3.7
1	E	1	MET	3.4
1	D	2	ALA	3.4
1	F	123	LEU	3.2
1	F	20	ILE	3.2
1	F	55	ASP	3.1
1	B	37	ILE	3.0
1	F	45	PHE	3.0
1	B	208	MET	2.9
1	B	56	VAL	2.8
1	F	127	PRO	2.8
1	B	60	TYR	2.7
1	D	52	LEU	2.7
1	F	71	ALA	2.6
1	F	53	GLY	2.6
1	E	123	LEU	2.6
1	D	194	HIS	2.5
1	E	178	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	194	HIS	2.5
1	F	57	VAL	2.5
1	F	22	GLU	2.4
1	B	34	LYS	2.4
1	F	83	ILE	2.4
1	B	196	GLY	2.3
1	F	27	PHE	2.3
1	F	161	PHE	2.3
1	E	153	PHE	2.3
1	B	27	PHE	2.3
1	B	2	ALA	2.2
1	F	108	LEU	2.2
1	F	31	LEU	2.2
1	B	31	LEU	2.2
1	F	62	TYR	2.1
1	C	79	CYS	2.1
1	F	40	VAL	2.1
1	F	134	GLN	2.0
1	E	2	ALA	2.0
1	C	95	LEU	2.0
1	F	2	ALA	2.0
1	E	95	LEU	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	MG	B	302	1/1	0.63	0.21	78,78,78,78	0

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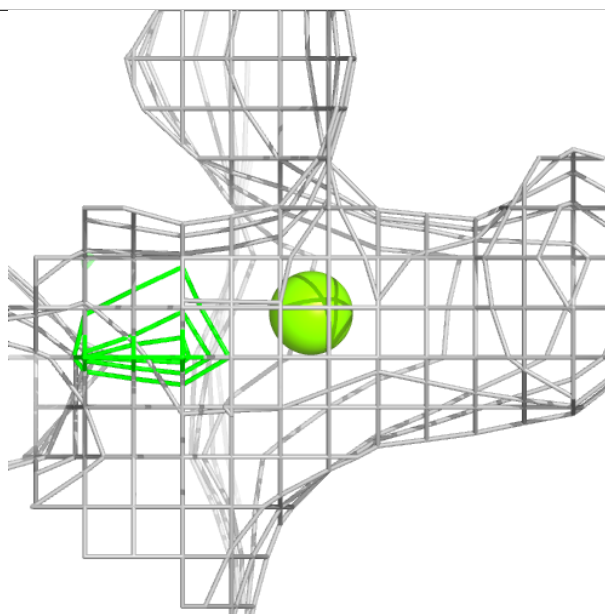
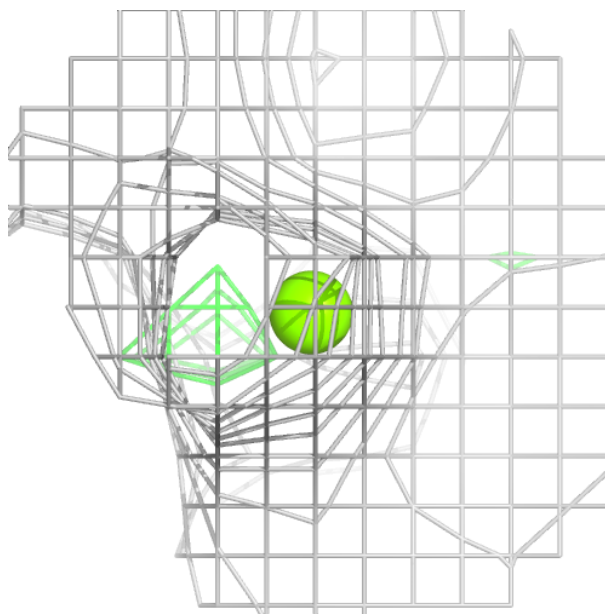
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NA	C	304	1/1	0.77	0.42	76,76,76,76	0
2	MG	D	301	1/1	0.84	0.15	81,81,81,81	0
2	MG	E	302	1/1	0.85	0.12	66,66,66,66	0
4	NA	A	304	1/1	0.86	0.28	64,64,64,64	0
2	MG	F	302	1/1	0.90	0.06	75,75,75,75	0
4	NA	C	303	1/1	0.91	0.38	71,71,71,71	0
3	CL	D	303	1/1	0.93	0.09	85,85,85,85	0
2	MG	A	302	1/1	0.95	0.06	51,51,51,51	0
2	MG	E	301	1/1	0.96	0.09	73,73,73,73	0
3	CL	A	303	1/1	0.97	0.13	42,42,42,42	0
4	NA	D	304	1/1	0.97	0.04	54,54,54,54	0
2	MG	F	301	1/1	0.97	0.05	86,86,86,86	0
3	CL	E	303	1/1	0.97	0.09	56,56,56,56	0
2	MG	D	302	1/1	0.98	0.06	56,56,56,56	0
2	MG	B	301	1/1	0.98	0.04	62,62,62,62	0
3	CL	C	302	1/1	0.99	0.13	42,42,42,42	0
2	MG	A	301	1/1	0.99	0.07	55,55,55,55	0
2	MG	C	301	1/1	0.99	0.03	51,51,51,51	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.

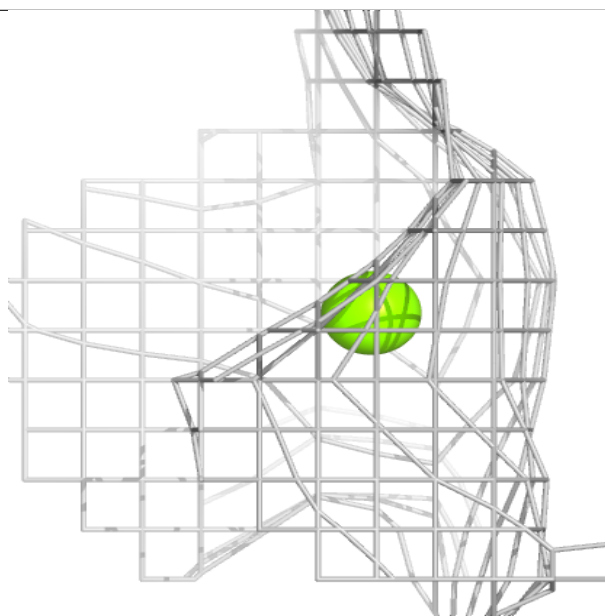
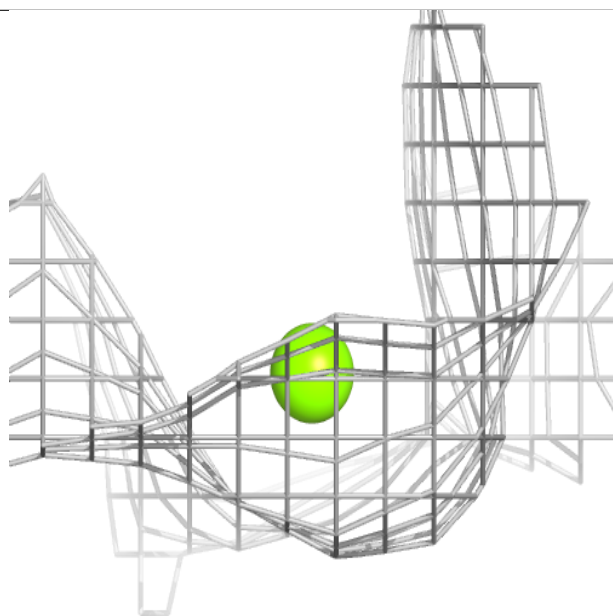
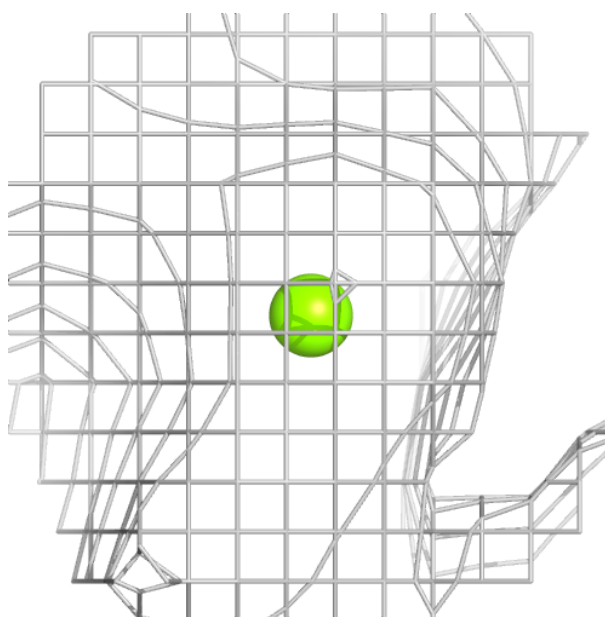
**Electron density around MG B 302:**

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



**Electron density around MG D 301:**

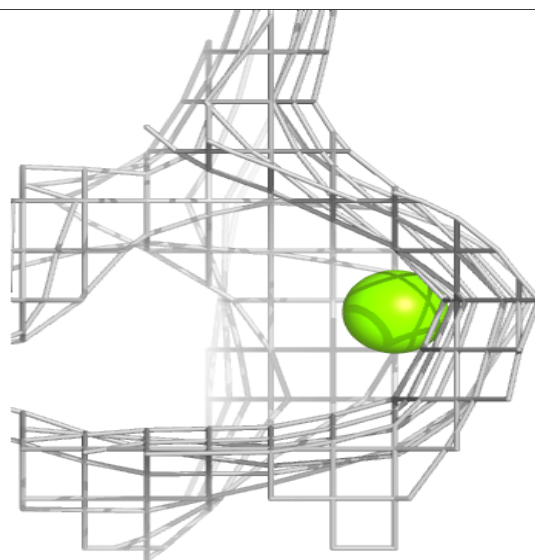
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





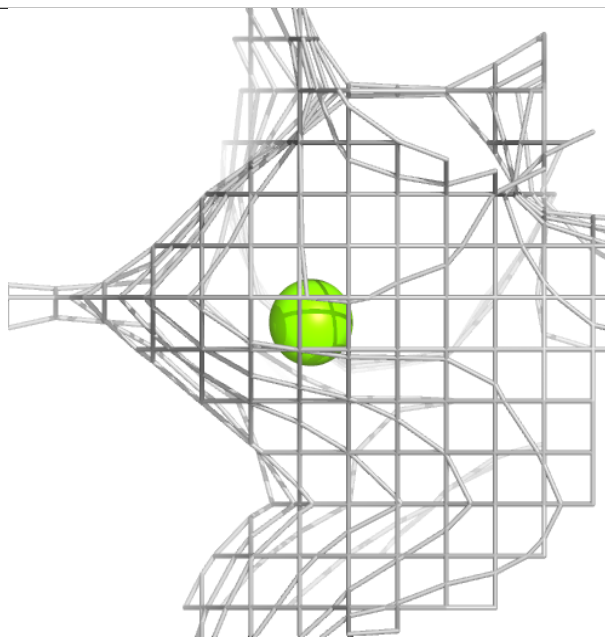
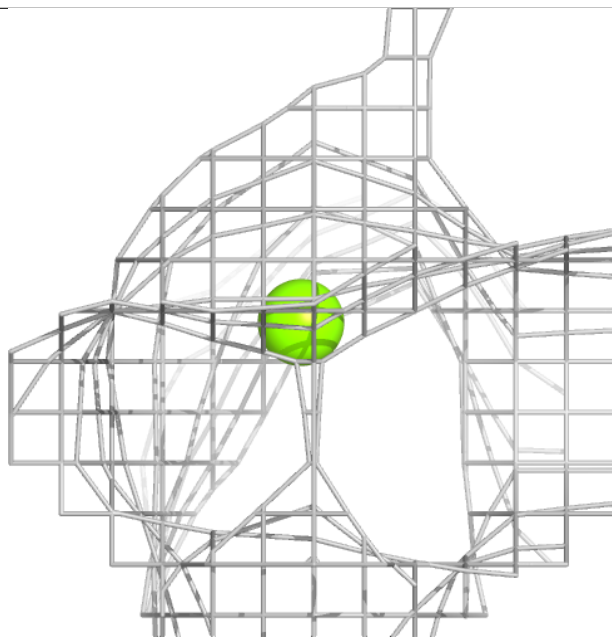
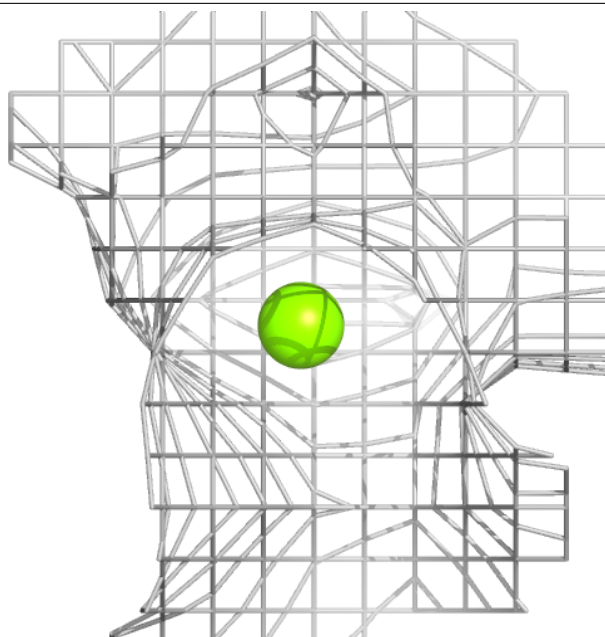
**Electron density around MG E 302:**

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



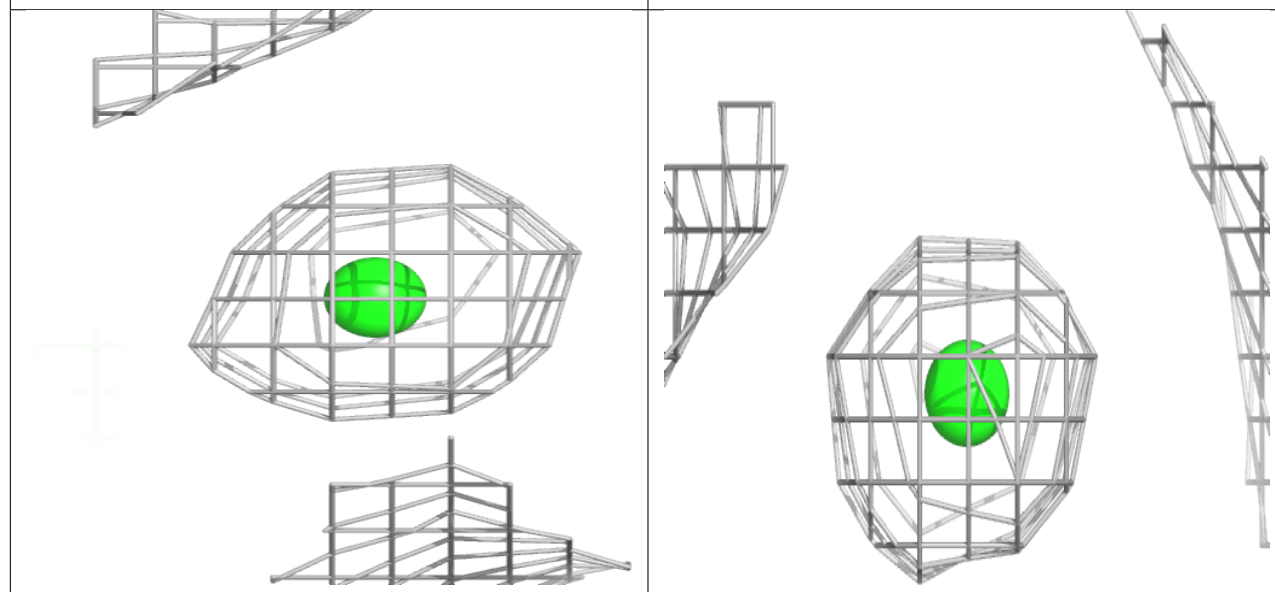
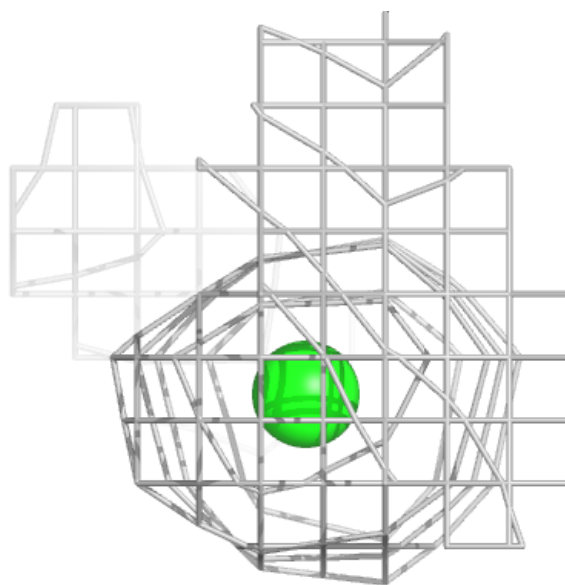
**Electron density around MG F 302:**

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



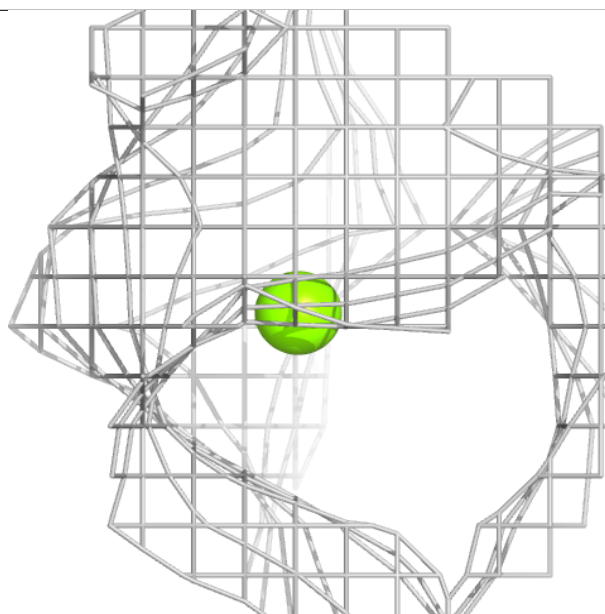
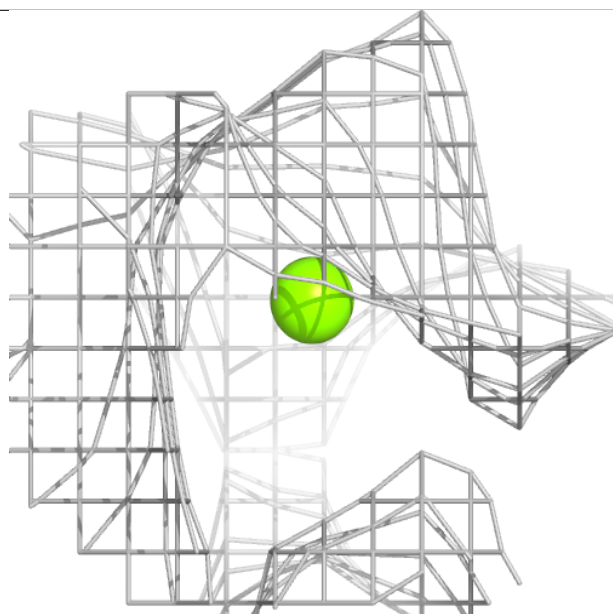
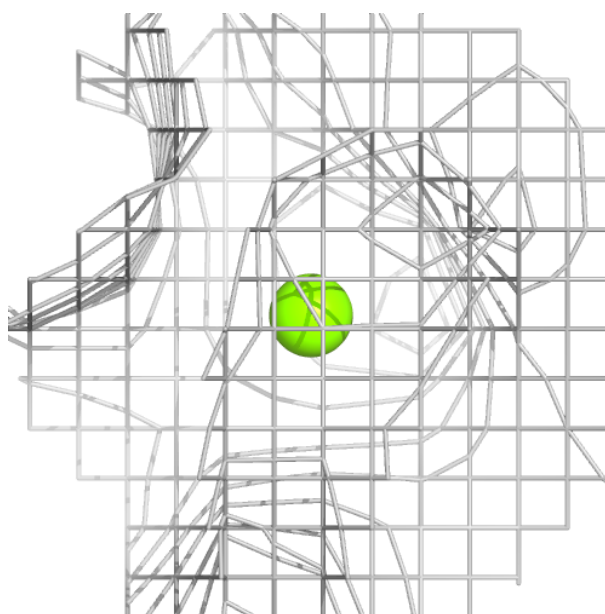
**Electron density around CL D 303:**

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



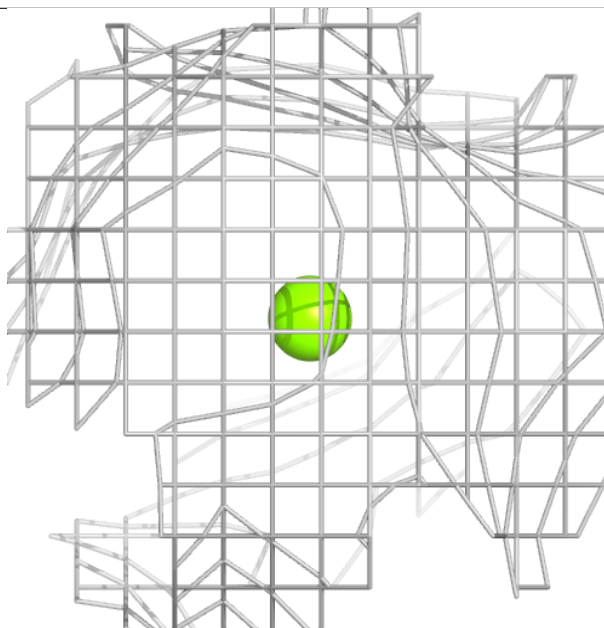
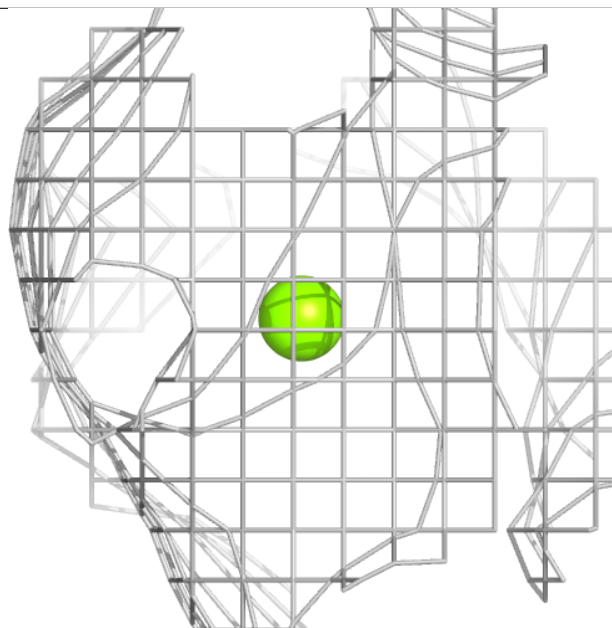
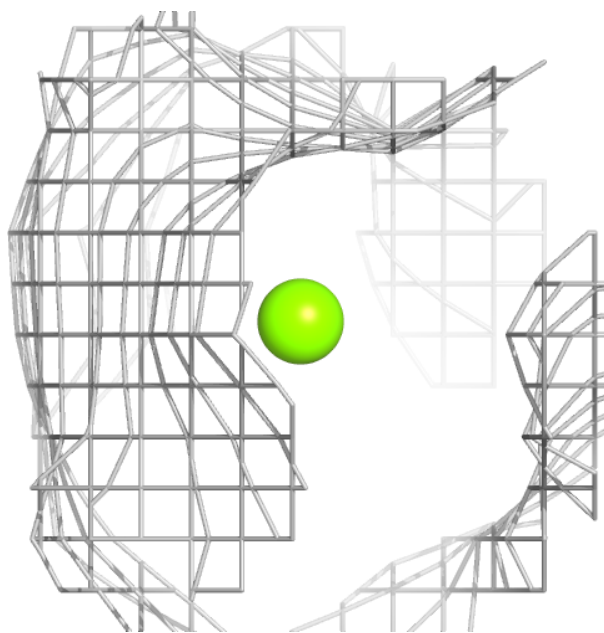
**Electron density around MG A 302:**

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



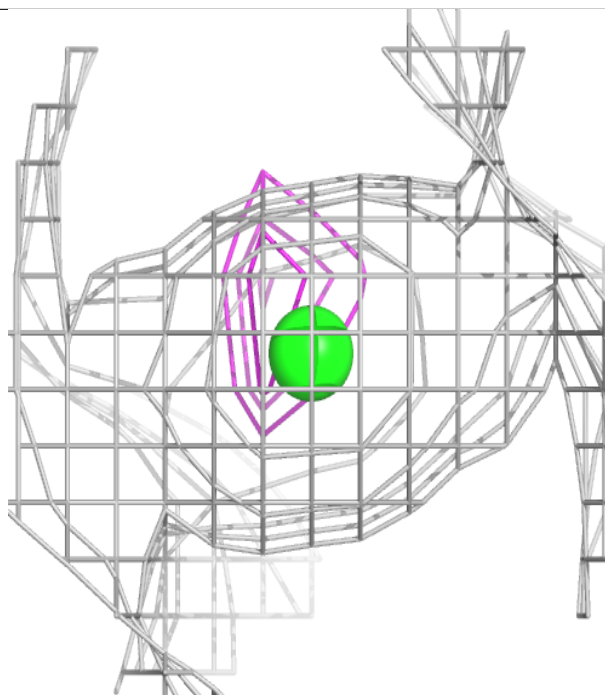
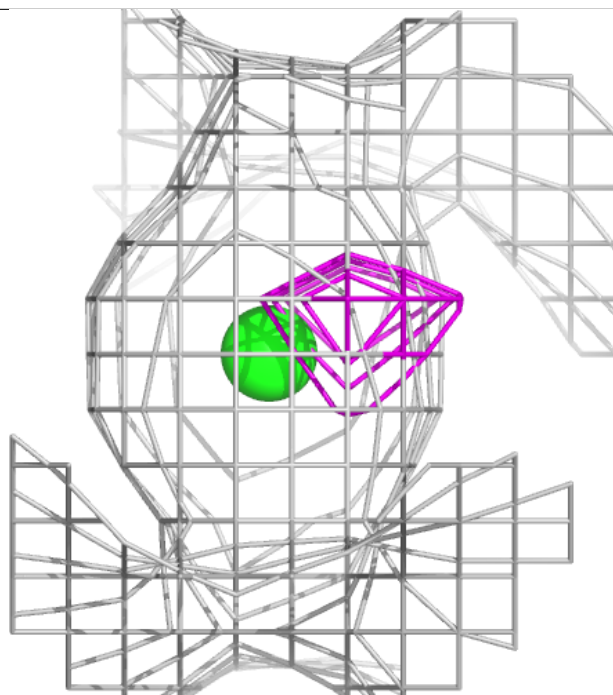
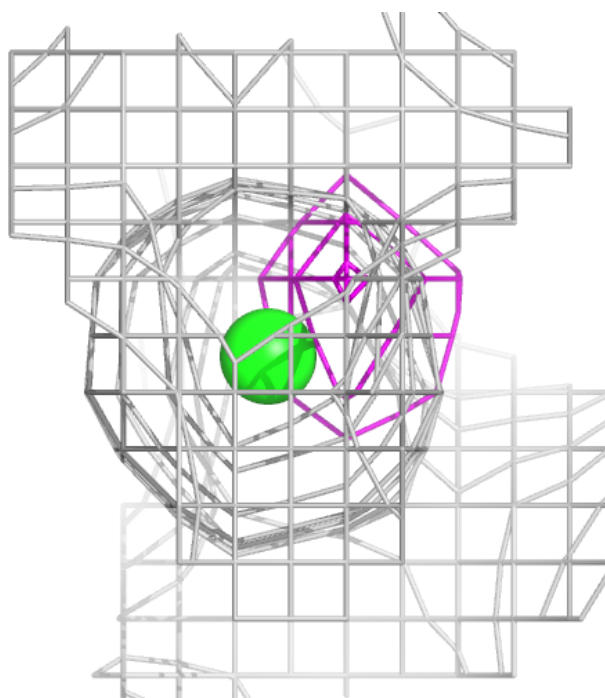
**Electron density around MG E 301:**

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



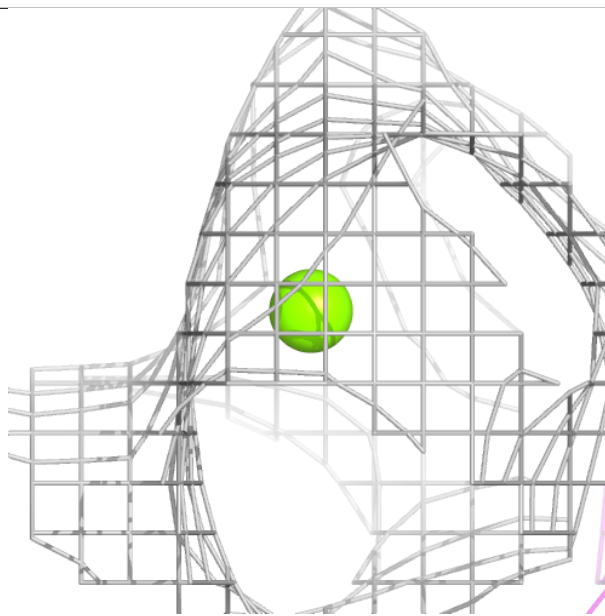
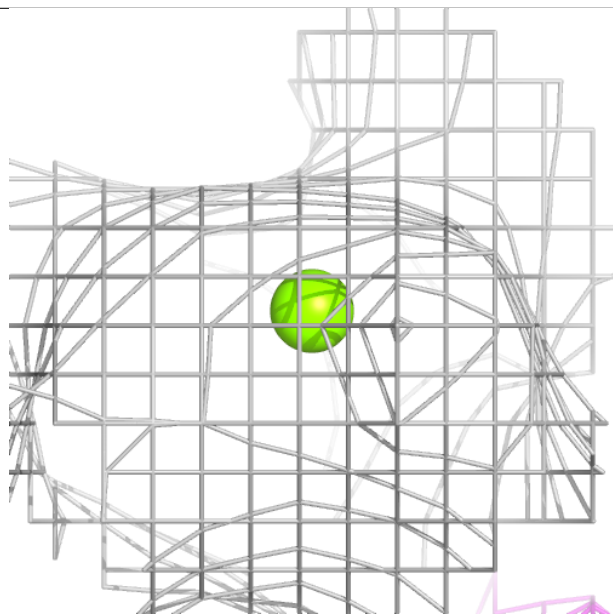
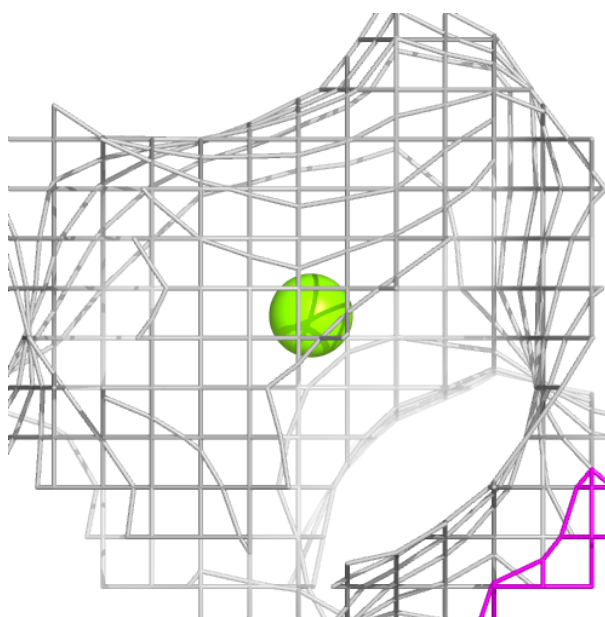
**Electron density around CL A 303:**

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



**Electron density around MG F 301:**

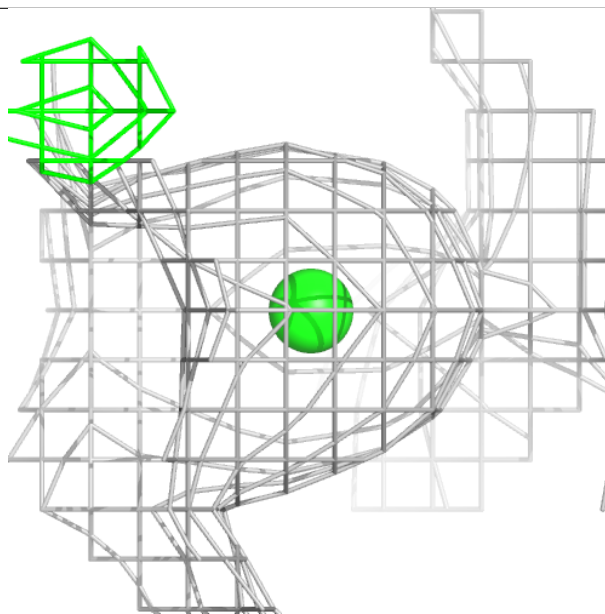
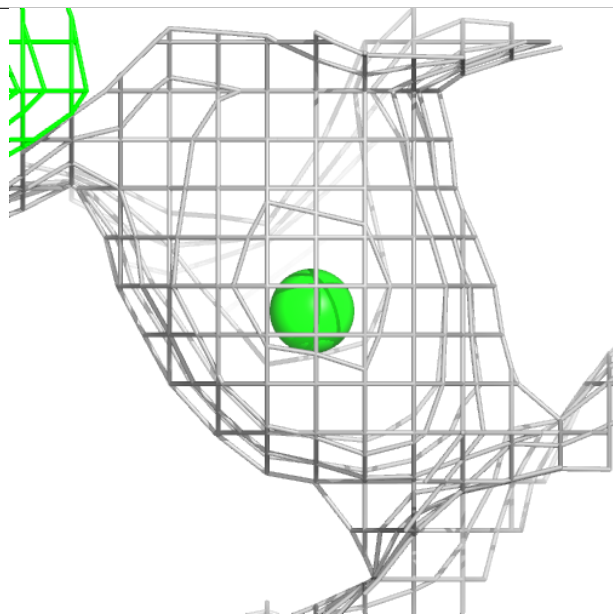
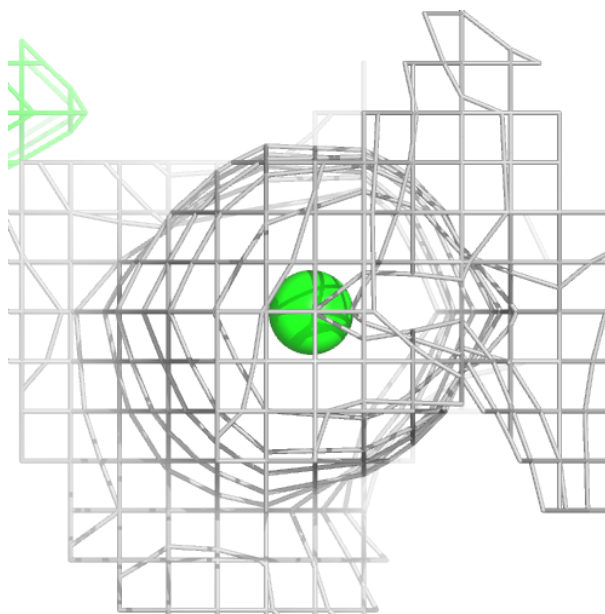
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CL E 303:**

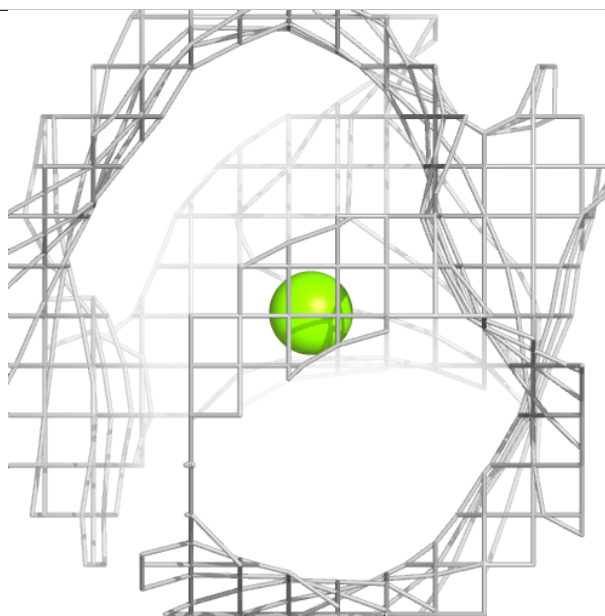
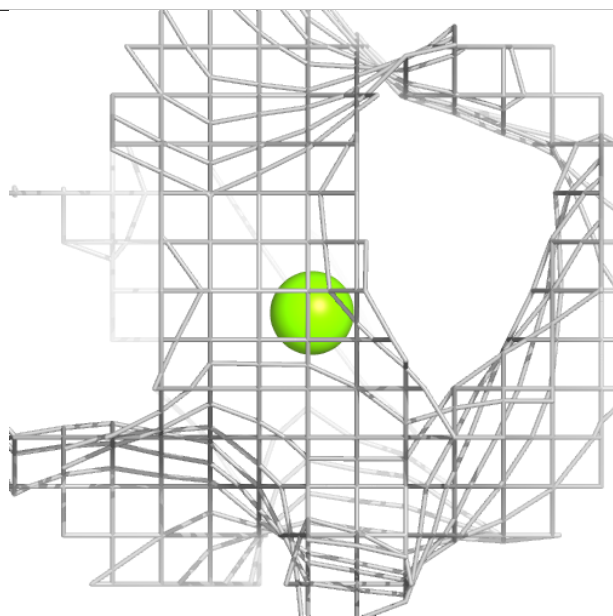
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





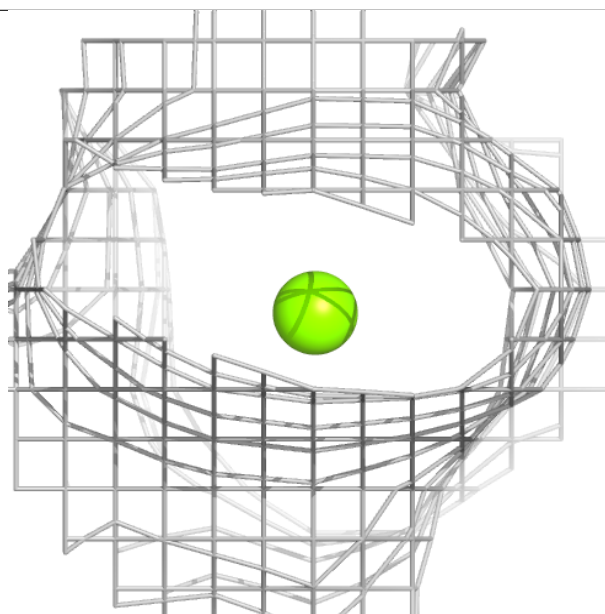
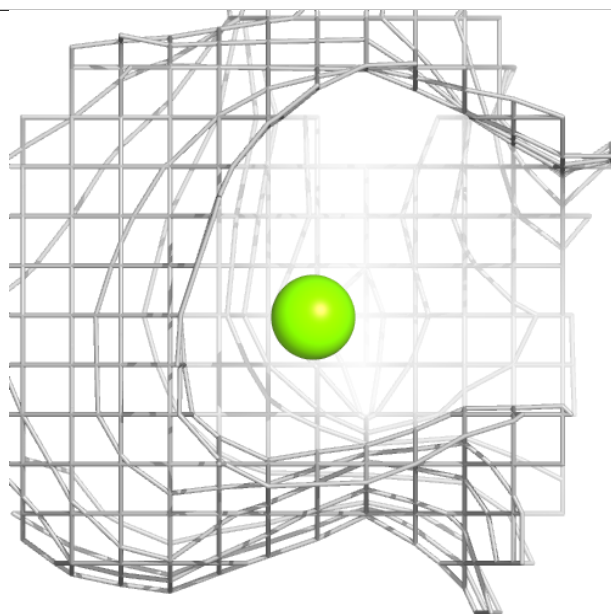
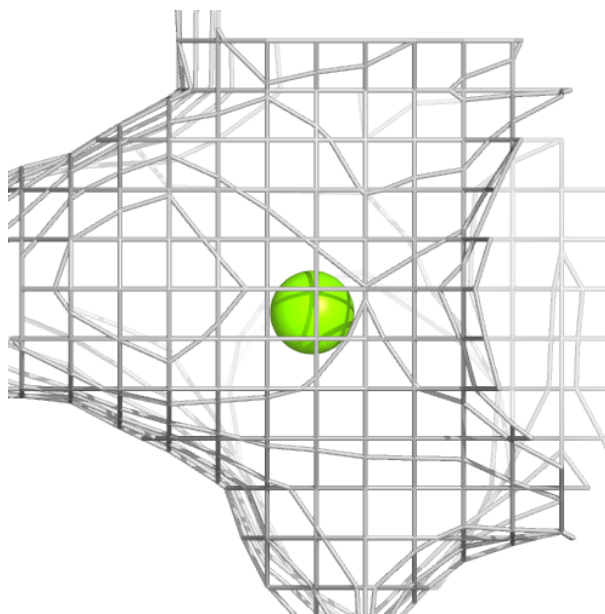
**Electron density around MG D 302:**

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



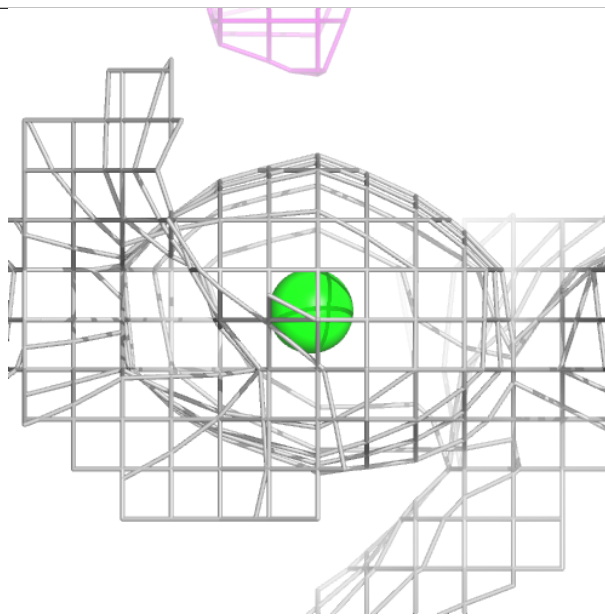
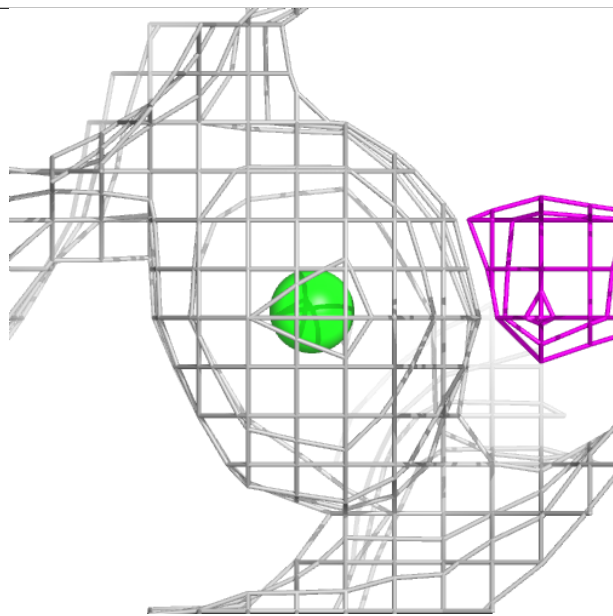
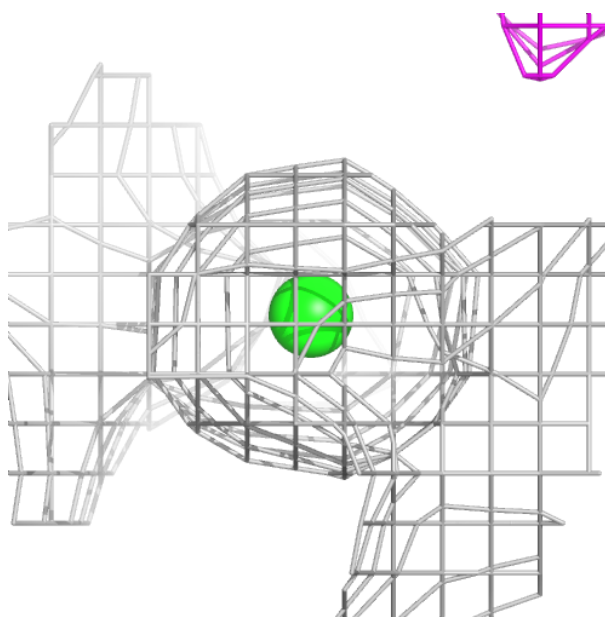
**Electron density around MG B 301:**

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



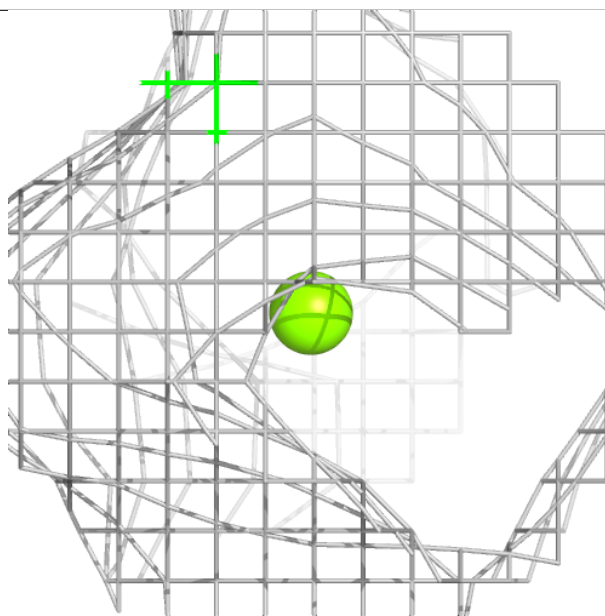
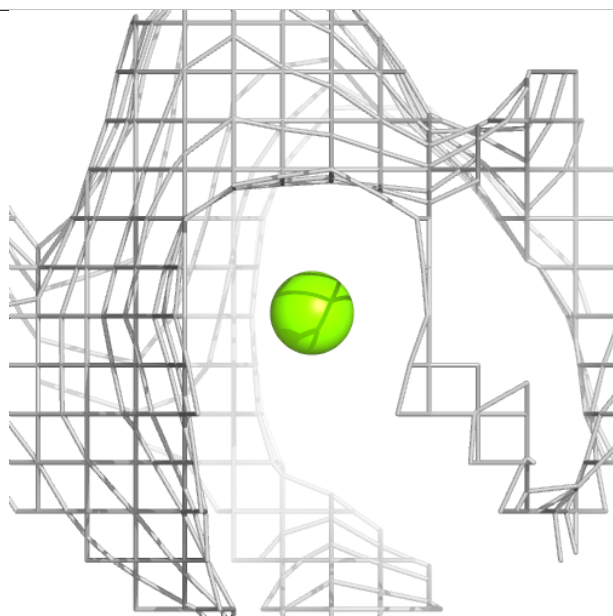
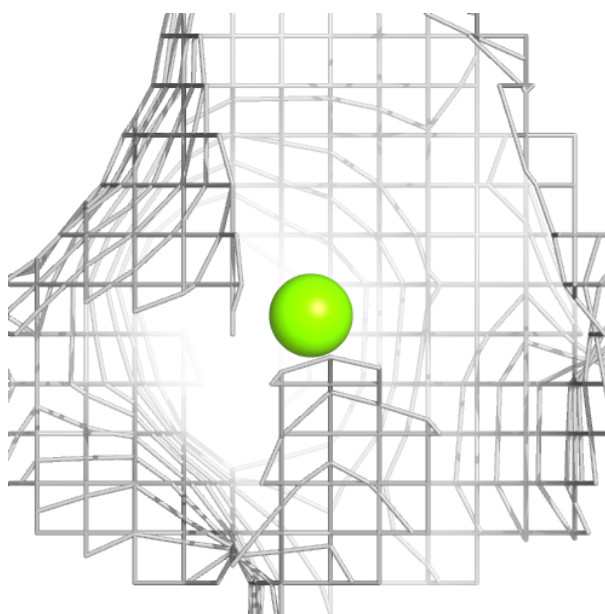
**Electron density around CL C 302:**

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



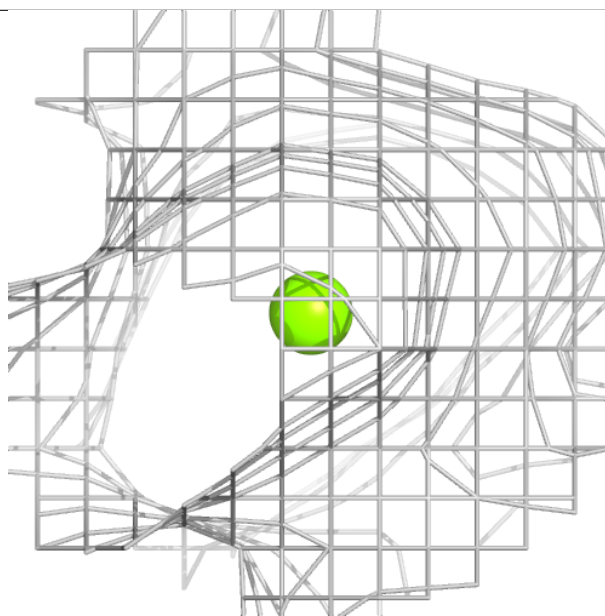
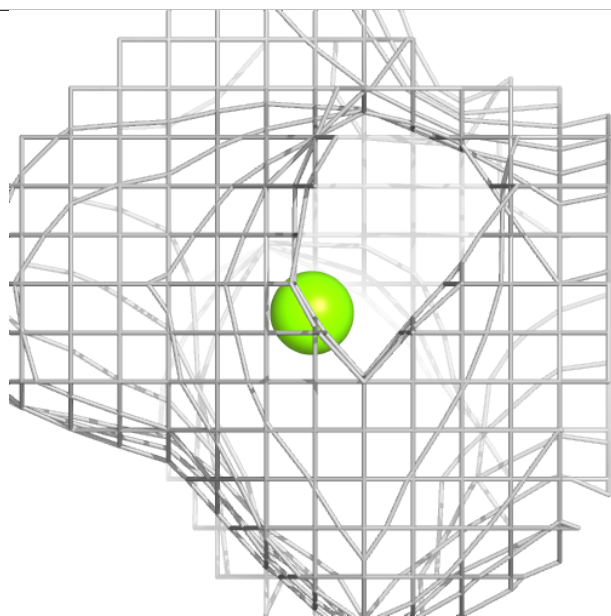
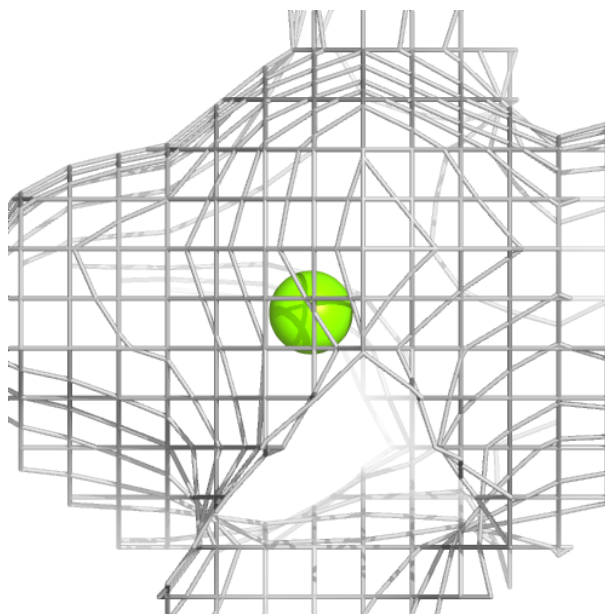
**Electron density around MG A 301:**

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



**Electron density around MG C 301:**

$2mF_o-DF_c$  (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.