Full wwPDB X-ray Structure Validation Report (i)

Mar 10, 2022 – 06:20 am GMT

PDB ID	:	7PU5
Title	:	Structure of SFPQ-NONO complex
Authors	:	Fribourg, S.
Deposited on	:	2021-09-28
Resolution	:	3.00 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

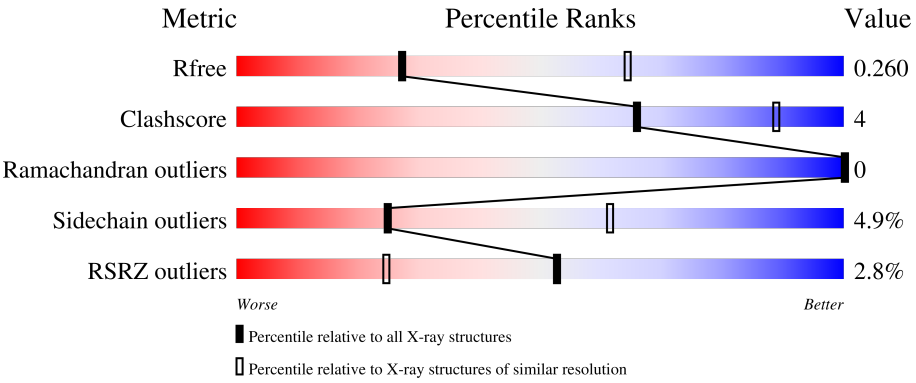
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	259	2% 81% 12% 7%
1	C	259	4% 79% 14% 7%
1	E	259	% 76% 15% 8%
1	G	259	4% 78% 13% • 8%
1	I	259	4% 81% 10% • 8%

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Mol	Chain	Length	Quality of chain
1	K	259	6% 77% 15% • 8%
2	B	259	79% 12% • 8%
2	D	259	2% 81% 11% • 8%
2	F	259	% 80% 11% • 8%
2	H	259	81% 11% • 7%
2	J	259	3% 80% 12% • 8%
2	L	259	2% 80% 12% 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 23285 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 Non-POU domain-containing octamer-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	0	0
			1963	1234	352	368	9			
1	C	242	Total	C	N	O	S	0	0	0
			1968	1238	353	368	9			
1	E	237	Total	C	N	O	S	0	0	0
			1929	1215	346	359	9			
1	G	237	Total	C	N	O	S	0	0	0
			1934	1219	347	359	9			
1	I	238	Total	C	N	O	S	0	0	0
			1930	1215	344	362	9			
1	K	239	Total	C	N	O	S	0	0	0
			1939	1221	346	363	9			

- Molecule 2 is a protein called Splicing factor, proline- and glutamine-rich.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	239	Total	C	N	O	S	0	0	0
			1932	1215	339	371	7			
2	D	239	Total	C	N	O	S	0	0	0
			1932	1215	339	371	7			
2	F	239	Total	C	N	O	S	0	0	0
			1932	1215	339	371	7			
2	H	240	Total	C	N	O	S	0	0	0
			1941	1220	340	374	7			
2	J	239	Total	C	N	O	S	0	0	0
			1932	1215	339	371	7			
2	L	240	Total	C	N	O	S	0	0	0
			1941	1220	340	374	7			

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

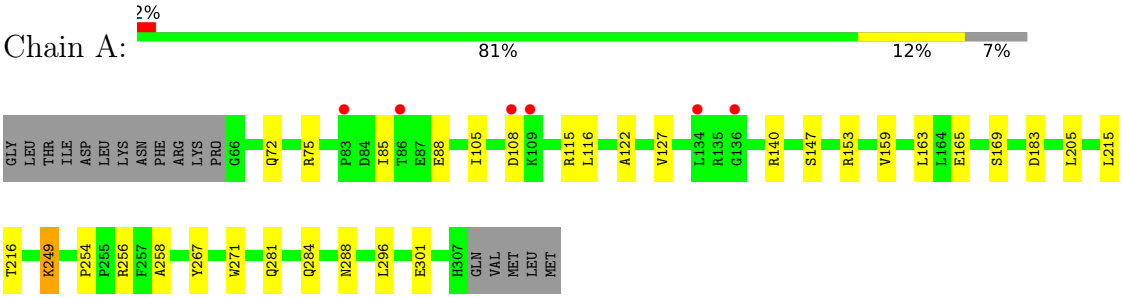
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Mg 2 2	0	0
3	D	2	Total Mg 2 2	0	0
3	F	2	Total Mg 2 2	0	0
3	H	2	Total Mg 2 2	0	0
3	J	2	Total Mg 2 2	0	0
3	K	1	Total Mg 1 1	0	0
3	L	1	Total Mg 1 1	0	0

3 Residue-property plots (i)

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

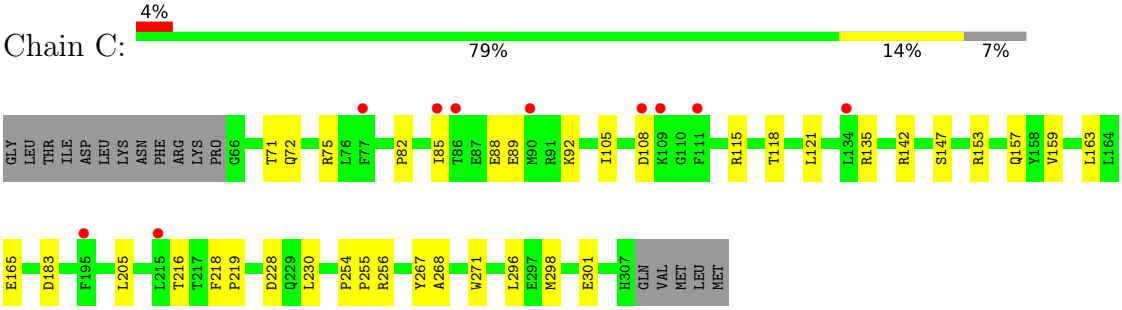
• Molecule 1: Non-POU domain-containing octamer-binding protein

Chain A:



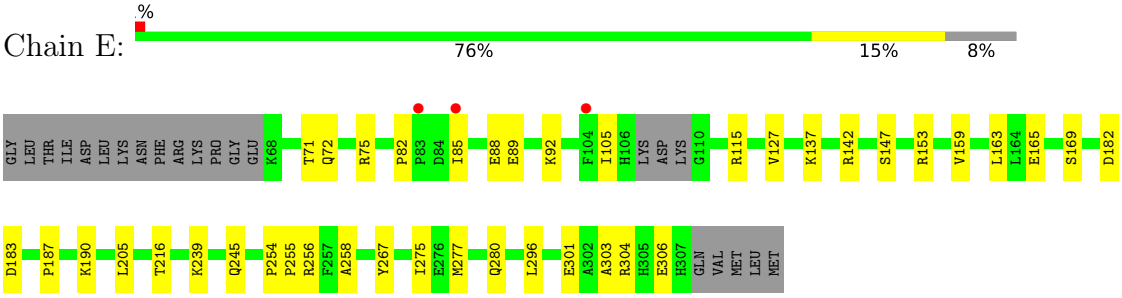
• Molecule 1: Non-POU domain-containing octamer-binding protein

Chain C:



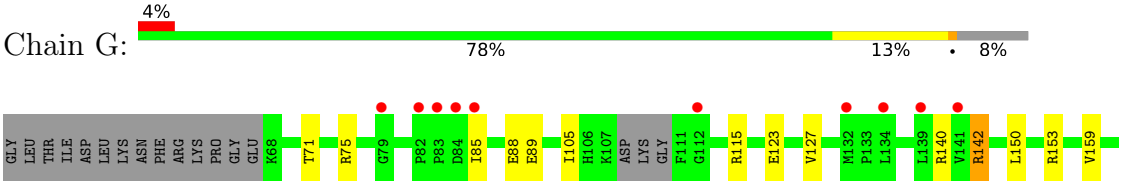
• Molecule 1: Non-POU domain-containing octamer-binding protein

Chain E:



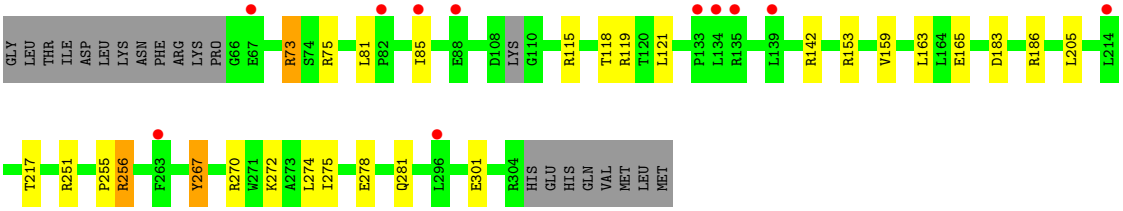
• Molecule 1: Non-POU domain-containing octamer-binding protein

Chain G:



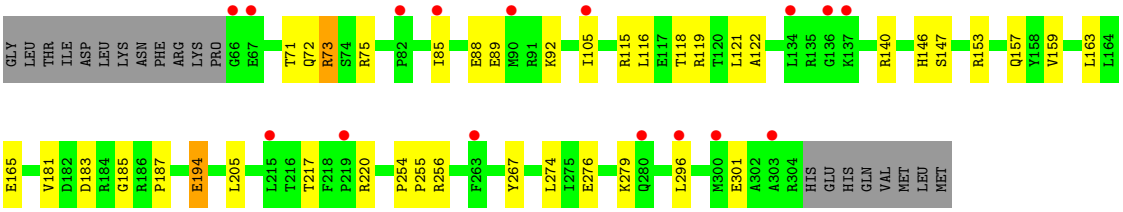
• Molecule 1: Non-POU domain-containing octamer-binding protein

Chain I:



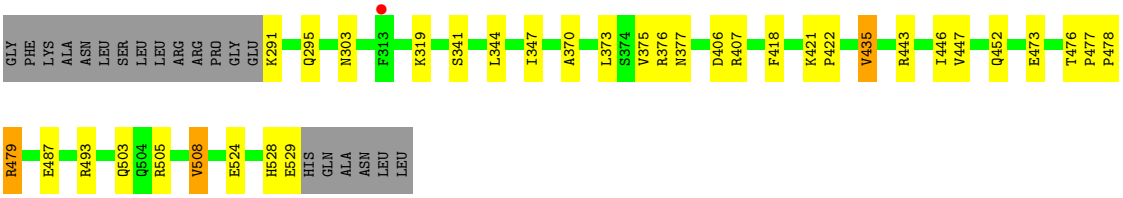
• Molecule 1: Non-POU domain-containing octamer-binding protein

Chain K:



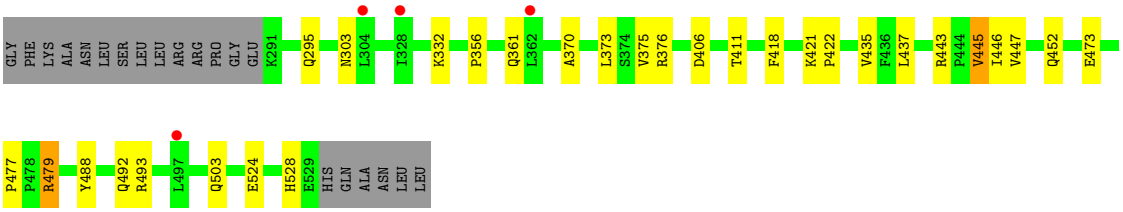
• Molecule 2: Splicing factor, proline- and glutamine-rich

Chain B:



• Molecule 2: Splicing factor, proline- and glutamine-rich

Chain D:

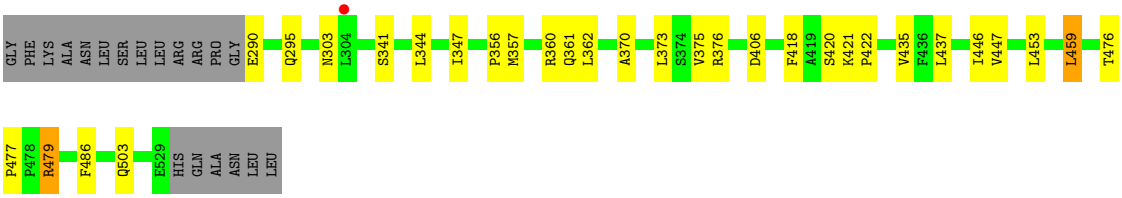


• Molecule 2: Splicing factor, proline- and glutamine-rich

Chain F:

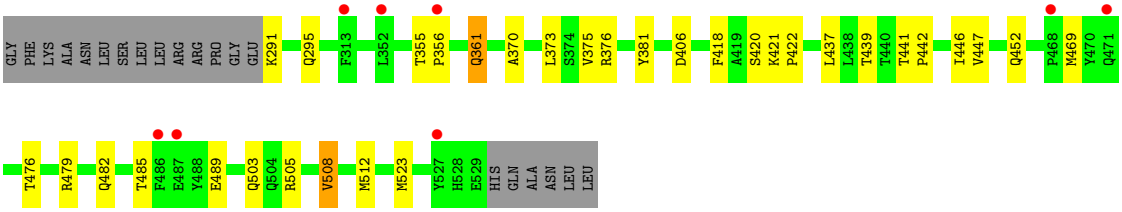
• Molecule 2: Splicing factor, proline- and glutamine-rich

Chain H:



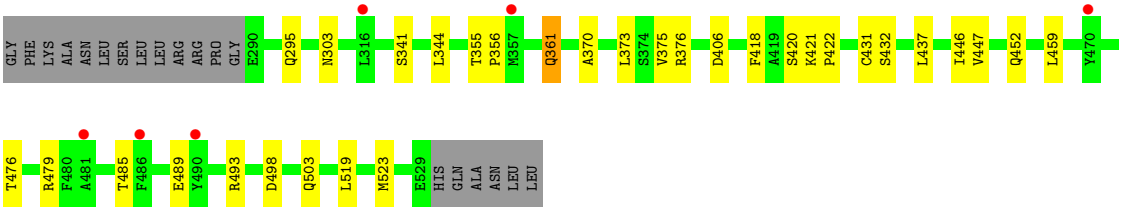
• Molecule 2: Splicing factor, proline- and glutamine-rich

Chain J:



• Molecule 2: Splicing factor, proline- and glutamine-rich

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	467.00Å 66.82Å 126.89Å 90.00° 105.89° 90.00°	Depositor
Resolution (Å)	48.45 – 3.00 48.45 – 3.00	Depositor EDS
% Data completeness (in resolution range)	77.2 (48.45-3.00) 77.2 (48.45-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.10.4 (16-JUL-2021)	Depositor
R, R_{free}	0.223 , 0.255 0.226 , 0.260	Depositor DCC
R_{free} test set	2903 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	80.7	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.022 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	23285	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 59.10 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8551e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.37	0/2001	0.54	0/2686
1	C	0.39	0/2006	0.53	0/2692
1	E	0.41	0/1966	0.55	0/2639
1	G	0.40	0/1971	0.54	0/2645
1	I	0.38	0/1965	0.55	0/2636
1	K	0.37	0/1975	0.56	0/2650
2	B	0.38	0/1970	0.52	0/2648
2	D	0.37	0/1970	0.50	0/2648
2	F	0.39	0/1970	0.52	0/2648
2	H	0.39	0/1979	0.52	0/2660
2	J	0.38	0/1970	0.52	0/2648
2	L	0.37	0/1979	0.52	0/2660
All	All	0.39	0/23722	0.53	0/31860

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1963	0	1945	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1968	0	1957	15	0
1	E	1929	0	1917	20	0
1	G	1934	0	1927	19	0
1	I	1930	0	1923	15	0
1	K	1939	0	1937	22	0
2	B	1932	0	1903	24	0
2	D	1932	0	1903	17	0
2	F	1932	0	1903	22	0
2	H	1941	0	1909	18	0
2	J	1932	0	1903	21	0
2	L	1941	0	1909	22	0
3	B	2	0	0	0	0
3	D	2	0	0	0	0
3	F	2	0	0	0	0
3	H	2	0	0	0	0
3	J	2	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
All	All	23285	0	23036	183	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 4.

All (183) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:THR:O	2:B:479:ARG:NH2	1.96	0.98
1:I:251:ARG:NH1	2:J:381:TYR:O	2.10	0.85
2:B:479:ARG:NH1	2:B:487:GLU:OE2	2.11	0.83
1:C:85:ILE:HG23	1:C:105:ILE:HD11	1.65	0.77
1:E:85:ILE:HG23	1:E:105:ILE:HD11	1.65	0.77
2:B:377:ASN:HB2	2:B:446:ILE:HD12	1.67	0.77
1:G:85:ILE:HG23	1:G:105:ILE:HD11	1.67	0.76
1:A:85:ILE:HG23	1:A:105:ILE:HD11	1.66	0.75
1:K:85:ILE:HG23	1:K:105:ILE:HD11	1.68	0.74
1:K:267:TYR:CZ	2:L:523:MET:HB2	2.22	0.74
2:L:431:CYS:HB2	2:L:447:VAL:HG21	1.68	0.74
1:E:258:ALA:HB3	2:F:435:VAL:HG23	1.69	0.74
2:L:375:VAL:HG12	2:L:447:VAL:HG12	1.69	0.73
1:I:217:THR:HG22	2:J:476:THR:HG23	1.69	0.73
2:J:482:GLN:O	2:J:485:THR:HG22	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:217:THR:HG22	2:L:476:THR:HG23	1.72	0.71
1:K:267:TYR:OH	2:L:523:MET:HB2	1.93	0.69
1:K:267:TYR:OH	2:L:519:LEU:O	2.11	0.68
1:G:140:ARG:HH11	1:G:142:ARG:NH2	1.93	0.66
2:J:361:GLN:H	2:J:361:GLN:CD	1.98	0.66
1:E:127:VAL:HG21	2:F:347:ILE:CG1	2.27	0.65
2:L:361:GLN:H	2:L:361:GLN:CD	2.00	0.65
1:A:296:LEU:HD13	2:B:493:ARG:HE	1.62	0.65
1:E:216:THR:OG1	2:F:473:GLU:HB3	1.97	0.65
1:K:146:HIS:NE2	1:K:194:GLU:HG3	2.12	0.64
2:L:431:CYS:HB2	2:L:447:VAL:CG2	2.28	0.64
1:E:258:ALA:HB3	2:F:435:VAL:CG2	2.28	0.62
1:E:127:VAL:HG21	2:F:347:ILE:HG13	1.81	0.62
2:B:377:ASN:CB	2:B:446:ILE:HD12	2.29	0.61
1:I:267:TYR:CZ	2:J:523:MET:HB2	2.36	0.61
1:A:284:GLN:HE21	1:A:288:ASN:HD21	1.48	0.59
1:G:258:ALA:HB3	2:H:435:VAL:HG23	1.85	0.59
1:K:276:GLU:HA	1:K:279:LYS:HG2	1.85	0.57
1:I:256:ARG:NH2	2:J:439:THR:O	2.38	0.57
1:G:140:ARG:HH11	1:G:142:ARG:HH21	1.52	0.56
2:H:357:MET:HE2	2:H:362:LEU:HD21	1.87	0.56
2:L:295:GLN:NE2	2:L:370:ALA:H	2.05	0.55
1:G:159:VAL:HG23	1:G:163:LEU:HD23	1.88	0.54
1:K:146:HIS:HE2	1:K:194:GLU:HG3	1.72	0.54
2:H:295:GLN:NE2	2:H:370:ALA:H	2.06	0.54
1:A:258:ALA:HB3	2:B:435:VAL:HG23	1.90	0.54
2:D:295:GLN:NE2	2:D:370:ALA:H	2.06	0.54
2:D:375:VAL:HG12	2:D:447:VAL:HG22	1.90	0.54
2:B:295:GLN:NE2	2:B:370:ALA:H	2.07	0.53
2:L:485:THR:O	2:L:489:GLU:HG2	2.09	0.53
1:E:277:MET:HA	1:E:280:GLN:HG2	1.90	0.53
1:E:296:LEU:HD13	2:F:493:ARG:HE	1.72	0.53
1:G:272:LYS:O	1:G:275:ILE:HG13	2.09	0.53
2:F:295:GLN:NE2	2:F:370:ALA:H	2.07	0.52
1:G:258:ALA:HB3	2:H:435:VAL:CG2	2.39	0.52
2:B:375:VAL:HG12	2:B:447:VAL:HG22	1.92	0.52
2:J:485:THR:O	2:J:489:GLU:HG2	2.09	0.52
2:J:375:VAL:HG12	2:J:447:VAL:HG22	1.92	0.51
2:F:375:VAL:HG12	2:F:447:VAL:HG22	1.92	0.51
1:C:82:PRO:HG2	1:C:135:ARG:HH21	1.74	0.51
1:C:296:LEU:HD13	2:D:493:ARG:HE	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:254:PRO:O	1:G:256:ARG:HD3	2.11	0.51
1:I:73:ARG:HH21	1:I:119:ARG:HB2	1.75	0.51
1:C:159:VAL:HG23	1:C:163:LEU:HD23	1.94	0.50
1:A:296:LEU:HD13	2:B:493:ARG:NE	2.25	0.50
1:K:296:LEU:HD13	2:L:493:ARG:HE	1.76	0.50
1:G:306:GLU:O	1:G:307:HIS:CD2	2.64	0.49
2:B:377:ASN:HB2	2:B:446:ILE:CD1	2.38	0.49
1:E:159:VAL:HG23	1:E:163:LEU:HD23	1.94	0.49
2:J:295:GLN:NE2	2:J:370:ALA:H	2.10	0.49
1:C:216:THR:OG1	2:D:473:GLU:HB3	2.11	0.49
1:A:271:TRP:CH2	2:B:443:ARG:HB3	2.48	0.49
1:K:73:ARG:HH21	1:K:119:ARG:HB2	1.76	0.49
2:D:445:VAL:HG23	2:D:447:VAL:HG23	1.95	0.48
1:I:270:ARG:O	1:I:274:LEU:HD13	2.14	0.48
1:G:217:THR:HA	2:H:476:THR:OG1	2.13	0.48
1:G:187:PRO:HG3	2:H:459:LEU:HD12	1.94	0.48
1:I:159:VAL:HG23	1:I:163:LEU:HD23	1.95	0.48
1:K:159:VAL:HG23	1:K:163:LEU:HD23	1.95	0.48
1:A:127:VAL:HG21	2:B:347:ILE:HG13	1.95	0.48
1:E:277:MET:O	1:E:280:GLN:HG2	2.13	0.48
1:E:303:ALA:HB3	2:F:486:PHE:HE1	1.78	0.48
2:H:375:VAL:HG12	2:H:447:VAL:HG22	1.94	0.48
1:A:159:VAL:HG23	1:A:163:LEU:HD23	1.96	0.48
1:E:254:PRO:O	1:E:256:ARG:HD3	2.13	0.47
2:F:307:ASP:OD1	2:F:358:ARG:NH1	2.47	0.47
1:A:216:THR:OG1	2:B:473:GLU:HB3	2.14	0.47
1:E:304:ARG:HG3	2:F:486:PHE:CZ	2.49	0.47
1:I:281:GLN:HB3	2:J:508:VAL:HG12	1.96	0.47
1:I:267:TYR:CE2	2:J:523:MET:HB2	2.50	0.46
1:G:127:VAL:HG11	2:H:347:ILE:CG1	2.46	0.46
2:L:373:LEU:HD12	2:L:418:PHE:HE2	1.81	0.46
2:F:373:LEU:HD12	2:F:418:PHE:HE2	1.81	0.46
1:K:276:GLU:OE1	1:K:279:LYS:HD2	2.14	0.46
2:L:421:LYS:N	2:L:422:PRO:HD2	2.31	0.46
2:B:505:ARG:HA	2:B:508:VAL:CG2	2.46	0.46
2:J:373:LEU:HD12	2:J:418:PHE:HE2	1.80	0.46
1:E:72:GLN:HE22	1:E:147:SER:H	1.62	0.46
1:K:118:THR:OG1	1:K:121:LEU:HD13	2.15	0.46
2:F:445:VAL:HG23	2:F:447:VAL:HG23	1.97	0.46
1:E:182:ASP:HA	2:F:453:LEU:HD23	1.98	0.45
2:D:376:ARG:HG3	2:D:446:ILE:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:182:ASP:HA	2:H:453:LEU:HD23	1.98	0.45
1:I:81:LEU:HD13	1:I:85:ILE:HD13	1.97	0.45
1:C:271:TRP:CH2	2:D:443:ARG:HB3	2.51	0.45
2:J:376:ARG:HG3	2:J:446:ILE:HB	1.98	0.45
1:K:187:PRO:HG3	2:L:459:LEU:HD22	1.99	0.45
2:H:477:PRO:O	2:H:479:ARG:HD3	2.17	0.45
1:C:118:THR:HG22	1:C:121:LEU:HD12	1.98	0.45
1:C:72:GLN:HE22	1:C:147:SER:H	1.65	0.45
1:A:254:PRO:O	1:A:256:ARG:HD3	2.17	0.45
2:J:421:LYS:N	2:J:422:PRO:HD2	2.32	0.45
2:B:376:ARG:HG3	2:B:446:ILE:HB	1.98	0.45
1:C:230:LEU:HD22	2:D:411:THR:HG21	1.99	0.45
2:F:420:SER:HB2	2:F:422:PRO:HD2	1.98	0.44
1:A:72:GLN:HE22	1:A:147:SER:H	1.66	0.44
1:C:254:PRO:O	1:C:256:ARG:HD3	2.18	0.44
2:H:421:LYS:N	2:H:422:PRO:HD2	2.32	0.44
1:I:272:LYS:O	1:I:275:ILE:HG13	2.17	0.44
2:H:356:PRO:HB3	2:H:361:GLN:HE22	1.82	0.44
2:L:376:ARG:HG3	2:L:446:ILE:HB	1.99	0.44
1:A:249:LYS:HE3	1:A:249:LYS:HB2	1.85	0.44
2:F:376:ARG:HG3	2:F:446:ILE:HB	2.00	0.44
1:G:123:GLU:O	1:G:127:VAL:HG12	2.17	0.44
2:B:421:LYS:N	2:B:422:PRO:HD2	2.33	0.44
2:H:376:ARG:HG3	2:H:446:ILE:HB	1.99	0.44
2:J:355:THR:HA	2:J:356:PRO:HD3	1.90	0.44
1:C:268:ALA:CB	2:D:435:VAL:HG11	2.48	0.44
1:I:255:PRO:HA	2:J:437:LEU:O	2.18	0.44
1:E:187:PRO:HG3	2:F:459:LEU:HD22	2.00	0.44
2:F:421:LYS:N	2:F:422:PRO:HD2	2.33	0.44
1:G:255:PRO:HA	2:H:437:LEU:O	2.17	0.44
1:E:75:ARG:HB2	1:E:115:ARG:HG3	2.00	0.43
2:B:373:LEU:HD12	2:B:418:PHE:HE2	1.83	0.43
2:F:477:PRO:O	2:F:479:ARG:HD3	2.18	0.43
1:A:127:VAL:HG21	2:B:347:ILE:CG1	2.47	0.43
1:C:75:ARG:HB2	1:C:115:ARG:HG3	2.01	0.43
1:C:255:PRO:HA	2:D:437:LEU:O	2.18	0.43
1:K:72:GLN:HE22	1:K:147:SER:H	1.66	0.43
1:K:255:PRO:HA	2:L:437:LEU:O	2.17	0.43
1:C:118:THR:HG23	1:C:121:LEU:H	1.84	0.43
2:H:420:SER:HB2	2:H:422:PRO:HD2	2.01	0.43
2:L:361:GLN:CD	2:L:361:GLN:N	2.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:GLN:HB3	2:B:508:VAL:HG12	2.01	0.43
1:I:118:THR:HG22	1:I:121:LEU:HD12	2.00	0.43
1:K:75:ARG:HB2	1:K:115:ARG:HG3	2.01	0.43
1:K:140:ARG:HA	1:K:140:ARG:HD2	1.88	0.43
1:A:75:ARG:HB2	1:A:115:ARG:HG3	2.01	0.43
1:C:218:PHE:HA	1:C:219:PRO:HD3	1.92	0.43
2:D:421:LYS:N	2:D:422:PRO:HD2	2.32	0.43
1:G:75:ARG:HB2	1:G:115:ARG:HG3	2.00	0.42
1:G:150:LEU:HD22	1:G:205:LEU:HD13	2.00	0.42
2:J:420:SER:HB2	2:J:422:PRO:HD2	2.01	0.42
1:K:220:ARG:NH2	2:L:498:ASP:OD1	2.52	0.42
2:D:477:PRO:O	2:D:479:ARG:HD3	2.20	0.42
1:I:75:ARG:HB2	1:I:115:ARG:HG3	2.02	0.42
2:J:441:THR:HA	2:J:442:PRO:HD3	1.89	0.42
1:E:82:PRO:HA	1:E:137:LYS:HE3	2.01	0.42
2:D:356:PRO:HB3	2:D:361:GLN:HE22	1.84	0.42
2:D:373:LEU:HD12	2:D:418:PHE:HE2	1.84	0.42
2:H:373:LEU:HD12	2:H:418:PHE:HE2	1.83	0.42
2:J:505:ARG:HA	2:J:508:VAL:CG2	2.50	0.42
1:K:181:VAL:CG1	1:K:185:GLY:HA2	2.50	0.42
1:K:254:PRO:O	1:K:256:ARG:HD3	2.20	0.42
1:A:140:ARG:HA	1:A:140:ARG:HD2	1.92	0.41
1:A:258:ALA:HB3	2:B:435:VAL:CG2	2.50	0.41
1:E:190:LYS:HB3	1:E:190:LYS:HE2	1.90	0.41
2:J:361:GLN:CD	2:J:361:GLN:N	2.69	0.41
2:H:341:SER:HB3	2:H:344:LEU:HD12	2.02	0.41
1:A:215:LEU:HA	2:B:478:PRO:HB3	2.01	0.41
1:I:278:GLU:HG3	2:J:512:MET:SD	2.60	0.41
2:B:476:THR:HA	2:B:477:PRO:HD3	1.95	0.41
2:L:295:GLN:HE22	2:L:370:ALA:H	1.68	0.41
2:F:356:PRO:HB3	2:F:361:GLN:HE22	1.86	0.41
2:D:295:GLN:HE22	2:D:370:ALA:H	1.69	0.41
1:E:255:PRO:HA	2:F:437:LEU:O	2.21	0.41
1:K:116:LEU:HD12	1:K:122:ALA:HA	2.03	0.41
2:L:341:SER:HB3	2:L:344:LEU:HD12	2.03	0.41
2:L:420:SER:HB2	2:L:422:PRO:HD2	2.02	0.41
2:D:488:TYR:O	2:D:492:GLN:HG2	2.21	0.41
1:A:116:LEU:HD12	1:A:122:ALA:HA	2.02	0.40
2:B:341:SER:HB3	2:B:344:LEU:HD12	2.03	0.40
2:B:524:GLU:OE2	2:B:528:HIS:HE1	2.05	0.40
2:D:524:GLU:OE2	2:D:528:HIS:HE1	2.05	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:355:THR:HA	2:L:356:PRO:HD3	1.92	0.40
2:F:355:THR:HA	2:F:356:PRO:HD3	1.91	0.40
1:G:190:LYS:HE2	1:G:190:LYS:HB3	1.88	0.40
1:G:303:ALA:HB3	2:H:486:PHE:HE1	1.86	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	240/259 (93%)	236 (98%)	4 (2%)	0	100	100
1	C	240/259 (93%)	235 (98%)	5 (2%)	0	100	100
1	E	233/259 (90%)	230 (99%)	3 (1%)	0	100	100
1	G	233/259 (90%)	229 (98%)	4 (2%)	0	100	100
1	I	234/259 (90%)	231 (99%)	3 (1%)	0	100	100
1	K	237/259 (92%)	234 (99%)	3 (1%)	0	100	100
2	B	237/259 (92%)	232 (98%)	5 (2%)	0	100	100
2	D	237/259 (92%)	230 (97%)	7 (3%)	0	100	100
2	F	237/259 (92%)	231 (98%)	6 (2%)	0	100	100
2	H	238/259 (92%)	232 (98%)	6 (2%)	0	100	100
2	J	237/259 (92%)	232 (98%)	5 (2%)	0	100	100
2	L	238/259 (92%)	233 (98%)	5 (2%)	0	100	100
All	All	2841/3108 (91%)	2785 (98%)	56 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	210/227 (92%)	200 (95%)	10 (5%)	25	62
1	C	211/227 (93%)	196 (93%)	15 (7%)	14	46
1	E	207/227 (91%)	191 (92%)	16 (8%)	13	42
1	G	208/227 (92%)	196 (94%)	12 (6%)	20	55
1	I	207/227 (91%)	197 (95%)	10 (5%)	25	62
1	K	208/227 (92%)	195 (94%)	13 (6%)	18	51
2	B	205/221 (93%)	194 (95%)	11 (5%)	22	57
2	D	205/221 (93%)	198 (97%)	7 (3%)	37	72
2	F	205/221 (93%)	199 (97%)	6 (3%)	42	76
2	H	206/221 (93%)	199 (97%)	7 (3%)	37	72
2	J	205/221 (93%)	197 (96%)	8 (4%)	32	69
2	L	206/221 (93%)	199 (97%)	7 (3%)	37	72
All	All	2483/2688 (92%)	2361 (95%)	122 (5%)	25	61

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	GLU
1	A	108	ASP
1	A	153	ARG
1	A	165	GLU
1	A	169	SER
1	A	183	ASP
1	A	205	LEU
1	A	249	LYS
1	A	267	TYR
1	A	301	GLU
2	B	291	LYS
2	B	303	ASN
2	B	319	LYS
2	B	406	ASP

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Mol	Chain	Res	Type
2	B	407	ARG
2	B	435	VAL
2	B	452	GLN
2	B	479	ARG
2	B	503	GLN
2	B	508	VAL
2	B	529	GLU
1	C	71	THR
1	C	88	GLU
1	C	89	GLU
1	C	92	LYS
1	C	108	ASP
1	C	142	ARG
1	C	153	ARG
1	C	157	GLN
1	C	165	GLU
1	C	183	ASP
1	C	205	LEU
1	C	228	ASP
1	C	267	TYR
1	C	298	MET
1	C	301	GLU
2	D	303	ASN
2	D	332	LYS
2	D	406	ASP
2	D	445	VAL
2	D	452	GLN
2	D	479	ARG
2	D	503	GLN
1	E	71	THR
1	E	88	GLU
1	E	89	GLU
1	E	92	LYS
1	E	142	ARG
1	E	153	ARG
1	E	165	GLU
1	E	169	SER
1	E	183	ASP
1	E	205	LEU
1	E	239	LYS
1	E	245	GLN
1	E	267	TYR

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Mol	Chain	Res	Type
1	E	275	ILE
1	E	301	GLU
1	E	306	GLU
2	F	303	ASN
2	F	406	ASP
2	F	445	VAL
2	F	452	GLN
2	F	479	ARG
2	F	503	GLN
1	G	71	THR
1	G	88	GLU
1	G	89	GLU
1	G	142	ARG
1	G	153	ARG
1	G	165	GLU
1	G	183	ASP
1	G	205	LEU
1	G	239	LYS
1	G	267	TYR
1	G	298	MET
1	G	301	GLU
2	H	290	GLU
2	H	303	ASN
2	H	360	ARG
2	H	406	ASP
2	H	459	LEU
2	H	479	ARG
2	H	503	GLN
1	I	73	ARG
1	I	142	ARG
1	I	153	ARG
1	I	165	GLU
1	I	183	ASP
1	I	186	ARG
1	I	205	LEU
1	I	256	ARG
1	I	267	TYR
1	I	301	GLU
2	J	291	LYS
2	J	361	GLN
2	J	406	ASP
2	J	452	GLN

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Mol	Chain	Res	Type
2	J	469	MET
2	J	479	ARG
2	J	503	GLN
2	J	508	VAL
1	K	71	THR
1	K	73	ARG
1	K	88	GLU
1	K	89	GLU
1	K	92	LYS
1	K	153	ARG
1	K	157	GLN
1	K	165	GLU
1	K	183	ASP
1	K	194	GLU
1	K	205	LEU
1	K	274	LEU
1	K	301	GLU
2	L	303	ASN
2	L	361	GLN
2	L	406	ASP
2	L	432	SER
2	L	452	GLN
2	L	479	ARG
2	L	503	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	245	GLN
1	A	288	ASN
1	A	307	HIS
2	B	295	GLN
1	C	72	GLN
1	C	106	HIS
2	D	295	GLN
1	E	72	GLN
2	F	295	GLN
2	F	471	GLN
1	G	307	HIS
2	H	295	GLN
1	I	245	GLN

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Mol	Chain	Res	Type
2	J	295	GLN
1	K	72	GLN
2	L	295	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 12 ligands modelled in this entry, 12 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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	242/259 (93%)	0.27	6 (2%) 57 29	67, 89, 125, 138	0
1	C	242/259 (93%)	0.28	10 (4%) 37 14	57, 85, 126, 141	0
1	E	237/259 (91%)	0.16	3 (1%) 77 51	60, 81, 124, 136	0
1	G	237/259 (91%)	0.28	10 (4%) 36 14	56, 83, 138, 151	0
1	I	238/259 (91%)	0.39	11 (4%) 32 12	64, 93, 135, 162	0
1	K	239/259 (92%)	0.41	16 (6%) 17 5	65, 102, 139, 213	0
2	B	239/259 (92%)	0.17	1 (0%) 92 79	46, 91, 120, 148	0
2	D	239/259 (92%)	0.10	4 (1%) 70 41	50, 84, 115, 143	0
2	F	239/259 (92%)	0.12	3 (1%) 77 51	43, 80, 112, 139	0
2	H	240/259 (92%)	0.15	1 (0%) 92 79	55, 85, 117, 142	0
2	J	239/259 (92%)	0.25	8 (3%) 46 20	52, 85, 133, 140	0
2	L	240/259 (92%)	0.25	6 (2%) 57 29	63, 98, 139, 144	0
All	All	2871/3108 (92%)	0.24	79 (2%) 53 25	43, 88, 130, 213	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	109	LYS	6.3
1	C	85	ILE	5.5
1	I	67	GLU	4.3
1	I	134	LEU	4.3
1	K	66	GLY	4.3
1	G	82	PRO	4.2
2	L	357	MET	3.9
2	L	470	TYR	3.9
1	K	219	PRO	3.7
2	J	486	PHE	3.6
1	K	67	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
2	L	490	TYR	3.6
1	A	136	GLY	3.6
1	E	85	ILE	3.6
1	G	112	GLY	3.5
1	G	139	LEU	3.5
1	A	109	LYS	3.4
1	A	108	ASP	3.3
1	K	136	GLY	3.3
1	A	86	THR	3.1
1	I	139	LEU	3.1
1	A	83	PRO	3.0
1	G	83	PRO	3.0
1	K	300	MET	3.0
1	G	85	ILE	3.0
2	J	527	TYR	2.9
2	L	481	ALA	2.9
2	F	490	TYR	2.8
2	J	356	PRO	2.8
1	G	84	ASP	2.8
1	C	90	MET	2.7
1	C	134	LEU	2.7
1	A	134	LEU	2.7
2	D	497	LEU	2.7
1	G	134	LEU	2.6
2	L	316	LEU	2.6
1	K	90	MET	2.6
1	I	82	PRO	2.5
1	I	133	PRO	2.5
1	K	105	ILE	2.5
2	L	486	PHE	2.5
1	K	85	ILE	2.5
2	J	471	GLN	2.4
2	J	487	GLU	2.4
2	F	526	ALA	2.4
2	D	362	LEU	2.4
2	J	468	PRO	2.4
1	K	134	LEU	2.4
1	G	79	GLY	2.3
1	K	137	LYS	2.3
1	C	108	ASP	2.3
1	C	215	LEU	2.3
1	I	214	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	304	LEU	2.3
1	G	141	VAL	2.3
1	I	85	ILE	2.3
1	K	280	GLN	2.3
1	K	215	LEU	2.2
1	C	195	PHE	2.2
2	J	352	LEU	2.2
1	E	104	PHE	2.2
1	I	135	ARG	2.2
1	I	88	GLU	2.2
1	E	83	PRO	2.2
1	C	77	PHE	2.2
1	K	303	ALA	2.2
1	C	111	PHE	2.2
2	B	313	PHE	2.2
2	J	313	PHE	2.1
1	G	132	MET	2.1
1	I	296	LEU	2.1
1	K	296	LEU	2.1
2	F	486	PHE	2.1
1	C	86	THR	2.1
1	K	263	PHE	2.0
1	I	263	PHE	2.0
2	D	328	ILE	2.0
1	K	82	PRO	2.0
2	H	304	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 monosaccharides in this entry.

6.4 Ligands (i)

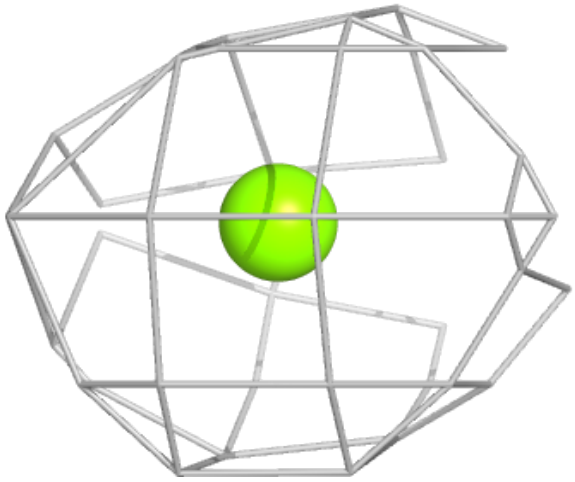
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

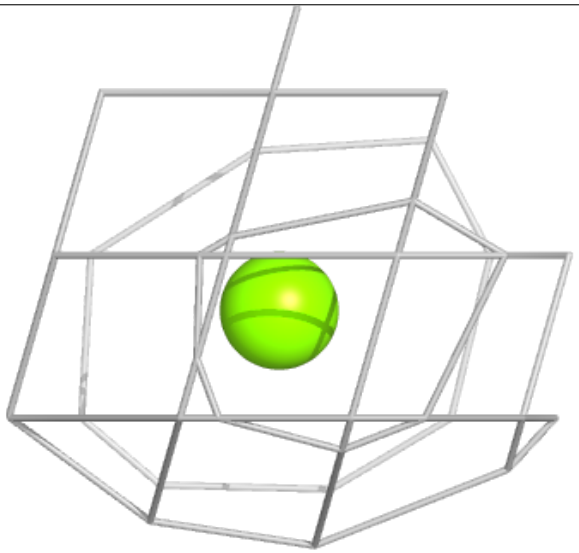
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	F	601	1/1	0.90	0.14	52,52,52,52	0
3	MG	H	602	1/1	0.90	0.19	62,62,62,62	0
3	MG	H	601	1/1	0.91	0.19	60,60,60,60	0
3	MG	D	601	1/1	0.91	0.16	70,70,70,70	0
3	MG	L	601	1/1	0.91	0.17	78,78,78,78	0
3	MG	F	602	1/1	0.92	0.12	48,48,48,48	0
3	MG	J	601	1/1	0.92	0.11	71,71,71,71	0
3	MG	B	602	1/1	0.92	0.21	41,41,41,41	0
3	MG	K	401	1/1	0.93	0.20	62,62,62,62	0
3	MG	J	602	1/1	0.95	0.18	45,45,45,45	0
3	MG	D	602	1/1	0.95	0.35	41,41,41,41	0
3	MG	B	601	1/1	0.95	0.14	82,82,82,82	0

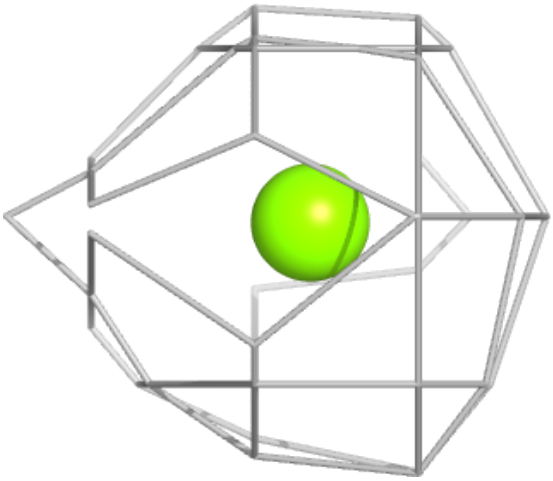
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MG F 601:

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

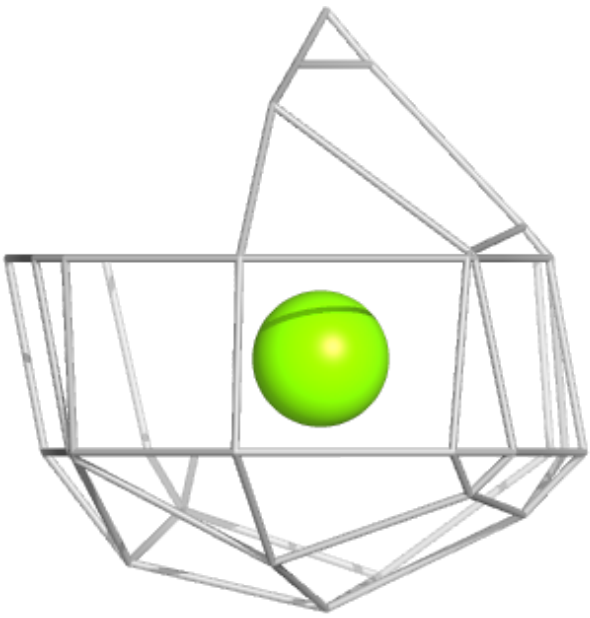


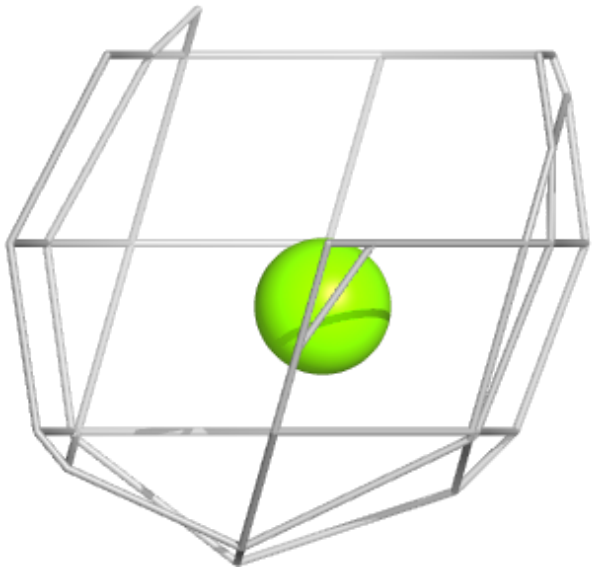


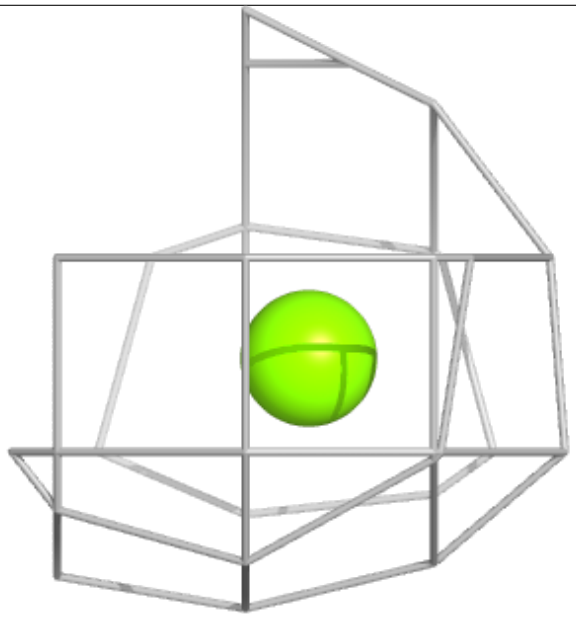


Electron density around MG H 602:

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

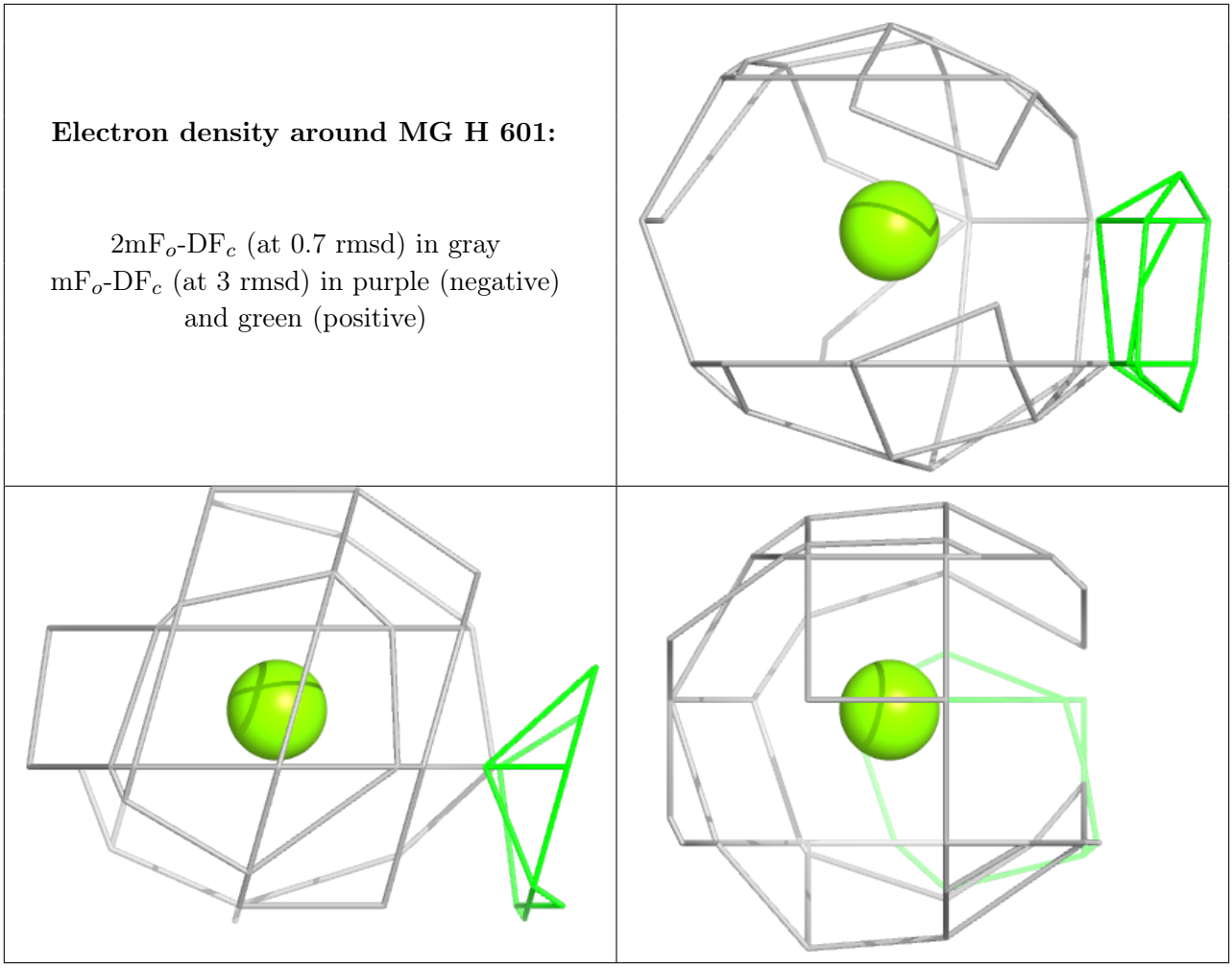






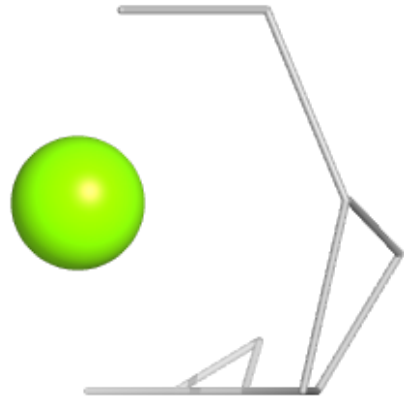
Electron density around MG H 601:

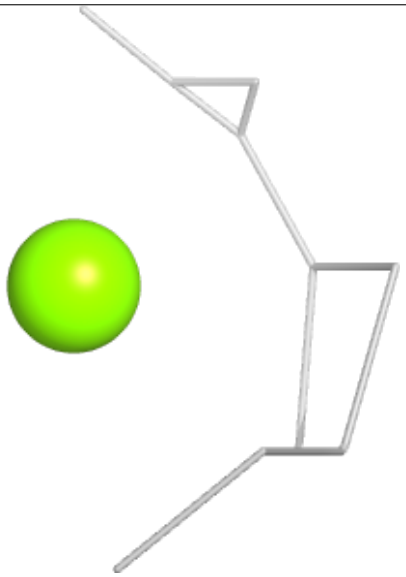
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

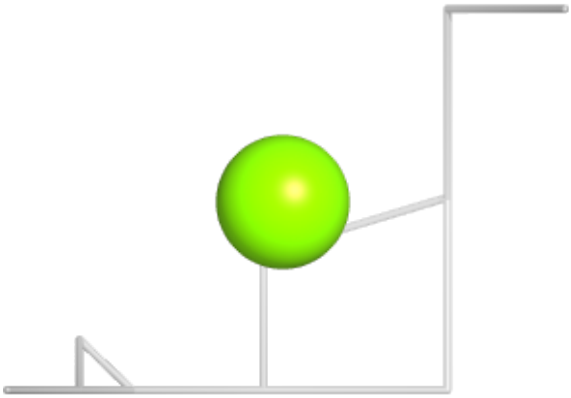


Electron density around MG D 601:

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

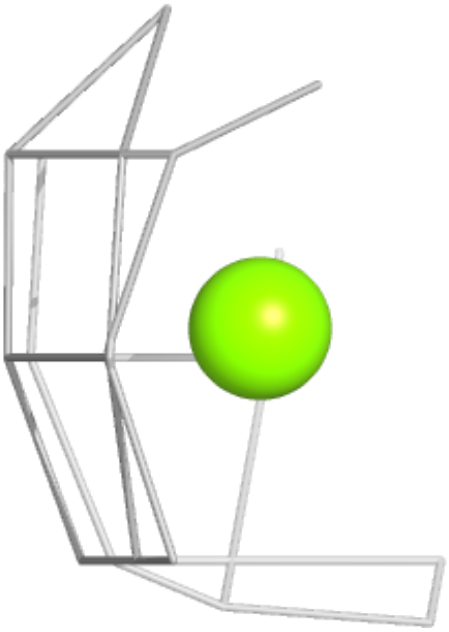


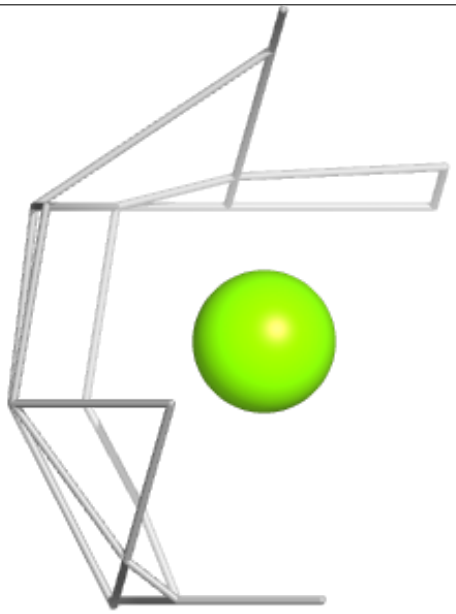


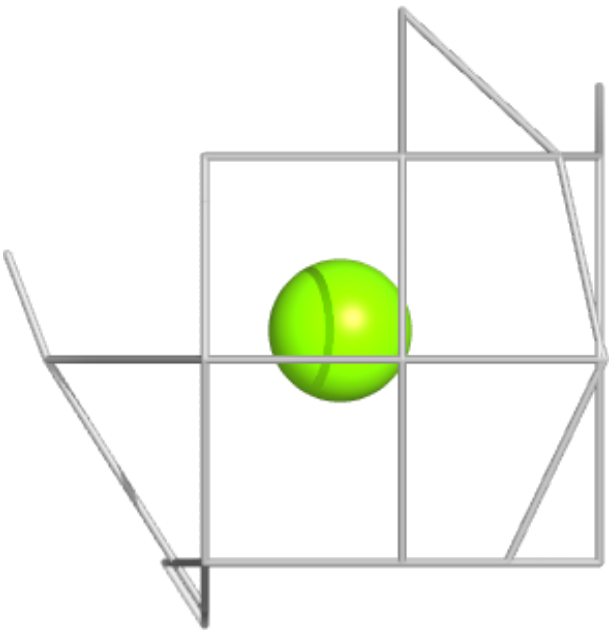


Electron density around MG L 601:

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

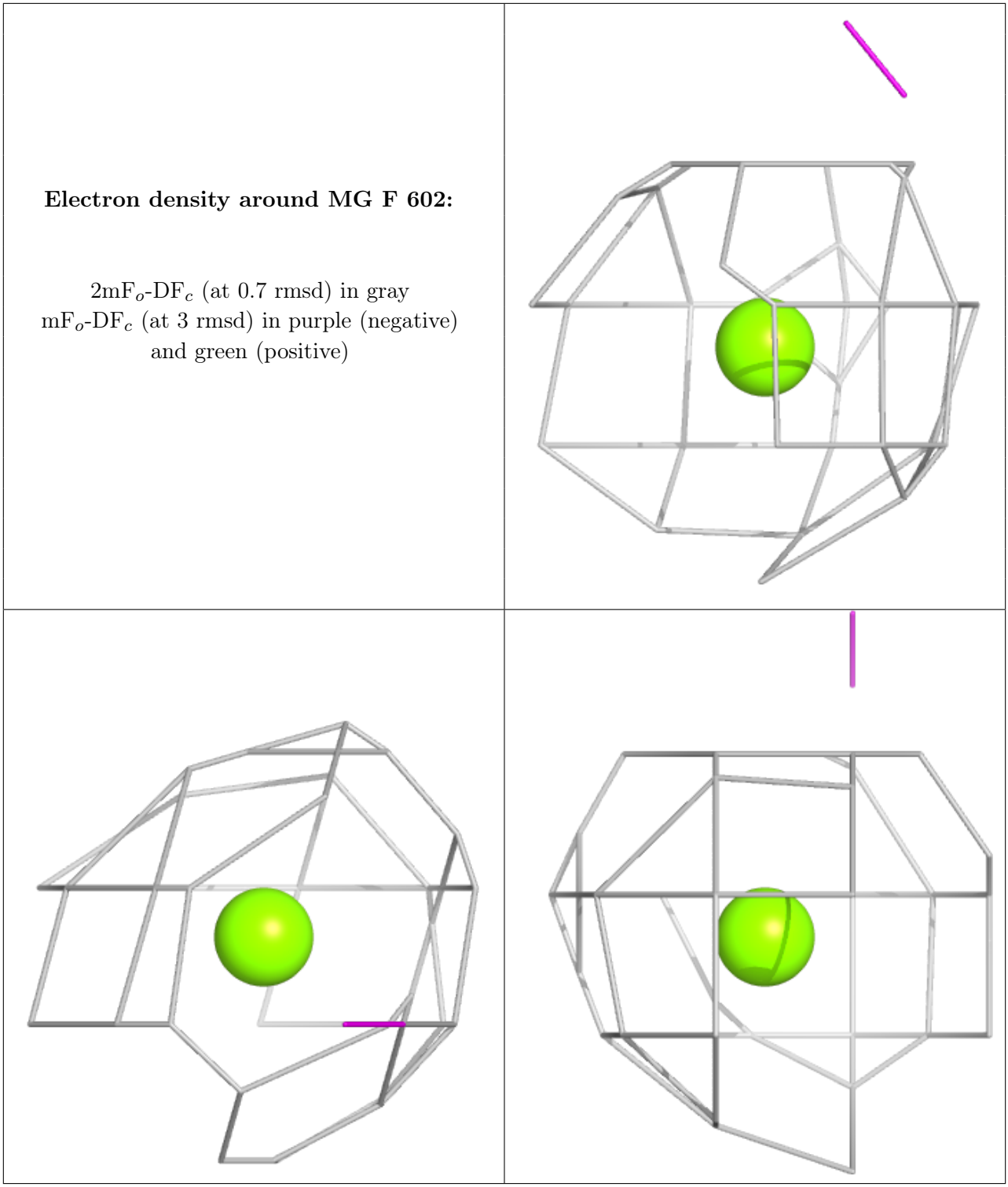






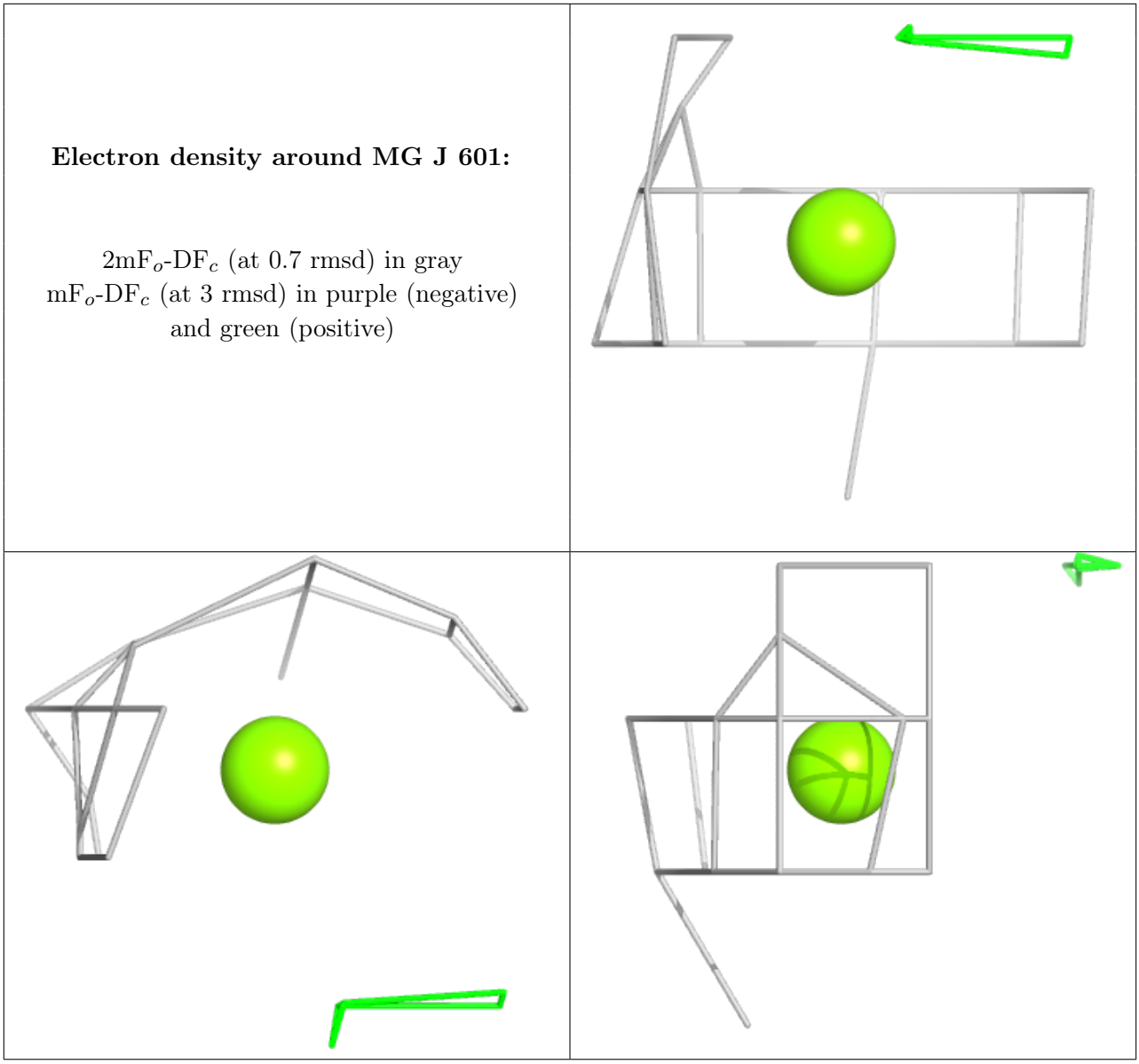
Electron density around MG F 602:

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



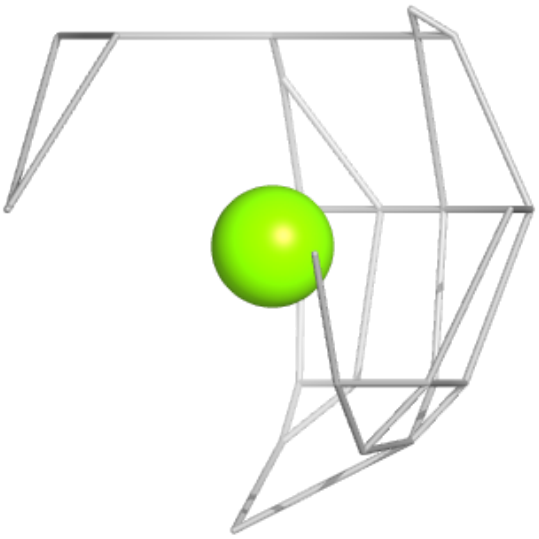
Electron density around MG J 601:

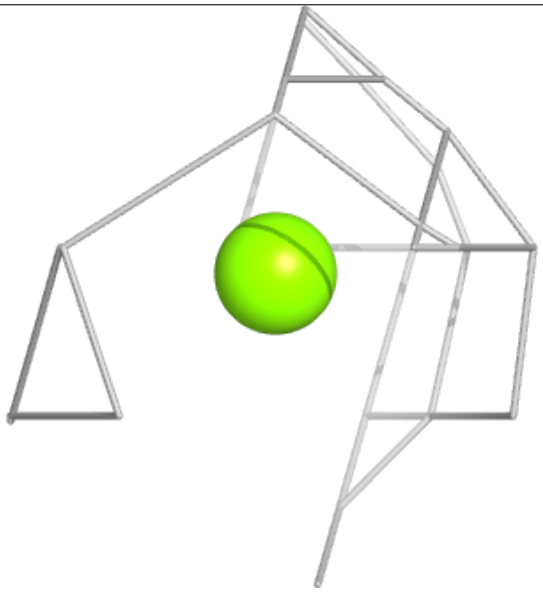
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

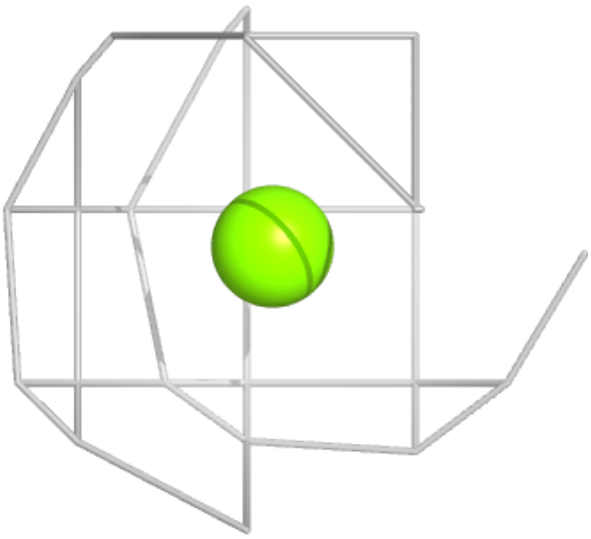


Electron density around MG B 602:

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

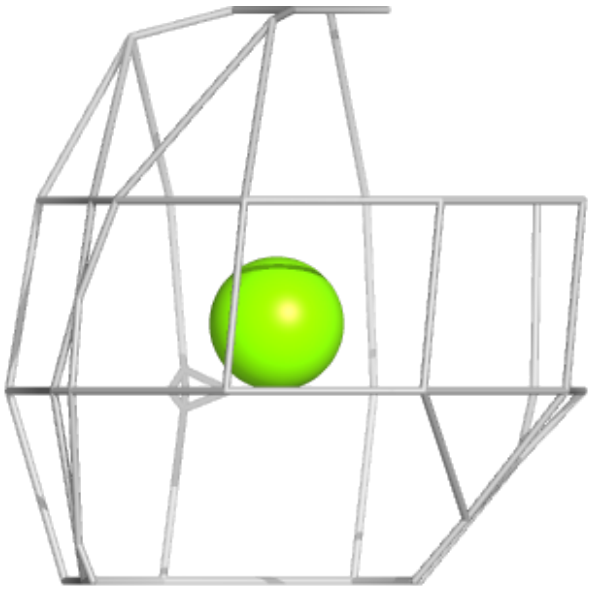


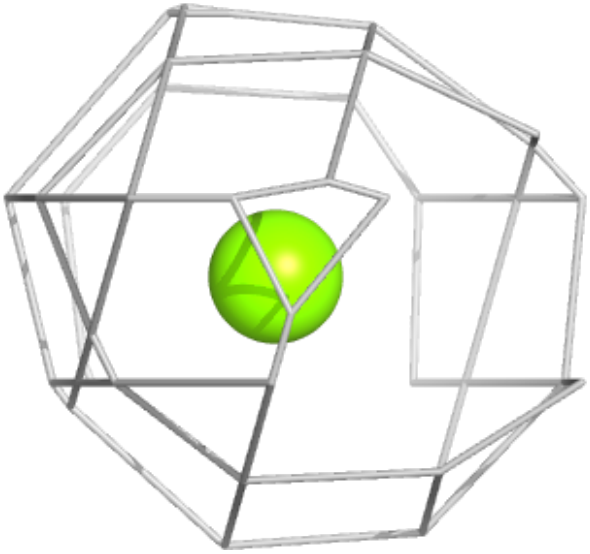


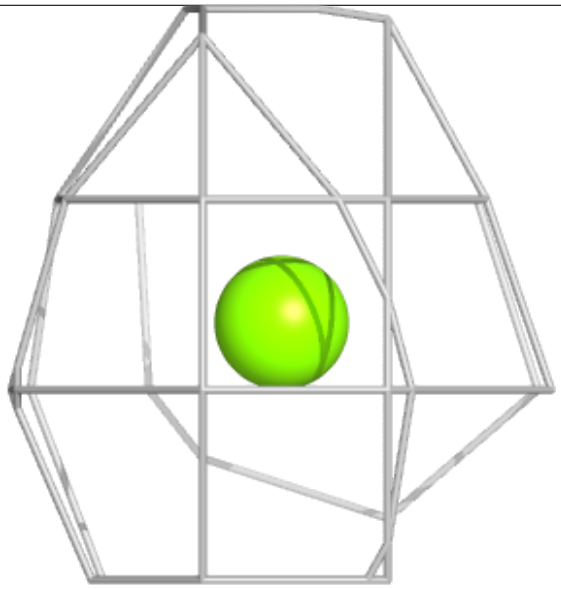


Electron density around MG K 401:

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

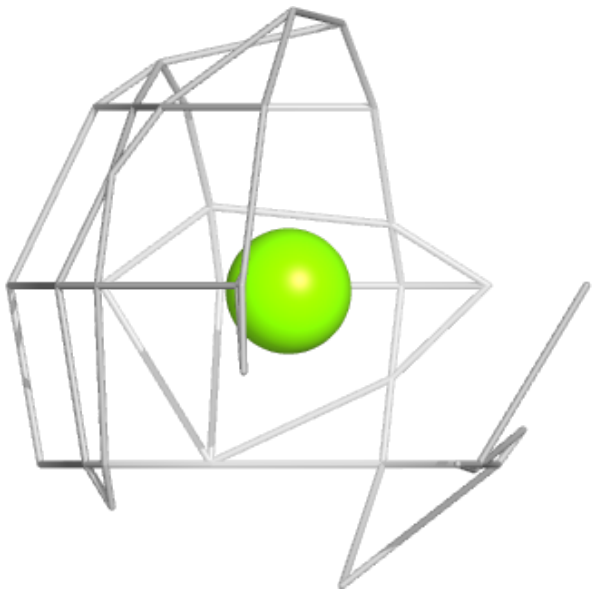


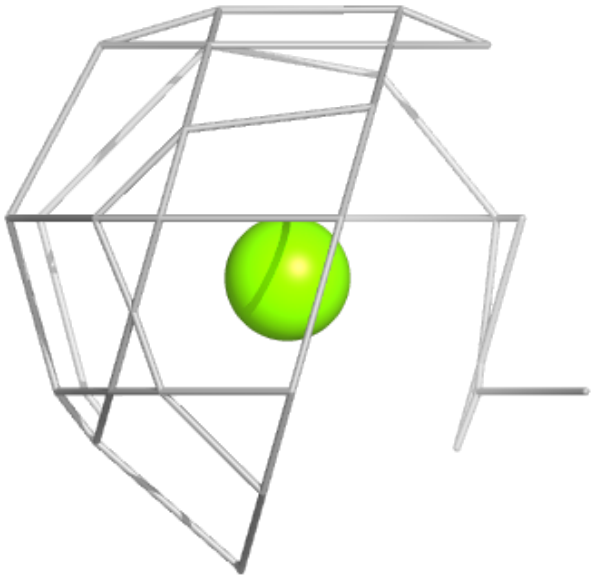


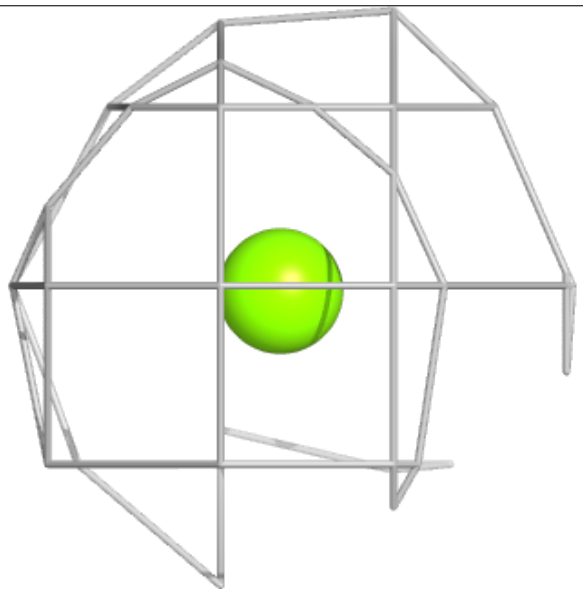


Electron density around MG J 602:

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

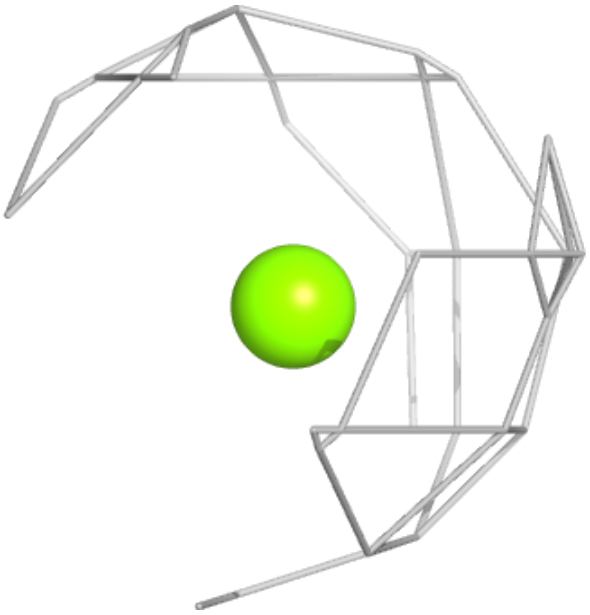


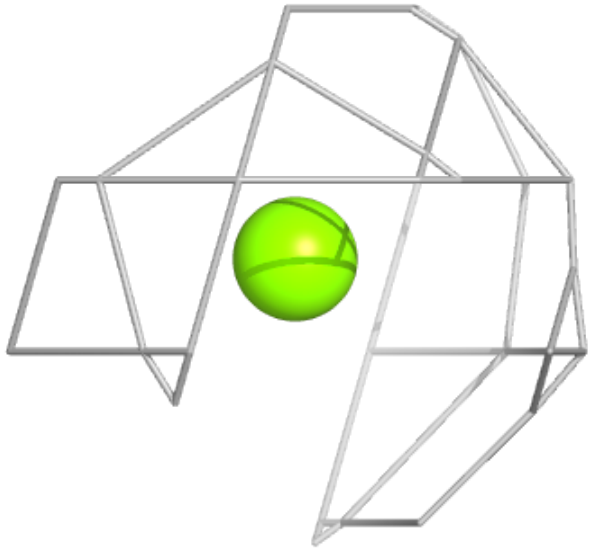


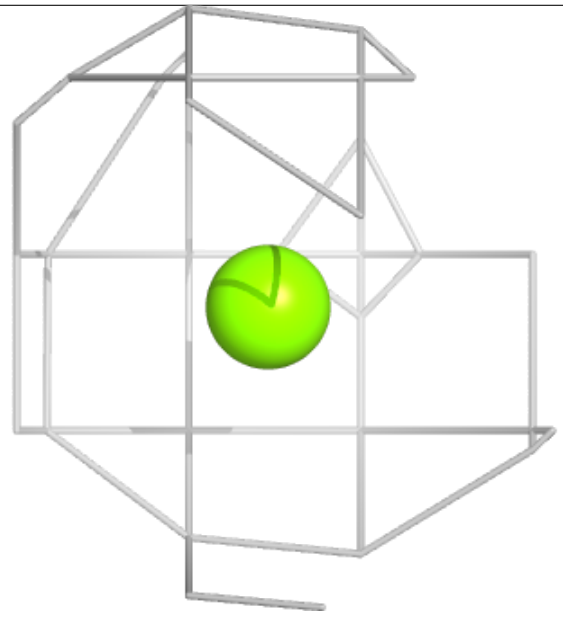


Electron density around MG D 602:

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

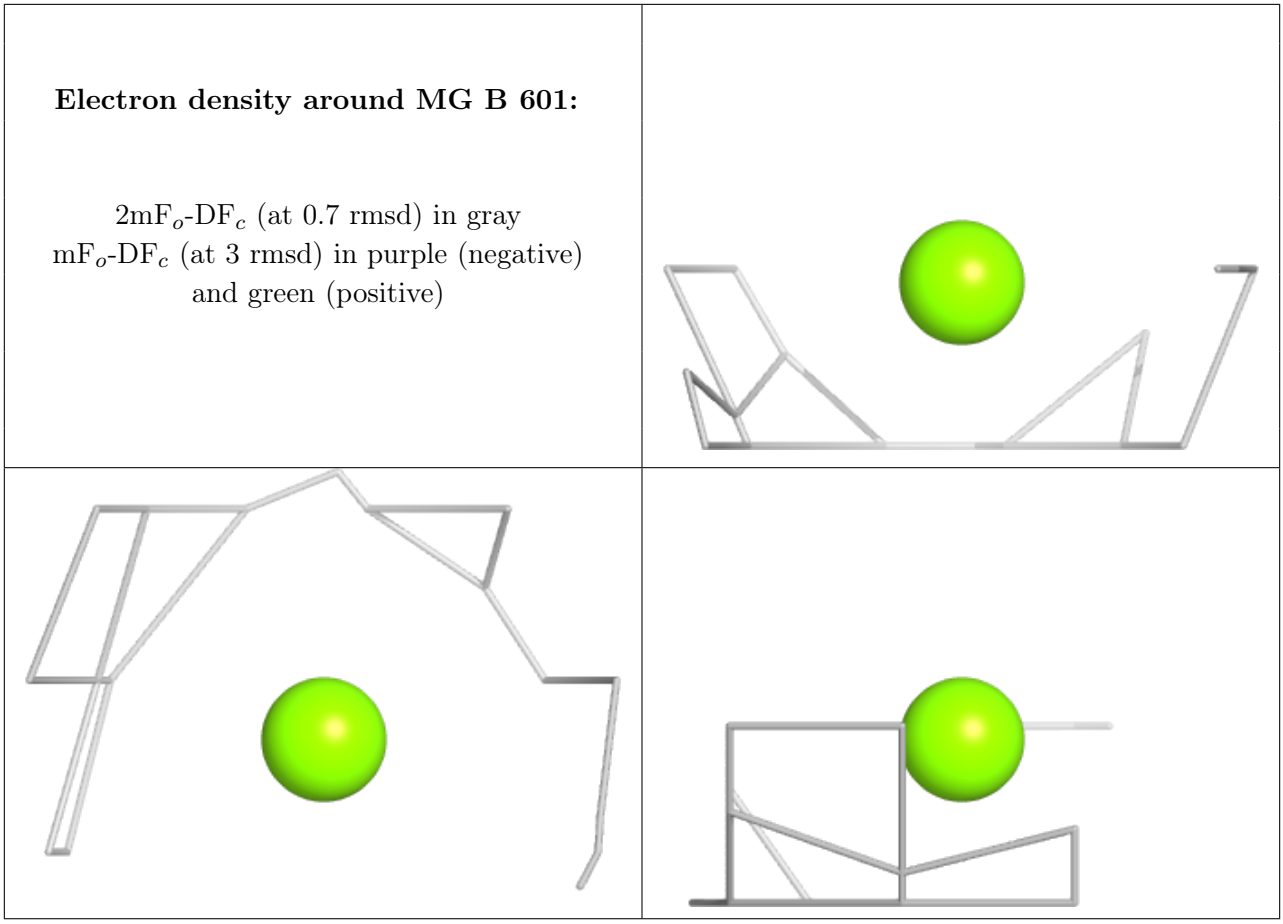






Electron density around MG B 601:

$2mF_o$-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.