wwPDB X-ray Structure Validation Summary Report (i)

Nov 21, 2023 – 02:22 AM JST

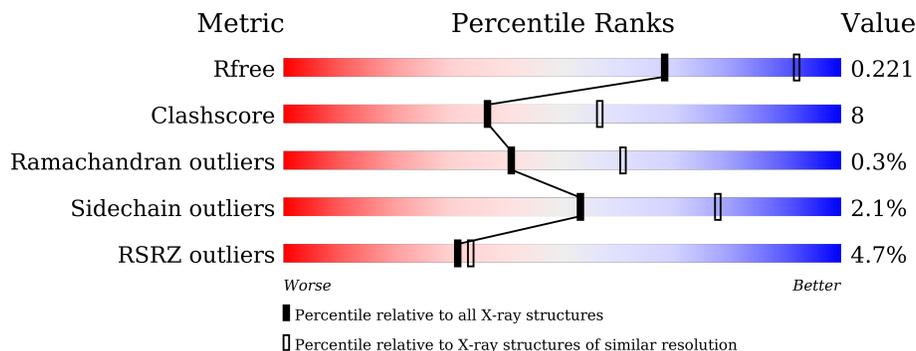|		
PDB ID	:	7EGR
Title	:	Co-crystal structure of Ac-AChBPP in complex with RgIA
Authors	:	Wang, X.Q.; Pan, S.; Fan, Y.X.; Xue, Y.; Zhu, X.P.; Luo, S.L.
Deposited on	:	2021-03-26
Resolution	:	2.50 Å(reported)

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 2.50 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.
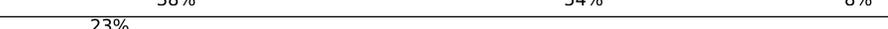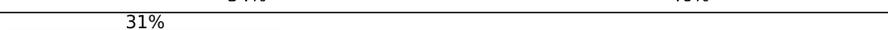
Metric	Percentile Ranks	Value
Rfree		0.221
Clashscore		8
Ramachandran outliers		0.3%
Sidechain outliers		2.1%
RSRZ outliers		4.7%

Worse — *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	206	4% / 85% / 14% ·
1	D	206	3% / 91% / 9%
1	G	206	4% / 73% / 25% ·
1	H	206	4% / 90% / 9%
1	I	206	3% / 81% / 18% ·
1	J	206	2% / 85% / 14% ·

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Mol	Chain	Length	Quality of chain
2	B	204	90% 9%
2	C	204	2% 87% 13%
3	E	205	3% 83% 15% ·
3	F	205	3% 88% 12%
4	K	13	46% 62% 38%
4	L	13	31% 38% 54% 8%
4	M	13	23% 54% 46%
4	N	13	62% 46% 23% 31%
4	O	13	46% 54% 46%
4	P	13	31% 62% 31% 8%
4	Q	13	8% 62% 23% 15%
4	R	13	54% 46% 46% 8%

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 17680 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 Soluble acetylcholine receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1638	1035	267	327	9			
1	D	206	Total	C	N	O	S	0	0	0
			1638	1035	267	327	9			
1	G	206	Total	C	N	O	S	0	0	0
			1638	1035	267	327	9			
1	H	206	Total	C	N	O	S	0	0	0
			1638	1035	267	327	9			
1	I	206	Total	C	N	O	S	0	0	0
			1638	1035	267	327	9			
1	J	206	Total	C	N	O	S	0	0	0
			1638	1035	267	327	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	VAL	ALA	conflict	UNP Q8WSF8
A	155	VAL	ALA	conflict	UNP Q8WSF8
D	60	VAL	ALA	conflict	UNP Q8WSF8
D	155	VAL	ALA	conflict	UNP Q8WSF8
G	60	VAL	ALA	conflict	UNP Q8WSF8
G	155	VAL	ALA	conflict	UNP Q8WSF8
H	60	VAL	ALA	conflict	UNP Q8WSF8
H	155	VAL	ALA	conflict	UNP Q8WSF8
I	60	VAL	ALA	conflict	UNP Q8WSF8
I	155	VAL	ALA	conflict	UNP Q8WSF8
J	60	VAL	ALA	conflict	UNP Q8WSF8
J	155	VAL	ALA	conflict	UNP Q8WSF8

- Molecule 2 is a protein called Soluble acetylcholine receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	204	Total 1621	C 1026	N 262	O 324	S 9	0	0	0
2	C	204	Total 1621	C 1026	N 262	O 324	S 9	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	60	VAL	ALA	conflict	UNP Q8WSF8
B	155	VAL	ALA	conflict	UNP Q8WSF8
C	60	VAL	ALA	conflict	UNP Q8WSF8
C	155	VAL	ALA	conflict	UNP Q8WSF8

- Molecule 3 is a protein called Soluble acetylcholine receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	205	Total 1627	C 1029	N 263	O 326	S 9	0	0	0
3	F	205	Total 1627	C 1029	N 263	O 326	S 9	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	60	VAL	ALA	conflict	UNP Q8WSF8
E	155	VAL	ALA	conflict	UNP Q8WSF8
F	60	VAL	ALA	conflict	UNP Q8WSF8
F	155	VAL	ALA	conflict	UNP Q8WSF8

- Molecule 4 is a protein called RgIA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	13	Total 105	C 59	N 25	O 17	S 4	0	0	0
4	L	13	Total 105	C 59	N 25	O 17	S 4	0	0	0
4	M	13	Total 105	C 59	N 25	O 17	S 4	0	0	0
4	N	13	Total 105	C 59	N 25	O 17	S 4	0	0	0
4	O	13	Total 105	C 59	N 25	O 17	S 4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	13	Total	C	N	O	S	0	0	0
			105	59	25	17	4			
4	R	13	Total	C	N	O	S	0	0	0
			105	59	25	17	4			
4	Q	13	Total	C	N	O	S	0	0	0
			105	59	25	17	4			

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	E	1	Total	Mg	0	0
			1	1		
5	H	1	Total	Mg	0	0
			1	1		
5	J	1	Total	Mg	0	0
			1	1		
5	N	1	Total	Mg	0	0
			1	1		
5	O	1	Total	Mg	0	0
			1	1		
5	R	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	47	Total	O	0	0
			47	47		
6	B	71	Total	O	0	0
			71	71		
6	C	50	Total	O	0	0
			50	50		
6	D	45	Total	O	0	0
			45	45		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	59	Total 59	O 59	0	0
6	F	47	Total 47	O 47	0	0
6	G	38	Total 38	O 38	0	0
6	H	46	Total 46	O 46	0	0
6	I	56	Total 56	O 56	0	0
6	J	44	Total 44	O 44	0	0
6	K	1	Total 1	O 1	0	0
6	P	1	Total 1	O 1	0	0
6	Q	1	Total 1	O 1	0	0

3   Residue-property plots ⓘ

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

• Molecule 1: Soluble acetylcholine receptor

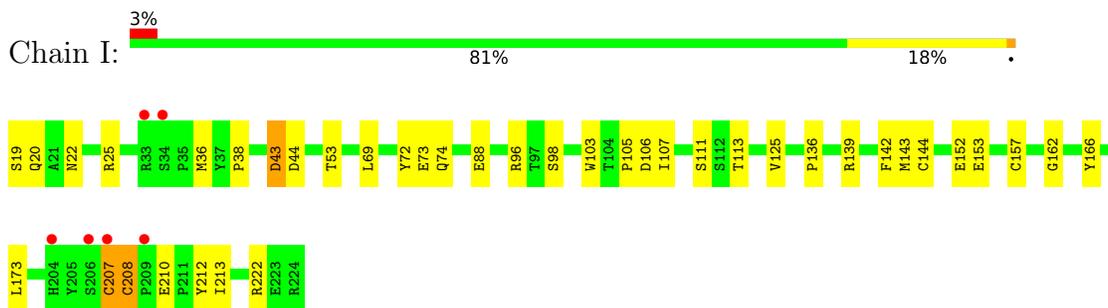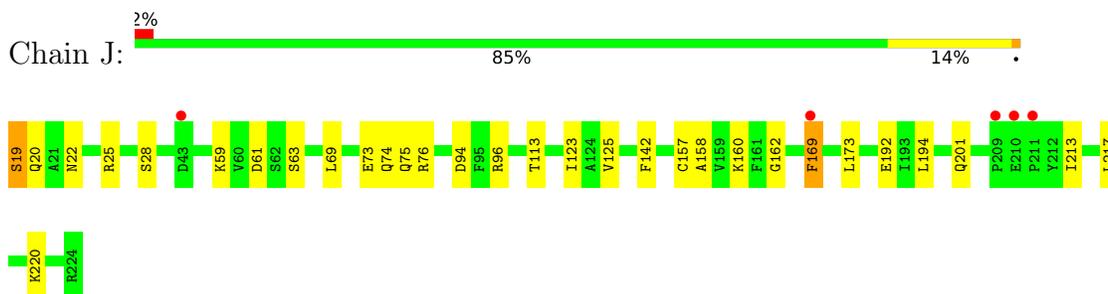• Molecule 1: Soluble acetylcholine receptor

• Molecule 1: Soluble acetylcholine receptor

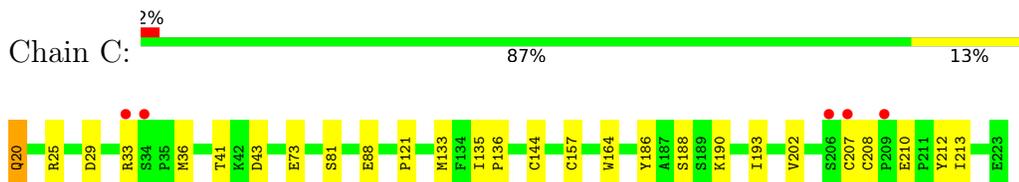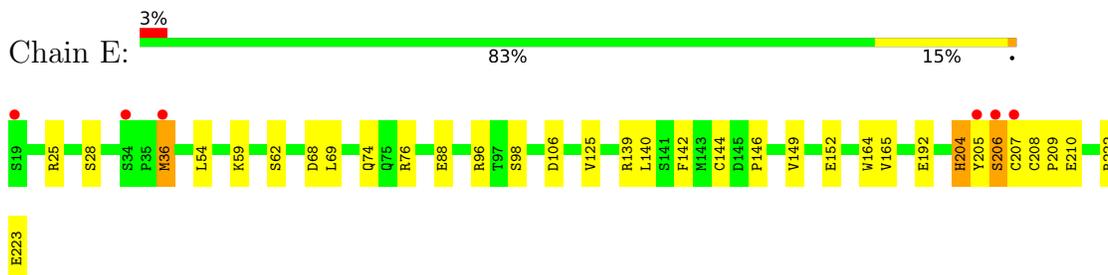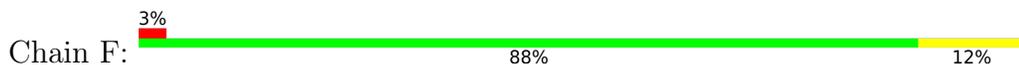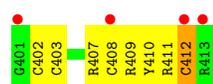• Molecule 1: Soluble acetylcholine receptor

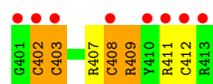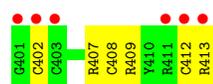• Molecule 1: Soluble acetylcholine receptor

Chain I:

3%

81%   18%

S19 Q20 A21 N22 R25 R33 S34 P35 M36 Y37 P38 D43 D44 T53 L69 Y72 E73 Q74 E88 R96 T97 S98 W103 T104 P105 D106 I107 S111 S112 T113 V125 P136 R139 F142 M143 C144 E152 E153 C157 G162 Y166

L173 H204 Y205 S206 C207 C208 P209 E210 P211 Y212 I213 R222 E223 R224

• Molecule 1: Soluble acetylcholine receptor

Chain J:

2%

85%   14%

S19 Q20 A21 N22 R25 S28 D43 K59 V60 D61 S62 S63 L69 E73 Q74 Q75 R76 D94 F95 R96 T113 I123 A124 V125 F142 C157 A158 V159 K160 F161 G162 F169 L173 E192 I193 L194 Q201 P209 E210 P211 Y212 I213 L217

K220 R224

• Molecule 2: Soluble acetylcholine receptor

Chain B:

90%   9%

Q20 R25 R33 S62 D68 L69 Y72 R76 E88 R96 D106 I123 A124 V125 R139 L140 S141 F142 M143 C144 E153 C157 D176 K190 E223

• Molecule 2: Soluble acetylcholine receptor

Chain C:

2%

87%   13%

Q20 R25 D29 R33 S34 P35 M36 T41 K42 D43 E73 S81 E88 P121 M133 F134 I135 P136 C144 C157 W164 Y186 A187 S188 S189 K190 I193 V202 S206 C207 C208 P209 E210 P211 Y212 I213 E223

• Molecule 3: Soluble acetylcholine receptor

Chain E:

3%

83%   15%

S19 R25 S28 S34 P35 M36 L54 K59 S62 D68 L69 Q74 Q75 R76 E88 R96 T97 S98 D106 V125 R139 L140 S141 F142 M143 C144 D145 P146 V149 E152 W164 V165 E192 H204 Y205 S206 C207 C208 P209 E210 R222

E223

• Molecule 3: Soluble acetylcholine receptor

Chain F:

3%

88%   12%

S19 N22 L23 M24 D29 R33 S34 T53 L54 Q55 N65 D68 L69 Y72 R96 V125 D129 G130 S131 L140 S141 F142 S163 W164 V165 D181 S195 Y205 S206 C207 C208 P209 E210 P211 Y212 E223

• Molecule 4: RgIA

Chain K:

46%

62%

38%

G401 C402 C403 R407 C408 R409 Y410 R411 C412 R413

• Molecule 4: RgIA

Chain L:

31%

38%

54%

8%

G401 C402 C403 R407 C408 R409 Y410 R411 C412 R413

• Molecule 4: RgIA

Chain M:

23%

54%

46%

G401 C402 R407 C408 R409 Y410 R411 C412 R413

• Molecule 4: RgIA

Chain N:

62%

46%

23%

31%

G401 C402 C403 R407 C408 R409 Y410 R411 C412 R413

• Molecule 4: RgIA

Chain O:

46%

54%

46%

G401 C402 C403 R407 C408 R409 Y410 R411 C412 R413

• Molecule 4: RgIA

Chain P:

31%

62%

31%

8%

G401 C402 C403 S404 D405 R409 Y410 R411 C412 R413

• Molecule 4: RgIA

Chain R:

• Molecule 4: RgIA

Chain Q:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	206.27Å 135.96Å 132.07Å 90.00° 101.16° 90.00°	Depositor
Resolution (Å)	35.40 – 2.50 35.40 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.4 (35.40-2.50) 98.4 (35.40-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.172 , 0.221 0.173 , 0.221	Depositor DCC
R_{free} test set	5894 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	35.0	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.0	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17680	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	0.44	0/1678	0.62	1/2289 (0.0%)
1	D	0.42	0/1678	0.60	0/2289
1	G	0.46	0/1678	0.66	1/2289 (0.0%)
1	H	0.42	0/1678	0.61	1/2289 (0.0%)
1	I	0.44	0/1678	0.65	3/2289 (0.1%)
1	J	0.41	0/1678	0.59	1/2289 (0.0%)
2	B	0.46	0/1661	0.63	1/2267 (0.0%)
2	C	0.47	0/1661	0.65	2/2267 (0.1%)
3	E	0.44	0/1667	0.60	0/2275
3	F	0.41	0/1667	0.60	0/2275
4	K	0.90	1/106 (0.9%)	0.76	0/139
4	L	0.47	0/106	0.79	0/139
4	M	0.65	0/106	0.78	0/139
4	N	0.89	1/106 (0.9%)	1.03	0/139
4	O	0.58	0/106	0.80	0/139
4	P	0.70	0/106	1.09	1/139 (0.7%)
4	Q	0.55	0/106	0.98	1/139 (0.7%)
4	R	0.58	0/106	0.80	0/139
All	All	0.45	2/17572 (0.0%)	0.64	12/23930 (0.1%)

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	A	0	1
1	I	0	1
3	E	0	1
3	F	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	408	CYS	CB-SG	-6.15	1.71	1.82
4	K	403	CYS	CB-SG	5.46	1.91	1.82

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	26	LEU	CA-CB-CG	7.26	132.01	115.30
1	A	157	CYS	CA-CB-SG	-7.21	101.02	114.00
1	I	208	CYS	CA-CB-SG	7.18	126.93	114.00
4	P	412	CYS	CA-CB-SG	6.71	126.08	114.00
4	Q	413	ARG	NE-CZ-NH1	6.65	123.62	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	207	CYS	Peptide
3	E	204	HIS	Peptide
3	F	207	CYS	Peptide
1	I	207	CYS	Peptide

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	1638	0	1560	22	0
1	D	1638	0	1560	20	0
1	G	1638	0	1560	53	0
1	H	1638	0	1562	22	0
1	I	1638	0	1560	40	0
1	J	1638	0	1560	20	0
2	B	1621	0	1544	18	0
2	C	1621	0	1544	21	0
3	E	1627	0	1549	26	0
3	F	1627	0	1547	18	0
4	K	105	0	94	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	105	0	96	8	0
4	M	105	0	96	11	0
4	N	105	0	98	12	0
4	O	105	0	97	5	0
4	P	105	0	94	7	0
4	Q	105	0	95	10	0
4	R	105	0	96	13	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	H	1	0	0	0	0
5	J	1	0	0	0	0
5	N	1	0	0	0	0
5	O	1	0	0	0	0
5	R	1	0	0	0	0
6	A	47	0	0	1	0
6	B	71	0	0	2	0
6	C	50	0	0	3	0
6	D	45	0	0	1	0
6	E	59	0	0	2	0
6	F	47	0	0	1	0
6	G	38	0	0	0	0
6	H	46	0	0	0	0
6	I	56	0	0	1	0
6	J	44	0	0	1	0
6	K	1	0	0	0	0
6	P	1	0	0	0	0
6	Q	1	0	0	0	0
All	All	17680	0	16312	256	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.

The worst 5 of 256 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)
3:F:96:ARG:HD2	3:F:125:VAL:HG22	1.26	1.15
1:H:74:GLN:OE1	4:R:409:ARG:HD3	1.61	1.00
1:G:202:VAL:HG22	1:G:213:ILE:HD12	1.42	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:208:CYS:HB3	3:E:210:GLU:OE1	1.62	0.98
1:J:160:LYS:HE2	1:J:201:GLN:HE22	1.28	0.97

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	204/206 (99%)	200 (98%)	4 (2%)	0	100	100
1	D	204/206 (99%)	199 (98%)	4 (2%)	1 (0%)	29	48
1	G	204/206 (99%)	199 (98%)	5 (2%)	0	100	100
1	H	204/206 (99%)	199 (98%)	4 (2%)	1 (0%)	29	48
1	I	204/206 (99%)	194 (95%)	9 (4%)	1 (0%)	29	48
1	J	204/206 (99%)	197 (97%)	7 (3%)	0	100	100
2	B	202/204 (99%)	198 (98%)	4 (2%)	0	100	100
2	C	202/204 (99%)	196 (97%)	6 (3%)	0	100	100
3	E	203/205 (99%)	196 (97%)	6 (3%)	1 (0%)	29	48
3	F	203/205 (99%)	196 (97%)	6 (3%)	1 (0%)	29	48
4	K	11/13 (85%)	11 (100%)	0	0	100	100
4	L	11/13 (85%)	10 (91%)	0	1 (9%)	1	0
4	M	11/13 (85%)	8 (73%)	3 (27%)	0	100	100
4	N	11/13 (85%)	8 (73%)	3 (27%)	0	100	100
4	O	11/13 (85%)	8 (73%)	3 (27%)	0	100	100
4	P	11/13 (85%)	7 (64%)	4 (36%)	0	100	100
4	Q	11/13 (85%)	10 (91%)	1 (9%)	0	100	100
4	R	11/13 (85%)	10 (91%)	1 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2122/2158 (98%)	2046 (96%)	70 (3%)	6 (0%)	41 61

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	206	SER
1	H	207	CYS
4	L	412	CYS
1	D	207	CYS
1	I	208	CYS

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	187/189 (99%)	183 (98%)	4 (2%)	53	78
1	D	187/189 (99%)	187 (100%)	0	100	100
1	G	187/189 (99%)	182 (97%)	5 (3%)	44	71
1	H	187/189 (99%)	183 (98%)	4 (2%)	53	78
1	I	187/189 (99%)	183 (98%)	4 (2%)	53	78
1	J	187/189 (99%)	180 (96%)	7 (4%)	34	60
2	B	185/187 (99%)	183 (99%)	2 (1%)	73	89
2	C	185/187 (99%)	184 (100%)	1 (0%)	88	96
3	E	186/188 (99%)	180 (97%)	6 (3%)	39	65
3	F	186/188 (99%)	185 (100%)	1 (0%)	88	96
4	K	12/12 (100%)	12 (100%)	0	100	100
4	L	12/12 (100%)	12 (100%)	0	100	100
4	M	12/12 (100%)	12 (100%)	0	100	100
4	N	12/12 (100%)	9 (75%)	3 (25%)	0	1
4	O	12/12 (100%)	11 (92%)	1 (8%)	11	22
4	P	12/12 (100%)	11 (92%)	1 (8%)	11	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Q	12/12 (100%)	10 (83%)	2 (17%)	2	4
4	R	12/12 (100%)	11 (92%)	1 (8%)	11	22
All	All	1960/1980 (99%)	1918 (98%)	42 (2%)	53	78

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	28	SER
4	N	403	CYS
1	J	59	LYS
1	J	169	PHE
4	O	413	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	22	ASN
1	J	201	GLN
3	F	74	GLN
1	G	74	GLN
1	H	20	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 10 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	206/206 (100%)	-0.23	9 (4%)	34	37	21, 33, 71, 98	0
1	D	206/206 (100%)	-0.18	7 (3%)	45	48	22, 34, 70, 106	0
1	G	206/206 (100%)	-0.16	9 (4%)	34	37	23, 38, 76, 109	0
1	H	206/206 (100%)	-0.21	8 (3%)	39	42	24, 37, 70, 117	0
1	I	206/206 (100%)	-0.22	6 (2%)	51	55	22, 35, 71, 130	0
1	J	206/206 (100%)	-0.31	5 (2%)	59	62	23, 37, 69, 94	0
2	B	204/204 (100%)	-0.54	0	100	100	21, 30, 54, 86	0
2	C	204/204 (100%)	-0.39	5 (2%)	57	61	20, 32, 71, 94	0
3	E	205/205 (100%)	-0.30	6 (2%)	51	55	21, 32, 82, 136	0
3	F	205/205 (100%)	-0.21	7 (3%)	45	48	25, 37, 74, 111	0
4	K	13/13 (100%)	1.75	6 (46%)	0	0	58, 74, 110, 116	0
4	L	13/13 (100%)	1.94	4 (30%)	0	0	55, 83, 108, 122	0
4	M	13/13 (100%)	1.47	3 (23%)	0	0	58, 90, 104, 119	0
4	N	13/13 (100%)	3.00	8 (61%)	0	0	62, 96, 123, 124	0
4	O	13/13 (100%)	1.77	6 (46%)	0	0	60, 91, 115, 129	0
4	P	13/13 (100%)	1.57	4 (30%)	0	0	63, 81, 113, 115	0
4	Q	13/13 (100%)	0.89	1 (7%)	13	13	64, 74, 99, 121	0
4	R	13/13 (100%)	2.50	7 (53%)	0	0	72, 100, 128, 143	0
All	All	2158/2158 (100%)	-0.17	101 (4%)	31	33	20, 35, 86, 143	0

The worst 5 of 101 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	L	413	ARG	7.4
4	N	412	CYS	7.1
4	R	413	ARG	7.0

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Mol	Chain	Res	Type	RSRZ
4	N	413	ARG	6.5
4	R	412	CYS	6.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	R	501	1/1	0.92	0.20	55,55,55,55	0
5	MG	N	501	1/1	0.93	0.30	58,58,58,58	0
5	MG	J	301	1/1	0.93	0.20	56,56,56,56	0
5	MG	E	301	1/1	0.96	0.27	30,30,30,30	0
5	MG	D	301	1/1	0.96	0.28	40,40,40,40	0
5	MG	H	301	1/1	0.97	0.22	43,43,43,43	0
5	MG	O	501	1/1	0.97	0.30	39,39,39,39	0
5	MG	C	301	1/1	0.97	0.35	44,44,44,44	0
5	MG	A	301	1/1	0.98	0.20	36,36,36,36	0
5	MG	B	301	1/1	1.00	0.40	23,23,23,23	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.
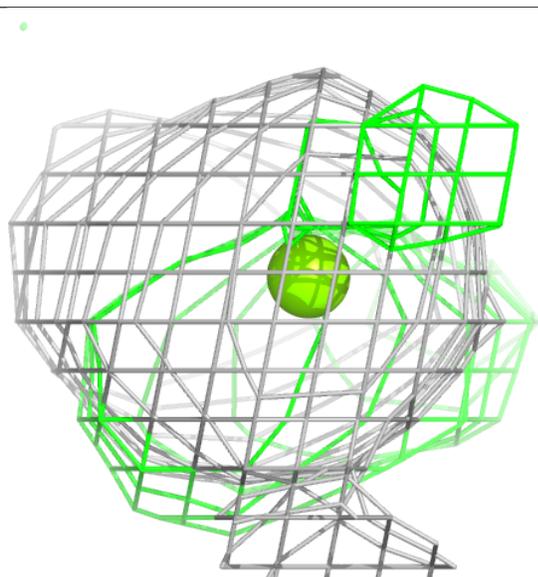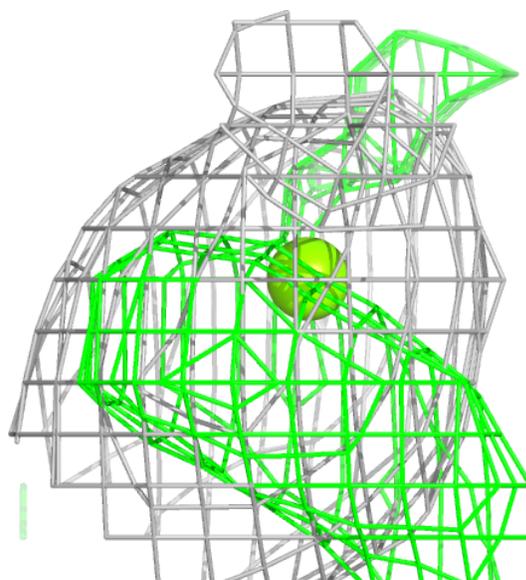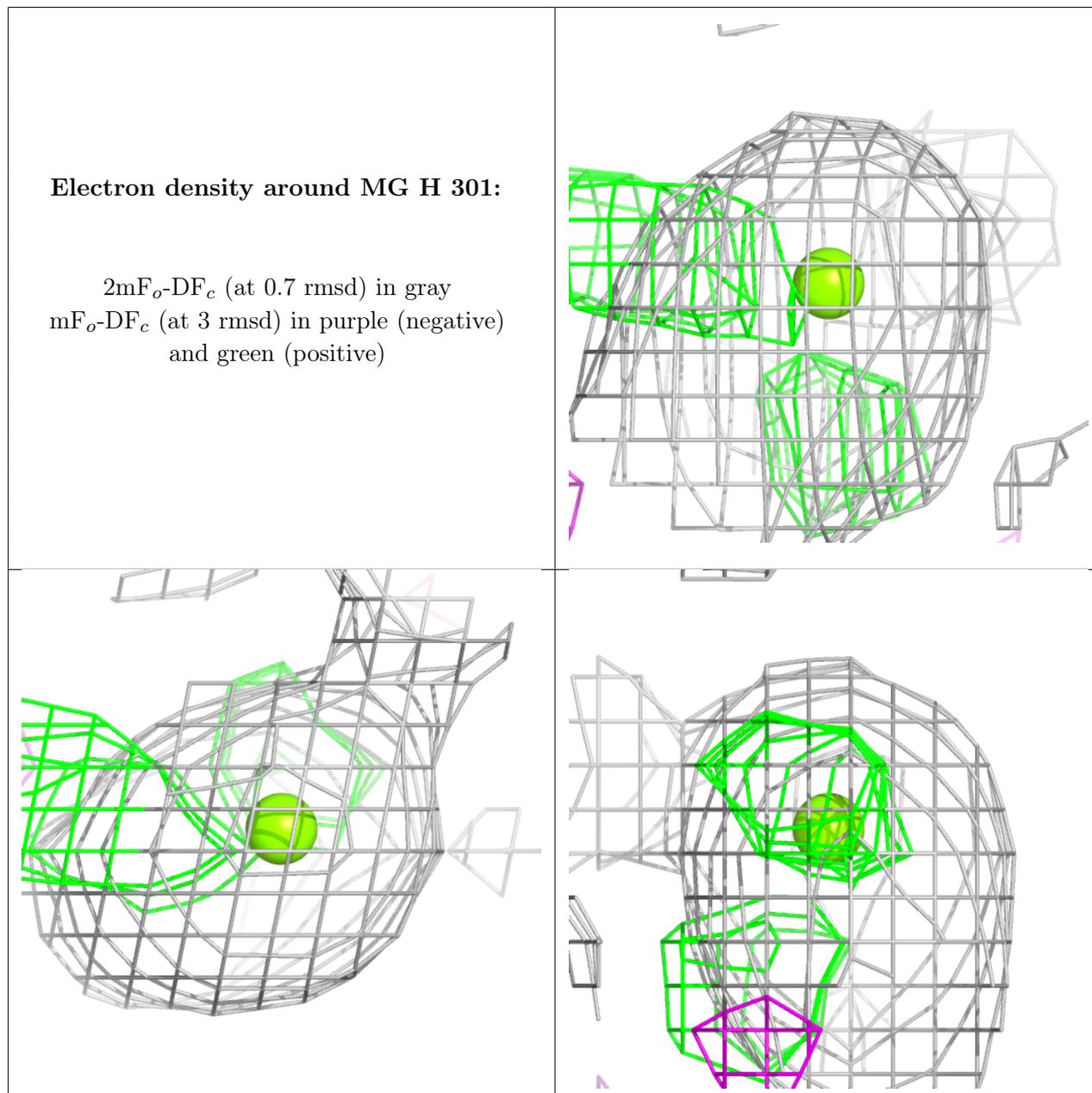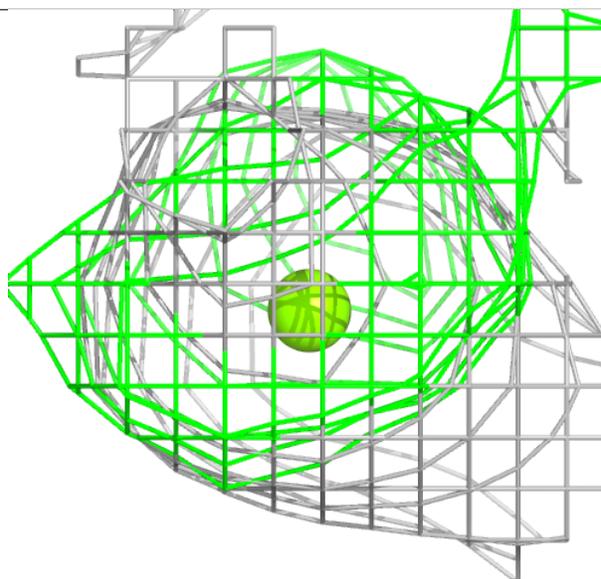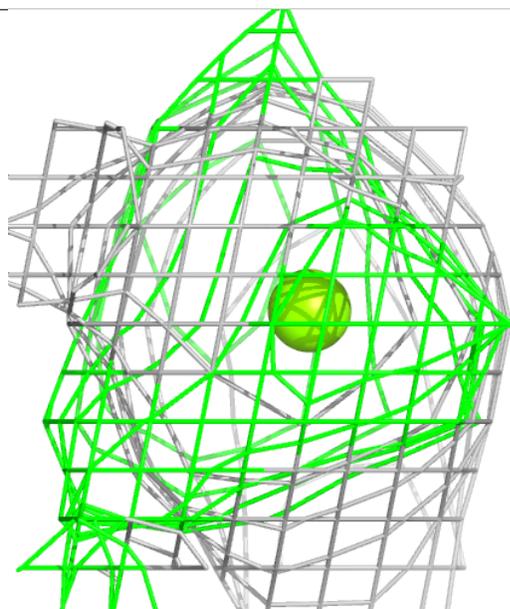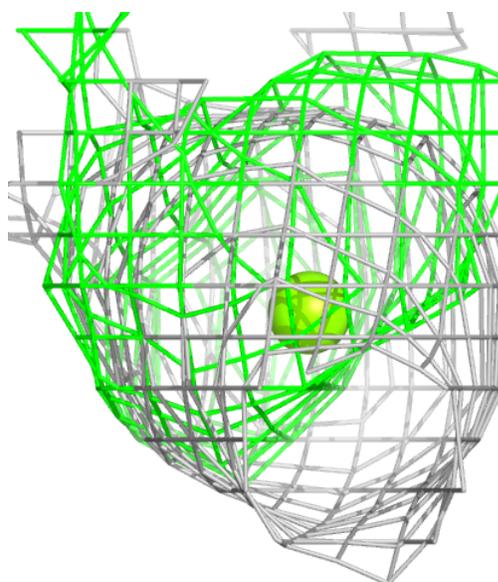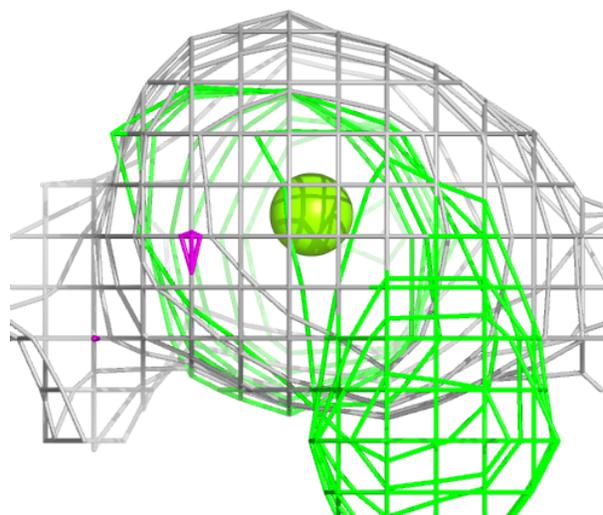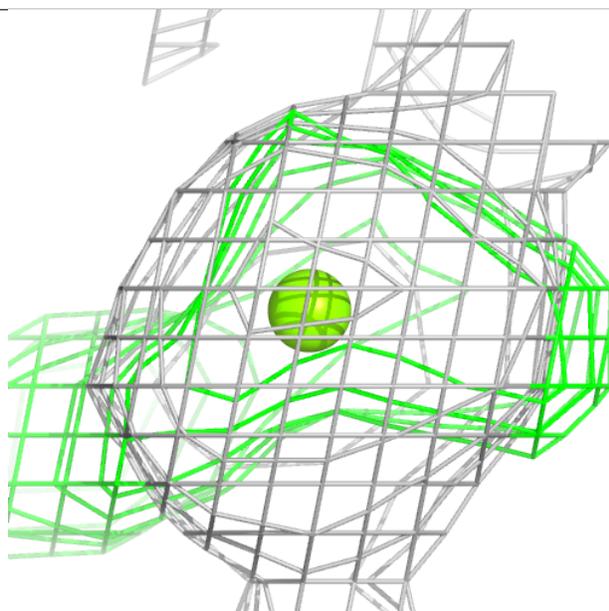
Electron density around MG R 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
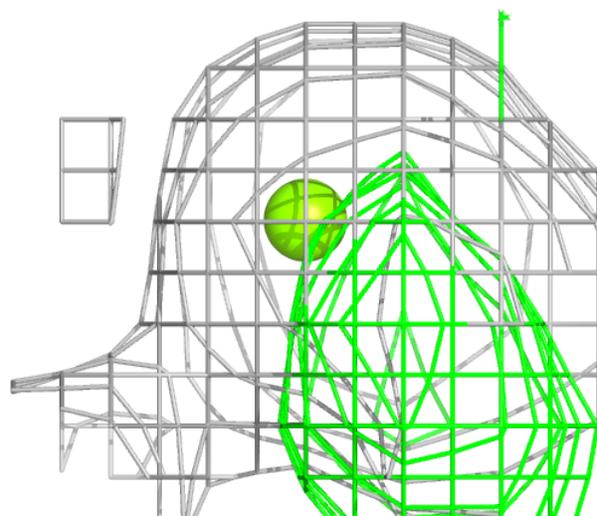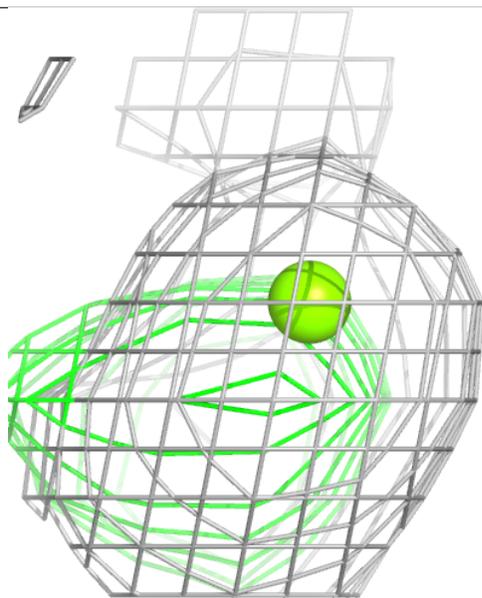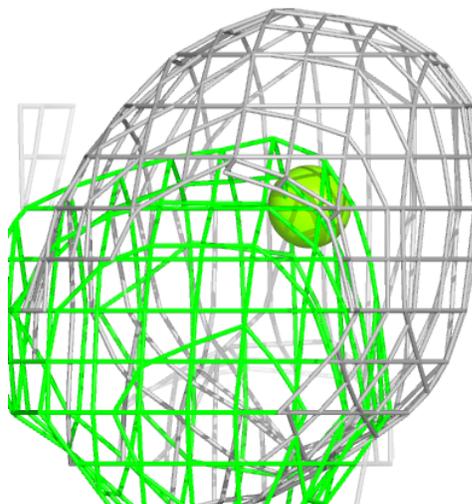
Electron density around MG N 501:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
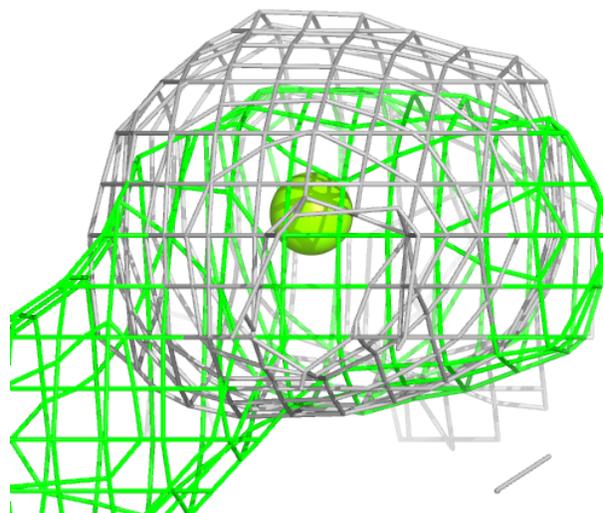and green (positive)
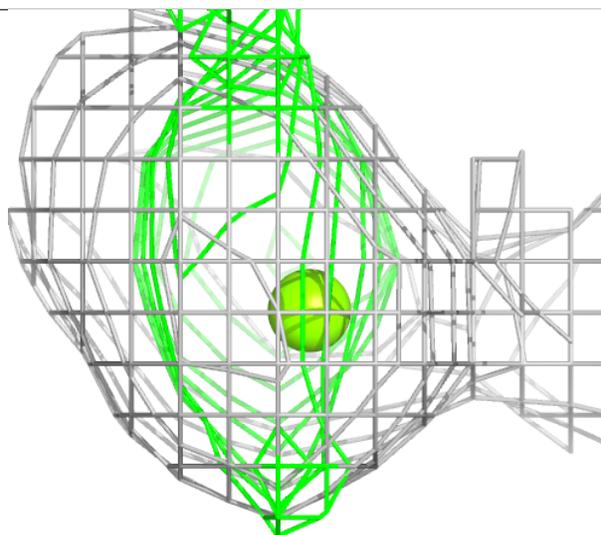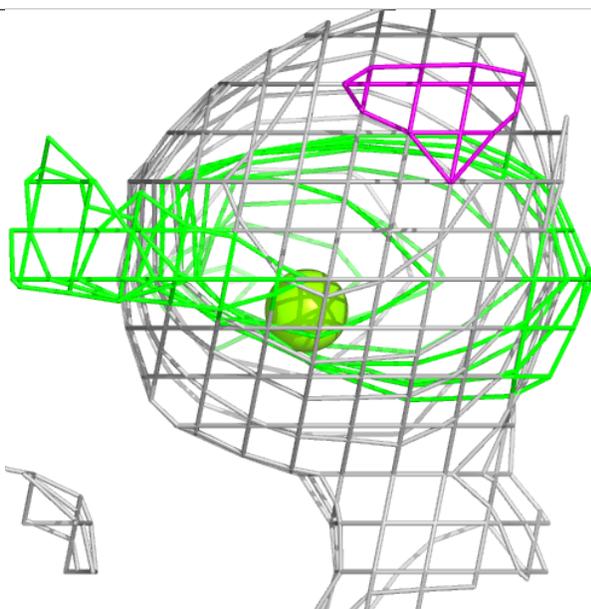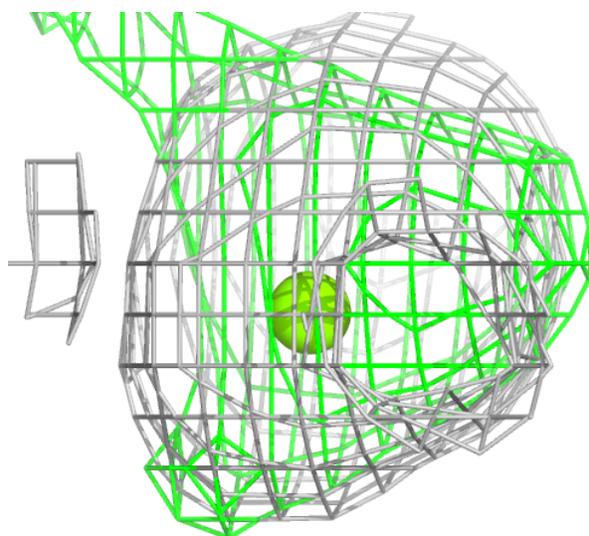
Electron density around MG J 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
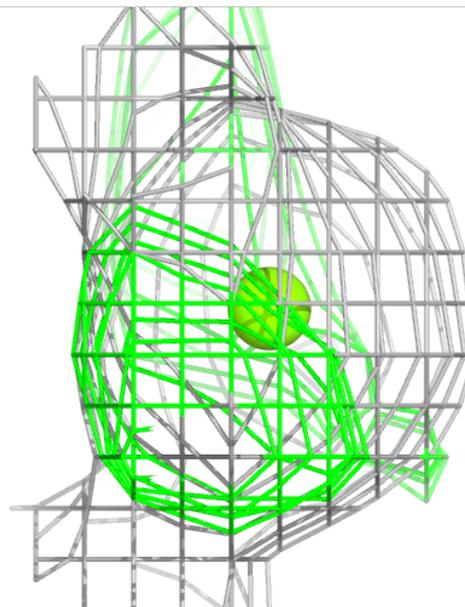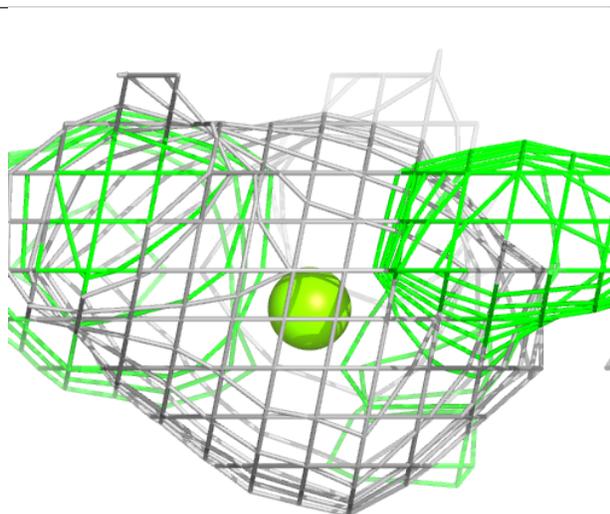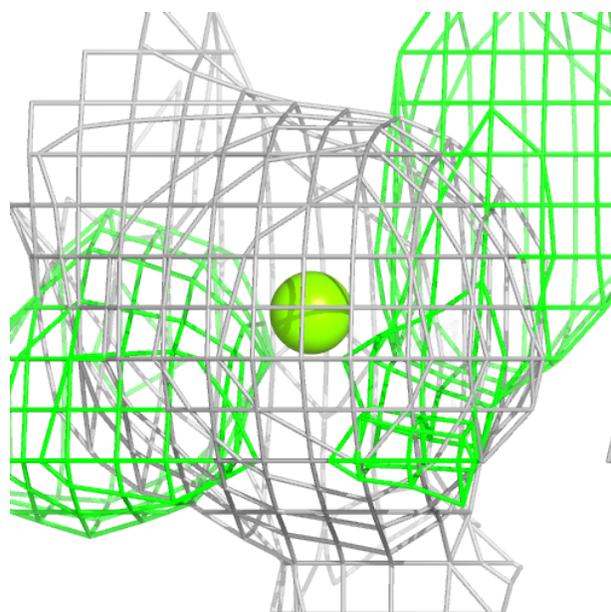
Electron density around MG E 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
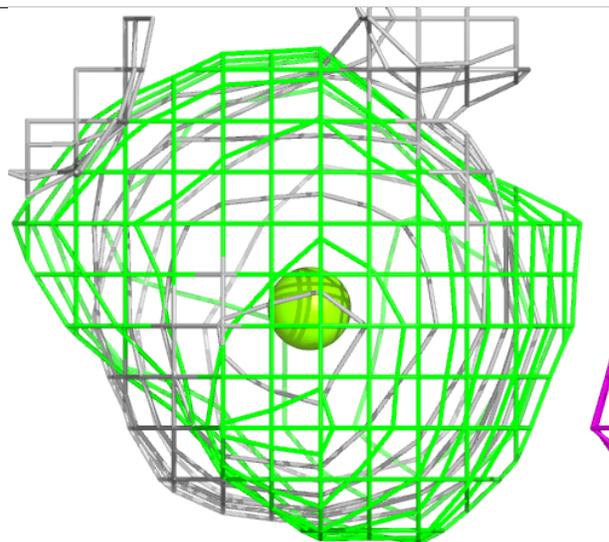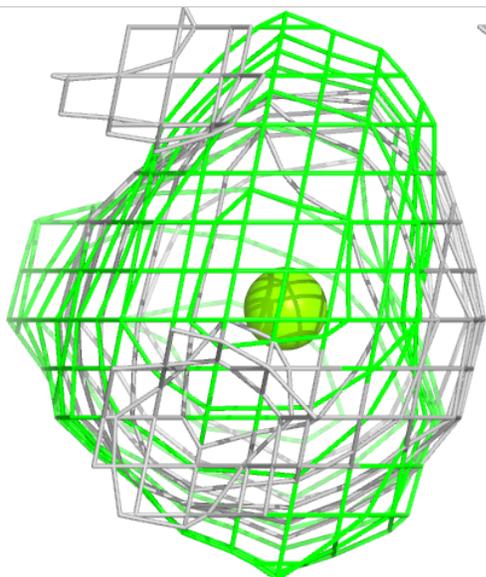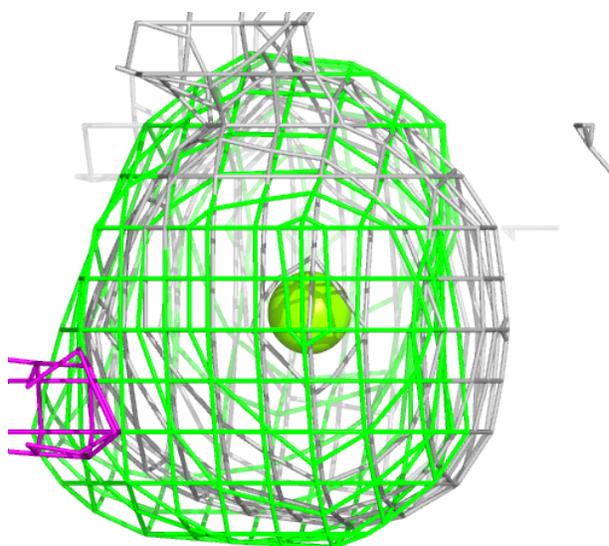
Electron density around MG D 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
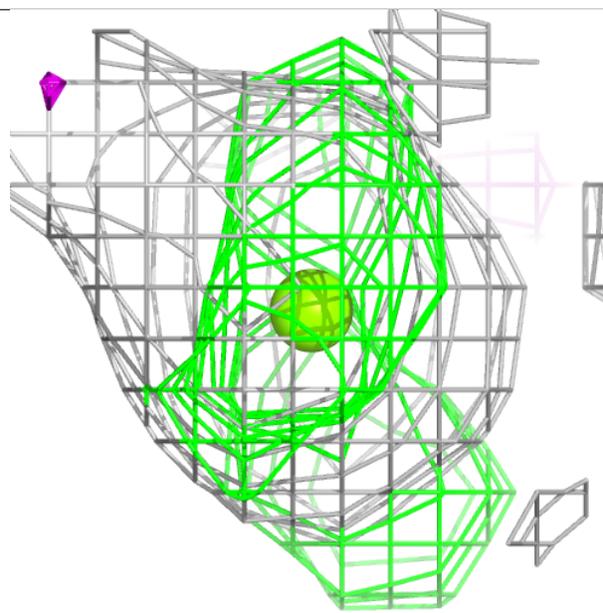$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
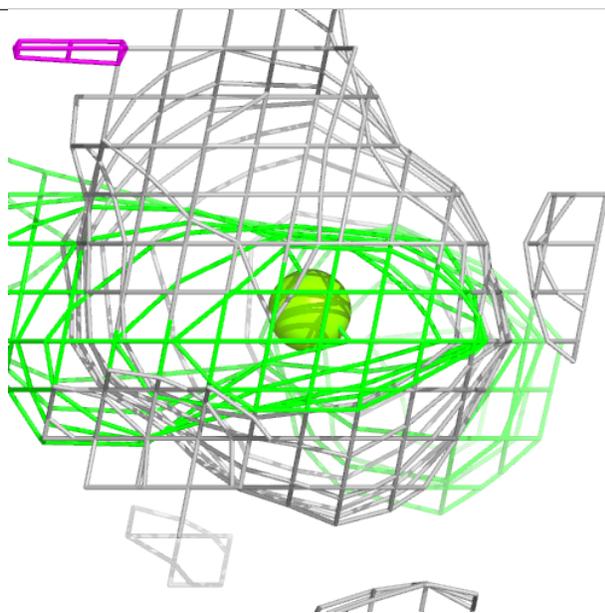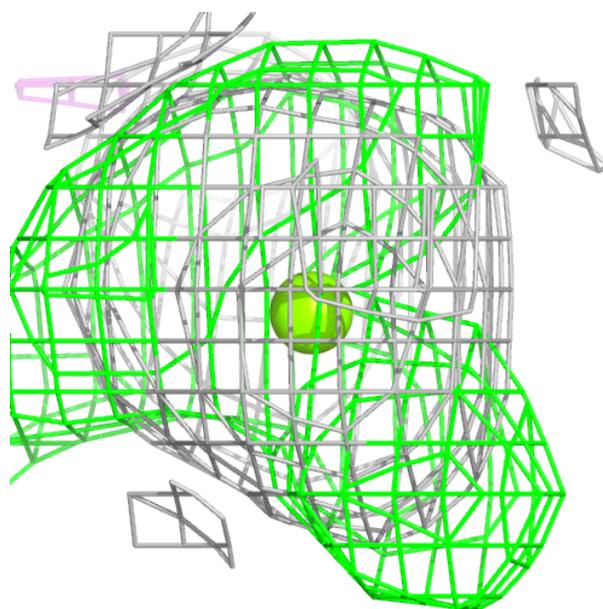and green (positive)
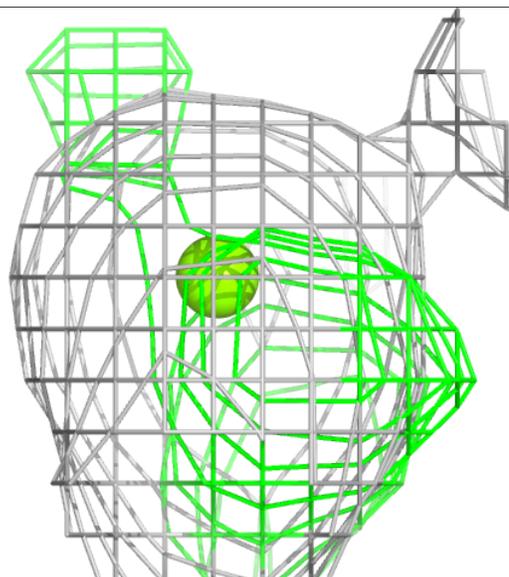
Electron density around MG H 301:

$2mF_o$-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 O 501:

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

Electron density around MG C 301:

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

Electron density around MG A 301:
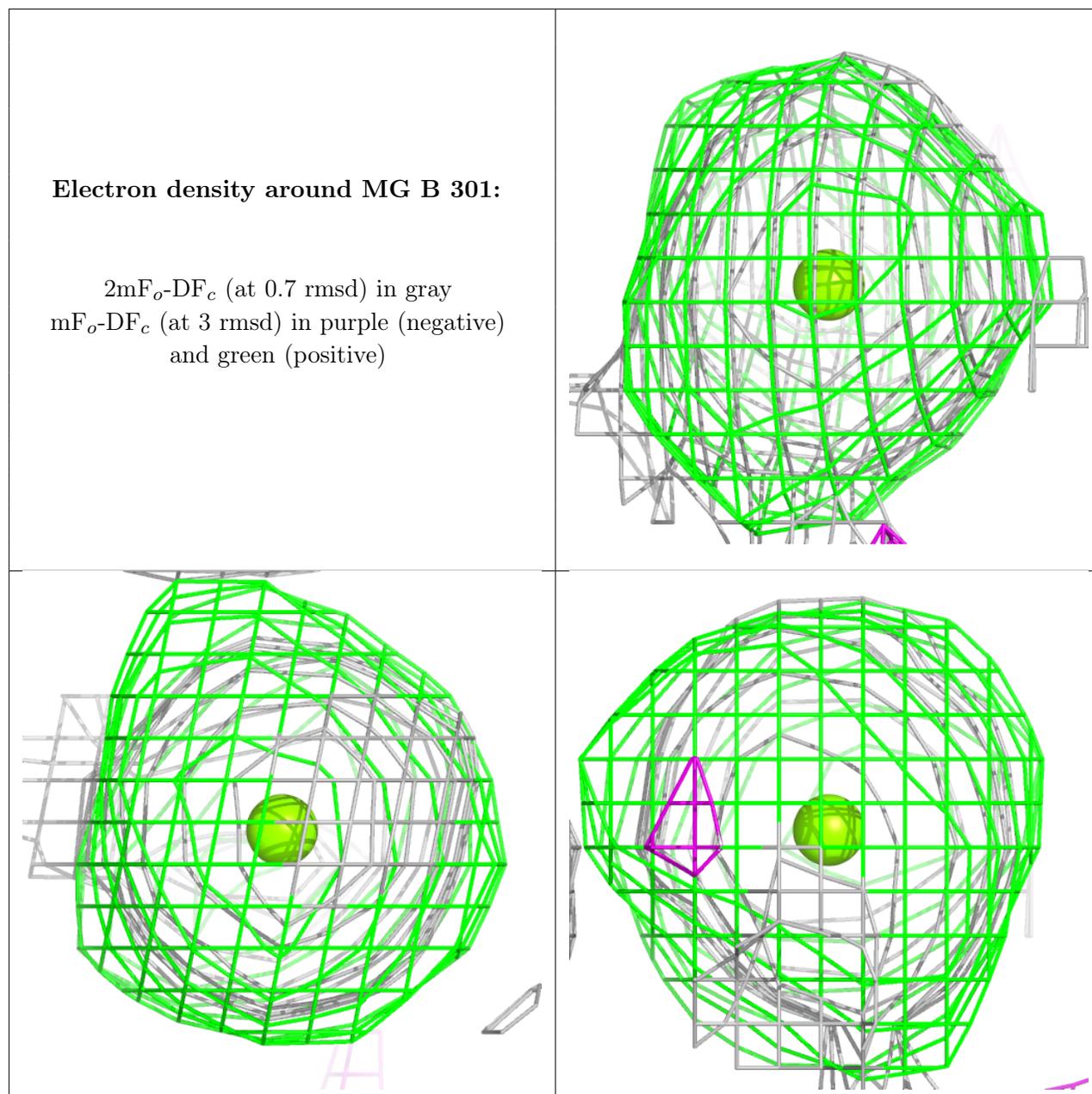
$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around MG B 301:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.