



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:03 PM UTC

PDB ID : 7EGR / pdb_00007egr
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)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

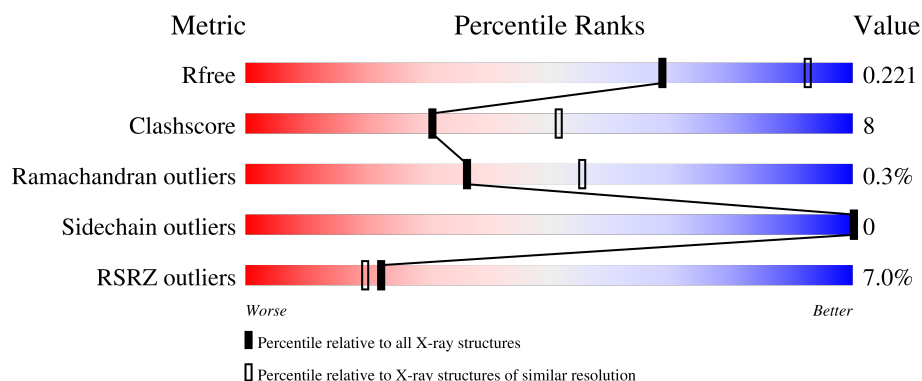
1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 $\leq 5\%$. 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	206	5% 86% 14%
1	D	206	4% 91% 9%
1	G	206	7% 75% 25%
1	H	206	4% 91% 9%
1	I	206	4% 82% 17%

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Mol	Chain	Length	Quality of chain
1	J	206	4% 86% 14%
2	B	204	% 91% 9%
2	C	204	5% 87% 12%
3	E	205	6% 84% 16%
3	F	205	5% 88% 12%
4	K	13	54% 62% 38%
4	L	13	54% 38% 54% 8%
4	M	13	54% 54% 46%
4	N	13	69% 38% 62%
4	O	13	54% 62% 38%
4	P	13	54% 62% 38%
4	Q	13	31% 69% 31%
4	R	13	69% 46% 54%

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	C	N	O	S	0	0	0
			1621	1026	262	324	9			
2	C	204	Total	C	N	O	S	0	0	0
			1621	1026	262	324	9			

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	C	N	O	S	0	0	0
			1627	1029	263	326	9			
3	F	205	Total	C	N	O	S	0	0	0
			1627	1029	263	326	9			

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	C	N	O	S	0	0	0
			105	59	25	17	4			
4	L	13	Total	C	N	O	S	0	0	0
			105	59	25	17	4			
4	M	13	Total	C	N	O	S	0	0	0
			105	59	25	17	4			
4	N	13	Total	C	N	O	S	0	0	0
			105	59	25	17	4			
4	O	13	Total	C	N	O	S	0	0	0
			105	59	25	17	4			

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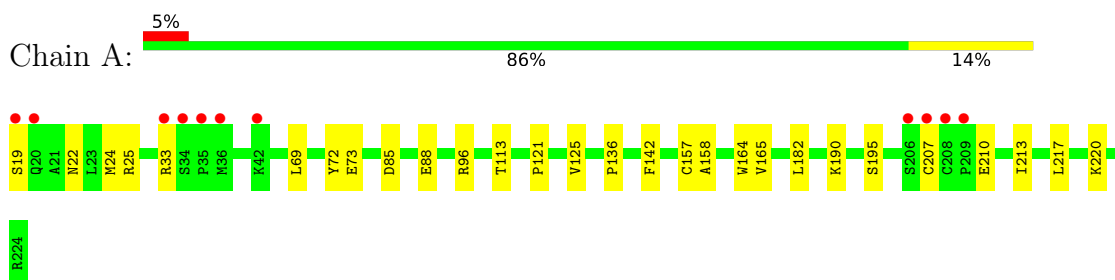
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	59	Total	O	0	0
			59	59		
6	F	47	Total	O	0	0
			47	47		
6	G	38	Total	O	0	0
			38	38		
6	H	46	Total	O	0	0
			46	46		
6	I	56	Total	O	0	0
			56	56		
6	J	44	Total	O	0	0
			44	44		
6	K	1	Total	O	0	0
			1	1	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

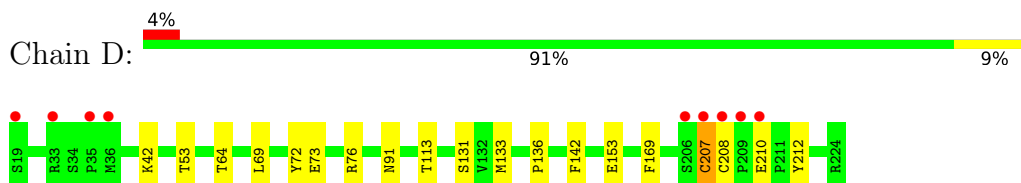
3 Residue-property plots [i](#)

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.

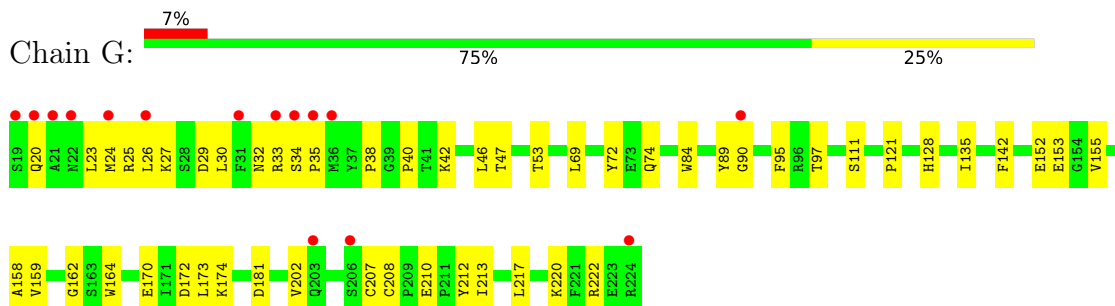
- Molecule 1: Soluble acetylcholine receptor



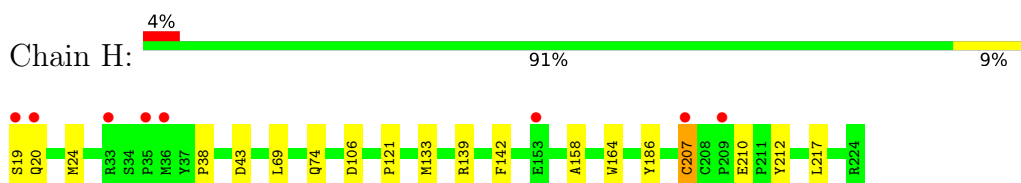
- Molecule 1: Soluble acetylcholine receptor



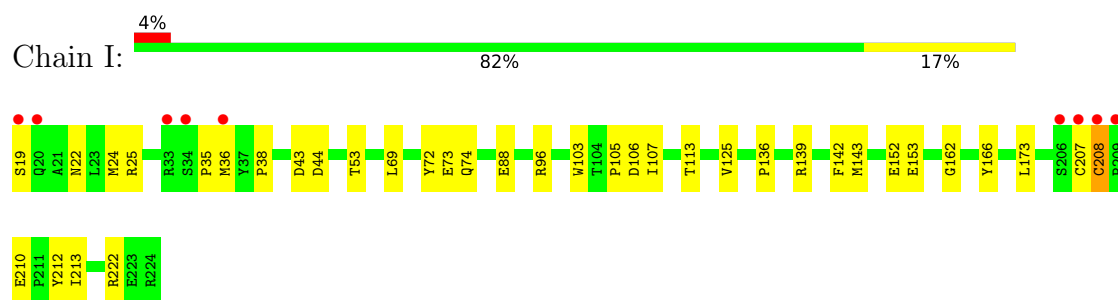
- Molecule 1: Soluble acetylcholine receptor



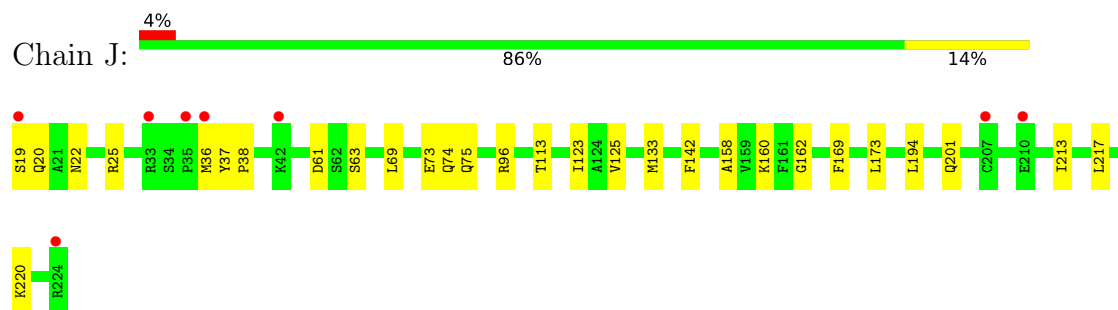
- Molecule 1: Soluble acetylcholine receptor



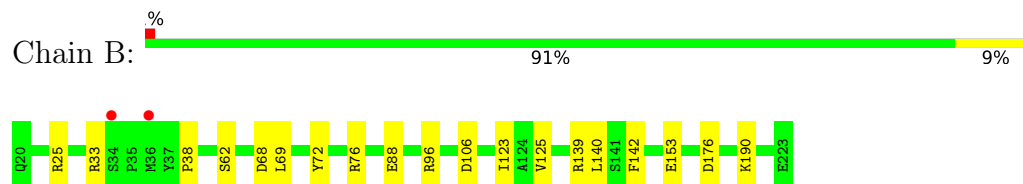
- Molecule 1: Soluble acetylcholine receptor



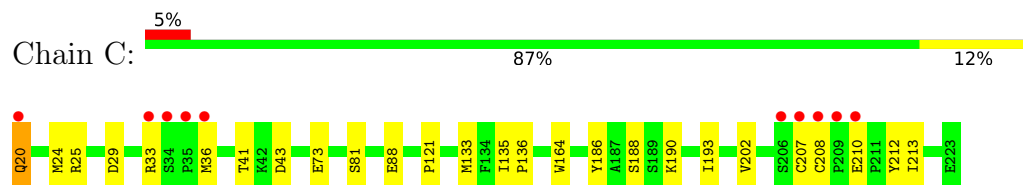
- Molecule 1: Soluble acetylcholine receptor



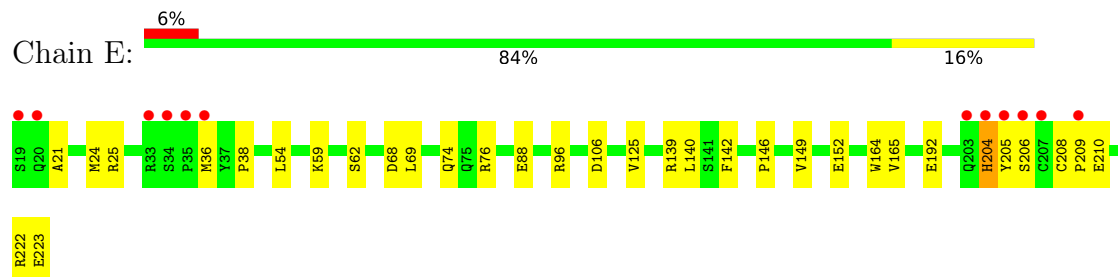
- Molecule 2: Soluble acetylcholine receptor



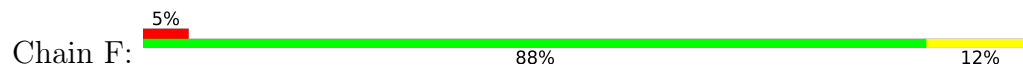
- Molecule 2: Soluble acetylcholine receptor



- Molecule 3: Soluble acetylcholine receptor

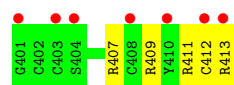


- Molecule 3: Soluble acetylcholine receptor

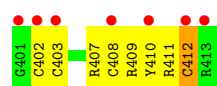




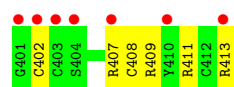
● Molecule 4: RgIA



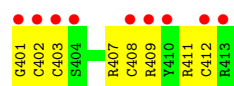
● Molecule 4: RgIA



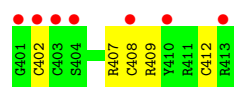
● Molecule 4: RgIA



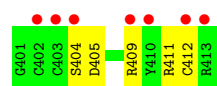
● Molecule 4: RgIA



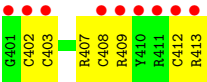
● Molecule 4: RgIA



● Molecule 4: RgIA



● Molecule 4: RgIA



● Molecule 4: RgIA



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.172 , 0.221 0.174 , 0.221	Depositor DCC
R_{free} test set	5895 reflections (4.79%)	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 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.36	0/1678	0.58	1/2289 (0.0%)
1	D	0.34	0/1678	0.53	0/2289
1	G	0.38	0/1678	0.60	0/2289
1	H	0.34	0/1678	0.57	2/2289 (0.1%)
1	I	0.37	0/1678	0.60	1/2289 (0.0%)
1	J	0.34	0/1678	0.54	0/2289
2	B	0.39	0/1661	0.55	0/2267
2	C	0.40	0/1661	0.61	1/2267 (0.0%)
3	E	0.37	0/1667	0.56	0/2275
3	F	0.34	0/1667	0.56	2/2275 (0.1%)
4	K	0.68	0/106	0.82	0/139
4	L	0.46	0/106	0.89	0/139
4	M	0.55	0/106	0.86	0/139
4	N	0.68	0/106	1.24	2/139 (1.4%)
4	O	0.53	0/106	0.92	0/139
4	P	0.53	0/106	1.09	1/139 (0.7%)
4	Q	0.56	0/106	0.81	0/139
4	R	0.45	0/106	0.93	0/139
All	All	0.37	0/17572	0.59	10/23930 (0.0%)

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

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	401	GLY	CA-C-N	-6.57	109.84	122.06
4	N	401	GLY	C-N-CA	-6.57	109.84	122.06
1	A	157	CYS	CA-CB-SG	-5.82	101.02	114.40
1	H	207	CYS	CA-C-N	5.56	135.36	121.80
1	H	207	CYS	C-N-CA	5.56	135.36	121.80
1	I	208	CYS	CA-CB-SG	5.45	126.93	114.40
3	F	64	THR	CA-C-N	-5.23	114.80	123.37
3	F	64	THR	C-N-CA	-5.23	114.80	123.37
4	P	412	CYS	CA-CB-SG	5.08	126.08	114.40
2	C	20	GLN	N-CA-C	5.04	125.11	111.00

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	23	0
1	D	1638	0	1560	21	0
1	G	1638	0	1560	53	0
1	H	1638	0	1562	26	0
1	I	1638	0	1560	44	0
1	J	1638	0	1560	24	0
2	B	1621	0	1544	19	0
2	C	1621	0	1544	22	0
3	E	1627	0	1549	29	0
3	F	1627	0	1547	18	0
4	K	105	0	94	10	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	13	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	14	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	269	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 (269) 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
1:H:74:GLN:OE1	4:R:409:ARG:CD	2.13	0.95
1:G:24:MET:SD	1:H:38:PRO:HB2	2.10	0.92
2:C:41:THR:HG22	2:C:43:ASP:H	1.35	0.89
3:F:96:ARG:CD	3:F:125:VAL:HG22	2.04	0.87
1:D:207:CYS:SG	1:D:208:CYS:N	2.49	0.85
1:H:20:GLN:HE21	1:I:38:PRO:HD2	1.45	0.80
1:J:22:ASN:HD22	1:J:25:ARG:HH21	1.28	0.80
1:H:20:GLN:NE2	1:I:38:PRO:HD2	1.98	0.79
1:J:19:SER:N	6:J:401:HOH:O	2.14	0.79
1:D:210:GLU:OE1	4:M:411:ARG:NE	2.16	0.79
4:N:402:CYS:HG	4:N:408:CYS:HG	1.08	0.77
3:E:59:LYS:NZ	6:E:402:HOH:O	2.16	0.77
1:D:210:GLU:OE1	4:M:411:ARG:CZ	2.34	0.75
1:H:20:GLN:HE21	1:I:38:PRO:CD	1.98	0.75
1:A:19:SER:HA	1:A:22:ASN:HD22	1.50	0.74
1:G:135:ILE:HD13	4:P:409:ARG:HD2	1.67	0.74
1:I:74:GLN:HE22	4:Q:409:ARG:HD2	1.52	0.74
3:F:19:SER:HA	3:F:22:ASN:HD22	1.53	0.73
1:H:74:GLN:OE1	4:R:409:ARG:HD2	1.89	0.73
1:A:195:SER:OG	1:A:220:LYS:HD2	1.89	0.73
1:G:40:PRO:HB3	1:G:46:LEU:HD22	1.71	0.73
1:J:96:ARG:HD2	1:J:125:VAL:HG22	1.71	0.73
1:G:202:VAL:HG22	1:G:213:ILE:CD1	2.19	0.72
1:A:22:ASN:OD1	1:A:25:ARG:NH2	2.23	0.72
1:G:20:GLN:HG2	1:H:43:ASP:HB2	1.73	0.70
1:J:74:GLN:HG2	4:N:409:ARG:HD3	1.72	0.70
1:J:133:MET:HE2	4:N:409:ARG:HB3	1.74	0.70
1:G:74:GLN:HE21	4:P:409:ARG:HD3	1.58	0.69
2:C:207:CYS:SG	6:C:403:HOH:O	2.50	0.69
1:G:181:ASP:OD2	4:P:404:SER:HB3	1.93	0.68
1:I:69:LEU:HG	1:I:142:PHE:HE1	1.59	0.67
1:J:69:LEU:HD13	1:J:142:PHE:HE1	1.60	0.66
4:Q:409:ARG:HD3	4:Q:412:CYS:HB2	1.79	0.65
3:F:19:SER:N	6:F:301:HOH:O	2.29	0.65
3:F:29:ASP:OD1	3:F:33:ARG:NH1	2.30	0.64
2:B:176:ASP:OD2	4:K:413:ARG:NH1	2.30	0.64
1:A:19:SER:N	6:A:401:HOH:O	2.31	0.62
2:B:69:LEU:HG	2:B:142:PHE:HE1	1.64	0.62
1:I:74:GLN:NE2	4:Q:409:ARG:HD2	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:413:ARG:NH1	4:Q:413:ARG:HG2	2.14	0.62
3:E:209:PRO:HD2	3:E:210:GLU:OE2	1.99	0.62
1:J:22:ASN:ND2	1:J:25:ARG:HH21	1.97	0.62
1:I:24:MET:HE3	1:J:38:PRO:HD3	1.82	0.62
1:J:160:LYS:HE2	1:J:201:GLN:NE2	2.10	0.62
3:E:223:GLU:O	6:E:401:HOH:O	2.16	0.62
1:A:19:SER:HA	1:A:22:ASN:ND2	2.14	0.61
1:I:96:ARG:HG3	1:I:125:VAL:HG22	1.82	0.61
1:J:36:MET:HE3	1:J:37:TYR:H	1.65	0.60
1:D:153:GLU:OE1	1:I:153:GLU:HG3	2.01	0.60
3:E:25:ARG:NH2	3:E:88:GLU:O	2.30	0.60
1:H:186:TYR:HB2	1:I:143:MET:HE3	1.82	0.60
6:B:420:HOH:O	2:C:20:GLN:HG3	2.00	0.60
1:G:142:PHE:CD2	1:G:159:VAL:HG22	2.36	0.60
1:G:135:ILE:CD1	4:P:409:ARG:HD2	2.32	0.59
4:P:405:ASP:O	4:P:409:ARG:HG3	2.03	0.59
2:C:133:MET:HE1	2:C:135:ILE:HD11	1.83	0.59
4:K:409:ARG:HH22	4:K:413:ARG:HH12	1.50	0.58
1:D:133:MET:HE3	4:L:410:TYR:HA	1.86	0.58
1:D:210:GLU:CD	4:M:411:ARG:NE	2.62	0.57
1:G:69:LEU:HG	1:G:142:PHE:HE1	1.67	0.57
1:H:20:GLN:HE21	1:I:38:PRO:CG	2.18	0.57
1:H:210:GLU:OE1	1:H:212:TYR:OH	2.14	0.57
1:G:155:VAL:O	1:G:220:LYS:HG2	2.04	0.57
1:A:210:GLU:OE2	4:K:411:ARG:NE	2.36	0.56
3:E:96:ARG:HD2	3:E:125:VAL:HG22	1.87	0.56
1:I:36:MET:HE3	1:I:103:TRP:HB2	1.88	0.56
1:G:74:GLN:NE2	4:P:409:ARG:HD3	2.19	0.56
1:G:207:CYS:SG	1:G:208:CYS:N	2.79	0.56
1:I:19:SER:HA	1:I:22:ASN:HD22	1.70	0.56
1:J:36:MET:HE3	1:J:37:TYR:N	2.21	0.56
1:I:44:ASP:OD1	6:I:301:HOH:O	2.18	0.56
4:N:403:CYS:HG	4:N:412:CYS:CB	2.16	0.56
2:C:25:ARG:NH2	2:C:88:GLU:O	2.39	0.56
4:N:402:CYS:HB2	4:N:408:CYS:SG	2.45	0.56
1:D:42:LYS:HG3	1:D:169:PHE:HB3	1.88	0.56
4:N:403:CYS:CB	4:N:412:CYS:HG	2.18	0.55
2:C:210:GLU:OE1	2:C:212:TYR:OH	2.18	0.55
1:D:210:GLU:CD	4:M:411:ARG:HE	2.14	0.55
4:R:403:CYS:HB3	4:R:412:CYS:SG	2.47	0.55
4:R:403:CYS:HG	4:R:412:CYS:HG	0.56	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:194:LEU:HD12	1:J:220:LYS:HG2	1.89	0.54
1:I:25:ARG:NH2	1:I:88:GLU:O	2.40	0.54
1:D:212:TYR:HE2	4:M:407:ARG:HB2	1.73	0.54
1:H:20:GLN:NE2	1:I:38:PRO:HG2	2.23	0.54
1:I:19:SER:HA	1:I:22:ASN:ND2	2.22	0.54
4:N:403:CYS:CB	4:N:412:CYS:SG	2.96	0.53
2:B:38:PRO:HD3	2:C:24:MET:HE3	1.89	0.53
1:G:47:THR:HG21	1:G:174:LYS:HD3	1.90	0.53
1:H:69:LEU:HG	1:H:142:PHE:HE1	1.73	0.53
4:N:402:CYS:CB	4:N:408:CYS:SG	2.96	0.53
2:B:153:GLU:CD	1:G:153:GLU:HG2	2.32	0.53
1:D:212:TYR:CE2	4:M:407:ARG:HB2	2.44	0.53
2:B:153:GLU:OE2	1:G:153:GLU:HG2	2.09	0.53
3:E:74:GLN:CD	4:M:409:ARG:HE	2.17	0.53
1:G:27:LYS:HB3	1:G:27:LYS:HZ1	1.74	0.52
1:A:72:TYR:CE1	3:E:164:TRP:HH2	2.27	0.52
3:F:19:SER:HA	3:F:22:ASN:ND2	2.22	0.52
1:J:73:GLU:OE2	1:J:75:GLN:NE2	2.41	0.52
1:D:64:THR:HG22	3:E:59:LYS:HB3	1.91	0.52
1:I:210:GLU:HG3	1:I:212:TYR:CE1	2.44	0.52
4:O:402:CYS:HG	4:O:408:CYS:HG	0.54	0.52
3:F:55:GLN:HE22	1:G:111:SER:HA	1.75	0.52
2:B:96:ARG:HG3	2:B:125:VAL:HG22	1.92	0.52
1:G:24:MET:SD	1:H:38:PRO:CB	2.92	0.52
3:E:204:HIS:N	3:E:205:TYR:HD1	2.08	0.51
3:F:69:LEU:HG	3:F:142:PHE:HE1	1.76	0.51
1:I:210:GLU:HG3	1:I:212:TYR:HE1	1.75	0.51
4:Q:409:ARG:HD3	4:Q:409:ARG:O	2.10	0.51
4:O:402:CYS:CB	4:O:408:CYS:HG	2.19	0.51
2:B:76:ARG:HD2	4:K:413:ARG:NE	2.25	0.51
1:G:26:LEU:O	1:G:30:LEU:HG	2.11	0.51
1:I:74:GLN:HE22	4:Q:409:ARG:CD	2.20	0.51
1:G:23:LEU:HD13	1:G:90:GLY:CA	2.41	0.51
3:E:204:HIS:N	3:E:205:TYR:CD1	2.79	0.51
4:Q:413:ARG:HG2	4:Q:413:ARG:HH11	1.74	0.51
4:N:402:CYS:O	4:N:408:CYS:HB3	2.11	0.51
1:G:208:CYS:SG	4:O:402:CYS:SG	3.09	0.50
3:E:69:LEU:HG	3:E:142:PHE:HE1	1.77	0.50
1:I:69:LEU:HG	1:I:142:PHE:CE1	2.45	0.50
3:F:53:THR:HA	3:F:181:ASP:HB3	1.93	0.50
1:H:24:MET:HE2	1:I:35:PRO:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ILE:O	4:K:407:ARG:NH1	2.45	0.50
1:G:32:ASN:C	1:G:33:ARG:HD3	2.37	0.49
1:G:23:LEU:HD23	1:G:26:LEU:HD12	1.94	0.49
4:N:409:ARG:C	4:N:411:ARG:H	2.18	0.49
4:R:402:CYS:O	4:R:408:CYS:HB3	2.11	0.49
1:H:133:MET:HE3	4:R:409:ARG:O	2.12	0.49
1:D:69:LEU:HG	1:D:142:PHE:HE1	1.77	0.49
1:G:42:LYS:HE2	1:G:170:GLU:OE2	2.12	0.49
2:B:76:ARG:CZ	4:K:413:ARG:HG2	2.43	0.49
4:R:403:CYS:CB	4:R:412:CYS:SG	3.01	0.49
1:H:20:GLN:NE2	1:I:38:PRO:CG	2.76	0.48
1:I:173:LEU:HB2	1:I:213:ILE:HG22	1.95	0.48
4:N:408:CYS:SG	4:N:408:CYS:O	2.71	0.48
1:J:69:LEU:HD13	1:J:142:PHE:CE1	2.46	0.48
1:A:113:THR:O	2:B:139:ARG:HD2	2.14	0.48
4:M:409:ARG:HH12	4:M:413:ARG:HB2	1.78	0.48
1:G:152:GLU:OE2	1:G:222:ARG:NH1	2.45	0.48
3:E:208:CYS:CB	3:E:210:GLU:OE1	2.48	0.47
2:B:153:GLU:OE1	1:G:153:GLU:HG2	2.15	0.47
1:I:166:TYR:O	4:R:407:ARG:HD2	2.14	0.47
3:E:192:GLU:OE2	3:E:222:ARG:NE	2.36	0.47
3:F:72:TYR:CE1	1:G:164:TRP:HH2	2.33	0.47
1:I:210:GLU:H	1:I:210:GLU:HG2	1.43	0.47
1:A:69:LEU:HG	1:A:142:PHE:HE1	1.80	0.47
1:A:24:MET:HE2	3:E:36:MET:O	2.15	0.47
2:B:76:ARG:HD2	4:K:413:ARG:HE	1.79	0.46
3:F:24:MET:HG3	1:G:38:PRO:HG3	1.97	0.46
1:G:162:GLY:HA2	1:G:173:LEU:HD11	1.97	0.46
4:R:403:CYS:HA	4:R:409:ARG:HG2	1.96	0.46
2:B:190:LYS:NZ	6:B:403:HOH:O	2.48	0.46
4:L:403:CYS:HG	4:L:412:CYS:CB	2.27	0.46
1:G:42:LYS:H	1:G:42:LYS:HD2	1.81	0.46
1:G:29:ASP:O	1:G:33:ARG:HG2	2.16	0.46
1:G:47:THR:CG2	1:G:174:LYS:HD3	2.46	0.46
1:J:61:ASP:OD1	1:J:63:SER:OG	2.32	0.46
4:L:402:CYS:O	4:L:408:CYS:HB3	2.16	0.46
1:D:42:LYS:HE2	1:D:169:PHE:CD2	2.51	0.46
1:D:113:THR:O	3:E:139:ARG:HD2	2.16	0.46
3:E:21:ALA:HA	3:E:24:MET:HE3	1.97	0.46
1:G:27:LYS:HB2	1:G:89:TYR:CD1	2.51	0.46
1:A:158:ALA:HA	1:A:217:LEU:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:152:GLU:O	3:E:222:ARG:NH1	2.49	0.45
1:I:53:THR:HB	1:I:72:TYR:HB2	1.97	0.45
1:G:34:SER:HB3	1:G:35:PRO:HD2	1.99	0.45
1:A:73:GLU:O	1:A:136:PRO:HD2	2.17	0.45
1:I:105:PRO:HB2	1:I:107:ILE:HG12	1.98	0.45
1:H:158:ALA:HA	1:H:217:LEU:O	2.16	0.45
1:I:74:GLN:HE22	4:Q:409:ARG:CZ	2.29	0.45
1:A:165:VAL:HG21	2:B:123:ILE:HG21	1.97	0.45
1:G:158:ALA:HA	1:G:217:LEU:O	2.17	0.45
2:B:106:ASP:HB2	2:C:121:PRO:HG2	1.99	0.45
2:C:212:TYR:HE2	4:L:407:ARG:HB2	1.82	0.45
3:F:165:VAL:HG21	1:J:123:ILE:HG21	1.99	0.45
1:A:96:ARG:HG3	1:A:125:VAL:HG22	2.00	0.44
2:C:36:MET:HE1	6:C:450:HOH:O	2.17	0.44
2:C:81:SER:OG	6:C:402:HOH:O	2.21	0.44
1:G:84:TRP:CZ3	1:G:128:HIS:HA	2.53	0.44
2:C:29:ASP:HA	2:C:33:ARG:HG3	1.98	0.44
3:F:212:TYR:HB3	4:N:407:ARG:NH2	2.33	0.44
1:H:19:SER:HB3	1:I:43:ASP:HB3	2.00	0.44
2:B:25:ARG:NH2	2:B:88:GLU:O	2.41	0.44
1:I:162:GLY:HA2	1:I:173:LEU:HD11	2.00	0.44
1:D:76:ARG:NH2	1:D:131:SER:OG	2.50	0.43
1:G:33:ARG:HD3	1:G:33:ARG:N	2.32	0.43
1:G:121:PRO:HG3	1:H:106:ASP:HB2	2.00	0.43
1:A:33:ARG:HA	1:A:33:ARG:HD2	1.51	0.43
1:A:85:ASP:HB3	1:A:88:GLU:HG3	1.98	0.43
1:G:95:PHE:CE1	1:G:97:THR:HB	2.54	0.43
3:F:68:ASP:HA	3:F:140:LEU:O	2.18	0.43
2:C:210:GLU:OE2	4:L:411:ARG:NE	2.51	0.43
1:G:27:LYS:HB3	1:G:27:LYS:NZ	2.32	0.43
4:M:402:CYS:CB	4:M:408:CYS:SG	3.05	0.43
4:K:413:ARG:NH1	4:K:413:ARG:HB2	2.34	0.43
4:R:409:ARG:HH21	4:R:413:ARG:HG2	1.83	0.43
1:D:73:GLU:O	1:D:136:PRO:HD2	2.19	0.43
1:D:91:ASN:ND2	6:D:401:HOH:O	2.17	0.43
1:G:210:GLU:HG2	1:G:212:TYR:CE1	2.53	0.43
3:F:129:ASP:OD1	3:F:131:SER:OG	2.34	0.43
1:H:186:TYR:CG	1:I:143:MET:HE3	2.54	0.43
1:G:172:ASP:OD2	1:G:174:LYS:HD2	2.19	0.42
1:H:210:GLU:OE2	4:P:411:ARG:NH1	2.52	0.42
1:A:195:SER:OG	1:A:220:LYS:CD	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:LYS:HE3	3:E:62:SER:O	2.19	0.42
1:I:212:TYR:HB3	4:R:407:ARG:NH2	2.35	0.42
1:I:139:ARG:HD2	1:J:113:THR:O	2.20	0.42
1:J:158:ALA:HA	1:J:217:LEU:O	2.20	0.42
4:O:409:ARG:HH11	4:O:412:CYS:HB2	1.84	0.42
2:C:164:TRP:HH2	1:D:72:TYR:CE1	2.37	0.42
1:G:53:THR:HB	1:G:72:TYR:HB2	2.01	0.42
1:H:139:ARG:HD2	1:I:113:THR:O	2.18	0.42
1:I:152:GLU:HG2	1:I:222:ARG:NH1	2.34	0.42
3:E:146:PRO:O	3:E:149:VAL:HG22	2.20	0.42
2:C:207:CYS:HB2	2:C:208:CYS:SG	2.60	0.42
3:E:205:TYR:HD1	3:E:205:TYR:N	2.18	0.42
3:E:205:TYR:CD1	3:E:205:TYR:N	2.88	0.42
1:G:95:PHE:HE1	1:G:97:THR:HB	1.83	0.42
1:I:173:LEU:HB2	1:I:213:ILE:CG2	2.48	0.42
2:C:73:GLU:O	2:C:136:PRO:HD2	2.20	0.42
4:K:413:ARG:HB2	4:K:413:ARG:HH11	1.85	0.42
1:G:27:LYS:HE2	1:G:84:TRP:CE2	2.54	0.42
1:J:213:ILE:O	4:Q:407:ARG:NH1	2.53	0.42
3:E:76:ARG:HD3	4:M:413:ARG:HD3	2.02	0.41
2:C:186:TYR:CZ	2:C:188:SER:HB2	2.55	0.41
1:G:84:TRP:CE3	1:G:128:HIS:HA	2.55	0.41
1:I:74:GLN:HE22	4:Q:409:ARG:NH1	2.18	0.41
3:F:65:ASN:HD22	3:F:65:ASN:HA	1.71	0.41
1:I:73:GLU:O	1:I:136:PRO:HD2	2.21	0.41
1:H:121:PRO:HG3	1:I:106:ASP:HB2	2.03	0.41
1:A:24:MET:HE3	3:E:38:PRO:HD3	2.02	0.41
1:I:212:TYR:HE2	4:R:407:ARG:HB2	1.85	0.41
1:J:169:PHE:HD1	1:J:169:PHE:HA	1.75	0.41
1:J:173:LEU:HB2	1:J:213:ILE:HG22	2.02	0.41
3:F:19:SER:O	3:F:19:SER:OG	2.37	0.41
3:E:68:ASP:HA	3:E:140:LEU:O	2.20	0.41
1:J:162:GLY:HA2	1:J:173:LEU:HD11	2.01	0.41
2:C:133:MET:CE	2:C:135:ILE:HD11	2.49	0.41
2:C:193:ILE:HD12	2:C:193:ILE:HG23	1.84	0.41
1:D:153:GLU:CD	1:I:153:GLU:HG3	2.45	0.41
1:G:25:ARG:HH11	1:H:38:PRO:HD3	1.86	0.41
1:G:212:TYR:CE2	4:O:407:ARG:HB2	2.56	0.41
1:J:20:GLN:H	1:J:20:GLN:HG3	1.58	0.41
2:B:62:SER:O	2:C:190:LYS:HE3	2.21	0.41
3:E:54:LEU:HD23	3:E:54:LEU:HA	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:72:TYR:CE1	1:H:164:TRP:HH2	2.38	0.41
4:K:411:ARG:O	4:K:412:CYS:C	2.64	0.41
2:B:33:ARG:HD2	2:B:33:ARG:HA	1.82	0.40
1:D:53:THR:HB	1:D:72:TYR:HB2	2.02	0.40
3:F:163:SER:O	4:N:407:ARG:HD3	2.21	0.40
1:G:40:PRO:CB	1:G:46:LEU:HD22	2.45	0.40
1:A:121:PRO:HG3	3:E:106:ASP:HB2	2.03	0.40
1:A:164:TRP:HH2	2:B:72:TYR:CE1	2.40	0.40
2:B:68:ASP:HA	2:B:140:LEU:O	2.21	0.40
2:C:212:TYR:CE2	4:L:407:ARG:HB2	2.56	0.40
1:D:210:GLU:OE1	4:M:411:ARG:NH2	2.54	0.40
3:E:106:ASP:OD2	3:E:165:VAL:HG22	2.22	0.40
1:I:36:MET:CE	1:I:103:TRP:HB2	2.50	0.40
2:C:202:VAL:HG22	2:C:213:ILE:HD12	2.02	0.40
3:E:209:PRO:HD2	3:E:210:GLU:CD	2.47	0.40
1:I:212:TYR:CE2	4:R:407:ARG:HB2	2.57	0.40
4:L:409:ARG:HH11	4:L:412:CYS:HB2	1.86	0.40
1:A:182:LEU:HD23	1:A:182:LEU:HA	1.84	0.40
1:G:30:LEU:HD12	1:G:89:TYR:CE1	2.57	0.40
4:L:409:ARG:NH1	4:L:412:CYS:HB2	2.37	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	204/206 (99%)	200 (98%)	4 (2%)	0	100	100
1	D	204/206 (99%)	199 (98%)	4 (2%)	1 (0%)	24	43
1	G	204/206 (99%)	199 (98%)	5 (2%)	0	100	100
1	H	204/206 (99%)	199 (98%)	4 (2%)	1 (0%)	24	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	204/206 (99%)	194 (95%)	9 (4%)	1 (0%)	24	43
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%)	24	43
3	F	203/205 (99%)	196 (97%)	6 (3%)	1 (0%)	24	43
4	K	11/13 (85%)	11 (100%)	0	0	100	100
4	L	11/13 (85%)	10 (91%)	0	1 (9%)	0	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
All	All	2122/2158 (98%)	2046 (96%)	70 (3%)	6 (0%)	36	55

All (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
3	F	34	SER

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%)	187 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	187/189 (99%)	187 (100%)	0	100	100
1	G	187/189 (99%)	187 (100%)	0	100	100
1	H	187/189 (99%)	187 (100%)	0	100	100
1	I	187/189 (99%)	187 (100%)	0	100	100
1	J	187/189 (99%)	187 (100%)	0	100	100
2	B	185/187 (99%)	185 (100%)	0	100	100
2	C	185/187 (99%)	185 (100%)	0	100	100
3	E	186/188 (99%)	186 (100%)	0	100	100
3	F	186/188 (99%)	186 (100%)	0	100	100
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%)	12 (100%)	0	100	100
4	O	12/12 (100%)	12 (100%)	0	100	100
4	P	12/12 (100%)	12 (100%)	0	100	100
4	Q	12/12 (100%)	12 (100%)	0	100	100
4	R	12/12 (100%)	12 (100%)	0	100	100
All	All	1960/1980 (99%)	1960 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	74	GLN
1	A	138	GLN
1	A	201	GLN
1	A	204	HIS
2	B	55	GLN
2	C	20	GLN
2	C	74	GLN
2	C	122	GLN
2	C	204	HIS
1	D	32	ASN
1	D	128	HIS

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Mol	Chain	Res	Type
1	D	138	GLN
1	D	203	GLN
3	E	138	GLN
3	F	74	GLN
3	F	138	GLN
3	F	179	GLN
1	G	32	ASN
1	G	74	GLN
1	G	128	HIS
1	G	204	HIS
1	H	20	GLN
1	I	20	GLN
1	I	74	GLN
1	I	87	ASN
1	I	138	GLN
1	I	179	GLN
1	J	22	ASN
1	J	87	ASN
1	J	201	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 oligosaccharides 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	206/206 (100%)	-0.31	11 (5%) 32 28	21, 33, 71, 98	0
1	D	206/206 (100%)	-0.26	9 (4%) 39 34	22, 34, 70, 106	0
1	G	206/206 (100%)	-0.01	15 (7%) 21 19	23, 38, 76, 109	0
1	H	206/206 (100%)	-0.20	8 (3%) 43 38	24, 37, 70, 117	0
1	I	206/206 (100%)	-0.27	9 (4%) 39 34	22, 35, 71, 130	0
1	J	206/206 (100%)	-0.24	8 (3%) 43 38	23, 37, 69, 94	0
2	B	204/204 (100%)	-0.51	2 (0%) 79 76	21, 30, 54, 86	0
2	C	204/204 (100%)	-0.32	10 (4%) 35 31	20, 32, 71, 94	0
3	E	205/205 (100%)	-0.29	12 (5%) 28 24	21, 32, 82, 136	0
3	F	205/205 (100%)	-0.18	11 (5%) 31 27	25, 37, 74, 111	0
4	K	13/13 (100%)	1.99	7 (53%) 0 0	58, 74, 110, 116	0
4	L	13/13 (100%)	2.16	7 (53%) 0 0	55, 83, 108, 122	0
4	M	13/13 (100%)	2.21	7 (53%) 0 0	58, 90, 104, 119	0
4	N	13/13 (100%)	2.87	9 (69%) 0 0	62, 96, 123, 124	0
4	O	13/13 (100%)	2.52	7 (53%) 0 0	60, 91, 115, 129	0
4	P	13/13 (100%)	2.12	7 (53%) 0 0	63, 81, 113, 115	0
4	Q	13/13 (100%)	2.00	4 (30%) 1 1	64, 74, 99, 121	0
4	R	13/13 (100%)	2.65	9 (69%) 0 0	72, 100, 128, 143	0
All	All	2158/2158 (100%)	-0.14	152 (7%) 22 20	20, 35, 86, 143	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	O	401	GLY	6.5
1	D	19	SER	6.2
4	N	410	TYR	6.2

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Mol	Chain	Res	Type	RSRZ
4	R	410	TYR	5.8
4	L	401	GLY	5.7
3	E	205	TYR	5.4
1	G	20	GLN	5.0
3	E	207	CYS	5.0
1	H	20	GLN	5.0
4	M	401	GLY	4.9
1	H	19	SER	4.8
4	K	413	ARG	4.8
1	A	36	MET	4.7
4	N	413	ARG	4.7
1	G	19	SER	4.7
1	H	207	CYS	4.6
4	Q	413	ARG	4.5
1	H	33	ARG	4.5
4	O	402	CYS	4.4
4	O	413	ARG	4.4
1	G	35	PRO	4.4
4	R	401	GLY	4.3
4	P	413	ARG	4.2
1	G	31	PHE	4.2
3	E	206	SER	4.1
3	E	36	MET	4.1
1	H	36	MET	4.0
1	D	35	PRO	3.9
3	F	209	PRO	3.9
4	N	403	CYS	3.8
1	D	207	CYS	3.8
4	K	403	CYS	3.8
3	F	210	GLU	3.7
4	M	413	ARG	3.7
4	N	401	GLY	3.6
1	G	26	LEU	3.6
4	L	410	TYR	3.6
1	G	21	ALA	3.6
4	L	413	ARG	3.5
1	I	20	GLN	3.5
4	R	412	CYS	3.4
1	I	209	PRO	3.4
4	N	412	CYS	3.4
3	E	204	HIS	3.4
4	P	410	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	36	MET	3.3
4	R	408	CYS	3.3
3	F	207	CYS	3.3
1	D	206	SER	3.2
1	I	207	CYS	3.2
1	I	206	SER	3.2
1	A	206	SER	3.2
4	R	413	ARG	3.2
2	B	36	MET	3.2
4	O	403	CYS	3.2
4	Q	401	GLY	3.2
1	D	36	MET	3.1
4	M	410	TYR	3.1
4	L	403	CYS	3.1
1	J	36	MET	3.1
4	O	410	TYR	3.1
4	N	404	SER	3.1
2	C	20	GLN	3.1
3	F	19	SER	3.1
4	P	412	CYS	3.0
3	E	19	SER	3.0
3	E	209	PRO	3.0
1	D	33	ARG	3.0
1	I	33	ARG	3.0
4	P	409	ARG	3.0
4	L	402	CYS	3.0
1	A	20	GLN	3.0
3	E	34	SER	3.0
3	F	34	SER	3.0
1	J	210	GLU	2.9
1	A	33	ARG	2.9
2	C	33	ARG	2.9
3	E	203	GLN	2.9
1	H	209	PRO	2.9
2	C	35	PRO	2.9
3	F	33	ARG	2.8
1	A	207	CYS	2.8
4	K	401	GLY	2.8
1	G	22	ASN	2.8
1	I	19	SER	2.8
4	M	402	CYS	2.8
1	I	36	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	210	GLU	2.8
4	R	402	CYS	2.8
1	A	19	SER	2.7
4	N	408	CYS	2.7
1	I	34	SER	2.7
2	C	34	SER	2.7
1	G	206	SER	2.7
1	A	208	CYS	2.7
1	J	19	SER	2.7
1	I	208	CYS	2.6
2	C	36	MET	2.6
1	D	209	PRO	2.6
2	C	206	SER	2.6
2	C	210	GLU	2.6
4	O	404	SER	2.6
1	J	35	PRO	2.5
2	C	208	CYS	2.5
1	G	34	SER	2.5
4	K	404	SER	2.5
1	G	33	ARG	2.5
1	J	207	CYS	2.5
3	F	96	ARG	2.5
4	N	409	ARG	2.5
4	Q	403	CYS	2.5
3	E	35	PRO	2.5
1	A	42	LYS	2.5
1	A	34	SER	2.5
1	G	24	MET	2.5
4	P	403	CYS	2.4
4	P	404	SER	2.4
4	N	402	CYS	2.4
4	R	403	CYS	2.4
4	K	408	CYS	2.4
4	K	412	CYS	2.3
4	M	407	ARG	2.3
1	A	35	PRO	2.3
1	H	35	PRO	2.3
2	C	209	PRO	2.3
4	P	402	CYS	2.3
4	R	411	ARG	2.3
4	M	404	SER	2.3
4	Q	404	SER	2.3

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Mol	Chain	Res	Type	RSRZ
4	L	408	CYS	2.3
1	G	203	GLN	2.2
1	G	224	ARG	2.2
3	F	206	SER	2.2
1	J	33	ARG	2.2
4	R	409	ARG	2.2
1	A	209	PRO	2.2
4	K	410	TYR	2.2
4	L	412	CYS	2.2
1	J	42	LYS	2.2
3	F	36	MET	2.1
2	B	34	SER	2.1
3	E	33	ARG	2.1
3	E	20	GLN	2.1
1	D	208	CYS	2.1
4	M	403	CYS	2.1
3	F	87	ASN	2.1
1	H	153	GLU	2.1
2	C	207	CYS	2.1
4	O	408	CYS	2.1
3	F	35	PRO	2.1
1	J	224	ARG	2.0
1	G	90	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

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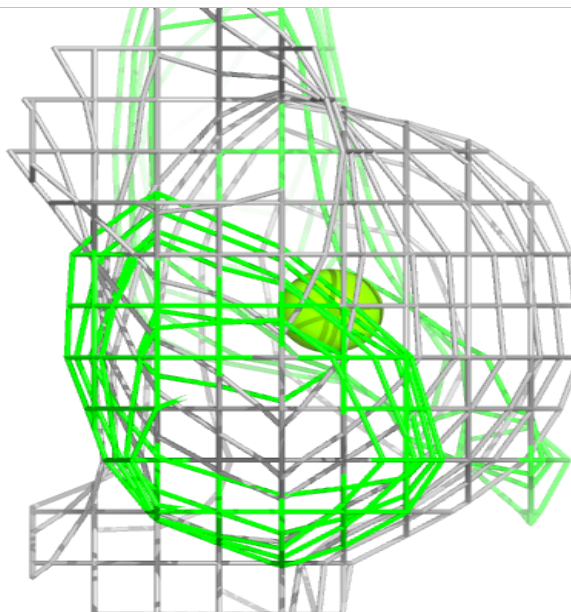
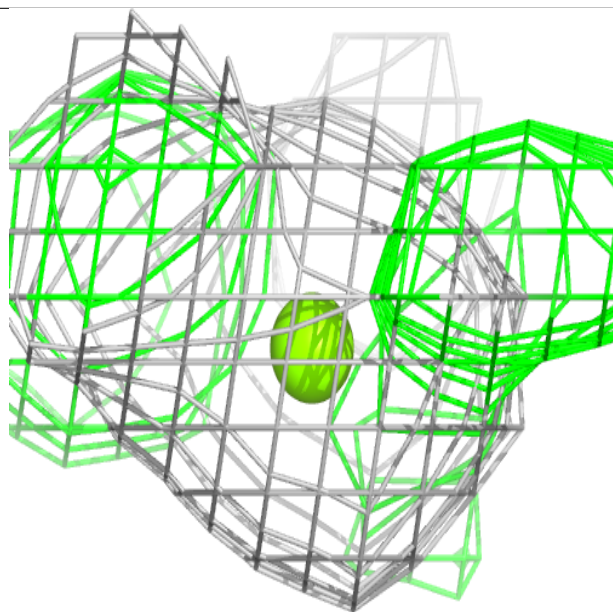
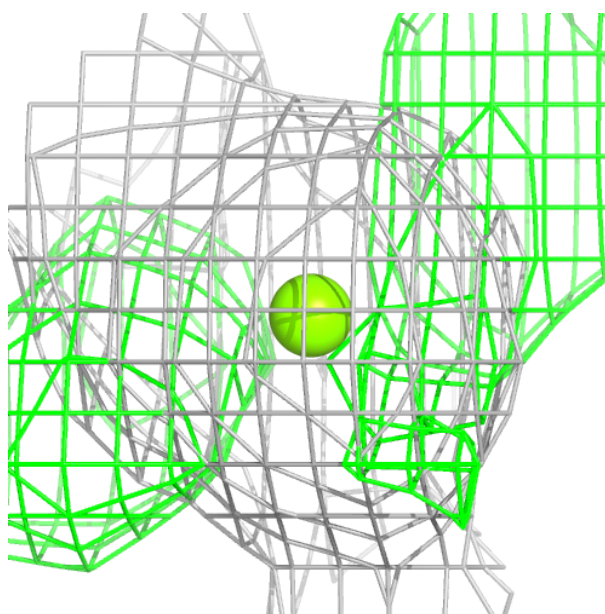
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	J	301	1/1	0.89	0.25	56,56,56,56	0
5	MG	N	501	1/1	0.90	0.22	58,58,58,58	0
5	MG	A	301	1/1	0.95	0.19	36,36,36,36	0
5	MG	R	501	1/1	0.95	0.14	55,55,55,55	0
5	MG	E	301	1/1	0.96	0.24	30,30,30,30	0
5	MG	C	301	1/1	0.96	0.26	44,44,44,44	0
5	MG	H	301	1/1	0.97	0.15	43,43,43,43	0
5	MG	O	501	1/1	0.97	0.22	39,39,39,39	0
5	MG	D	301	1/1	0.97	0.17	40,40,40,40	0
5	MG	B	301	1/1	1.00	0.30	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.

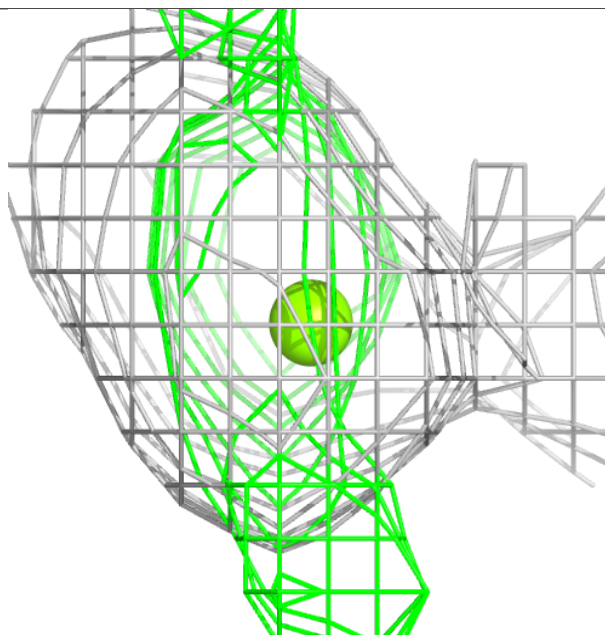
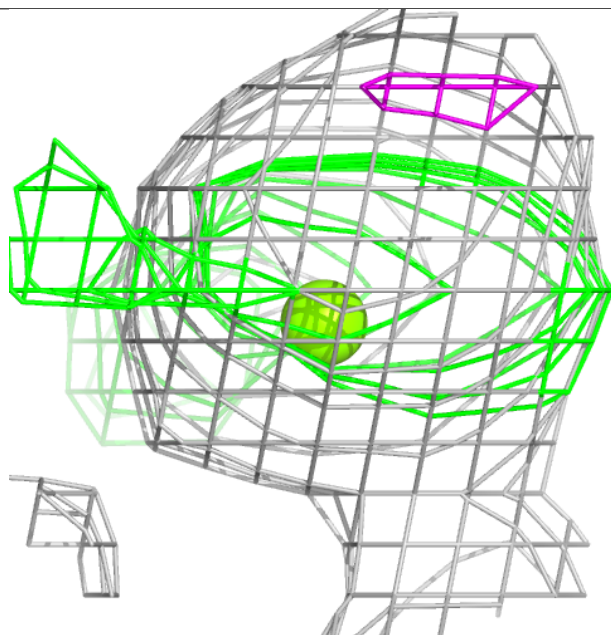
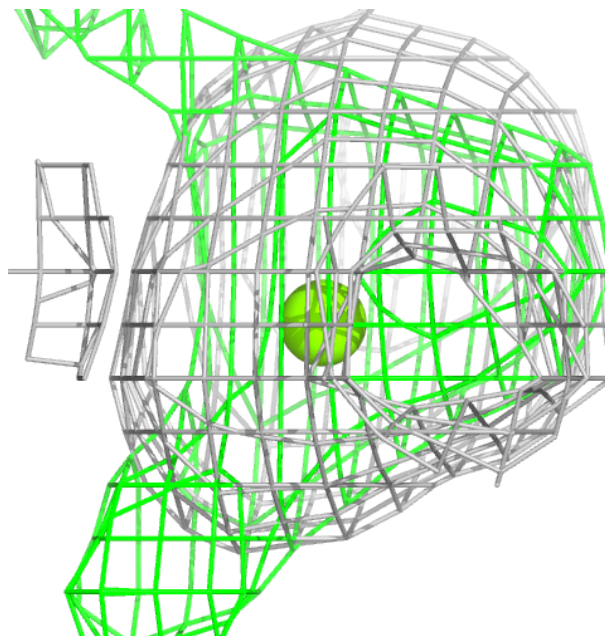
Electron density around MG J 301:

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



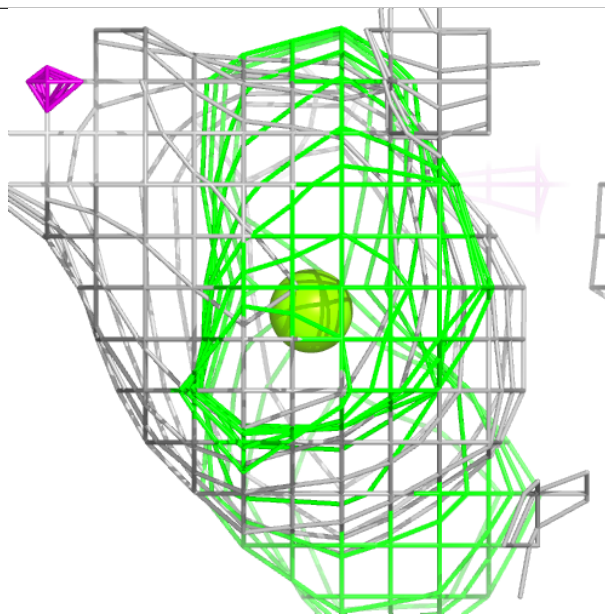
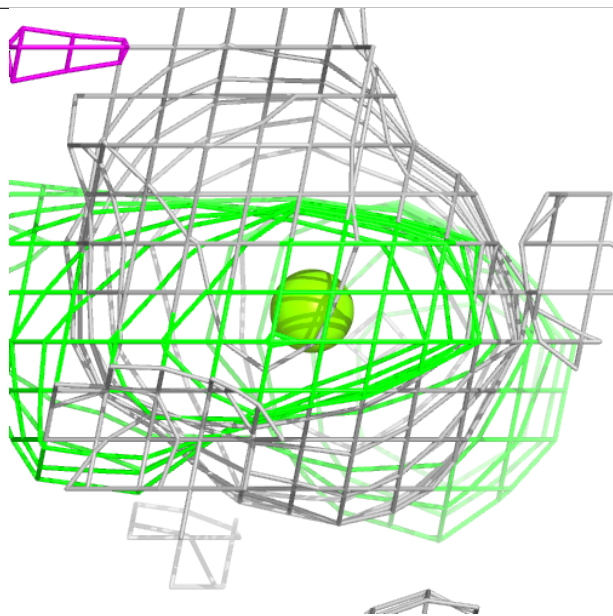
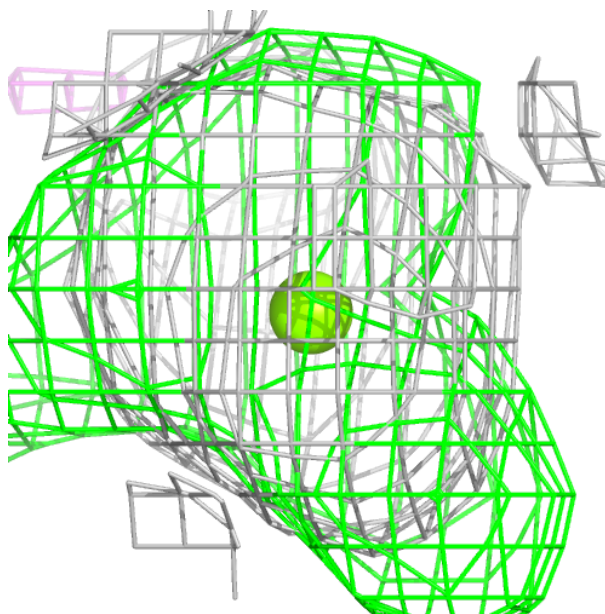
Electron density around MG N 501:

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



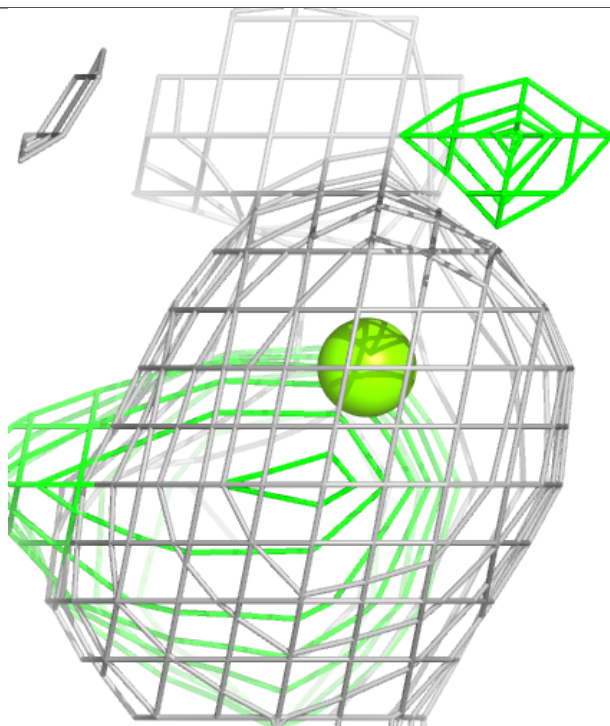
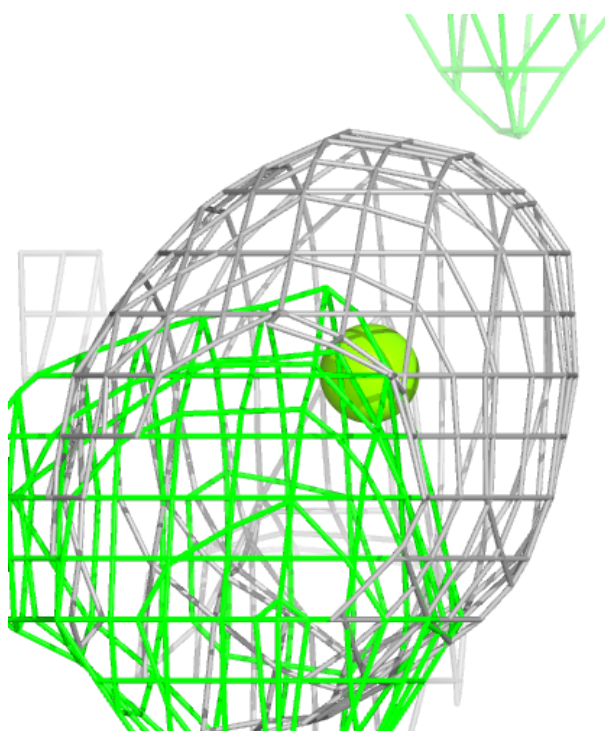
Electron density around MG A 301:

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



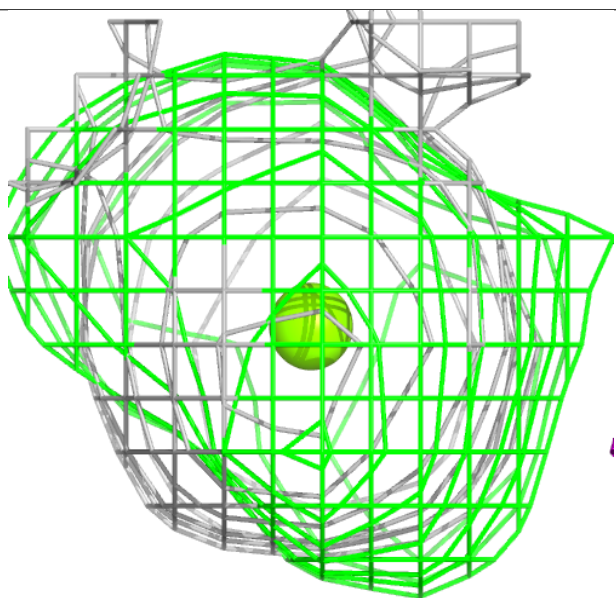
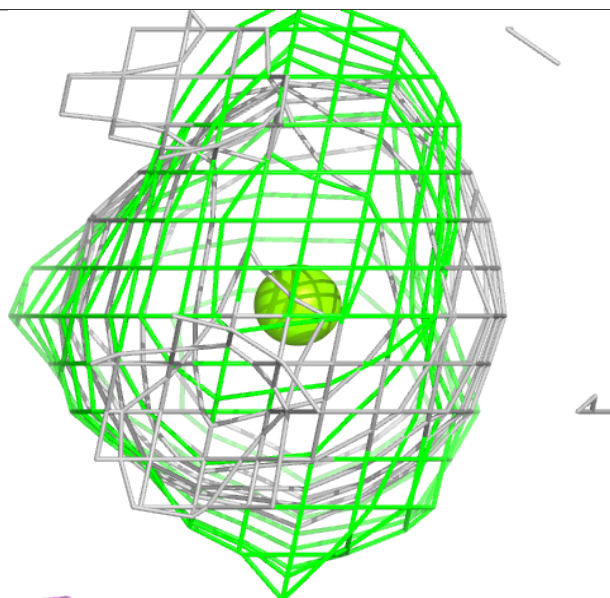
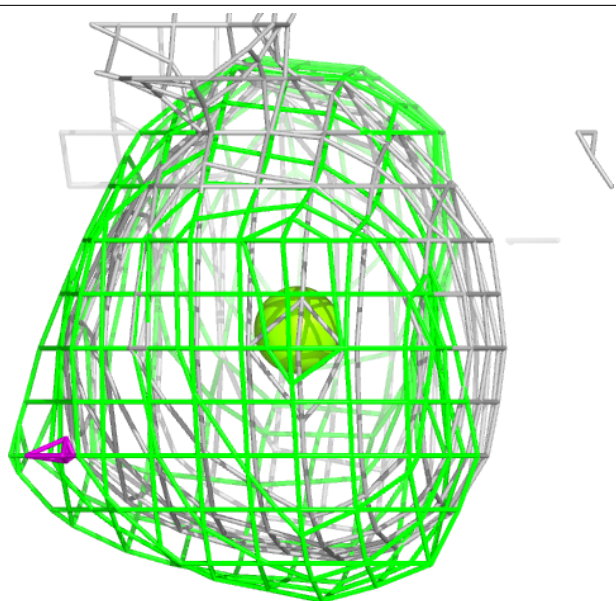
Electron density around MG R 501:

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



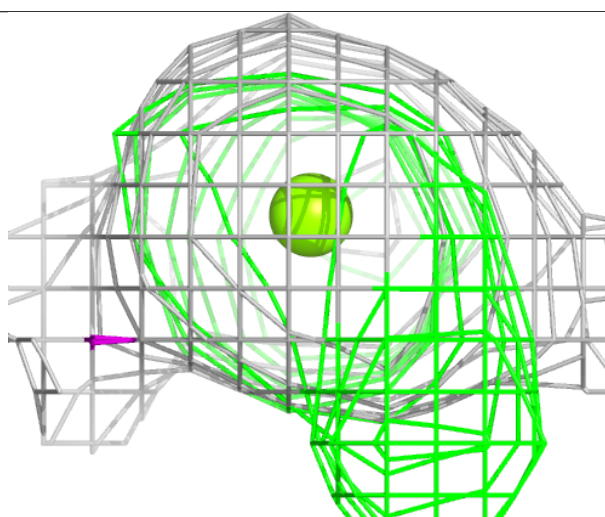
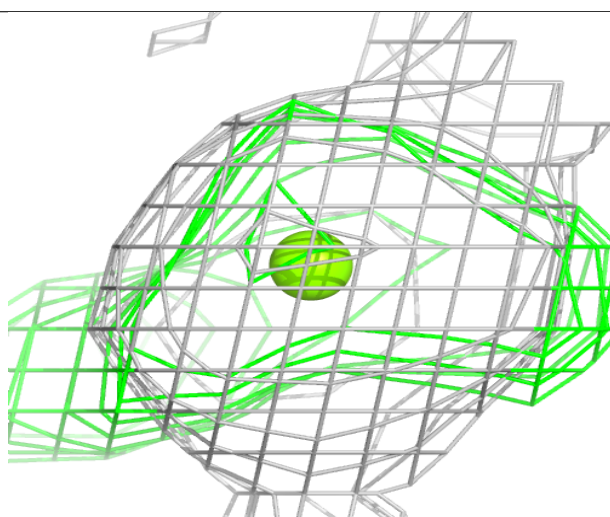
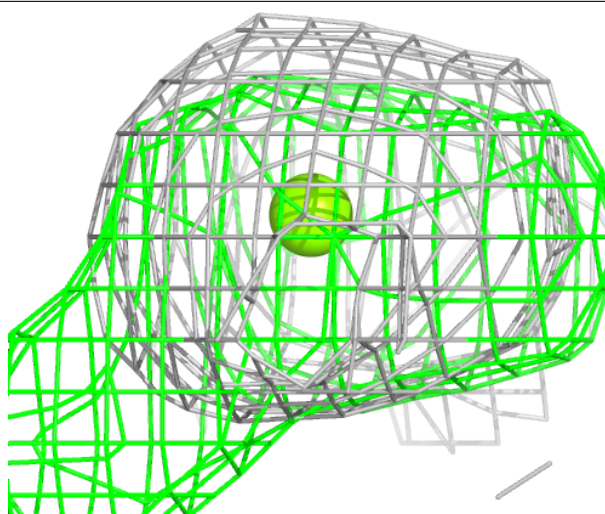
Electron density around MG E 301:

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



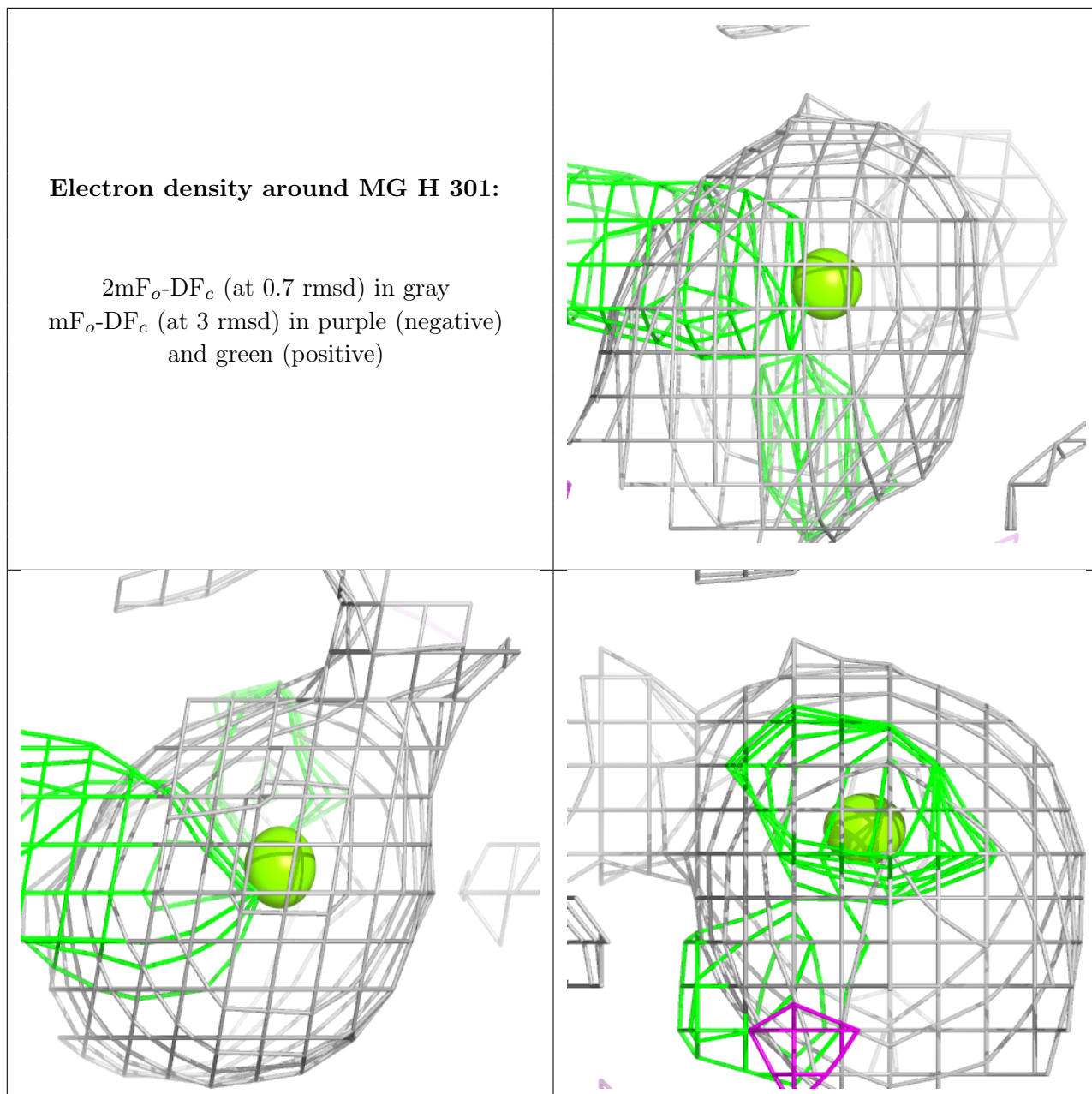
Electron density around MG C 301:

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



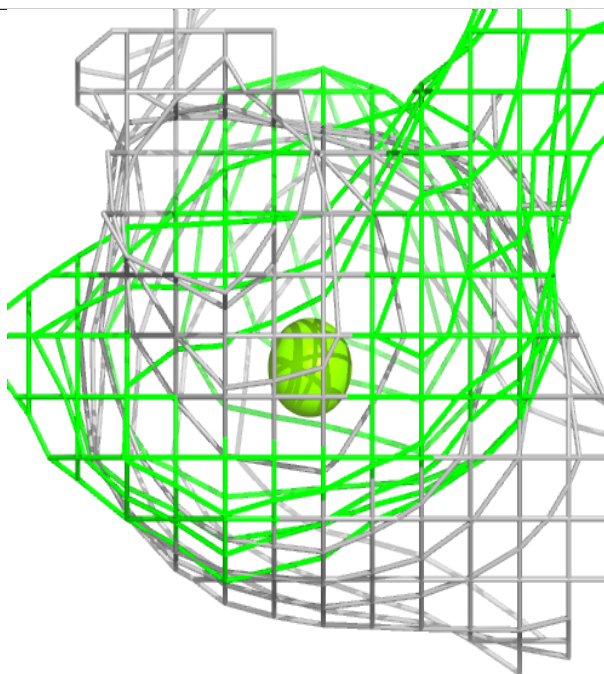
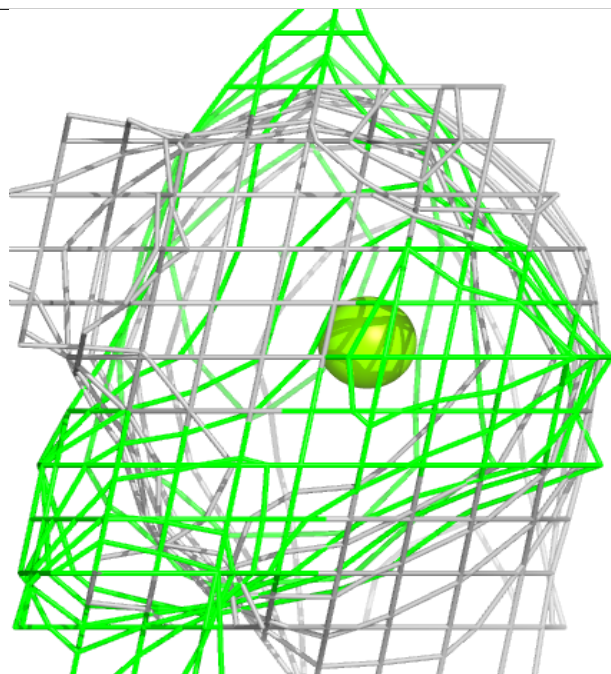
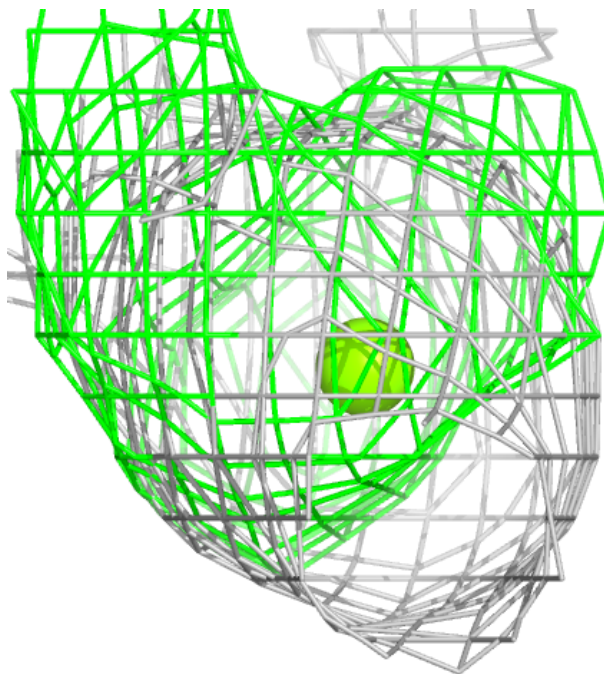
Electron density around MG H 301:

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



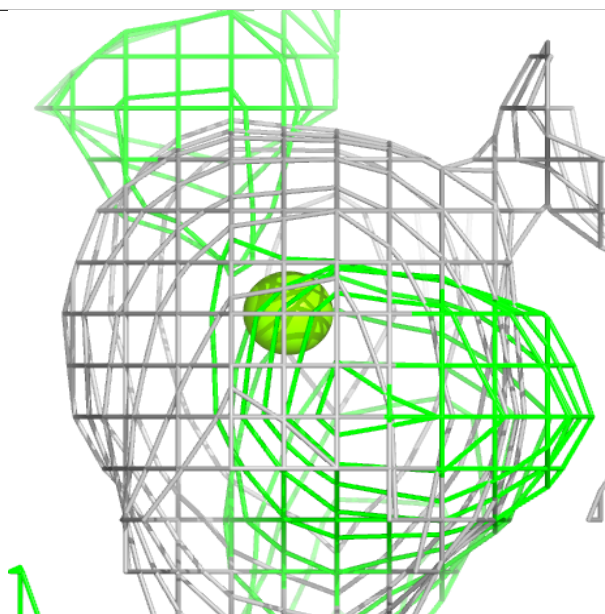
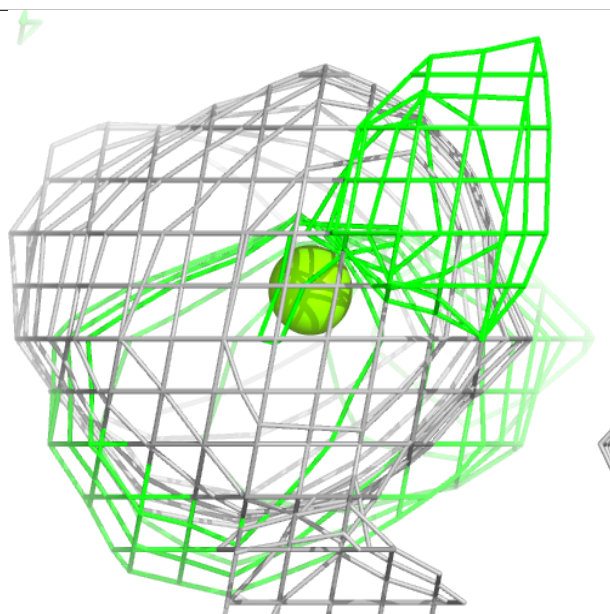
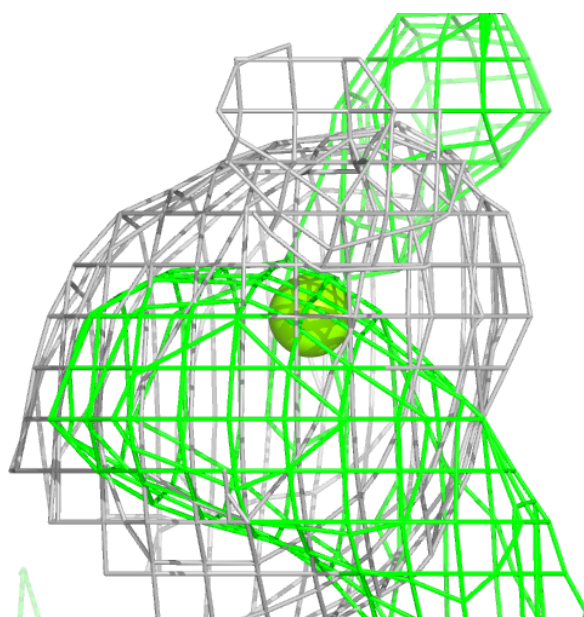
Electron density around MG O 501:

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



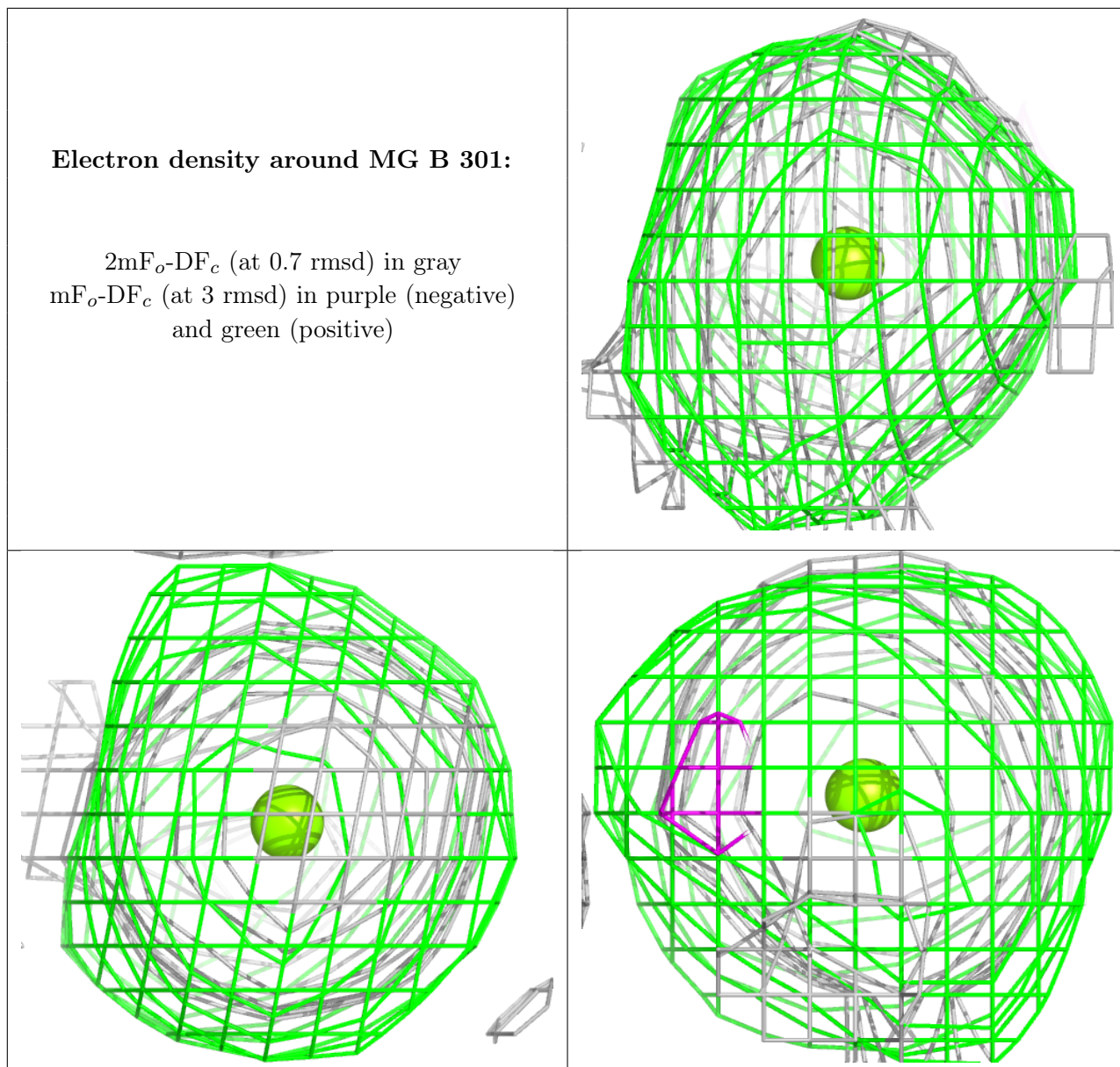
Electron density around MG D 301:

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



Electron density around MG 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.