



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 03:20 AM UTC

PDB ID : 9WF6 / pdb_00009wf6
Title : Crystal Structure of Escherichia coli GroEL with Magnesium Ions and a Phosphorylated Serine Residue-3.0 Å
Authors : Guo, Y.; Zhang, L.; Zheng, H.; Li, J.; Han, Q.
Deposited on : 2025-08-21
Resolution : 2.99 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

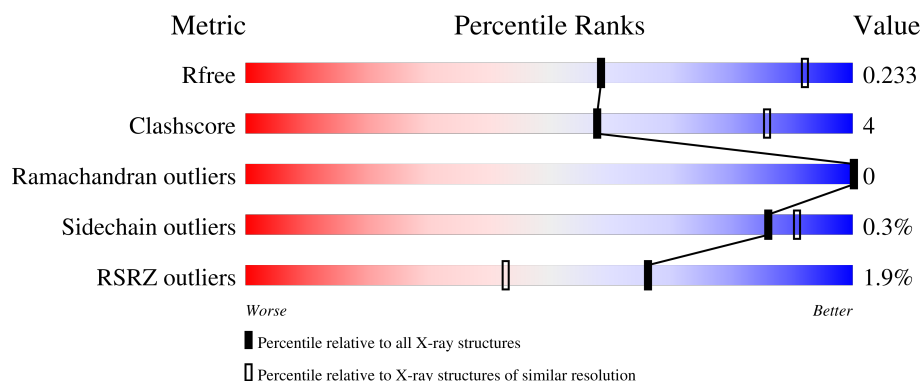
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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.



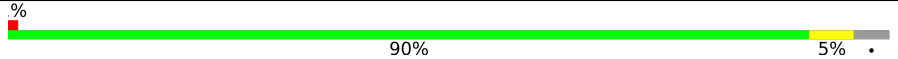
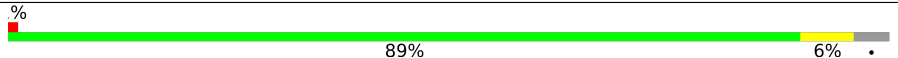
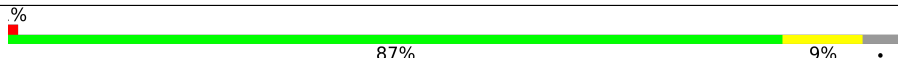
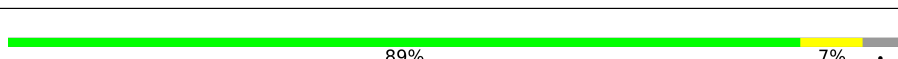
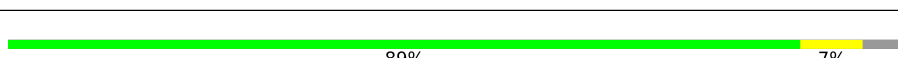
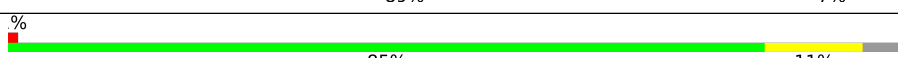
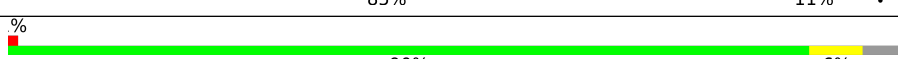
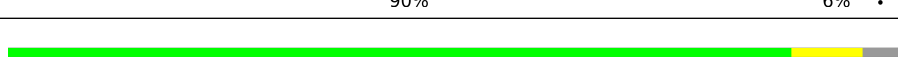
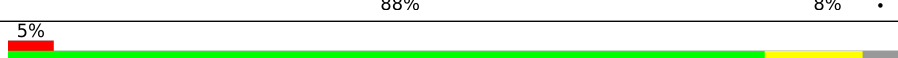
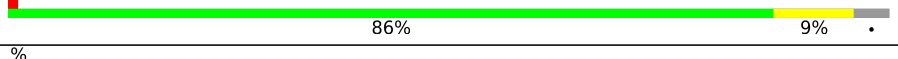
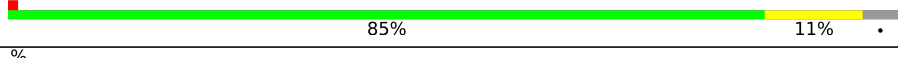
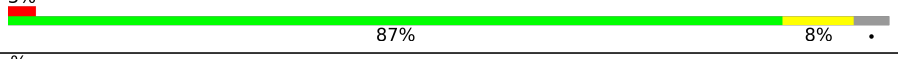
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 $\leq 5\%$. 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	548	5% 85% 10% .
1	B	548	% 89% 7% .
1	C	548	2% 87% 9% .
1	F	548	4% 86% 9% .
1	G	548	3% 85% 10% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	548	
1	I	548	
1	J	548	
1	M	548	
1	N	548	
1	P	548	
1	Q	548	
1	T	548	
1	U	548	
1	Y	548	
1	a	548	
1	b	548	
2	D	548	
2	E	548	
2	K	548	
2	L	548	
2	O	548	
2	R	548	
2	V	548	
2	W	548	
2	X	548	
2	Z	548	
2	c	548	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 108950 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 Chaperonin GroEL.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	P	S	0	0	0
			3868	2403	667	777	1	20			
1	B	525	Total	C	N	O	P	S	0	0	0
			3868	2403	667	777	1	20			
1	C	525	Total	C	N	O	P	S	0	0	0
			3868	2403	667	777	1	20			
1	F	524	Total	C	N	O	P	S	0	0	0
			3859	2397	665	776	1	20			
1	G	525	Total	C	N	O	P	S	0	0	0
			3868	2403	667	777	1	20			
1	H	525	Total	C	N	O	P	S	0	0	0
			3868	2403	667	777	1	20			
1	I	524	Total	C	N	O	P	S	0	0	0
			3859	2397	665	776	1	20			
1	J	525	Total	C	N	O	P	S	0	0	0
			3868	2403	667	777	1	20			
1	M	525	Total	C	N	O	P	S	0	0	0
			3868	2403	667	777	1	20			
1	N	525	Total	C	N	O	P	S	0	0	0
			3868	2403	667	777	1	20			
1	P	525	Total	C	N	O	P	S	0	0	0
			3868	2403	667	777	1	20			
1	Q	525	Total	C	N	O	P	S	0	0	0
			3868	2403	667	777	1	20			
1	T	525	Total	C	N	O	P	S	0	0	0
			3868	2403	667	777	1	20			
1	U	525	Total	C	N	O	P	S	0	0	0
			3868	2403	667	777	1	20			
1	Y	525	Total	C	N	O	P	S	0	0	0
			3868	2403	667	777	1	20			
1	a	525	Total	C	N	O	P	S	0	0	0
			3868	2403	667	777	1	20			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	b	525	Total	C	N	O	P	S	0	0	0
			3868	2403	667	777	1	20			

- Molecule 2 is a protein called Chaperonin GroEL.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	525	Total	C	N	O	S		0	0	0
			3864	2403	667	774	20				
2	E	525	Total	C	N	O	S		0	0	0
			3864	2403	667	774	20				
2	K	525	Total	C	N	O	S		0	0	0
			3864	2403	667	774	20				
2	L	525	Total	C	N	O	S		0	0	0
			3864	2403	667	774	20				
2	O	525	Total	C	N	O	S		0	0	0
			3864	2403	667	774	20				
2	R	525	Total	C	N	O	S		0	0	0
			3864	2403	667	774	20				
2	V	525	Total	C	N	O	S		0	0	0
			3864	2403	667	774	20				
2	W	525	Total	C	N	O	S		0	0	0
			3864	2403	667	774	20				
2	X	525	Total	C	N	O	S		0	0	0
			3864	2403	667	774	20				
2	Z	525	Total	C	N	O	S		0	0	0
			3864	2403	667	774	20				
2	c	525	Total	C	N	O	S		0	0	0
			3864	2403	667	774	20				

- Molecule 3 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		
3	C	1	Total	C	O	S	0	0
			4	2	1	1		
3	D	1	Total	C	O	S	0	0
			4	2	1	1		
3	D	1	Total	C	O	S	0	0
			4	2	1	1		
3	D	1	Total	C	O	S	0	0
			4	2	1	1		
3	E	1	Total	C	O	S	0	0
			4	2	1	1		
3	E	1	Total	C	O	S	0	0
			4	2	1	1		
3	E	1	Total	C	O	S	0	0
			4	2	1	1		
3	F	1	Total	C	O	S	0	0
			4	2	1	1		
3	G	1	Total	C	O	S	0	0
			4	2	1	1		
3	G	1	Total	C	O	S	0	0
			4	2	1	1		
3	G	1	Total	C	O	S	0	0
			4	2	1	1		

Continued on next page...

Continued from previous page...

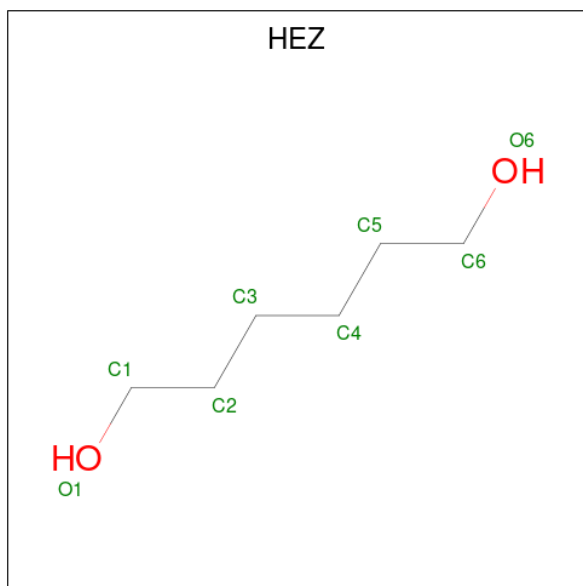
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	G	1	Total 4	C 2	O 1	S 1	0	0
3	H	1	Total 4	C 2	O 1	S 1	0	0
3	J	1	Total 4	C 2	O 1	S 1	0	0
3	K	1	Total 4	C 2	O 1	S 1	0	0
3	M	1	Total 4	C 2	O 1	S 1	0	0
3	N	1	Total 4	C 2	O 1	S 1	0	0
3	O	1	Total 4	C 2	O 1	S 1	0	0
3	O	1	Total 4	C 2	O 1	S 1	0	0
3	O	1	Total 4	C 2	O 1	S 1	0	0
3	P	1	Total 4	C 2	O 1	S 1	0	0
3	P	1	Total 4	C 2	O 1	S 1	0	0
3	Q	1	Total 4	C 2	O 1	S 1	0	0
3	Q	1	Total 4	C 2	O 1	S 1	0	0
3	Q	1	Total 4	C 2	O 1	S 1	0	0
3	R	1	Total 4	C 2	O 1	S 1	0	0
3	R	1	Total 4	C 2	O 1	S 1	0	0
3	T	1	Total 4	C 2	O 1	S 1	0	0
3	U	1	Total 4	C 2	O 1	S 1	0	0
3	U	1	Total 4	C 2	O 1	S 1	0	0
3	U	1	Total 4	C 2	O 1	S 1	0	0
3	V	1	Total 4	C 2	O 1	S 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	X	1	Total 4	C 2	O 1	S 1	0	0
3	X	1	Total 4	C 2	O 1	S 1	0	0
3	Y	1	Total 4	C 2	O 1	S 1	0	0
3	Z	1	Total 4	C 2	O 1	S 1	0	0
3	a	1	Total 4	C 2	O 1	S 1	0	0
3	b	1	Total 4	C 2	O 1	S 1	0	0
3	c	1	Total 4	C 2	O 1	S 1	0	0
3	c	1	Total 4	C 2	O 1	S 1	0	0
3	c	1	Total 4	C 2	O 1	S 1	0	0

- Molecule 4 is HEXANE-1,6-DIOL (CCD ID: HEZ) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 8	C 6	O 2	0	0
4	A	1	Total 8	C 6	O 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		
4	C	1	Total	C	O	0	0
			8	6	2		
4	D	1	Total	C	O	0	0
			8	6	2		
4	D	1	Total	C	O	0	0
			8	6	2		
4	E	1	Total	C	O	0	0
			8	6	2		
4	E	1	Total	C	O	0	0
			8	6	2		
4	E	1	Total	C	O	0	0
			8	6	2		
4	F	1	Total	C	O	0	0
			8	6	2		
4	F	1	Total	C	O	0	0
			8	6	2		
4	G	1	Total	C	O	0	0
			8	6	2		
4	H	1	Total	C	O	0	0
			8	6	2		
4	I	1	Total	C	O	0	0
			8	6	2		
4	I	1	Total	C	O	0	0
			8	6	2		
4	J	1	Total	C	O	0	0
			8	6	2		
4	K	1	Total	C	O	0	0
			8	6	2		
4	L	1	Total	C	O	0	0
			8	6	2		
4	M	1	Total	C	O	0	0
			8	6	2		
4	N	1	Total	C	O	0	0
			8	6	2		
4	O	1	Total	C	O	0	0
			8	6	2		
4	O	1	Total	C	O	0	0
			8	6	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	P	1	Total	C	O	0	0
			8	6	2		
4	Q	1	Total	C	O	0	0
			8	6	2		
4	R	1	Total	C	O	0	0
			8	6	2		
4	R	1	Total	C	O	0	0
			8	6	2		
4	T	1	Total	C	O	0	0
			8	6	2		
4	T	1	Total	C	O	0	0
			8	6	2		
4	U	1	Total	C	O	0	0
			8	6	2		
4	V	1	Total	C	O	0	0
			8	6	2		
4	V	1	Total	C	O	0	0
			8	6	2		
4	W	1	Total	C	O	0	0
			8	6	2		
4	W	1	Total	C	O	0	0
			8	6	2		
4	X	1	Total	C	O	0	0
			8	6	2		
4	Y	1	Total	C	O	0	0
			8	6	2		
4	Z	1	Total	C	O	0	0
			8	6	2		
4	a	1	Total	C	O	0	0
			8	6	2		
4	b	1	Total	C	O	0	0
			8	6	2		
4	c	1	Total	C	O	0	0
			8	6	2		
4	c	1	Total	C	O	0	0
			8	6	2		
4	c	1	Total	C	O	0	0
			8	6	2		

- 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 1 1	0	0
5	D	1	Total Mg 1 1	0	0
5	E	1	Total Mg 1 1	0	0
5	F	1	Total Mg 1 1	0	0
5	G	1	Total Mg 1 1	0	0
5	H	2	Total Mg 2 2	0	0
5	M	1	Total Mg 1 1	0	0
5	N	1	Total Mg 1 1	0	0
5	T	1	Total Mg 1 1	0	0
5	U	1	Total Mg 1 1	0	0
5	V	1	Total Mg 1 1	0	0
5	b	1	Total Mg 1 1	0	0
5	c	1	Total Mg 1 1	0	0

- Molecule 6 is water.

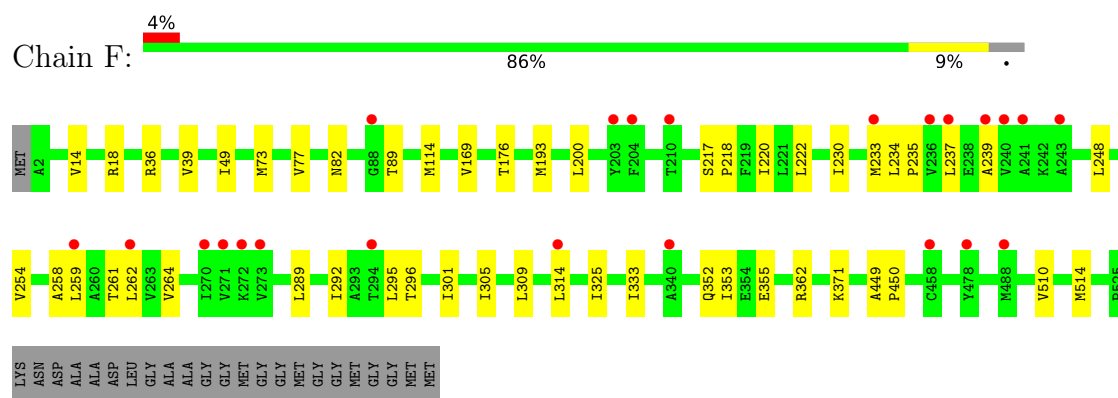
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	8	Total O 8 8	0	0
6	B	7	Total O 7 7	0	0
6	C	3	Total O 3 3	0	0
6	D	9	Total O 9 9	0	0
6	E	6	Total O 6 6	0	0
6	F	6	Total O 6 6	0	0
6	G	5	Total O 5 5	0	0

Continued on next page...

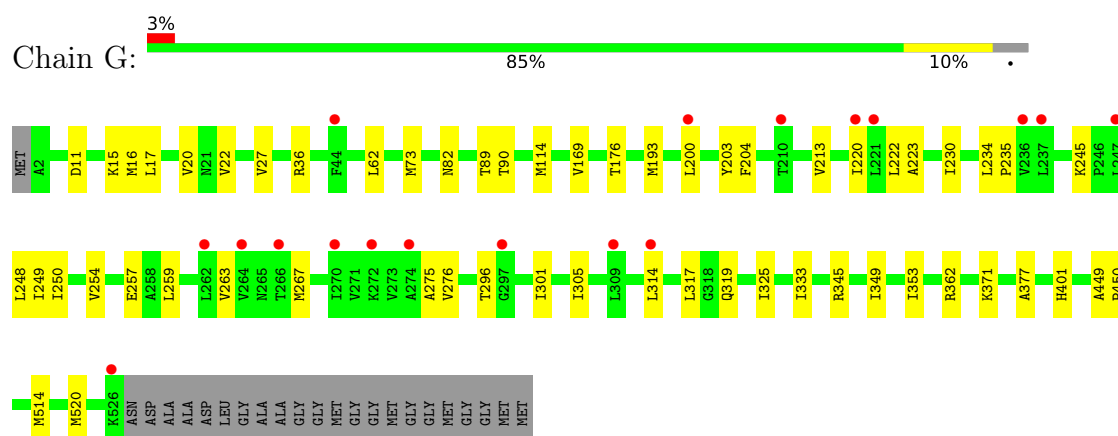
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	13	Total 13	O 13	0	0
6	I	6	Total 6	O 6	0	0
6	J	4	Total 4	O 4	0	0
6	K	5	Total 5	O 5	0	0
6	L	3	Total 3	O 3	0	0
6	M	8	Total 8	O 8	0	0
6	N	11	Total 11	O 11	0	0
6	O	9	Total 9	O 9	0	0
6	P	3	Total 3	O 3	0	0
6	Q	8	Total 8	O 8	0	0
6	R	5	Total 5	O 5	0	0
6	T	7	Total 7	O 7	0	0
6	U	9	Total 9	O 9	0	0
6	V	3	Total 3	O 3	0	0
6	W	1	Total 1	O 1	0	0
6	X	5	Total 5	O 5	0	0
6	Y	6	Total 6	O 6	0	0
6	Z	8	Total 8	O 8	0	0
6	a	9	Total 9	O 9	0	0
6	b	7	Total 7	O 7	0	0
6	c	8	Total 8	O 8	0	0

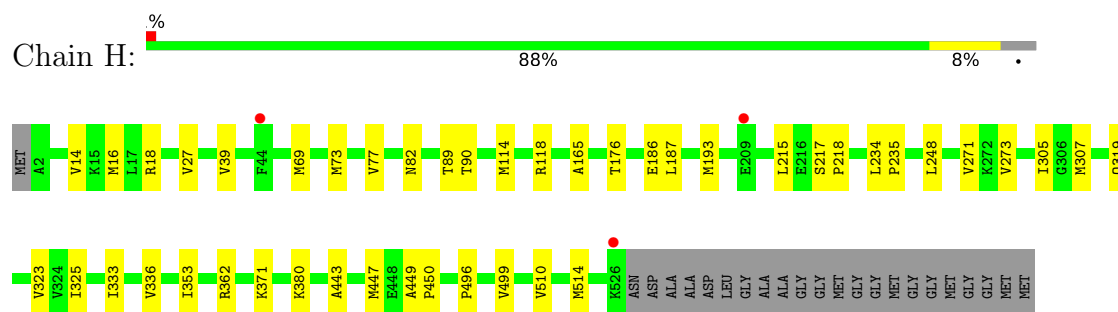
- Molecule 1: Chaperonin GroEL



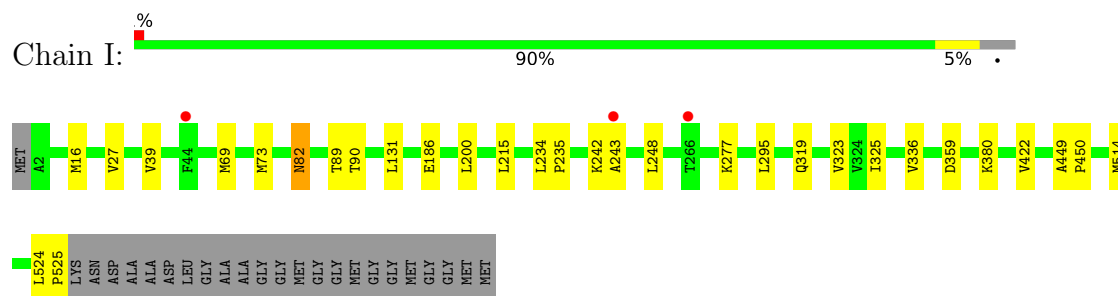
- Molecule 1: Chaperonin GroEL



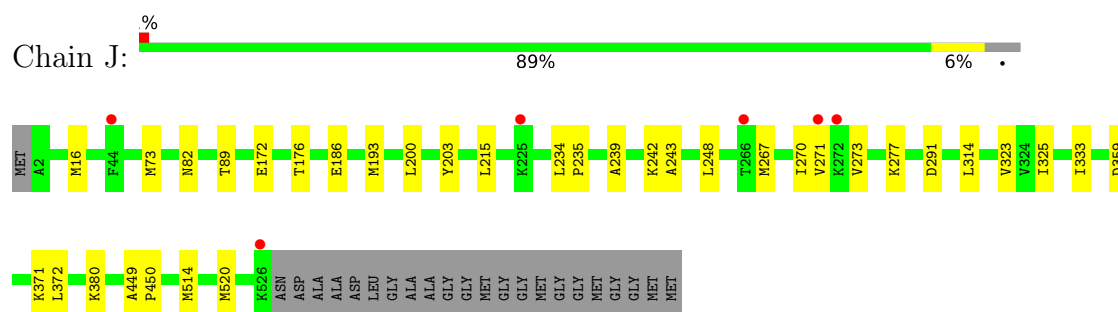
- Molecule 1: Chaperonin GroEL



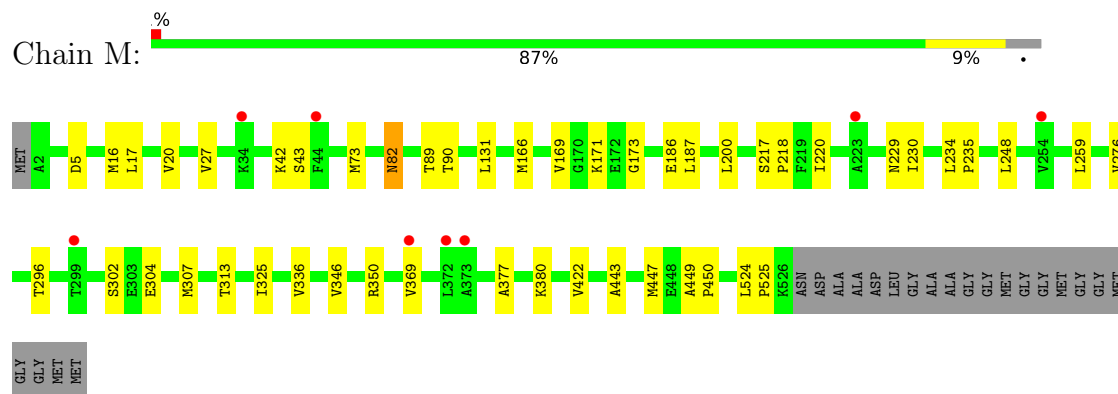
- Molecule 1: Chaperonin GroEL



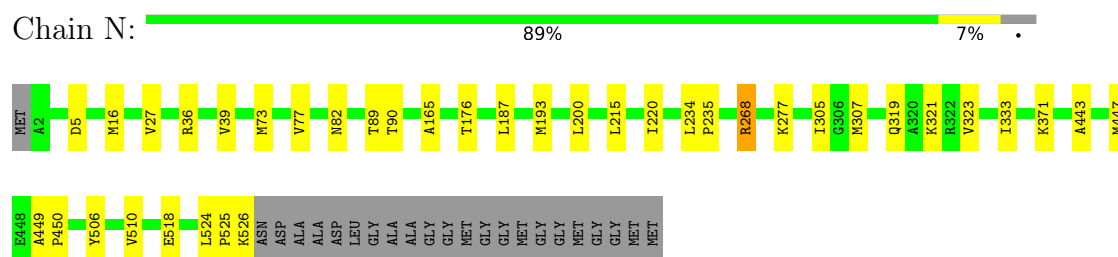
- Molecule 1: Chaperonin GroEL



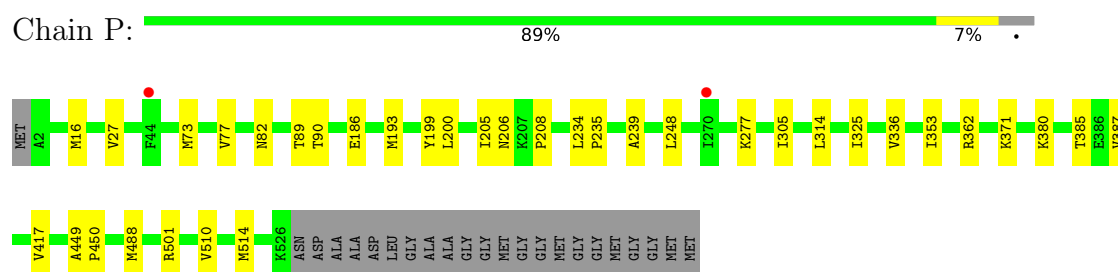
• Molecule 1: Chaperonin GroEL



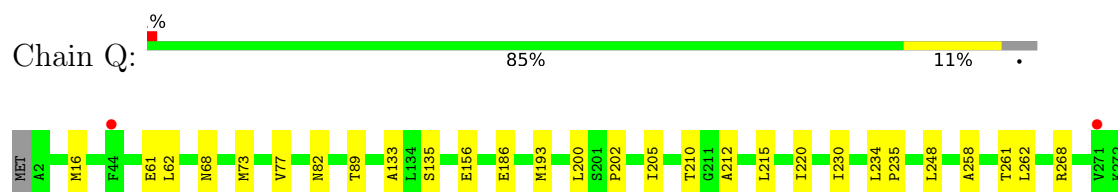
• Molecule 1: Chaperonin GroEL

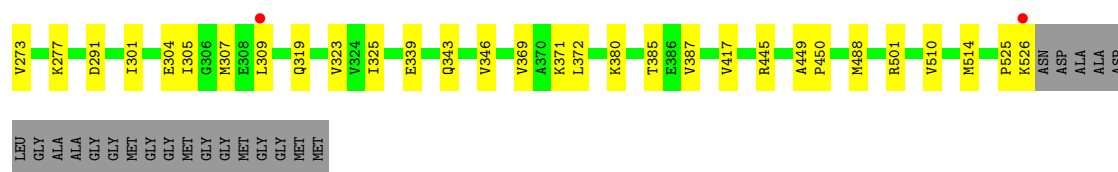


• Molecule 1: Chaperonin GroEL

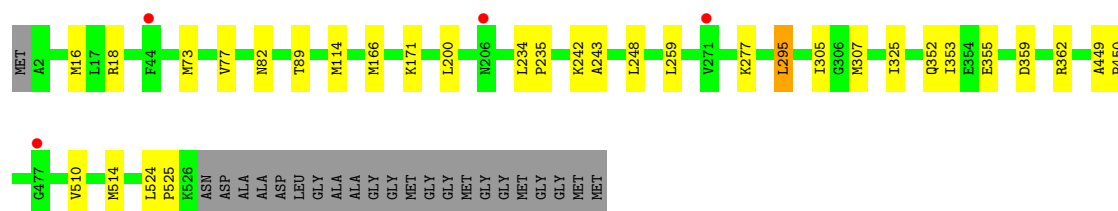
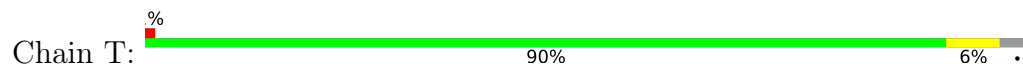


• Molecule 1: Chaperonin GroEL

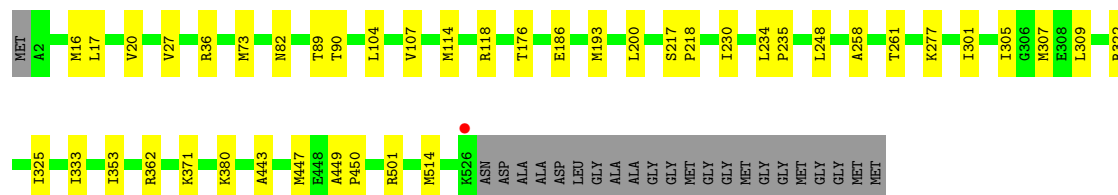




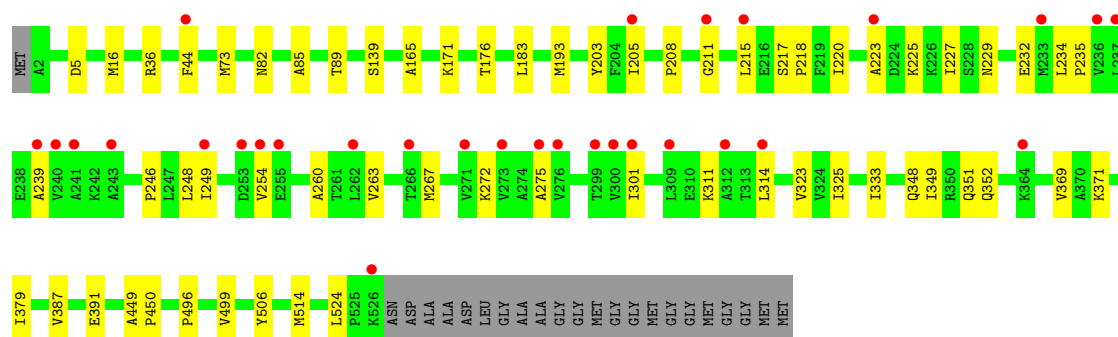
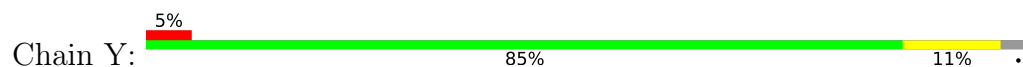
• Molecule 1: Chaperonin GroEL



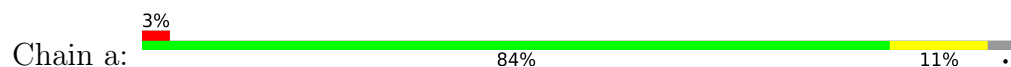
• Molecule 1: Chaperonin GroEL

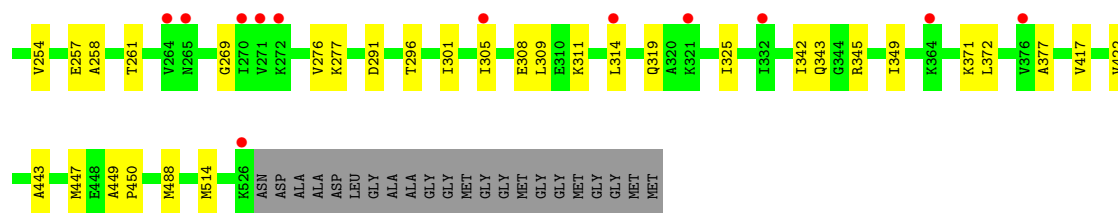


• Molecule 1: Chaperonin GroEL

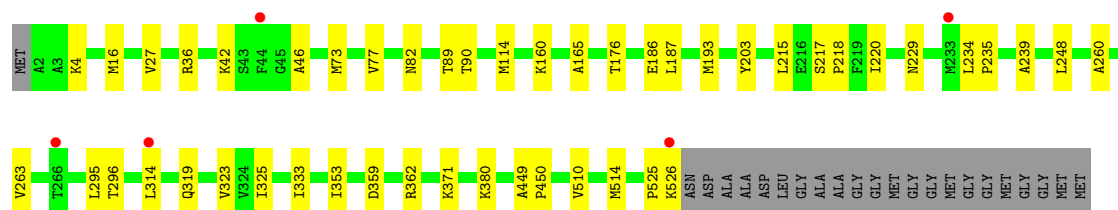
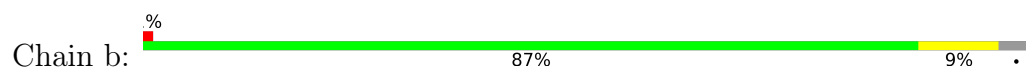


• Molecule 1: Chaperonin GroEL

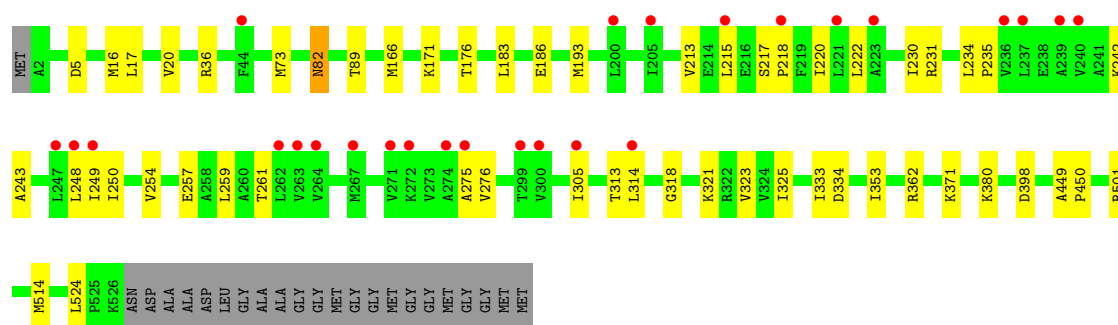
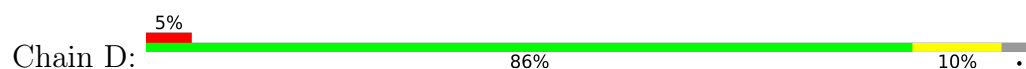




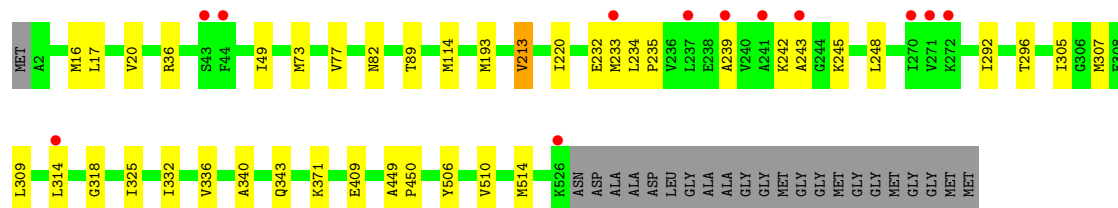
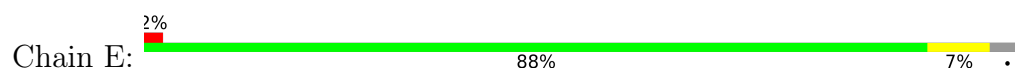
• Molecule 1: Chaperonin GroEL



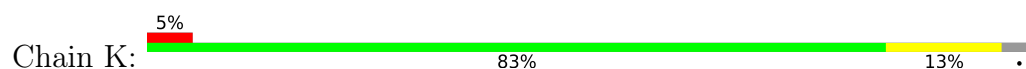
• Molecule 2: Chaperonin GroEL

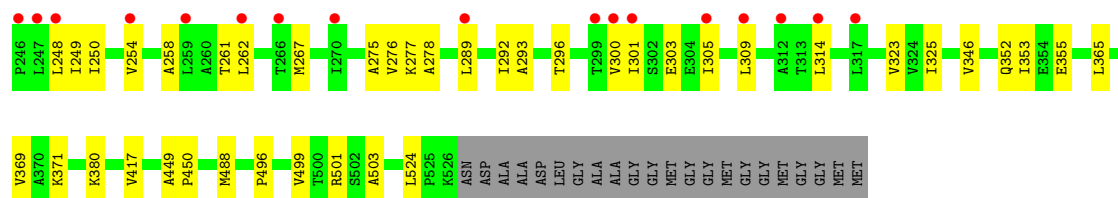


• Molecule 2: Chaperonin GroEL

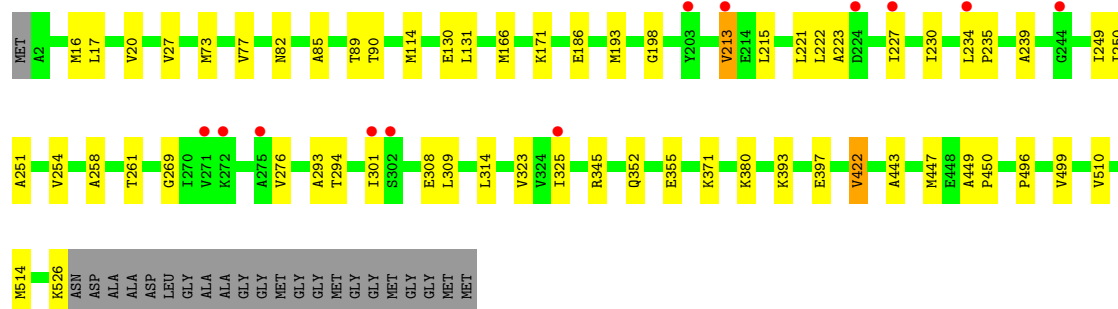
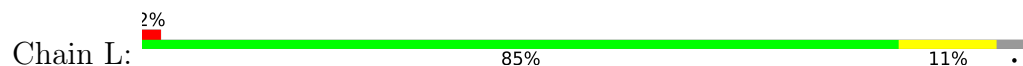


• Molecule 2: Chaperonin GroEL

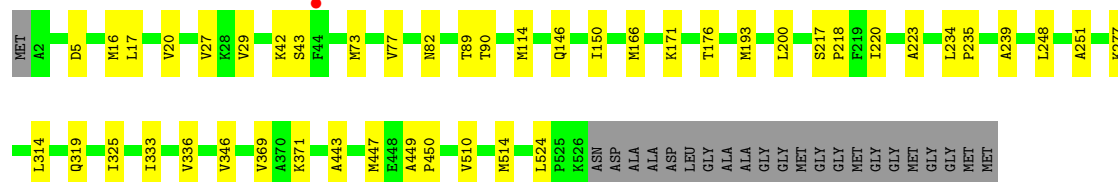
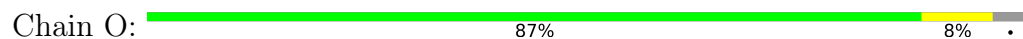




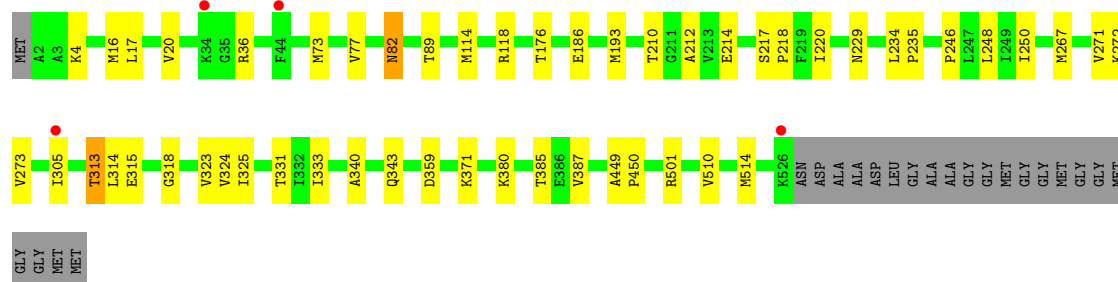
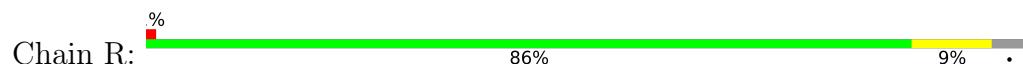
• Molecule 2: Chaperonin GroEL



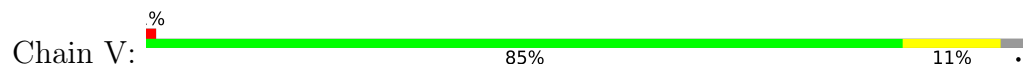
• Molecule 2: Chaperonin GroEL

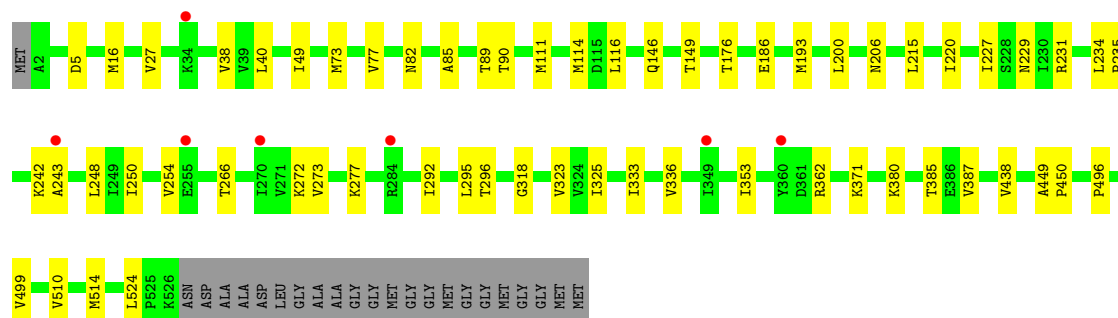


• Molecule 2: Chaperonin GroEL

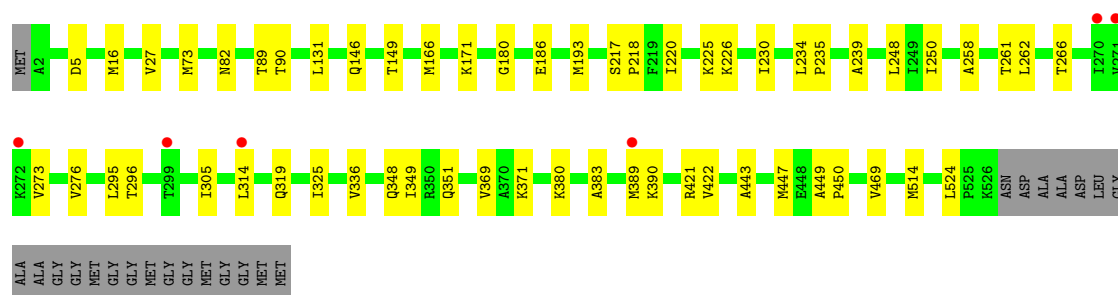
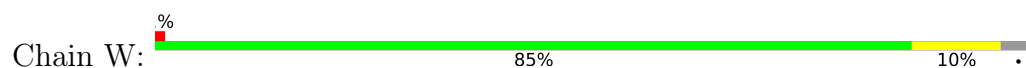


• Molecule 2: Chaperonin GroEL

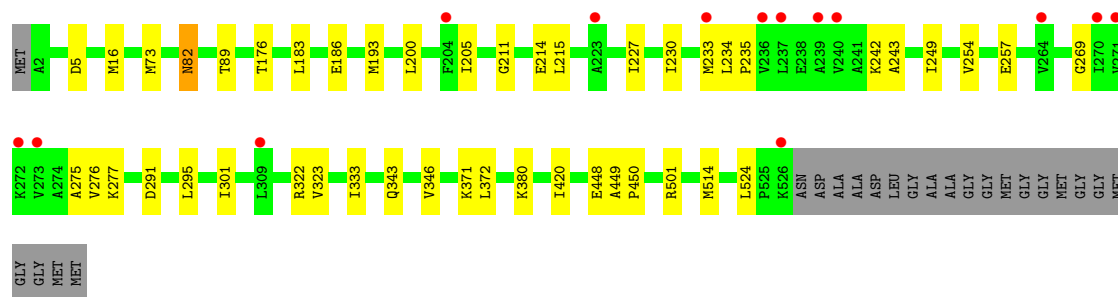
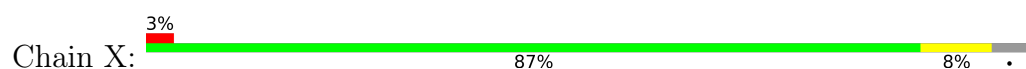




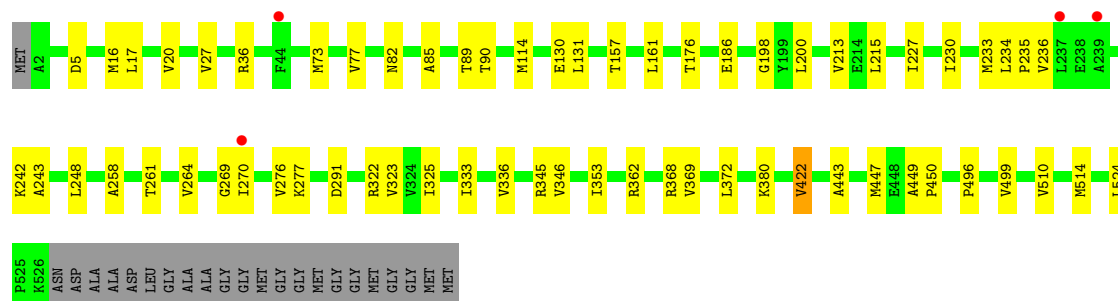
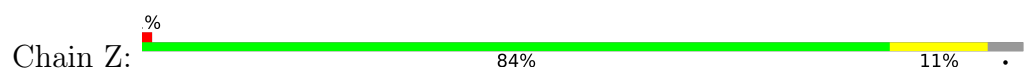
• Molecule 2: Chaperonin GroEL



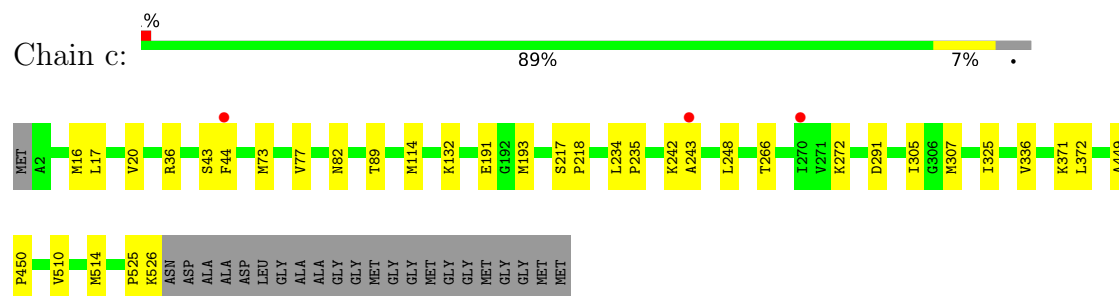
• Molecule 2: Chaperonin GroEL



• Molecule 2: Chaperonin GroEL



- Molecule 2: Chaperonin GroEL



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	285.87Å 136.26Å 287.80Å 90.00° 117.11° 90.00°	Depositor
Resolution (Å)	49.74 – 2.99 49.74 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.74-2.99) 99.0 (49.74-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.38 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.205 , 0.236 0.203 , 0.233	Depositor DCC
R_{free} test set	19672 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	66.1	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.001 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	108950	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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: SEP, BME, HEZ, 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	0.51	0/3885	0.89	0/5243
1	B	0.52	0/3885	0.89	0/5243
1	C	0.51	0/3885	0.89	0/5243
1	F	0.51	0/3876	0.89	0/5232
1	G	0.51	0/3885	0.90	0/5243
1	H	0.54	0/3885	0.90	0/5243
1	I	0.55	0/3876	0.88	0/5232
1	J	0.53	0/3885	0.89	0/5243
1	M	0.52	0/3885	0.90	0/5243
1	N	0.53	0/3885	0.90	0/5243
1	P	0.52	0/3885	0.88	0/5243
1	Q	0.53	0/3885	0.88	0/5243
1	T	0.52	0/3885	0.89	0/5243
1	U	0.53	0/3885	0.88	0/5243
1	Y	0.52	0/3885	0.89	0/5243
1	a	0.52	0/3885	0.89	0/5243
1	b	0.52	0/3885	0.89	1/5243 (0.0%)
2	D	0.51	0/3892	0.89	0/5254
2	E	0.52	0/3892	0.89	0/5254
2	K	0.52	0/3892	0.90	0/5254
2	L	0.51	0/3892	0.89	0/5254
2	O	0.53	0/3892	0.89	0/5254
2	R	0.52	0/3892	0.89	0/5254
2	V	0.51	0/3892	0.89	0/5254
2	W	0.50	0/3892	0.88	0/5254
2	X	0.51	0/3892	0.89	0/5254
2	Z	0.53	0/3892	0.89	0/5254
2	c	0.52	0/3892	0.88	0/5254
All	All	0.52	0/108839	0.89	1/146903 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	359	ASP	CA-CB-CG	5.02	117.62	112.60

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	3868	0	3988	39	0
1	B	3868	0	3987	28	0
1	C	3868	0	3988	34	0
1	F	3859	0	3974	43	0
1	G	3868	0	3988	50	0
1	H	3868	0	3988	29	0
1	I	3859	0	3975	23	0
1	J	3868	0	3988	25	0
1	M	3868	0	3988	34	0
1	N	3868	0	3988	28	0
1	P	3868	0	3987	23	0
1	Q	3868	0	3987	35	0
1	T	3868	0	3988	19	0
1	U	3868	0	3988	27	0
1	Y	3868	0	3987	41	0
1	a	3868	0	3987	51	0
1	b	3868	0	3987	30	0
2	D	3864	0	3989	47	0
2	E	3864	0	3989	32	0
2	K	3864	0	3989	69	0
2	L	3864	0	3989	45	0
2	O	3864	0	3989	30	0
2	R	3864	0	3989	41	0
2	V	3864	0	3989	41	0
2	W	3864	0	3989	43	0
2	X	3864	0	3989	34	0
2	Z	3864	0	3989	51	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	c	3864	0	3989	26	0
3	A	4	0	6	0	0
3	B	8	0	12	0	0
3	C	4	0	6	0	0
3	D	12	0	18	0	0
3	E	12	0	18	1	0
3	F	4	0	6	0	0
3	G	16	0	24	1	0
3	H	4	0	6	0	0
3	J	4	0	6	0	0
3	K	4	0	6	2	0
3	M	4	0	6	1	0
3	N	4	0	6	0	0
3	O	12	0	18	1	0
3	P	8	0	12	0	0
3	Q	12	0	18	3	0
3	R	8	0	12	0	0
3	T	4	0	6	0	0
3	U	12	0	18	0	0
3	V	4	0	6	0	0
3	X	8	0	12	0	0
3	Y	4	0	6	0	0
3	Z	4	0	6	0	0
3	a	4	0	6	0	0
3	b	4	0	6	0	0
3	c	12	0	18	2	0
4	A	16	0	28	0	0
4	B	16	0	28	2	0
4	C	8	0	14	0	0
4	D	16	0	28	1	0
4	E	24	0	42	1	0
4	F	16	0	28	0	0
4	G	8	0	14	0	0
4	H	8	0	14	0	0
4	I	16	0	28	0	0
4	J	8	0	14	0	0
4	K	8	0	14	1	0
4	L	8	0	14	0	0
4	M	8	0	14	0	0
4	N	8	0	14	1	0
4	O	16	0	28	0	0
4	P	8	0	14	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Q	8	0	14	1	0
4	R	16	0	28	2	0
4	T	16	0	28	0	0
4	U	8	0	14	1	0
4	V	16	0	28	0	0
4	W	16	0	28	0	0
4	X	8	0	14	1	0
4	Y	8	0	14	1	0
4	Z	8	0	14	0	0
4	a	8	0	14	0	0
4	b	8	0	14	0	0
4	c	24	0	42	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	2	0	0	0	0
5	M	1	0	0	0	0
5	N	1	0	0	0	0
5	T	1	0	0	0	0
5	U	1	0	0	0	0
5	V	1	0	0	0	0
5	b	1	0	0	0	0
5	c	1	0	0	0	0
6	A	8	0	0	0	0
6	B	7	0	0	0	0
6	C	3	0	0	0	0
6	D	9	0	0	1	0
6	E	6	0	0	0	0
6	F	6	0	0	0	0
6	G	5	0	0	1	0
6	H	13	0	0	0	0
6	I	6	0	0	0	0
6	J	4	0	0	0	0
6	K	5	0	0	2	0
6	L	3	0	0	0	0
6	M	8	0	0	1	0
6	N	11	0	0	0	0
6	O	9	0	0	0	0
6	P	3	0	0	0	0
6	Q	8	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	R	5	0	0	1	0
6	T	7	0	0	1	0
6	U	9	0	0	0	0
6	V	3	0	0	0	0
6	W	1	0	0	0	0
6	X	5	0	0	0	0
6	Y	6	0	0	0	0
6	Z	8	0	0	0	0
6	a	9	0	0	0	0
6	b	7	0	0	0	0
6	c	8	0	0	0	0
All	All	108950	0	112494	984	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.

The worst 5 of 984 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)
2:D:230:ILE:HG13	2:D:261:THR:HG21	1.29	1.09
1:F:230:ILE:HD11	1:F:261:THR:HB	1.46	0.97
2:D:230:ILE:CG1	2:D:261:THR:HG21	1.95	0.95
1:F:230:ILE:CD1	1:F:261:THR:HB	1.98	0.94
2:Z:230:ILE:HG21	2:Z:261:THR:HG21	1.51	0.93

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	522/548 (95%)	511 (98%)	11 (2%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	522/548 (95%)	516 (99%)	6 (1%)	0	100	100
1	C	522/548 (95%)	517 (99%)	5 (1%)	0	100	100
1	F	521/548 (95%)	513 (98%)	8 (2%)	0	100	100
1	G	522/548 (95%)	514 (98%)	8 (2%)	0	100	100
1	H	522/548 (95%)	517 (99%)	5 (1%)	0	100	100
1	I	521/548 (95%)	514 (99%)	7 (1%)	0	100	100
1	J	522/548 (95%)	516 (99%)	6 (1%)	0	100	100
1	M	522/548 (95%)	517 (99%)	5 (1%)	0	100	100
1	N	522/548 (95%)	516 (99%)	6 (1%)	0	100	100
1	P	522/548 (95%)	514 (98%)	8 (2%)	0	100	100
1	Q	522/548 (95%)	516 (99%)	6 (1%)	0	100	100
1	T	522/548 (95%)	515 (99%)	7 (1%)	0	100	100
1	U	522/548 (95%)	517 (99%)	5 (1%)	0	100	100
1	Y	522/548 (95%)	514 (98%)	8 (2%)	0	100	100
1	a	522/548 (95%)	514 (98%)	8 (2%)	0	100	100
1	b	522/548 (95%)	514 (98%)	8 (2%)	0	100	100
2	D	523/548 (95%)	514 (98%)	9 (2%)	0	100	100
2	E	523/548 (95%)	513 (98%)	10 (2%)	0	100	100
2	K	523/548 (95%)	516 (99%)	7 (1%)	0	100	100
2	L	523/548 (95%)	515 (98%)	8 (2%)	0	100	100
2	O	523/548 (95%)	516 (99%)	7 (1%)	0	100	100
2	R	523/548 (95%)	515 (98%)	8 (2%)	0	100	100
2	V	523/548 (95%)	515 (98%)	8 (2%)	0	100	100
2	W	523/548 (95%)	515 (98%)	8 (2%)	0	100	100
2	X	523/548 (95%)	514 (98%)	9 (2%)	0	100	100
2	Z	523/548 (95%)	512 (98%)	11 (2%)	0	100	100
2	c	523/548 (95%)	515 (98%)	8 (2%)	0	100	100
All	All	14625/15344 (95%)	14415 (99%)	210 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	404/414 (98%)	403 (100%)	1 (0%)	87	92
1	B	404/414 (98%)	402 (100%)	2 (0%)	81	89
1	C	404/414 (98%)	401 (99%)	3 (1%)	76	86
1	F	403/414 (97%)	403 (100%)	0	100	100
1	G	404/414 (98%)	403 (100%)	1 (0%)	87	92
1	H	404/414 (98%)	404 (100%)	0	100	100
1	I	403/414 (97%)	401 (100%)	2 (0%)	81	89
1	J	404/414 (98%)	402 (100%)	2 (0%)	81	89
1	M	404/414 (98%)	402 (100%)	2 (0%)	81	89
1	N	404/414 (98%)	402 (100%)	2 (0%)	81	89
1	P	404/414 (98%)	404 (100%)	0	100	100
1	Q	404/414 (98%)	402 (100%)	2 (0%)	81	89
1	T	404/414 (98%)	402 (100%)	2 (0%)	81	89
1	U	404/414 (98%)	404 (100%)	0	100	100
1	Y	404/414 (98%)	403 (100%)	1 (0%)	87	92
1	a	404/414 (98%)	403 (100%)	1 (0%)	87	92
1	b	404/414 (98%)	403 (100%)	1 (0%)	87	92
2	D	405/415 (98%)	404 (100%)	1 (0%)	87	92
2	E	405/415 (98%)	403 (100%)	2 (0%)	81	89
2	K	405/415 (98%)	405 (100%)	0	100	100
2	L	405/415 (98%)	402 (99%)	3 (1%)	76	86
2	O	405/415 (98%)	405 (100%)	0	100	100
2	R	405/415 (98%)	402 (99%)	3 (1%)	76	86
2	V	405/415 (98%)	405 (100%)	0	100	100
2	W	405/415 (98%)	405 (100%)	0	100	100
2	X	405/415 (98%)	404 (100%)	1 (0%)	87	92

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Z	405/415 (98%)	404 (100%)	1 (0%)	87	92
2	c	405/415 (98%)	405 (100%)	0	100	100
All	All	11321/11603 (98%)	11288 (100%)	33 (0%)	86	91

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	X	82	ASN
1	Y	352	GLN
1	b	160	LYS
1	J	172	GLU
1	I	359	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 135 such sidechains are listed below:

Mol	Chain	Res	Type
2	X	479	ASN
1	Y	348	GLN
1	b	453	GLN
1	J	366	GLN
1	J	348	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

17 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SEP	G	43	1	8,9,10	0.76	0	7,12,14	0.61	0
1	SEP	T	43	1	8,9,10	0.79	0	7,12,14	0.54	0
1	SEP	Q	43	1	8,9,10	0.76	0	7,12,14	0.58	0
1	SEP	B	43	1	8,9,10	0.71	0	7,12,14	0.60	0
1	SEP	M	43	1	8,9,10	0.76	0	7,12,14	0.59	0
1	SEP	J	43	1	8,9,10	0.78	0	7,12,14	0.57	0
1	SEP	a	43	1	8,9,10	0.73	0	7,12,14	0.62	0
1	SEP	b	43	1	8,9,10	0.64	0	7,12,14	0.63	0
1	SEP	C	43	1	8,9,10	0.82	0	7,12,14	0.62	0
1	SEP	Y	43	1	8,9,10	0.66	0	7,12,14	0.60	0
1	SEP	H	43	1	8,9,10	0.76	0	7,12,14	0.60	0
1	SEP	U	43	1	8,9,10	0.78	0	7,12,14	0.57	0
1	SEP	I	43	1	8,9,10	0.81	0	7,12,14	0.55	0
1	SEP	F	43	1	8,9,10	0.68	0	7,12,14	0.61	0
1	SEP	A	43	1	8,9,10	0.80	0	7,12,14	0.54	0
1	SEP	P	43	1	8,9,10	0.69	0	7,12,14	0.59	0
1	SEP	N	43	1	8,9,10	0.80	0	7,12,14	0.59	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	G	43	1	-	3/6/8/10	-
1	SEP	T	43	1	-	3/6/8/10	-
1	SEP	Q	43	1	-	3/6/8/10	-
1	SEP	B	43	1	-	1/6/8/10	-
1	SEP	M	43	1	-	5/6/8/10	-
1	SEP	J	43	1	-	3/6/8/10	-
1	SEP	a	43	1	-	2/6/8/10	-
1	SEP	b	43	1	-	1/6/8/10	-
1	SEP	C	43	1	-	4/6/8/10	-
1	SEP	Y	43	1	-	4/6/8/10	-
1	SEP	H	43	1	-	2/6/8/10	-
1	SEP	U	43	1	-	3/6/8/10	-
1	SEP	I	43	1	-	3/6/8/10	-
1	SEP	F	43	1	-	3/6/8/10	-
1	SEP	A	43	1	-	4/6/8/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	P	43	1	-	3/6/8/10	-
1	SEP	N	43	1	-	2/6/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	43	SEP	N-CA-CB-OG
1	A	43	SEP	C-CA-CB-OG
1	A	43	SEP	CA-CB-OG-P
1	C	43	SEP	CB-OG-P-O2P
1	C	43	SEP	CB-OG-P-O3P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	M	43	SEP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 100 ligands modelled in this entry, 14 are monoatomic - leaving 86 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	HEZ	T	603	-	7,7,7	0.06	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BME	E	602	-	3,3,3	0.24	0	2,2,2	0.33	0
3	BME	U	603	-	3,3,3	0.19	0	2,2,2	0.16	0
4	HEZ	O	604	-	7,7,7	0.12	0	6,6,6	0.11	0
4	HEZ	a	602	-	7,7,7	0.16	0	6,6,6	0.13	0
3	BME	R	601	-	3,3,3	0.24	0	2,2,2	0.30	0
4	HEZ	F	602	-	7,7,7	0.19	0	6,6,6	0.13	0
3	BME	Y	601	-	3,3,3	0.21	0	2,2,2	0.28	0
4	HEZ	V	602	-	7,7,7	0.09	0	6,6,6	0.12	0
4	HEZ	E	606	-	7,7,7	0.16	0	6,6,6	0.13	0
3	BME	O	603	-	3,3,3	0.24	0	2,2,2	0.28	0
4	HEZ	c	605	-	7,7,7	0.10	0	6,6,6	0.11	0
4	HEZ	J	602	-	7,7,7	0.24	0	6,6,6	0.13	0
3	BME	O	602	-	3,3,3	0.26	0	2,2,2	0.30	0
3	BME	A	601	-	3,3,3	0.20	0	2,2,2	0.35	0
3	BME	J	601	-	3,3,3	0.25	0	2,2,2	0.26	0
3	BME	c	603	-	3,3,3	0.21	0	2,2,2	0.30	0
3	BME	T	601	-	3,3,3	0.17	0	2,2,2	0.16	0
3	BME	b	601	-	3,3,3	0.21	0	2,2,2	0.23	0
4	HEZ	F	603	-	7,7,7	0.19	0	6,6,6	0.13	0
4	HEZ	N	602	-	7,7,7	0.19	0	6,6,6	0.14	0
3	BME	V	601	-	3,3,3	0.16	0	2,2,2	0.19	0
3	BME	c	602	-	3,3,3	0.18	0	2,2,2	0.22	0
3	BME	E	603	-	3,3,3	0.20	0	2,2,2	0.28	0
4	HEZ	c	606	-	7,7,7	0.26	0	6,6,6	0.14	0
3	BME	a	601	-	3,3,3	0.20	0	2,2,2	0.25	0
4	HEZ	B	604	-	7,7,7	0.18	0	6,6,6	0.12	0
4	HEZ	I	601	-	7,7,7	0.16	0	6,6,6	0.11	0
3	BME	Z	601	-	3,3,3	0.25	0	2,2,2	0.23	0
4	HEZ	W	601	-	7,7,7	0.12	0	6,6,6	0.13	0
4	HEZ	A	603	-	7,7,7	0.10	0	6,6,6	0.11	0
4	HEZ	Y	602	-	7,7,7	0.20	0	6,6,6	0.12	0
3	BME	N	601	-	3,3,3	0.18	0	2,2,2	0.14	0
4	HEZ	B	603	-	7,7,7	0.27	0	6,6,6	0.14	0
4	HEZ	M	602	-	7,7,7	0.15	0	6,6,6	0.12	0
4	HEZ	X	603	-	7,7,7	0.10	0	6,6,6	0.13	0
4	HEZ	U	604	-	7,7,7	0.19	0	6,6,6	0.14	0
4	HEZ	L	601	-	7,7,7	0.20	0	6,6,6	0.12	0
4	HEZ	V	603	-	7,7,7	0.07	0	6,6,6	0.10	0
3	BME	G	601	-	3,3,3	0.25	0	2,2,2	0.25	0
3	BME	Q	602	-	3,3,3	0.24	0	2,2,2	0.33	0
4	HEZ	H	602	-	7,7,7	0.09	0	6,6,6	0.11	0
4	HEZ	C	602	-	7,7,7	0.15	0	6,6,6	0.12	0
3	BME	C	601	-	3,3,3	0.21	0	2,2,2	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	HEZ	b	602	-	7,7,7	0.13	0	6,6,6	0.14	0
4	HEZ	c	604	-	7,7,7	0.22	0	6,6,6	0.14	0
3	BME	D	602	-	3,3,3	0.20	0	2,2,2	0.24	0
4	HEZ	T	602	-	7,7,7	0.24	0	6,6,6	0.13	0
4	HEZ	P	603	-	7,7,7	0.27	0	6,6,6	0.16	0
4	HEZ	R	604	-	7,7,7	0.18	0	6,6,6	0.10	0
4	HEZ	O	605	-	7,7,7	0.12	0	6,6,6	0.11	0
4	HEZ	D	605	-	7,7,7	0.15	0	6,6,6	0.13	0
3	BME	H	601	-	3,3,3	0.31	0	2,2,2	0.33	0
3	BME	M	601	-	3,3,3	0.27	0	2,2,2	0.49	0
3	BME	Q	601	-	3,3,3	0.22	0	2,2,2	0.35	0
4	HEZ	E	605	-	7,7,7	0.09	0	6,6,6	0.13	0
3	BME	G	603	-	3,3,3	0.18	0	2,2,2	0.40	0
3	BME	X	601	-	3,3,3	0.32	0	2,2,2	0.38	0
4	HEZ	D	604	-	7,7,7	0.11	0	6,6,6	0.13	0
3	BME	G	602	-	3,3,3	0.19	0	2,2,2	0.26	0
3	BME	c	601	-	3,3,3	0.24	0	2,2,2	0.28	0
4	HEZ	W	602	-	7,7,7	0.17	0	6,6,6	0.08	0
3	BME	B	601	-	3,3,3	0.42	0	2,2,2	0.42	0
3	BME	Q	603	-	3,3,3	0.17	0	2,2,2	0.18	0
3	BME	D	603	-	3,3,3	0.22	0	2,2,2	0.31	0
4	HEZ	I	602	-	7,7,7	0.11	0	6,6,6	0.11	0
3	BME	B	602	-	3,3,3	0.17	0	2,2,2	0.30	0
4	HEZ	A	602	-	7,7,7	0.07	0	6,6,6	0.10	0
3	BME	R	602	-	3,3,3	0.21	0	2,2,2	0.18	0
3	BME	D	601	-	3,3,3	0.27	0	2,2,2	0.29	0
3	BME	E	601	-	3,3,3	0.21	0	2,2,2	0.24	0
3	BME	P	602	-	3,3,3	0.26	0	2,2,2	0.32	0
4	HEZ	G	605	-	7,7,7	0.17	0	6,6,6	0.12	0
4	HEZ	K	602	-	7,7,7	0.15	0	6,6,6	0.13	0
3	BME	U	601	-	3,3,3	0.35	0	2,2,2	0.36	0
3	BME	O	601	-	3,3,3	0.26	0	2,2,2	0.31	0
3	BME	X	602	-	3,3,3	0.21	0	2,2,2	0.26	0
4	HEZ	R	603	-	7,7,7	0.17	0	6,6,6	0.14	0
3	BME	U	602	-	3,3,3	0.23	0	2,2,2	0.27	0
3	BME	P	601	-	3,3,3	0.28	0	2,2,2	0.36	0
3	BME	K	601	-	3,3,3	0.17	0	2,2,2	0.23	0
4	HEZ	E	604	-	7,7,7	0.10	0	6,6,6	0.11	0
4	HEZ	Z	602	-	7,7,7	0.18	0	6,6,6	0.12	0
3	BME	G	604	-	3,3,3	0.20	0	2,2,2	0.27	0
4	HEZ	Q	604	-	7,7,7	0.22	0	6,6,6	0.12	0
3	BME	F	601	-	3,3,3	0.23	0	2,2,2	0.33	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEZ	T	603	-	-	3/5/5/5	-
3	BME	E	602	-	-	1/1/1/1	-
3	BME	U	603	-	-	0/1/1/1	-
4	HEZ	O	604	-	-	3/5/5/5	-
4	HEZ	a	602	-	-	3/5/5/5	-
3	BME	R	601	-	-	0/1/1/1	-
4	HEZ	F	602	-	-	2/5/5/5	-
3	BME	Y	601	-	-	1/1/1/1	-
4	HEZ	V	602	-	-	3/5/5/5	-
4	HEZ	E	606	-	-	0/5/5/5	-
3	BME	O	603	-	-	1/1/1/1	-
4	HEZ	c	605	-	-	4/5/5/5	-
4	HEZ	J	602	-	-	4/5/5/5	-
3	BME	O	602	-	-	0/1/1/1	-
3	BME	A	601	-	-	1/1/1/1	-
3	BME	J	601	-	-	0/1/1/1	-
3	BME	c	603	-	-	1/1/1/1	-
3	BME	T	601	-	-	0/1/1/1	-
3	BME	b	601	-	-	0/1/1/1	-
4	HEZ	F	603	-	-	4/5/5/5	-
4	HEZ	N	602	-	-	1/5/5/5	-
3	BME	V	601	-	-	1/1/1/1	-
3	BME	c	602	-	-	0/1/1/1	-
3	BME	E	603	-	-	1/1/1/1	-
4	HEZ	c	606	-	-	1/5/5/5	-
3	BME	a	601	-	-	1/1/1/1	-
4	HEZ	B	604	-	-	4/5/5/5	-
4	HEZ	I	601	-	-	2/5/5/5	-
3	BME	Z	601	-	-	0/1/1/1	-
4	HEZ	W	601	-	-	2/5/5/5	-
4	HEZ	A	603	-	-	3/5/5/5	-
4	HEZ	Y	602	-	-	2/5/5/5	-
3	BME	N	601	-	-	1/1/1/1	-
4	HEZ	B	603	-	-	5/5/5/5	-
4	HEZ	M	602	-	-	3/5/5/5	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEZ	X	603	-	-	2/5/5/5	-
4	HEZ	U	604	-	-	4/5/5/5	-
4	HEZ	L	601	-	-	4/5/5/5	-
4	HEZ	V	603	-	-	3/5/5/5	-
3	BME	G	601	-	-	0/1/1/1	-
3	BME	Q	602	-	-	1/1/1/1	-
4	HEZ	H	602	-	-	4/5/5/5	-
4	HEZ	C	602	-	-	4/5/5/5	-
3	BME	C	601	-	-	1/1/1/1	-
4	HEZ	b	602	-	-	2/5/5/5	-
4	HEZ	c	604	-	-	2/5/5/5	-
3	BME	D	602	-	-	0/1/1/1	-
4	HEZ	T	602	-	-	1/5/5/5	-
4	HEZ	P	603	-	-	4/5/5/5	-
4	HEZ	R	604	-	-	3/5/5/5	-
4	HEZ	O	605	-	-	2/5/5/5	-
4	HEZ	D	605	-	-	3/5/5/5	-
3	BME	H	601	-	-	0/1/1/1	-
3	BME	M	601	-	-	1/1/1/1	-
3	BME	Q	601	-	-	1/1/1/1	-
4	HEZ	E	605	-	-	4/5/5/5	-
3	BME	G	603	-	-	1/1/1/1	-
3	BME	X	601	-	-	0/1/1/1	-
4	HEZ	D	604	-	-	3/5/5/5	-
3	BME	G	602	-	-	1/1/1/1	-
3	BME	c	601	-	-	0/1/1/1	-
4	HEZ	W	602	-	-	2/5/5/5	-
3	BME	B	601	-	-	1/1/1/1	-
3	BME	Q	603	-	-	0/1/1/1	-
3	BME	D	603	-	-	1/1/1/1	-
4	HEZ	I	602	-	-	1/5/5/5	-
3	BME	B	602	-	-	1/1/1/1	-
4	HEZ	A	602	-	-	4/5/5/5	-
3	BME	R	602	-	-	0/1/1/1	-
3	BME	D	601	-	-	1/1/1/1	-
3	BME	E	601	-	-	0/1/1/1	-
3	BME	P	602	-	-	1/1/1/1	-
4	HEZ	G	605	-	-	3/5/5/5	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEZ	K	602	-	-	0/5/5/5	-
3	BME	U	601	-	-	0/1/1/1	-
3	BME	O	601	-	-	1/1/1/1	-
3	BME	X	602	-	-	0/1/1/1	-
4	HEZ	R	603	-	-	2/5/5/5	-
3	BME	U	602	-	-	1/1/1/1	-
3	BME	P	601	-	-	1/1/1/1	-
3	BME	K	601	-	-	0/1/1/1	-
4	HEZ	E	604	-	-	3/5/5/5	-
4	HEZ	Z	602	-	-	4/5/5/5	-
3	BME	G	604	-	-	1/1/1/1	-
4	HEZ	Q	604	-	-	4/5/5/5	-
3	BME	F	601	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 141 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	603	BME	O1-C1-C2-S2
3	E	603	BME	O1-C1-C2-S2
3	G	602	BME	O1-C1-C2-S2
3	O	603	BME	O1-C1-C2-S2
3	P	601	BME	O1-C1-C2-S2

There are no ring outliers.

21 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	602	BME	1	0
3	O	602	BME	1	0
4	N	602	HEZ	1	0
3	c	602	BME	1	0
4	B	604	HEZ	2	0
4	Y	602	HEZ	1	0
4	X	603	HEZ	1	0
4	U	604	HEZ	1	0
4	P	603	HEZ	1	0
4	R	604	HEZ	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	601	BME	1	0
3	Q	601	BME	2	0
3	G	603	BME	1	0
4	D	604	HEZ	1	0
3	c	601	BME	1	0
3	Q	603	BME	1	0
4	K	602	HEZ	1	0
4	R	603	HEZ	1	0
3	K	601	BME	2	0
4	E	604	HEZ	1	0
4	Q	604	HEZ	1	0

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	524/548 (95%)	0.21	27 (5%) 33 17	42, 76, 141, 183	0
1	B	524/548 (95%)	-0.02	3 (0%) 85 69	37, 66, 119, 161	0
1	C	524/548 (95%)	0.15	13 (2%) 58 35	37, 73, 143, 194	0
1	F	523/548 (95%)	0.20	23 (4%) 39 21	42, 80, 151, 217	0
1	G	524/548 (95%)	0.19	18 (3%) 48 27	42, 78, 152, 189	0
1	H	524/548 (95%)	-0.22	3 (0%) 85 69	35, 58, 89, 141	0
1	I	523/548 (95%)	-0.34	3 (0%) 85 69	33, 53, 80, 144	0
1	J	524/548 (95%)	-0.17	6 (1%) 78 57	37, 63, 101, 159	0
1	M	524/548 (95%)	0.02	8 (1%) 72 49	39, 72, 111, 143	0
1	N	524/548 (95%)	-0.14	0 100 100	36, 63, 93, 136	0
1	P	524/548 (95%)	-0.11	2 (0%) 88 76	38, 69, 112, 146	0
1	Q	524/548 (95%)	0.05	4 (0%) 82 64	35, 70, 125, 153	0
1	T	524/548 (95%)	-0.15	4 (0%) 82 64	42, 71, 99, 152	0
1	U	524/548 (95%)	-0.27	1 (0%) 91 83	36, 60, 95, 133	0
1	Y	524/548 (95%)	0.20	30 (5%) 29 15	37, 69, 148, 200	0
1	a	524/548 (95%)	0.15	17 (3%) 50 29	36, 73, 147, 193	0
1	b	524/548 (95%)	0.02	5 (0%) 79 59	41, 77, 126, 159	0
2	D	525/548 (95%)	0.24	26 (4%) 34 18	38, 74, 159, 225	0
2	E	525/548 (95%)	0.09	12 (2%) 61 38	39, 72, 151, 212	0
2	K	525/548 (95%)	0.28	30 (5%) 29 15	39, 84, 163, 194	0
2	L	525/548 (95%)	0.15	12 (2%) 61 38	41, 80, 144, 173	0
2	O	525/548 (95%)	-0.26	1 (0%) 91 83	38, 60, 90, 144	0
2	R	525/548 (95%)	-0.02	4 (0%) 82 64	41, 74, 114, 144	0
2	V	525/548 (95%)	0.16	7 (1%) 75 53	43, 82, 129, 168	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	W	525/548 (95%)	0.12	6 (1%) 78 57	43, 82, 139, 170	0
2	X	525/548 (95%)	0.14	14 (2%) 56 33	39, 74, 155, 223	0
2	Z	525/548 (95%)	-0.14	4 (0%) 82 64	34, 63, 116, 154	0
2	c	525/548 (95%)	-0.24	3 (0%) 85 69	42, 60, 89, 143	0
All	All	14681/15344 (95%)	0.01	286 (1%) 66 43	33, 69, 136, 225	0

The worst 5 of 286 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	271	VAL	4.7
1	C	237	LEU	4.6
1	C	271	VAL	4.5
1	A	239	ALA	4.4
2	L	271	VAL	4.3

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

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
1	SEP	A	43	10/11	0.56	0.16	109,129,159,163	0
1	SEP	H	43	10/11	0.57	0.16	102,132,157,160	0
1	SEP	I	43	10/11	0.58	0.15	111,138,166,174	0
1	SEP	M	43	10/11	0.60	0.17	101,123,141,162	0
1	SEP	U	43	10/11	0.60	0.17	107,139,163,169	0
1	SEP	T	43	10/11	0.61	0.16	113,132,163,165	0
1	SEP	N	43	10/11	0.61	0.15	102,117,129,135	0
1	SEP	J	43	10/11	0.63	0.14	106,127,161,164	0
1	SEP	G	43	10/11	0.64	0.19	120,138,154,168	0
1	SEP	C	43	10/11	0.66	0.15	106,131,158,161	0
1	SEP	Q	43	10/11	0.67	0.17	102,138,164,176	0
1	SEP	b	43	10/11	0.68	0.15	115,137,161,174	0
1	SEP	F	43	10/11	0.70	0.15	107,129,145,149	0
1	SEP	a	43	10/11	0.72	0.15	114,125,142,148	0
1	SEP	Y	43	10/11	0.74	0.17	107,126,139,148	0
1	SEP	B	43	10/11	0.75	0.19	101,113,130,136	0
1	SEP	P	43	10/11	0.78	0.15	113,131,150,157	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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
3	BME	E	602	4/4	0.57	0.19	116,142,142,145	0
3	BME	V	601	4/4	0.59	0.14	132,133,134,135	0
3	BME	G	604	4/4	0.70	0.23	99,107,113,125	0
3	BME	G	603	4/4	0.73	0.14	78,87,94,109	0
4	HEZ	V	603	8/8	0.78	0.19	96,109,115,116	0
5	MG	N	603	1/1	0.78	0.10	80,80,80,80	0
3	BME	U	603	4/4	0.79	0.19	98,100,107,122	0
3	BME	O	603	4/4	0.80	0.20	95,109,113,115	0
3	BME	D	602	4/4	0.81	0.12	102,104,104,106	0
4	HEZ	B	604	8/8	0.83	0.23	79,107,110,110	0
5	MG	c	607	1/1	0.83	0.09	76,76,76,76	0
5	MG	G	606	1/1	0.84	0.13	110,110,110,110	0
3	BME	R	602	4/4	0.84	0.17	106,107,108,112	0
3	BME	X	602	4/4	0.84	0.19	93,104,113,116	0
3	BME	c	602	4/4	0.85	0.14	71,84,85,86	0
4	HEZ	D	605	8/8	0.85	0.19	79,97,104,107	0
3	BME	Q	603	4/4	0.86	0.14	79,79,84,94	0
4	HEZ	O	605	8/8	0.86	0.20	79,96,112,114	0
3	BME	E	601	4/4	0.87	0.12	103,115,119,121	0
4	HEZ	V	602	8/8	0.87	0.18	76,87,109,110	0
4	HEZ	A	603	8/8	0.87	0.17	98,103,107,107	0
4	HEZ	F	603	8/8	0.88	0.20	79,85,90,93	0
3	BME	c	603	4/4	0.88	0.16	57,69,75,97	0
4	HEZ	T	602	8/8	0.88	0.16	60,86,109,114	0
5	MG	T	604	1/1	0.88	0.14	94,94,94,94	0
5	MG	b	603	1/1	0.88	0.11	92,92,92,92	0
3	BME	c	601	4/4	0.88	0.11	72,87,88,99	0
3	BME	Q	602	4/4	0.89	0.22	70,74,89,116	0
3	BME	C	601	4/4	0.89	0.19	69,78,81,98	0
4	HEZ	E	606	8/8	0.89	0.15	77,82,85,87	0
4	HEZ	B	603	8/8	0.89	0.18	56,73,91,92	0
4	HEZ	c	606	8/8	0.89	0.17	77,84,88,90	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BME	O	602	4/4	0.90	0.20	87,91,97,97	0
4	HEZ	E	604	8/8	0.90	0.12	61,64,73,78	0
4	HEZ	E	605	8/8	0.90	0.15	61,66,81,89	0
4	HEZ	C	602	8/8	0.91	0.12	56,63,82,94	0
3	BME	G	601	4/4	0.91	0.14	70,73,74,82	0
4	HEZ	G	605	8/8	0.91	0.12	67,77,83,85	0
4	HEZ	H	602	8/8	0.91	0.12	59,63,67,71	0
3	BME	X	601	4/4	0.91	0.16	55,68,76,86	0
4	HEZ	P	603	8/8	0.91	0.14	46,65,88,91	0
5	MG	U	605	1/1	0.91	0.08	77,77,77,77	0
4	HEZ	R	604	8/8	0.91	0.14	67,87,94,96	0
3	BME	P	601	4/4	0.91	0.15	62,69,76,83	0
4	HEZ	c	604	8/8	0.92	0.12	53,73,86,90	0
4	HEZ	c	605	8/8	0.92	0.16	63,70,84,85	0
4	HEZ	A	602	8/8	0.92	0.13	78,81,89,96	0
5	MG	D	606	1/1	0.92	0.09	82,82,82,82	0
3	BME	D	601	4/4	0.92	0.15	77,80,80,81	0
4	HEZ	R	603	8/8	0.92	0.10	62,63,74,80	0
3	BME	M	601	4/4	0.92	0.13	54,63,67,87	0
3	BME	E	603	4/4	0.92	0.13	67,67,72,79	0
4	HEZ	K	602	8/8	0.92	0.12	59,65,79,84	0
4	HEZ	N	602	8/8	0.92	0.15	50,62,94,97	0
4	HEZ	U	604	8/8	0.93	0.12	55,58,74,81	0
4	HEZ	J	602	8/8	0.93	0.12	51,60,75,78	0
3	BME	Z	601	4/4	0.93	0.14	49,58,65,80	0
4	HEZ	W	601	8/8	0.93	0.12	61,78,92,95	0
4	HEZ	Z	602	8/8	0.93	0.16	53,62,81,84	0
4	HEZ	L	601	8/8	0.93	0.13	56,69,88,88	0
4	HEZ	M	602	8/8	0.93	0.13	64,71,83,84	0
3	BME	K	601	4/4	0.93	0.18	76,80,81,86	0
3	BME	F	601	4/4	0.93	0.12	57,65,69,83	0
5	MG	E	607	1/1	0.93	0.11	95,95,95,95	0
4	HEZ	F	602	8/8	0.93	0.12	58,62,76,83	0
4	HEZ	Q	604	8/8	0.93	0.12	53,62,80,82	0
3	BME	T	601	4/4	0.93	0.15	63,76,84,106	0
4	HEZ	D	604	8/8	0.93	0.12	60,67,82,87	0
3	BME	U	601	4/4	0.93	0.12	64,71,73,85	0
4	HEZ	T	603	8/8	0.93	0.16	82,91,107,110	0
3	BME	b	601	4/4	0.94	0.15	88,88,89,91	0
4	HEZ	b	602	8/8	0.94	0.14	53,71,102,108	0
3	BME	A	601	4/4	0.94	0.23	71,75,75,76	0
4	HEZ	I	602	8/8	0.94	0.16	71,77,82,93	0

Continued on next page...

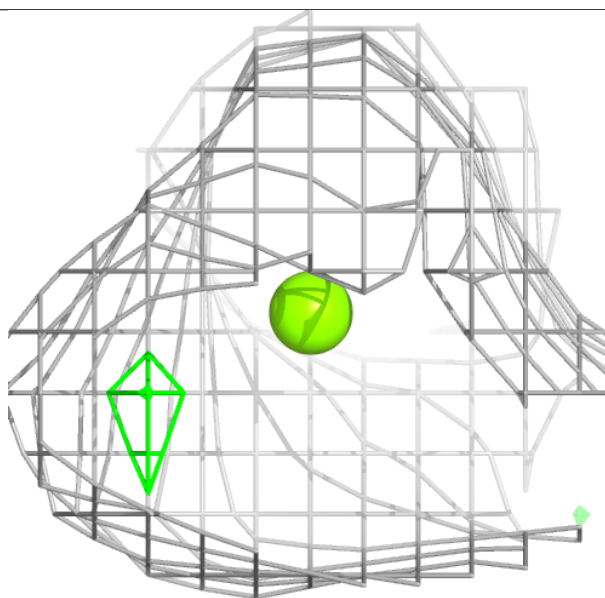
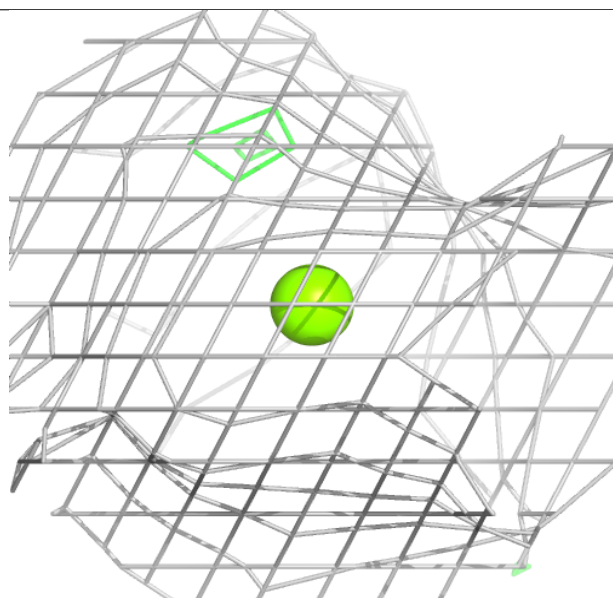
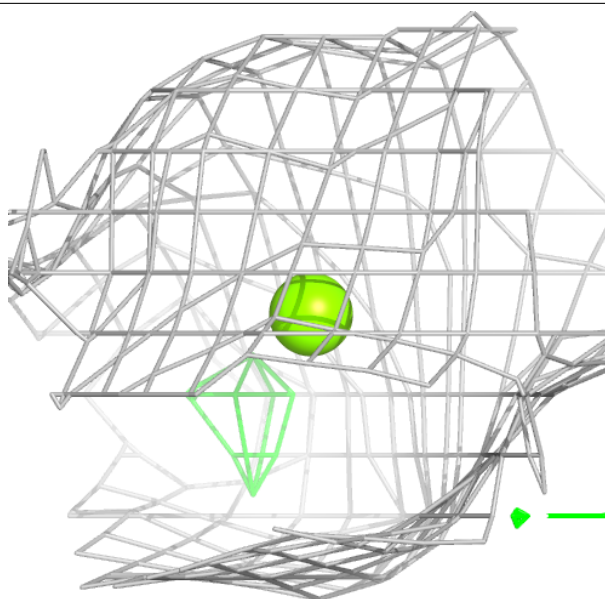
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BME	H	601	4/4	0.94	0.16	64,68,72,74	0
3	BME	J	601	4/4	0.94	0.15	81,84,87,95	0
3	BME	P	602	4/4	0.94	0.14	57,69,72,83	0
3	BME	B	601	4/4	0.94	0.16	54,60,65,82	0
3	BME	B	602	4/4	0.94	0.15	50,62,67,85	0
4	HEZ	O	604	8/8	0.94	0.14	52,59,69,76	0
3	BME	N	601	4/4	0.94	0.17	76,91,92,95	0
4	HEZ	W	602	8/8	0.94	0.12	68,82,99,101	0
4	HEZ	Y	602	8/8	0.94	0.12	54,57,75,78	0
3	BME	G	602	4/4	0.95	0.12	59,68,74,93	0
5	MG	H	603	1/1	0.95	0.15	74,74,74,74	0
5	MG	M	603	1/1	0.95	0.05	59,59,59,59	0
3	BME	O	601	4/4	0.95	0.11	62,75,83,95	0
4	HEZ	X	603	8/8	0.95	0.12	54,62,85,93	0
4	HEZ	I	601	8/8	0.95	0.11	53,60,76,84	0
5	MG	V	604	1/1	0.95	0.05	77,77,77,77	0
3	BME	R	601	4/4	0.95	0.14	82,87,88,91	0
4	HEZ	a	602	8/8	0.95	0.12	52,63,83,85	0
5	MG	H	604	1/1	0.96	0.30	39,39,39,39	0
3	BME	a	601	4/4	0.96	0.13	56,71,83,94	0
3	BME	U	602	4/4	0.96	0.16	76,78,79,86	0
3	BME	D	603	4/4	0.96	0.12	85,86,90,90	0
3	BME	Y	601	4/4	0.97	0.12	64,67,76,84	0
5	MG	F	604	1/1	0.97	0.05	87,87,87,87	0
3	BME	Q	601	4/4	0.97	0.08	57,61,64,69	0
5	MG	A	604	1/1	0.98	0.09	78,78,78,78	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.

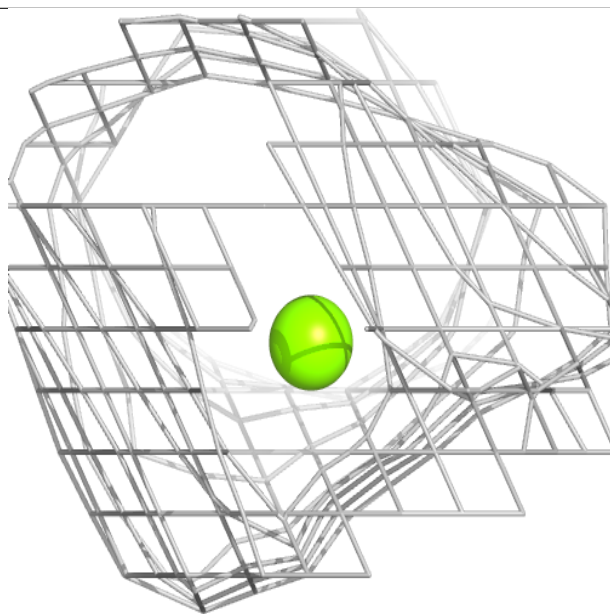
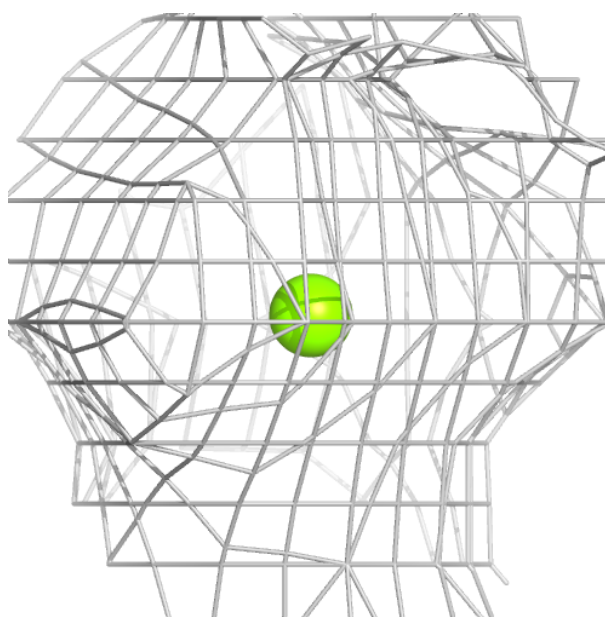
Electron density around MG N 603:

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



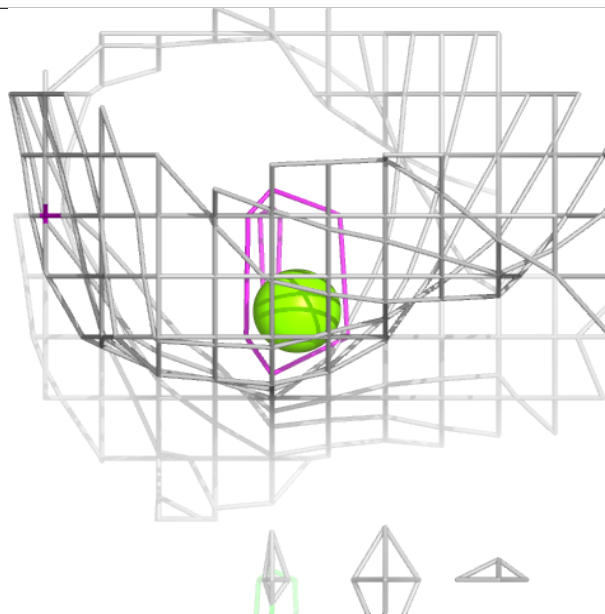
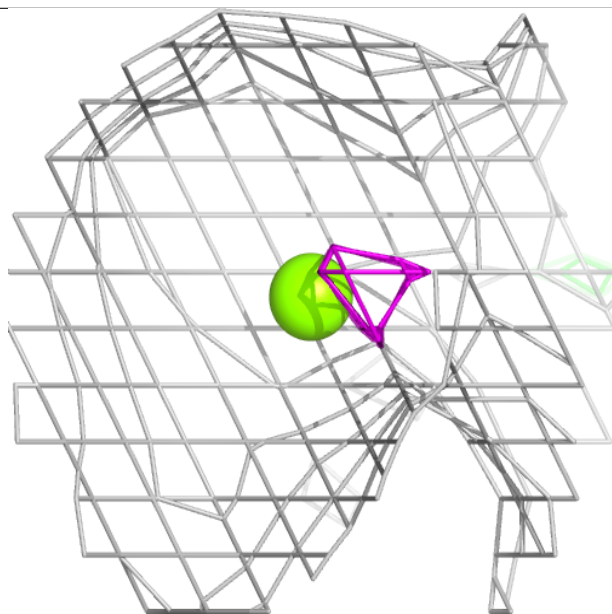
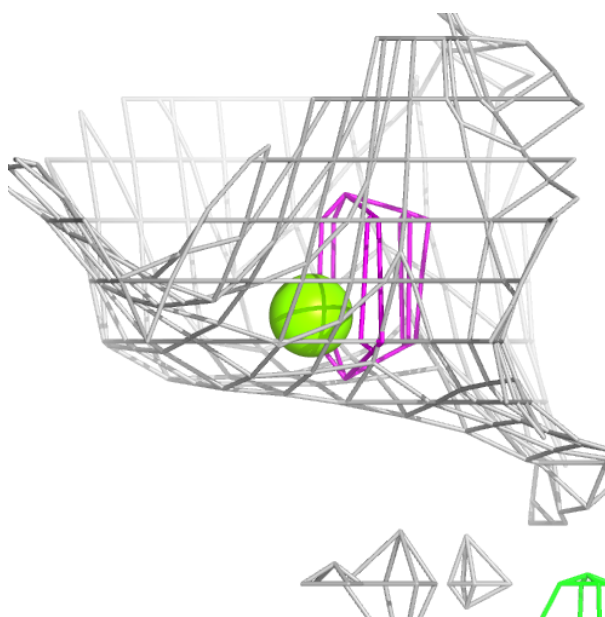
Electron density around MG c 607:

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



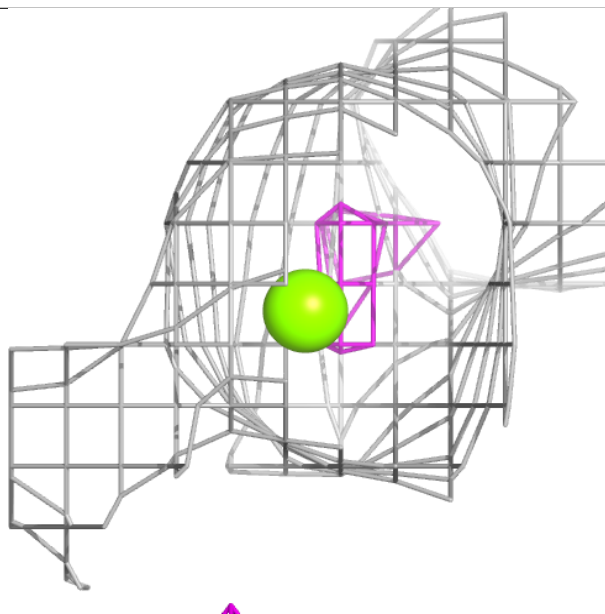
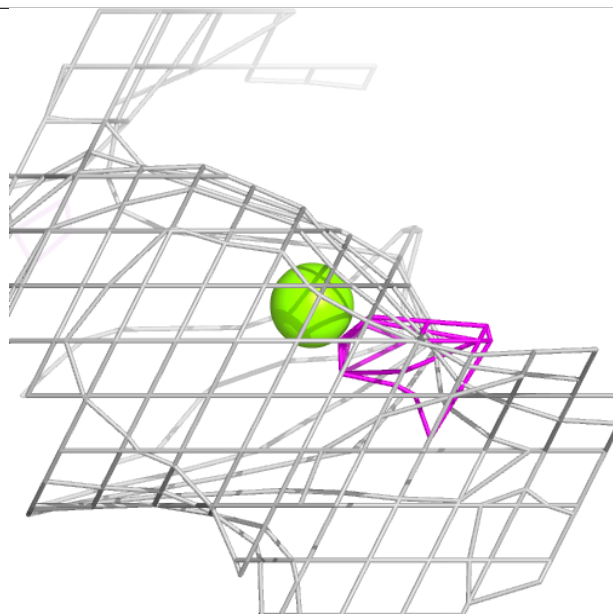
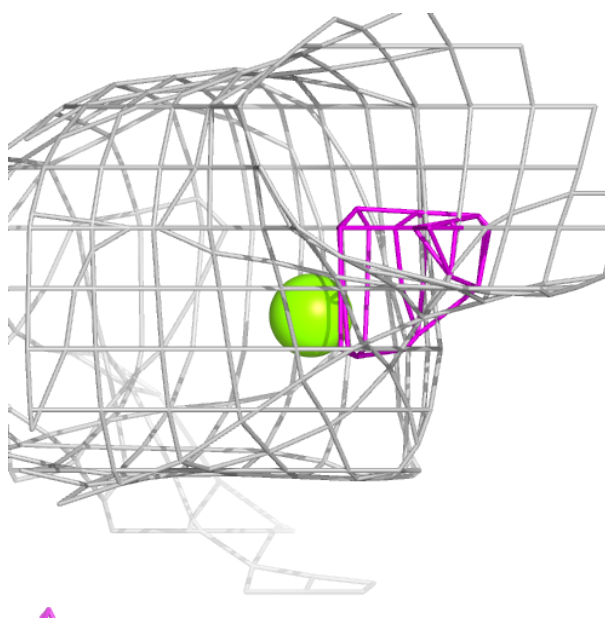
Electron density around MG G 606:

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



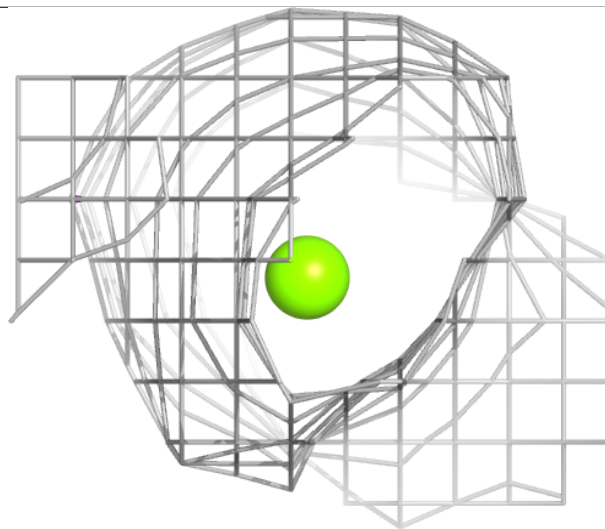
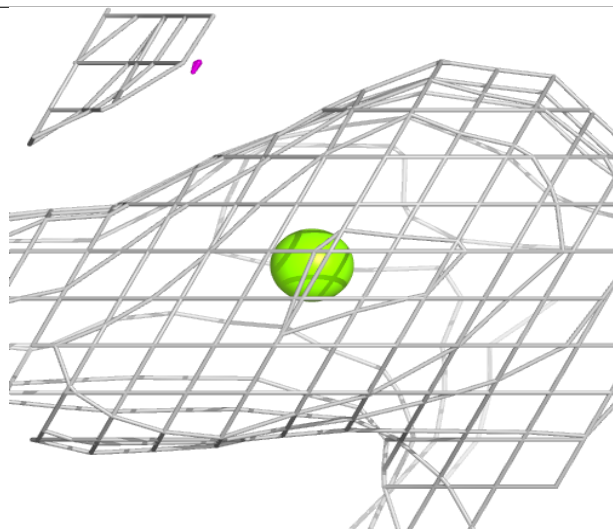
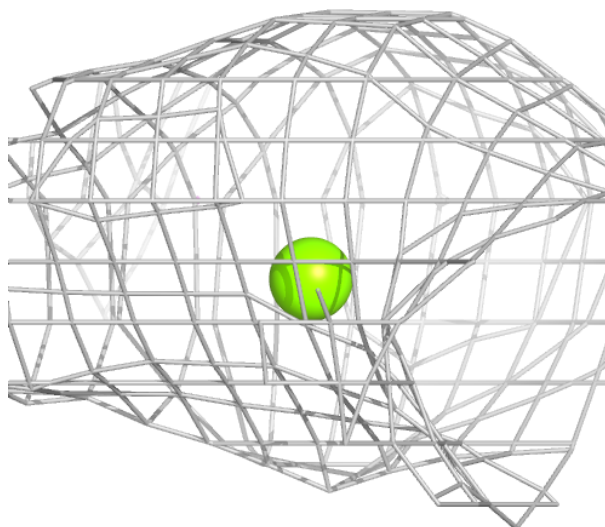
Electron density around MG T 604:

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



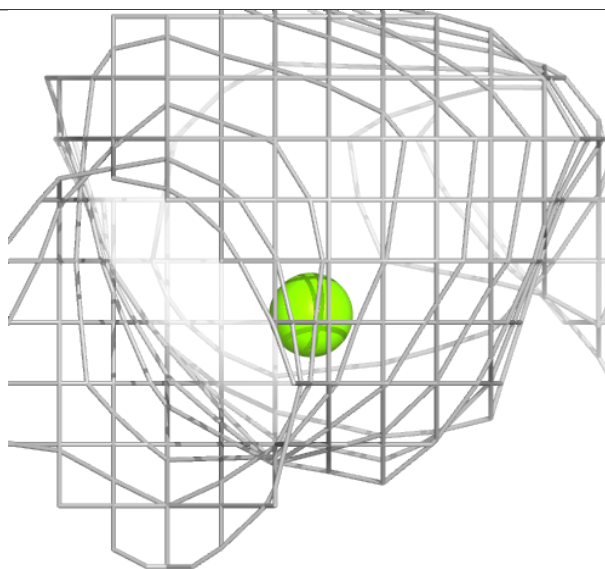
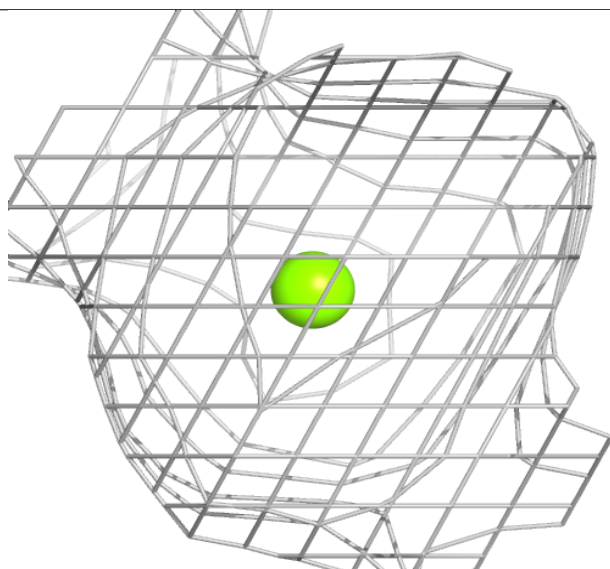
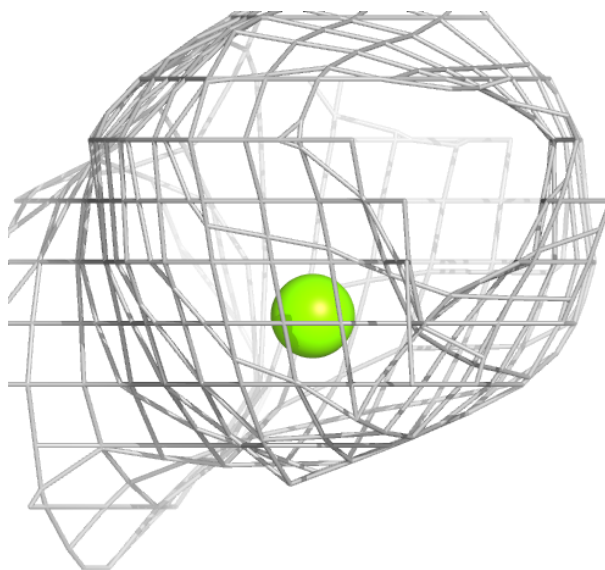
Electron density around MG b 603:

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



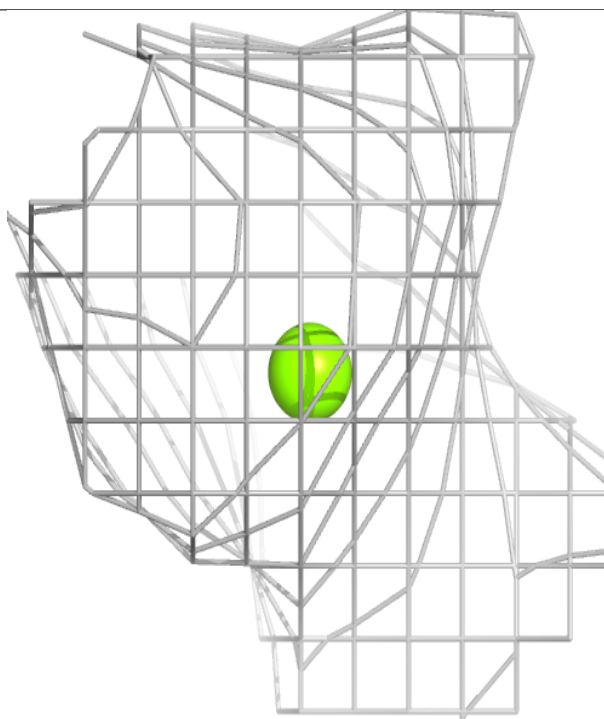
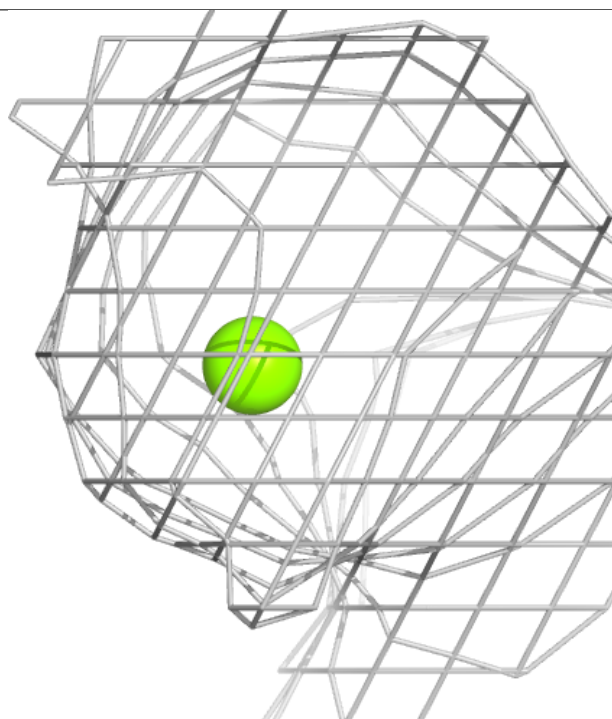
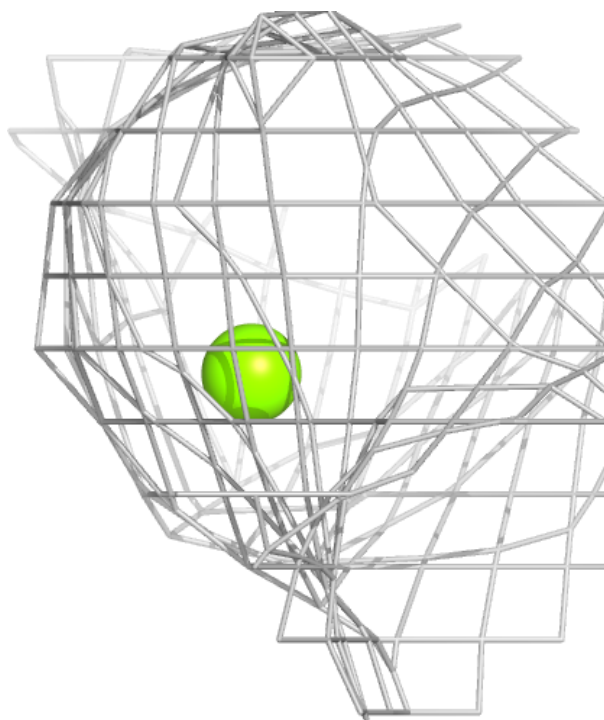
Electron density around MG U 605:

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



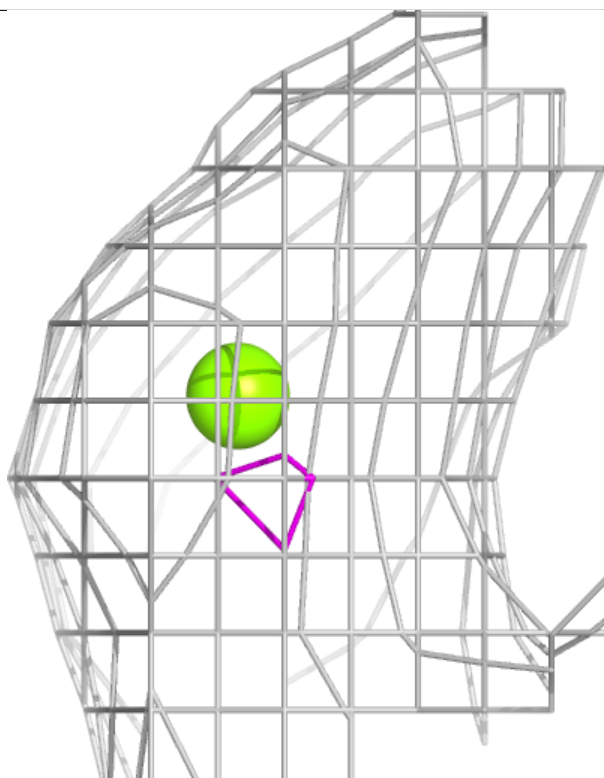
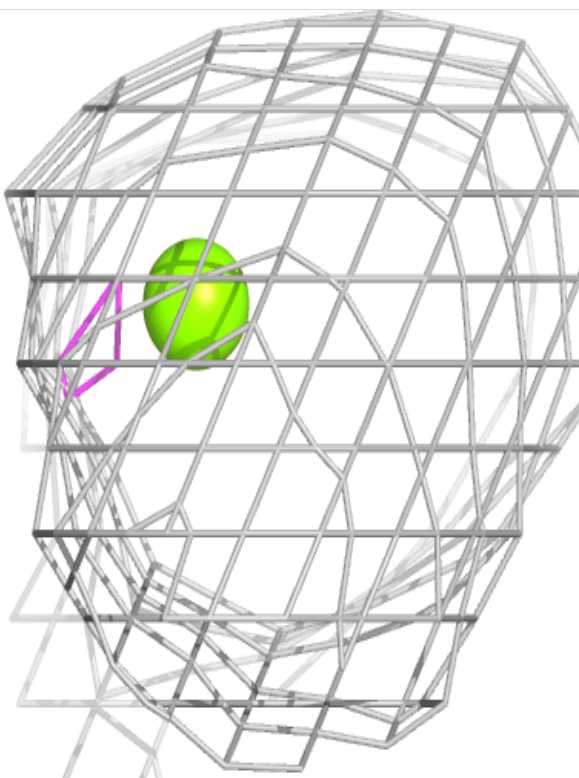
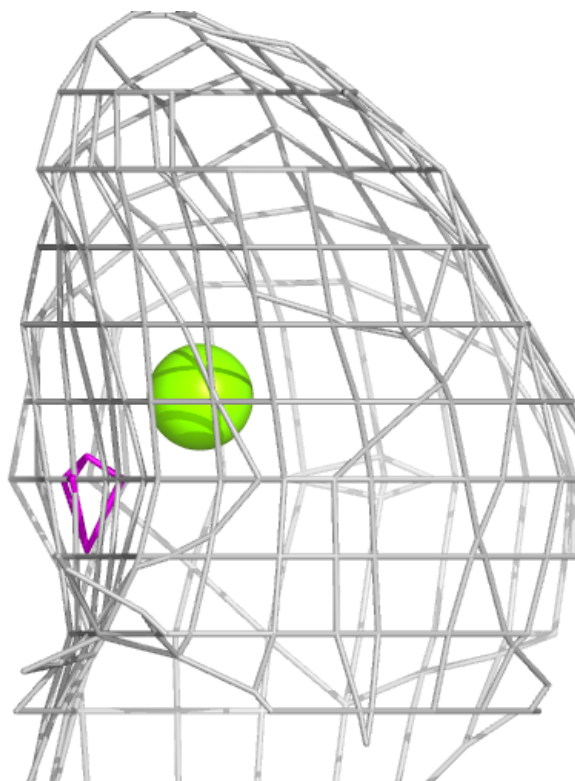
Electron density around MG D 606:

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



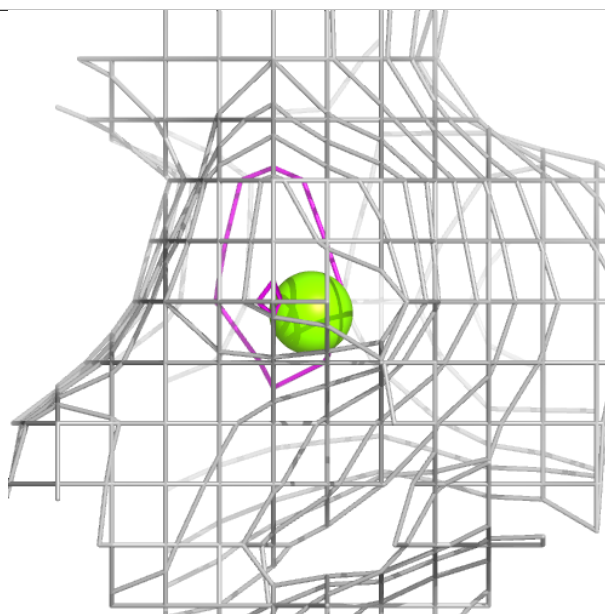
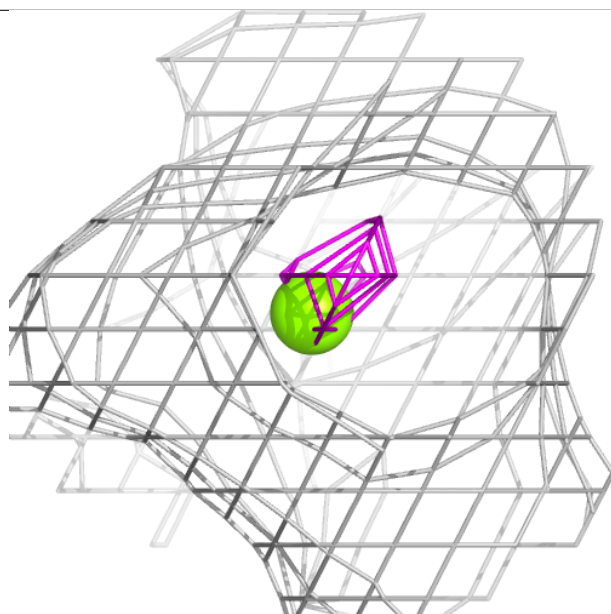
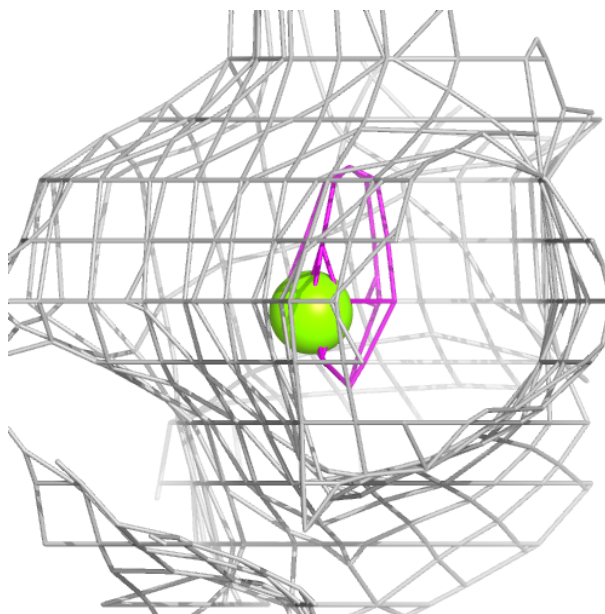
Electron density around MG E 607:

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



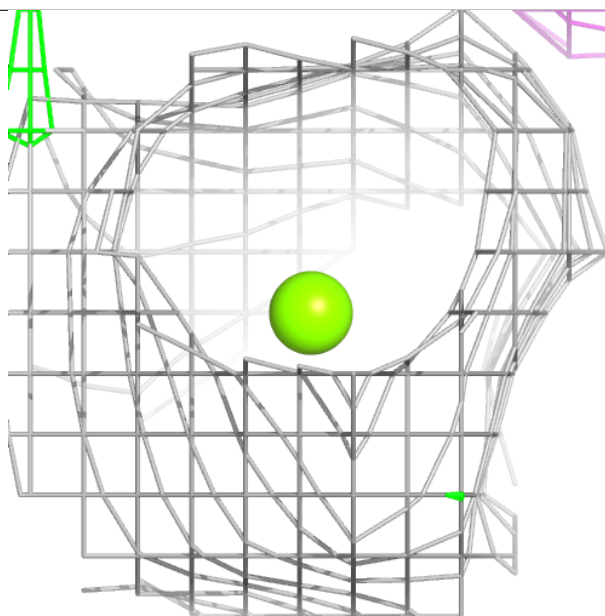
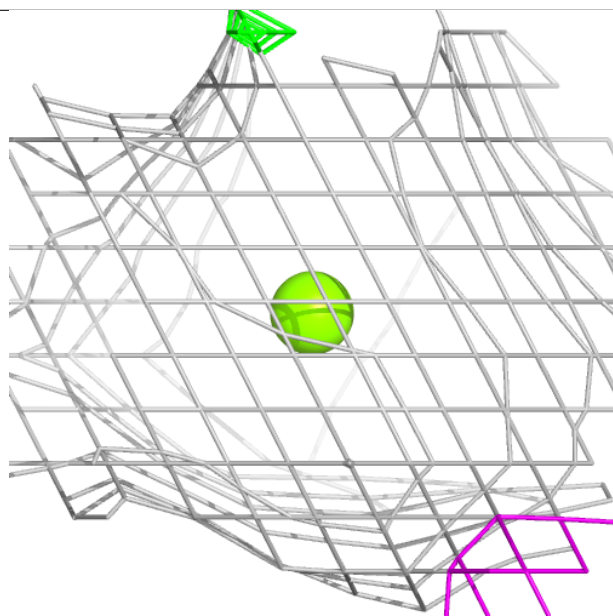
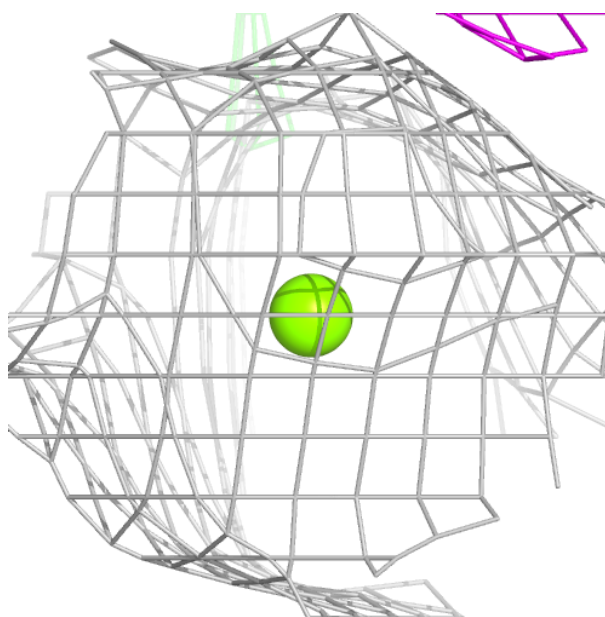
Electron density around MG H 603:

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



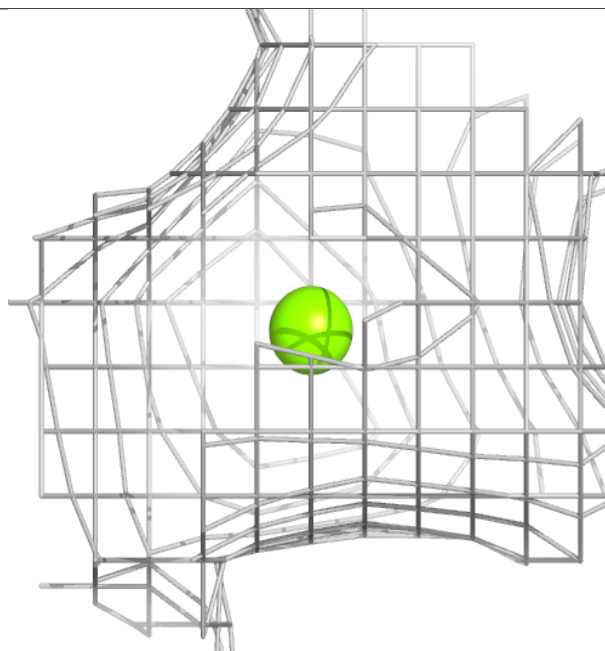
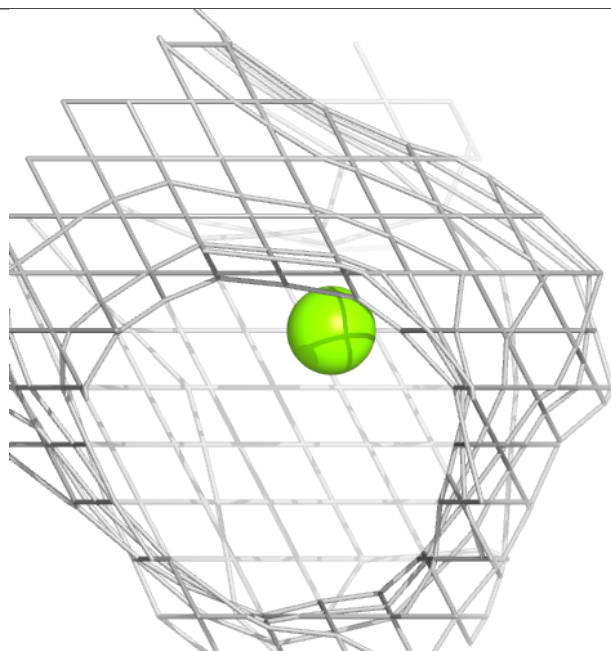
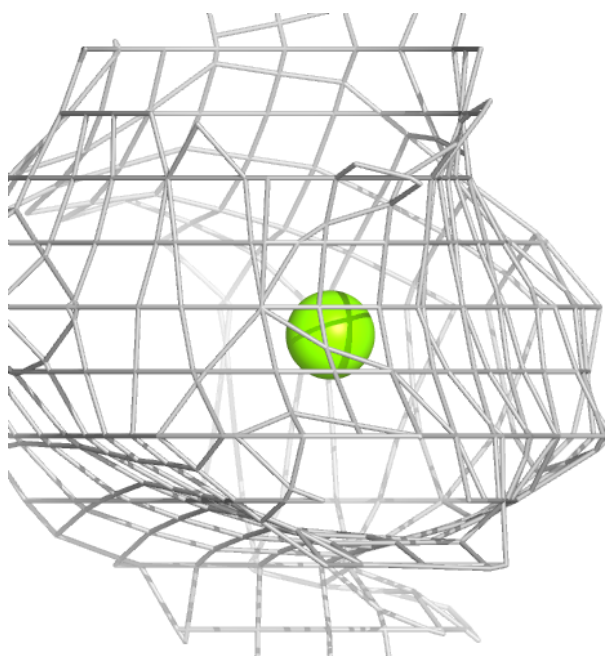
Electron density around MG M 603:

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



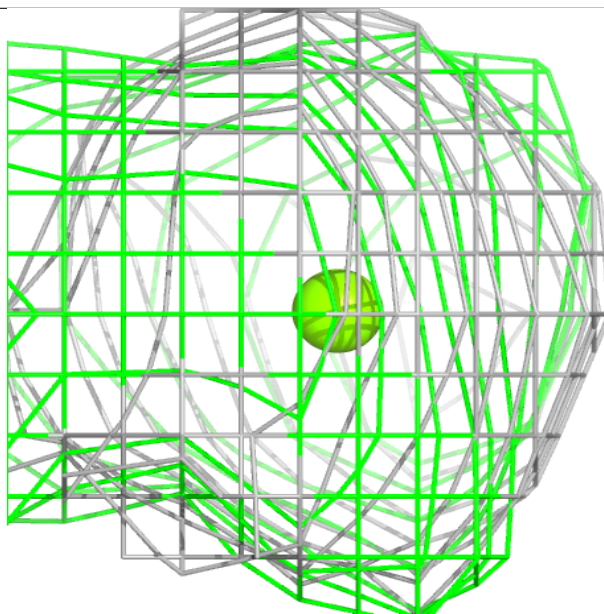
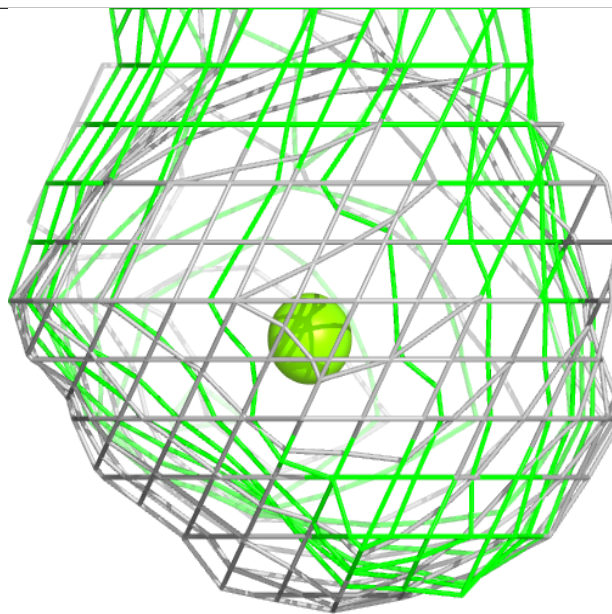
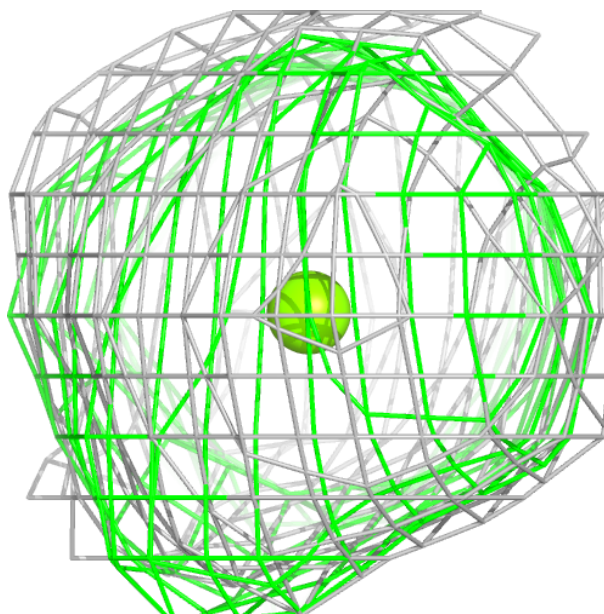
Electron density around MG V 604:

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



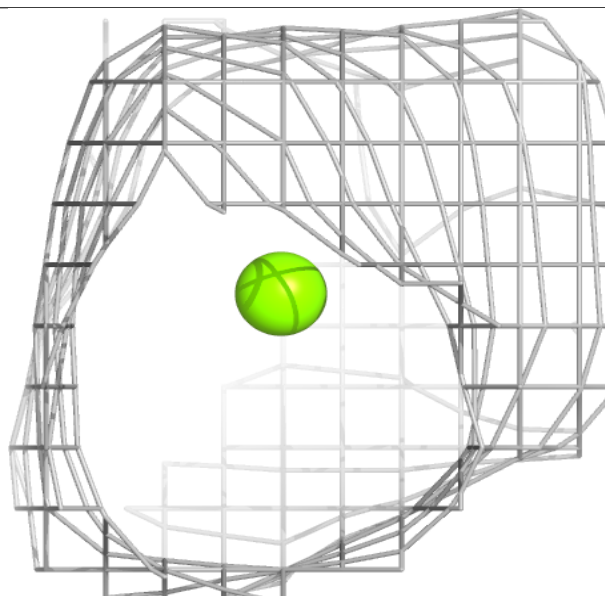
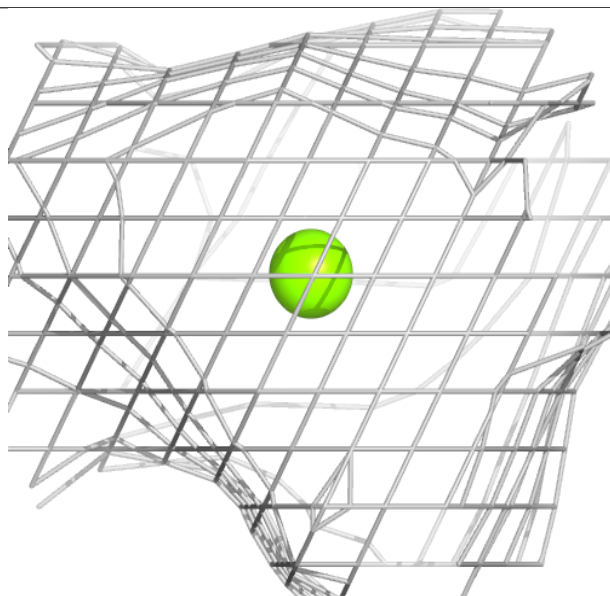
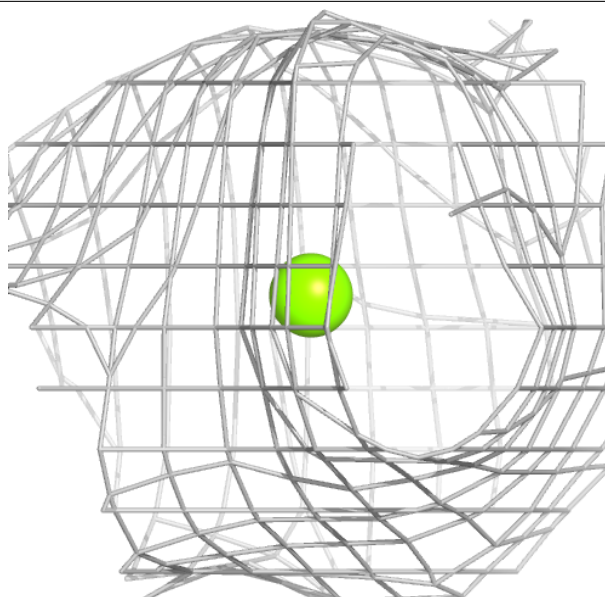
Electron density around MG H 604:

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



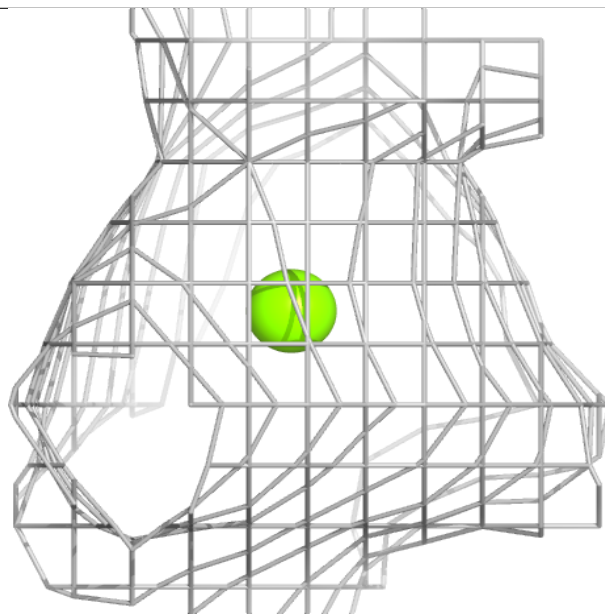
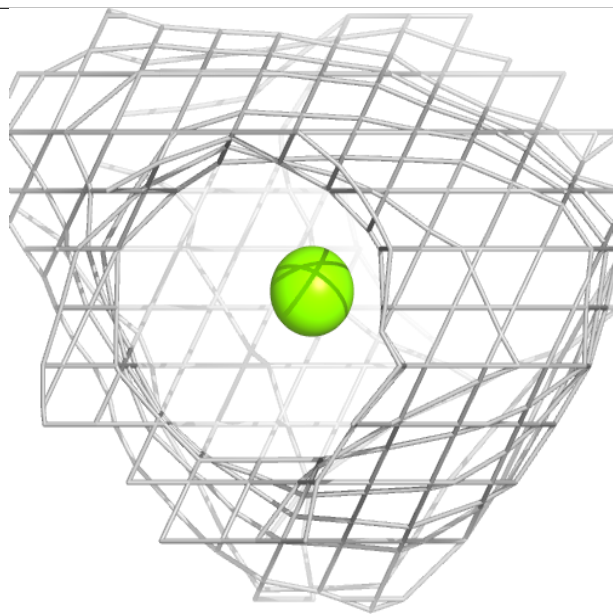
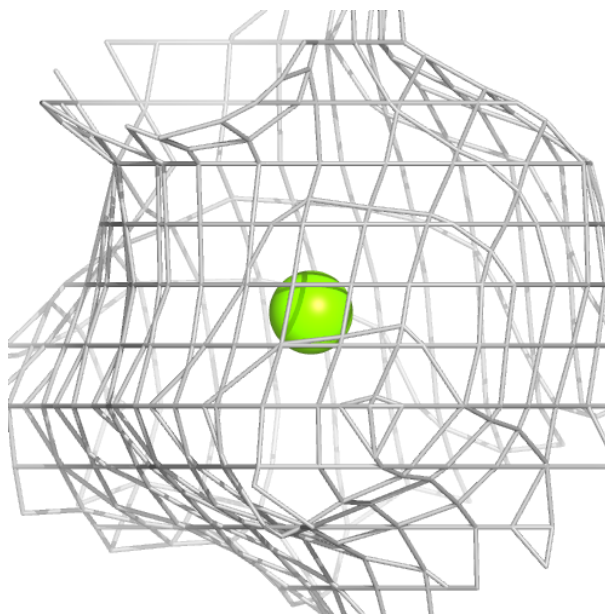
Electron density around MG F 604:

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



Electron density around MG A 604:

$2mF_o-DF_c$ (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.