



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 24, 2025 – 04:41 PM JST

PDB ID : 9WBT / pdb_00009wbt
Title : Crystal Structure of Escherichia coli GroEL with Magnesium Ions and a Phosphorylated Serine Residue-3.2A
Authors : Guo, Y.; Zhang, L.; Zheng, H.; Li, J.; Han, Q.
Deposited on : 2025-08-15
Resolution : 3.20 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 Phenix2.0rc1
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

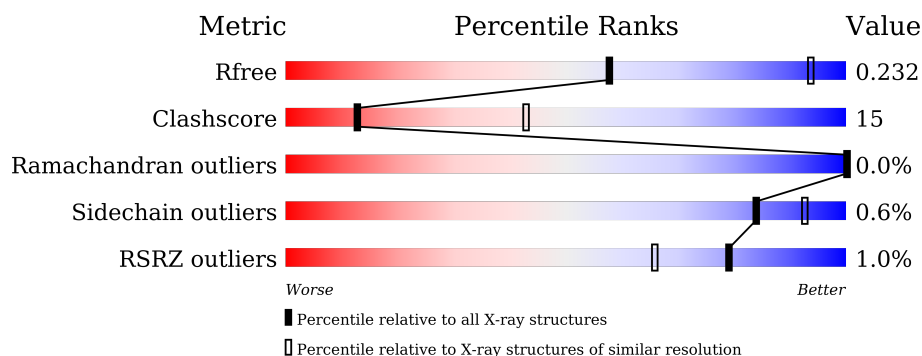
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	164625	1370 (3.20-3.20)
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (3.20-3.20)

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	<div><div></div><div>74%</div><div>22%</div><div>.</div></div>
1	B	548	<div><div></div><div>74%</div><div>22%</div><div>.</div></div>
1	E	548	<div><div>%</div><div></div><div>75%</div><div>21%</div><div>.</div></div>
1	F	548	<div><div></div><div>74%</div><div>22%</div><div>.</div></div>
1	H	548	<div><div></div><div>75%</div><div>20%</div><div>.</div></div>
1	J	548	<div><div></div><div>71%</div><div>25%</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
1	M	548	<div> <div>7%</div> <div>68%</div> <div>28%</div> <div>..</div> </div>
2	C	548	<div> <div>73%</div> <div>22%</div> <div>.</div> </div>
2	D	548	<div> <div>2%</div> <div>71%</div> <div>24%</div> <div>..</div> </div>
2	G	548	<div> <div>73%</div> <div>23%</div> <div>.</div> </div>
2	I	548	<div> <div>73%</div> <div>23%</div> <div>.</div> </div>
2	K	548	<div> <div>3%</div> <div>66%</div> <div>29%</div> <div>..</div> </div>
2	L	548	<div> <div>68%</div> <div>27%</div> <div>..</div> </div>
2	N	548	<div> <div>74%</div> <div>22%</div> <div>..</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 54517 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.

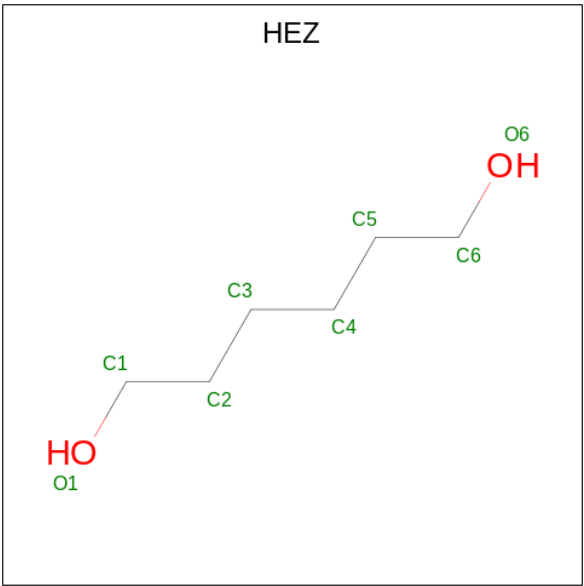
- Molecule 1 is a protein called Chaperonin GroEL.

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	524	Total	C	N	O	P	S	0	0	0
			3859	2397	665	776	1	20			
1	E	525	Total	C	N	O	P	S	0	0	0
			3868	2403	667	777	1	20			
1	F	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	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			

- Molecule 2 is a protein called Chaperonin GroEL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	525	Total	C	N	O	S	0	0	0
			3864	2403	667	774	20			
2	D	525	Total	C	N	O	S	0	0	0
			3864	2403	667	774	20			
2	G	525	Total	C	N	O	S	0	0	0
			3864	2403	667	774	20			
2	I	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	N	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			

- Molecule 3 is HEXANE-1,6-DIOL (CCD ID: HEZ) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	E	1	Total	C	O	0	0
			8	6	2		
3	E	1	Total	C	O	0	0
			8	6	2		
3	E	1	Total	C	O	0	0
			8	6	2		
3	F	1	Total	C	O	0	0
			8	6	2		
3	F	1	Total	C	O	0	0
			8	6	2		

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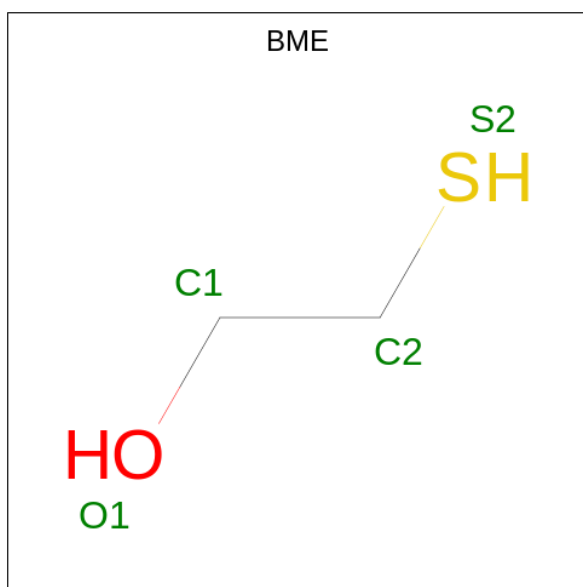
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	C	O	0	0
			8	6	2		
3	H	1	Total	C	O	0	0
			8	6	2		
3	H	1	Total	C	O	0	0
			8	6	2		
3	I	1	Total	C	O	0	0
			8	6	2		
3	I	1	Total	C	O	0	0
			8	6	2		
3	J	1	Total	C	O	0	0
			8	6	2		
3	K	1	Total	C	O	0	0
			8	6	2		
3	L	1	Total	C	O	0	0
			8	6	2		
3	M	1	Total	C	O	0	0
			8	6	2		
3	N	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		
4	G	1	Total	Mg	0	0
			1	1		
4	H	1	Total	Mg	0	0
			1	1		
4	N	1	Total	Mg	0	0
			1	1		

- Molecule 5 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C₂H₆OS).



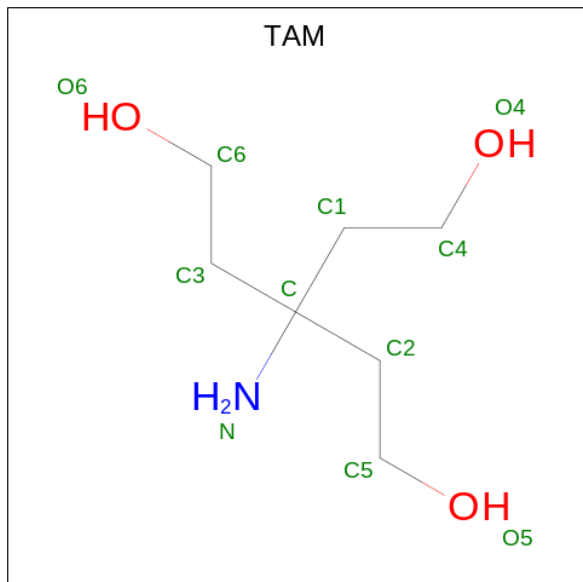
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	E	1	Total 4	C 2	O 1	S 1	0	0
5	E	1	Total 4	C 2	O 1	S 1	0	0
5	E	1	Total 4	C 2	O 1	S 1	0	0
5	E	1	Total 4	C 2	O 1	S 1	0	0
5	F	1	Total 4	C 2	O 1	S 1	0	0
5	G	1	Total 4	C 2	O 1	S 1	0	0
5	G	1	Total 4	C 2	O 1	S 1	0	0
5	G	1	Total 4	C 2	O 1	S 1	0	0
5	G	1	Total 4	C 2	O 1	S 1	0	0
5	H	1	Total 4	C 2	O 1	S 1	0	0
5	H	1	Total 4	C 2	O 1	S 1	0	0
5	I	1	Total 4	C 2	O 1	S 1	0	0
5	I	1	Total 4	C 2	O 1	S 1	0	0
5	J	1	Total 4	C 2	O 1	S 1	0	0
5	J	1	Total 4	C 2	O 1	S 1	0	0
5	J	1	Total 4	C 2	O 1	S 1	0	0
5	K	1	Total 4	C 2	O 1	S 1	0	0
5	L	1	Total 4	C 2	O 1	S 1	0	0
5	M	1	Total 4	C 2	O 1	S 1	0	0
5	N	1	Total 4	C 2	O 1	S 1	0	0
5	N	1	Total 4	C 2	O 1	S 1	0	0

- Molecule 6 is TRIS(HYDROXYETHYL)AMINOMETHANE (CCD ID: TAM) (formula: $C_7H_{17}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	G	1	Total	C	N	O	0	0
			11	7	1	3		
6	I	1	Total	C	N	O	0	0
			11	7	1	3		
6	J	1	Total	C	N	O	0	0
			11	7	1	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	5	Total	O	0	0
			5	5		
7	B	8	Total	O	0	0
			8	8		
7	C	5	Total	O	0	0
			5	5		
7	D	4	Total	O	0	0
			4	4		
7	E	5	Total	O	0	0
			5	5		
7	F	2	Total	O	0	0
			2	2		
7	G	5	Total	O	0	0
			5	5		

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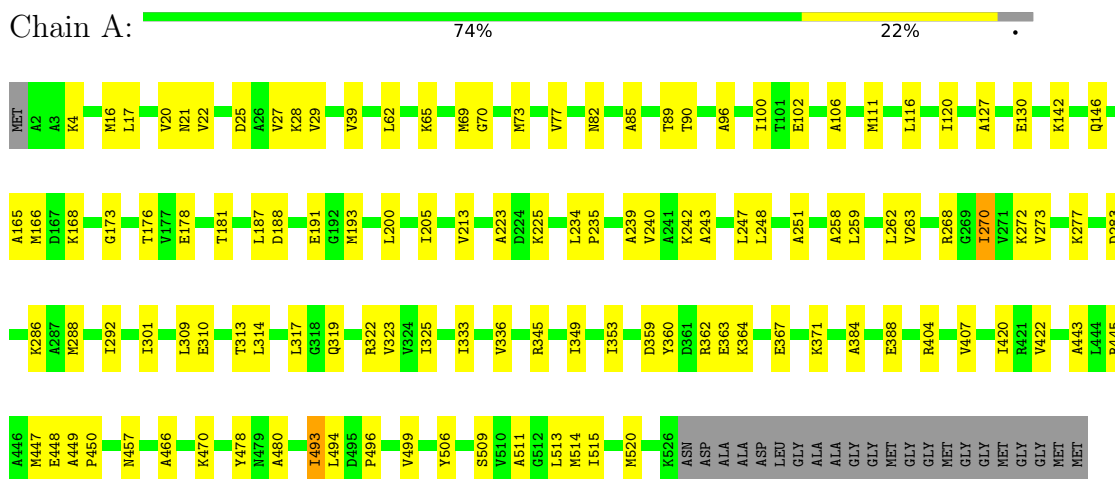
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	3	Total 3	O 3	0	0
7	I	1	Total 1	O 1	0	0
7	J	2	Total 2	O 2	0	0
7	K	2	Total 2	O 2	0	0
7	L	1	Total 1	O 1	0	0
7	N	4	Total 4	O 4	0	0

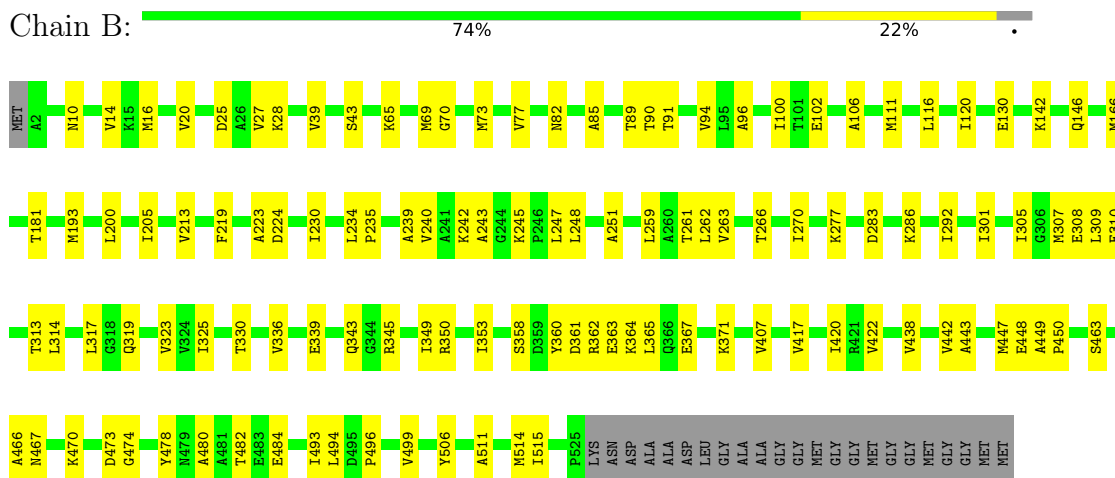
3 Residue-property plots

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

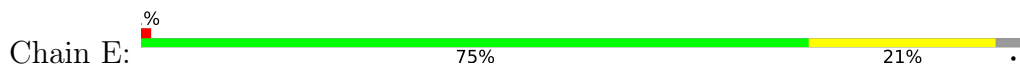
• Molecule 1: Chaperonin GroEL

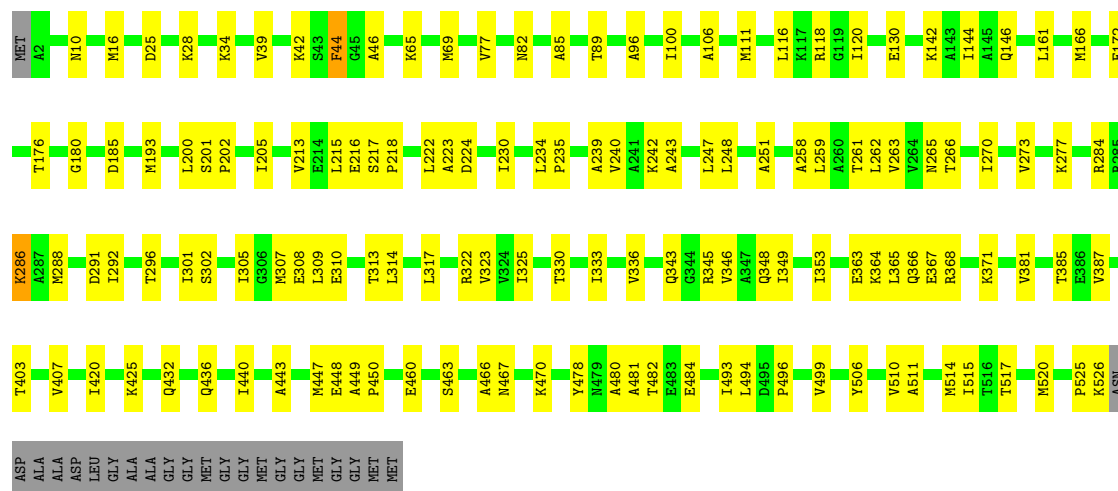


• Molecule 1: Chaperonin GroEL

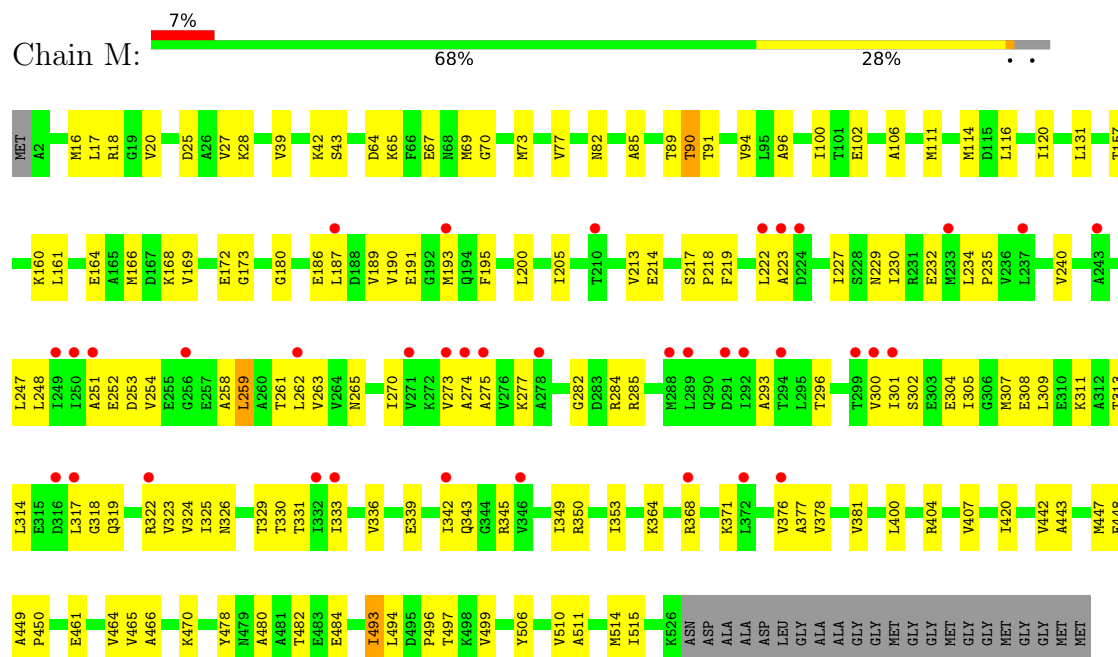


• Molecule 1: Chaperonin GroEL

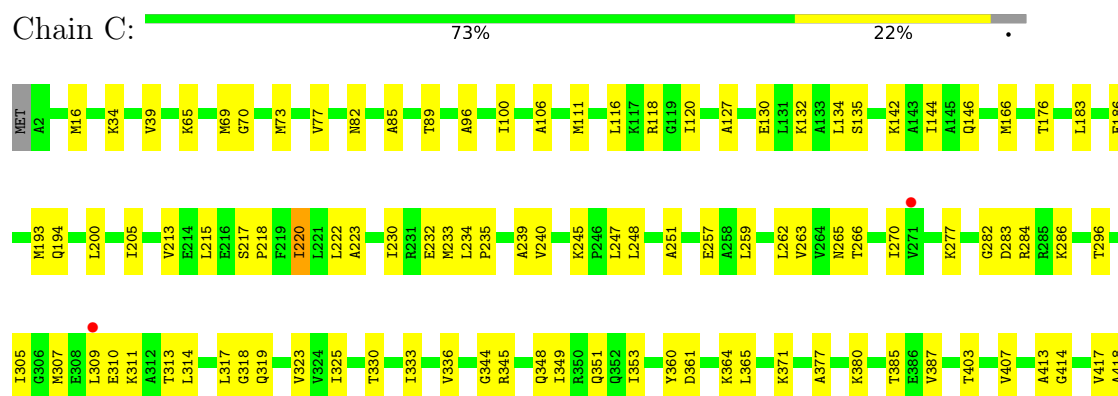


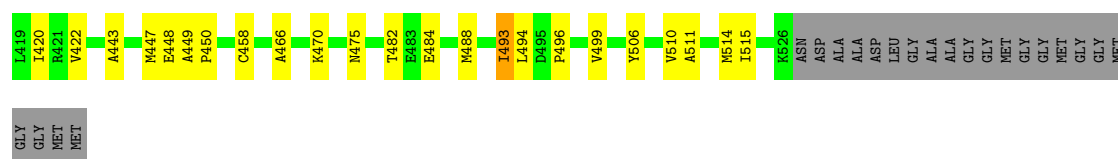


• Molecule 1: Chaperonin GroEL

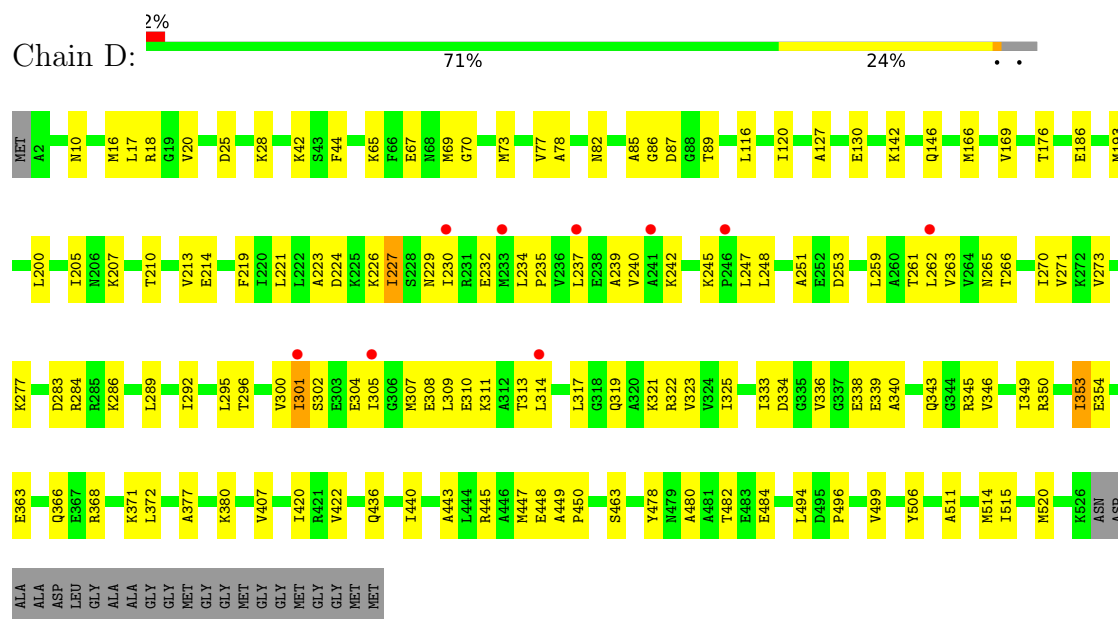


• Molecule 2: Chaperonin GroEL

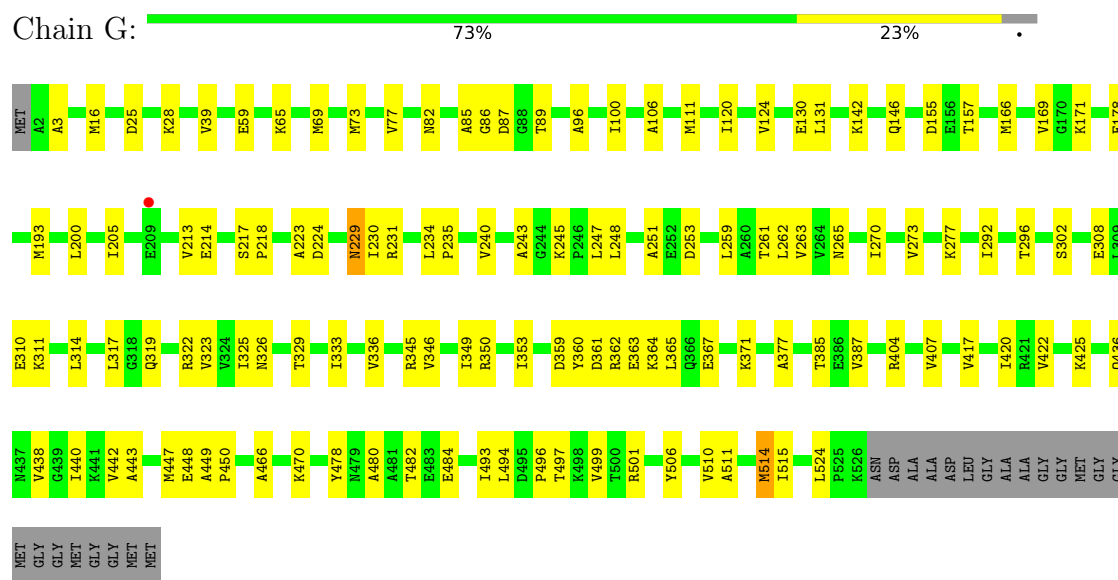




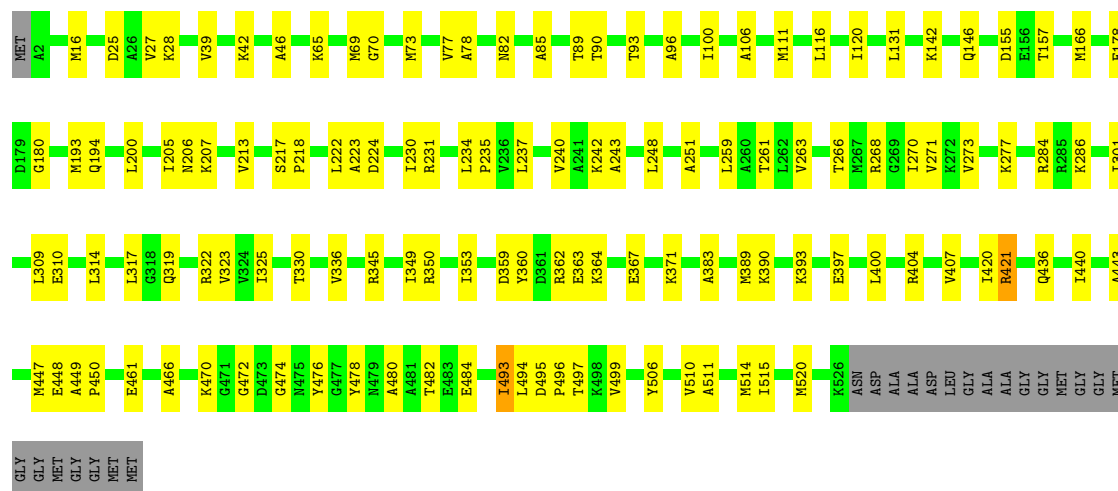
• Molecule 2: Chaperonin GroEL



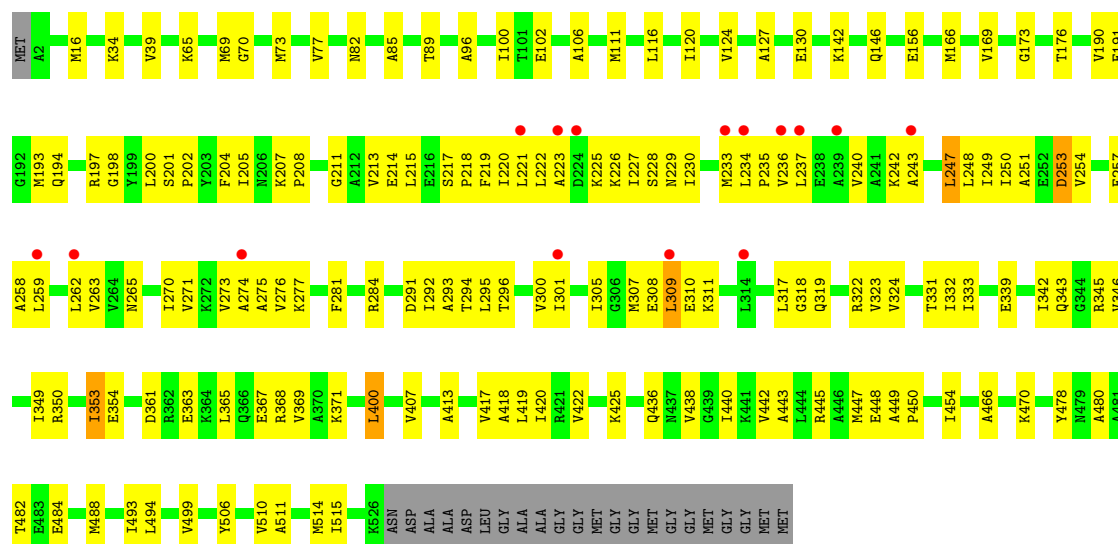
• Molecule 2: Chaperonin GroEL



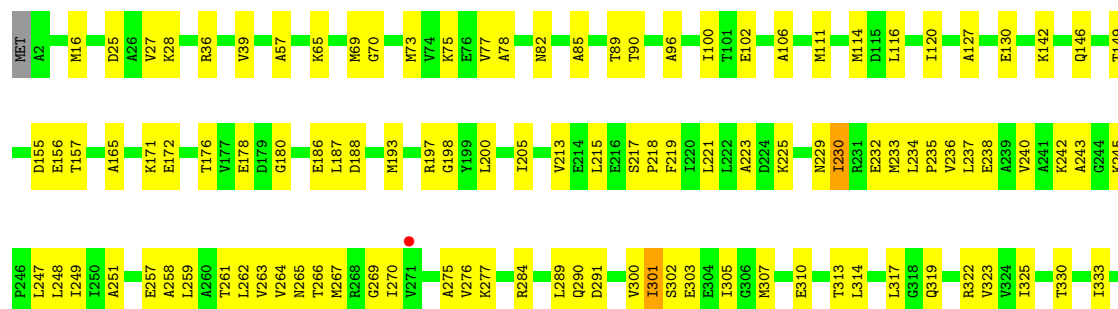
• Molecule 2: Chaperonin GroEL

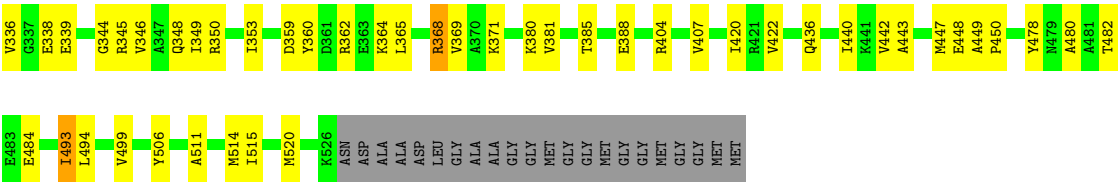


• Molecule 2: Chaperonin GroEL

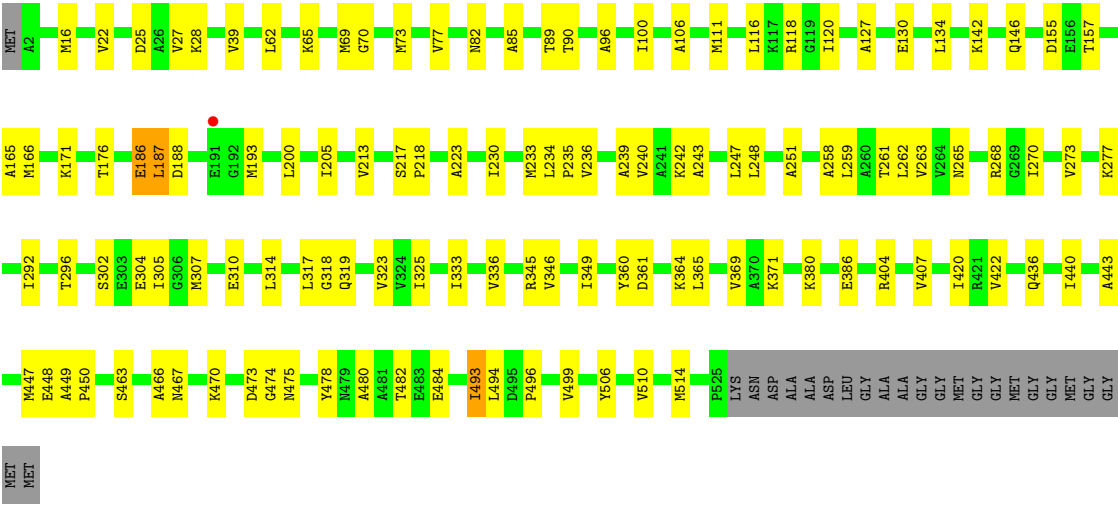


• Molecule 2: Chaperonin GroEL





• Molecule 2: Chaperonin GroEL



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	135.84Å 262.17Å 284.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.20 – 3.20 49.20 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.20-3.20) 99.3 (49.20-3.20)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.43 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.196 , 0.236 0.196 , 0.232	Depositor DCC
R_{free} test set	8340 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	66.4	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 34.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	54517	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BME, TAM, MG, SEP, HEZ

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	0.48	0/3885	0.96	0/5243
1	B	0.49	0/3876	0.95	0/5232
1	E	0.49	0/3885	0.95	0/5243
1	F	0.47	0/3885	0.94	1/5243 (0.0%)
1	H	0.47	0/3885	0.93	0/5243
1	J	0.48	0/3885	0.94	0/5243
1	M	0.47	0/3885	0.97	1/5243 (0.0%)
2	C	0.48	0/3892	0.94	1/5254 (0.0%)
2	D	0.47	0/3892	0.95	0/5254
2	G	0.48	0/3892	0.94	0/5254
2	I	0.47	0/3892	0.94	2/5254 (0.0%)
2	K	0.46	0/3892	0.94	1/5254 (0.0%)
2	L	0.46	0/3892	0.94	0/5254
2	N	0.47	0/3883	0.94	0/5243
All	All	0.48	0/54421	0.94	6/73457 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	I	0	1
2	K	0	1
2	L	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	351	GLN	N-CA-C	-7.47	102.82	112.23
1	F	91	THR	CA-CB-OG1	-6.19	100.31	109.60
2	I	93	THR	CA-CB-OG1	-6.17	100.35	109.60
2	I	495	ASP	CA-CB-CG	6.00	118.61	112.60
2	K	253	ASP	CA-CB-CG	5.61	118.21	112.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	I	421	ARG	Sidechain
2	K	368	ARG	Sidechain
2	L	368	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3868	0	3987	96	0
1	B	3859	0	3974	90	0
1	E	3868	0	3987	95	0
1	F	3868	0	3988	104	0
1	H	3868	0	3988	94	0
1	J	3868	0	3987	113	0
1	M	3868	0	3988	184	0
2	C	3864	0	3989	137	0
2	D	3864	0	3989	112	0
2	G	3864	0	3989	93	0
2	I	3864	0	3989	104	0
2	K	3864	0	3989	221	0
2	L	3864	0	3989	162	0
2	N	3855	0	3976	94	0
3	A	16	0	28	0	0
3	B	16	0	28	0	0
3	C	16	0	28	1	0
3	D	16	0	28	0	0
3	E	24	0	42	0	0
3	F	16	0	28	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	8	0	14	1	0
3	H	16	0	28	0	0
3	I	16	0	28	0	0
3	J	8	0	14	0	0
3	K	8	0	14	0	0
3	L	8	0	14	0	0
3	M	8	0	14	1	0
3	N	8	0	14	0	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	N	1	0	0	0	0
5	A	16	0	24	2	0
5	B	16	0	24	0	0
5	C	16	0	24	2	0
5	D	8	0	12	0	0
5	E	16	0	24	3	0
5	F	4	0	6	0	0
5	G	16	0	24	0	0
5	H	8	0	12	1	0
5	I	8	0	12	0	0
5	J	12	0	18	0	0
5	K	4	0	6	0	0
5	L	4	0	6	0	0
5	M	4	0	6	0	0
5	N	8	0	12	0	0
6	G	11	0	17	0	0
6	I	11	0	17	0	0
6	J	11	0	17	1	0
7	A	5	0	0	0	0
7	B	8	0	0	0	0
7	C	5	0	0	0	0
7	D	4	0	0	0	0
7	E	5	0	0	0	0
7	F	2	0	0	0	0
7	G	5	0	0	0	0
7	H	3	0	0	0	0
7	I	1	0	0	0	0
7	J	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	K	2	0	0	0	0
7	L	1	0	0	0	0
7	N	4	0	0	0	0
All	All	54517	0	56392	1655	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 15.

The worst 5 of 1655 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:E:16:MET:HE2	1:E:514:MET:HE3	1.21	1.20
1:E:16:MET:CE	1:E:73:MET:HE1	1.70	1.19
2:D:193:MET:HE1	2:D:292:ILE:HG12	1.23	1.18
1:M:227:ILE:HD12	1:M:227:ILE:O	1.44	1.18
1:H:16:MET:CE	1:H:73:MET:HE1	1.74	1.17

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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
1	B	521/548 (95%)	513 (98%)	8 (2%)	0	100	100
1	E	522/548 (95%)	514 (98%)	8 (2%)	0	100	100
1	F	522/548 (95%)	513 (98%)	9 (2%)	0	100	100
1	H	522/548 (95%)	511 (98%)	11 (2%)	0	100	100
1	J	522/548 (95%)	510 (98%)	11 (2%)	1 (0%)	44	75
1	M	522/548 (95%)	513 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	523/548 (95%)	516 (99%)	7 (1%)	0	100	100
2	D	523/548 (95%)	514 (98%)	9 (2%)	0	100	100
2	G	523/548 (95%)	515 (98%)	8 (2%)	0	100	100
2	I	523/548 (95%)	514 (98%)	9 (2%)	0	100	100
2	K	523/548 (95%)	515 (98%)	8 (2%)	0	100	100
2	L	523/548 (95%)	514 (98%)	9 (2%)	0	100	100
2	N	522/548 (95%)	514 (98%)	8 (2%)	0	100	100
All	All	7313/7672 (95%)	7187 (98%)	125 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	44	PHE

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%)	401 (99%)	3 (1%)	81	92
1	B	403/414 (97%)	403 (100%)	0	100	100
1	E	404/414 (98%)	404 (100%)	0	100	100
1	F	404/414 (98%)	402 (100%)	2 (0%)	86	93
1	H	404/414 (98%)	403 (100%)	1 (0%)	92	97
1	J	404/414 (98%)	401 (99%)	3 (1%)	81	92
1	M	404/414 (98%)	401 (99%)	3 (1%)	81	92
2	C	405/415 (98%)	402 (99%)	3 (1%)	81	92
2	D	405/415 (98%)	401 (99%)	4 (1%)	73	87
2	G	405/415 (98%)	402 (99%)	3 (1%)	81	92
2	I	405/415 (98%)	403 (100%)	2 (0%)	86	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	405/415 (98%)	400 (99%)	5 (1%)	67	85
2	L	405/415 (98%)	402 (99%)	3 (1%)	81	92
2	N	404/415 (97%)	400 (99%)	4 (1%)	73	87
All	All	5661/5803 (98%)	5625 (99%)	36 (1%)	84	92

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	493	ILE
2	N	510	VAL
1	M	259	LEU
2	N	186	GLU
2	G	229	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
2	K	475	ASN
2	N	21	ASN
2	L	112	ASN
1	M	97	GLN
2	N	153	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

7 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	H	43	1	8,9,10	0.65	0	8,12,14	0.54	0
1	SEP	M	43	1	8,9,10	0.67	0	8,12,14	0.55	0
1	SEP	B	43	1	8,9,10	0.65	0	8,12,14	0.54	0
1	SEP	A	43	1	8,9,10	0.61	0	8,12,14	0.60	0
1	SEP	F	43	1	8,9,10	0.68	0	8,12,14	0.66	0
1	SEP	J	43	1	8,9,10	0.67	0	8,12,14	0.60	0
1	SEP	E	43	1	8,9,10	0.69	0	8,12,14	0.66	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	H	43	1	-	5/5/8/10	-
1	SEP	M	43	1	-	3/5/8/10	-
1	SEP	B	43	1	-	3/5/8/10	-
1	SEP	A	43	1	-	2/5/8/10	-
1	SEP	F	43	1	-	3/5/8/10	-
1	SEP	J	43	1	-	2/5/8/10	-
1	SEP	E	43	1	-	1/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	43	SEP	N-CA-CB-OG
1	H	43	SEP	N-CA-CB-OG
1	H	43	SEP	CA-CB-OG-P
1	J	43	SEP	CA-CB-OG-P
1	M	43	SEP	N-CA-CB-OG

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	H	43	SEP	1	0

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 68 ligands modelled in this entry, 7 are monoatomic - leaving 61 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	$\# Z > 2$
3	HEZ	B	601	-	7,7,7	0.12	0	6,6,6	0.14	0
3	HEZ	D	601	-	7,7,7	0.09	0	6,6,6	0.15	0
5	BME	C	604	-	3,3,3	0.20	0	1,2,2	0.01	0
3	HEZ	E	602	-	7,7,7	0.12	0	6,6,6	0.15	0
5	BME	D	605	-	3,3,3	0.27	0	1,2,2	0.40	0
3	HEZ	G	602	-	7,7,7	0.13	0	6,6,6	0.18	0
5	BME	B	605	-	3,3,3	0.14	0	1,2,2	0.15	0
6	TAM	J	601	-	7,10,10	0.57	0	9,12,12	0.48	0
5	BME	B	603	-	3,3,3	0.27	0	1,2,2	0.50	0
3	HEZ	C	601	-	7,7,7	0.13	0	6,6,6	0.11	0
5	BME	A	604	-	3,3,3	0.10	0	1,2,2	0.18	0
3	HEZ	B	602	-	7,7,7	0.16	0	6,6,6	0.16	0
3	HEZ	L	601	-	7,7,7	0.08	0	6,6,6	0.14	0
3	HEZ	A	602	-	7,7,7	0.11	0	6,6,6	0.15	0
5	BME	B	604	-	3,3,3	0.20	0	1,2,2	0.59	0
5	BME	I	605	-	3,3,3	0.15	0	1,2,2	0.07	0
3	HEZ	M	601	-	7,7,7	0.10	0	6,6,6	0.14	0
5	BME	M	602	-	3,3,3	0.18	0	1,2,2	0.03	0
5	BME	C	605	-	3,3,3	0.25	0	1,2,2	0.21	0
5	BME	E	606	-	3,3,3	0.31	0	1,2,2	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BME	E	605	-	3,3,3	0.23	0	1,2,2	0.33	0
5	BME	E	607	-	3,3,3	0.22	0	1,2,2	0.25	0
5	BME	L	602	-	3,3,3	0.19	0	1,2,2	0.20	0
3	HEZ	E	601	-	7,7,7	0.13	0	6,6,6	0.09	0
5	BME	A	605	-	3,3,3	0.30	0	1,2,2	0.97	0
5	BME	C	606	-	3,3,3	0.16	0	1,2,2	0.09	0
5	BME	N	603	-	3,3,3	0.12	0	1,2,2	0.01	0
5	BME	N	604	-	3,3,3	0.15	0	1,2,2	0.20	0
5	BME	A	607	-	3,3,3	0.17	0	1,2,2	0.04	0
6	TAM	I	601	-	7,10,10	0.60	0	9,12,12	0.68	0
5	BME	E	608	-	3,3,3	0.21	0	1,2,2	0.43	0
3	HEZ	J	602	-	7,7,7	0.10	0	6,6,6	0.12	0
5	BME	B	606	-	3,3,3	0.21	0	1,2,2	0.49	0
3	HEZ	F	602	-	7,7,7	0.10	0	6,6,6	0.12	0
3	HEZ	N	601	-	7,7,7	0.09	0	6,6,6	0.11	0
5	BME	F	604	-	3,3,3	0.16	0	1,2,2	0.31	0
5	BME	G	604	-	3,3,3	0.24	0	1,2,2	0.74	0
5	BME	G	606	-	3,3,3	0.26	0	1,2,2	0.55	0
5	BME	J	604	-	3,3,3	0.17	0	1,2,2	0.12	0
3	HEZ	I	603	-	7,7,7	0.07	0	6,6,6	0.13	0
3	HEZ	F	601	-	7,7,7	0.08	0	6,6,6	0.15	0
5	BME	D	604	-	3,3,3	0.33	0	1,2,2	0.30	0
6	TAM	G	601	-	7,10,10	0.47	0	9,12,12	0.74	0
5	BME	G	605	-	3,3,3	0.16	0	1,2,2	0.06	0
5	BME	H	604	-	3,3,3	0.24	0	1,2,2	0.66	0
5	BME	A	606	-	3,3,3	0.17	0	1,2,2	1.05	0
3	HEZ	I	602	-	7,7,7	0.15	0	6,6,6	0.22	0
3	HEZ	K	601	-	7,7,7	0.12	0	6,6,6	0.16	0
3	HEZ	A	601	-	7,7,7	0.13	0	6,6,6	0.15	0
5	BME	I	604	-	3,3,3	0.16	0	1,2,2	0.16	0
3	HEZ	H	602	-	7,7,7	0.07	0	6,6,6	0.12	0
5	BME	G	607	-	3,3,3	0.15	0	1,2,2	0.39	0
3	HEZ	H	601	-	7,7,7	0.07	0	6,6,6	0.15	0
5	BME	J	605	-	3,3,3	0.23	0	1,2,2	0.44	0
5	BME	J	603	-	3,3,3	0.15	0	1,2,2	0.32	0
5	BME	C	603	-	3,3,3	0.17	0	1,2,2	0.21	0
5	BME	K	602	-	3,3,3	0.14	0	1,2,2	0.05	0
3	HEZ	D	602	-	7,7,7	0.10	0	6,6,6	0.13	0
3	HEZ	C	602	-	7,7,7	0.11	0	6,6,6	0.11	0
5	BME	H	605	-	3,3,3	0.15	0	1,2,2	0.30	0
3	HEZ	E	603	-	7,7,7	0.12	0	6,6,6	0.11	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
3	HEZ	B	601	-	-	3/5/5/5	-
3	HEZ	D	601	-	-	3/5/5/5	-
5	BME	C	604	-	-	1/1/1/1	-
3	HEZ	E	602	-	-	2/5/5/5	-
5	BME	D	605	-	-	1/1/1/1	-
3	HEZ	G	602	-	-	3/5/5/5	-
5	BME	B	605	-	-	1/1/1/1	-
6	TAM	J	601	-	-	4/12/12/12	-
5	BME	B	603	-	-	0/1/1/1	-
3	HEZ	C	601	-	-	4/5/5/5	-
5	BME	A	604	-	-	0/1/1/1	-
3	HEZ	B	602	-	-	3/5/5/5	-
3	HEZ	L	601	-	-	3/5/5/5	-
3	HEZ	A	602	-	-	1/5/5/5	-
5	BME	B	604	-	-	0/1/1/1	-
5	BME	I	605	-	-	0/1/1/1	-
3	HEZ	M	601	-	-	4/5/5/5	-
5	BME	M	602	-	-	1/1/1/1	-
5	BME	C	605	-	-	1/1/1/1	-
5	BME	E	606	-	-	1/1/1/1	-
5	BME	E	605	-	-	1/1/1/1	-
5	BME	E	607	-	-	1/1/1/1	-
5	BME	L	602	-	-	1/1/1/1	-
3	HEZ	E	601	-	-	4/5/5/5	-
5	BME	A	605	-	-	1/1/1/1	-
5	BME	C	606	-	-	1/1/1/1	-
5	BME	N	603	-	-	0/1/1/1	-
5	BME	N	604	-	-	1/1/1/1	-
5	BME	A	607	-	-	1/1/1/1	-
6	TAM	I	601	-	-	4/12/12/12	-
5	BME	E	608	-	-	1/1/1/1	-
3	HEZ	J	602	-	-	3/5/5/5	-
5	BME	B	606	-	-	1/1/1/1	-
3	HEZ	F	602	-	-	2/5/5/5	-
3	HEZ	N	601	-	-	3/5/5/5	-
5	BME	F	604	-	-	1/1/1/1	-
5	BME	G	604	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BME	G	606	-	-	1/1/1/1	-
5	BME	J	604	-	-	1/1/1/1	-
3	HEZ	I	603	-	-	2/5/5/5	-
3	HEZ	F	601	-	-	3/5/5/5	-
5	BME	D	604	-	-	1/1/1/1	-
6	TAM	G	601	-	-	3/12/12/12	-
5	BME	G	605	-	-	0/1/1/1	-
5	BME	H	604	-	-	0/1/1/1	-
5	BME	A	606	-	-	0/1/1/1	-
3	HEZ	I	602	-	-	2/5/5/5	-
3	HEZ	K	601	-	-	4/5/5/5	-
3	HEZ	A	601	-	-	3/5/5/5	-
5	BME	I	604	-	-	1/1/1/1	-
3	HEZ	H	602	-	-	2/5/5/5	-
5	BME	G	607	-	-	0/1/1/1	-
3	HEZ	H	601	-	-	3/5/5/5	-
5	BME	J	605	-	-	0/1/1/1	-
5	BME	J	603	-	-	0/1/1/1	-
5	BME	C	603	-	-	1/1/1/1	-
5	BME	K	602	-	-	0/1/1/1	-
3	HEZ	D	602	-	-	1/5/5/5	-
3	HEZ	C	602	-	-	3/5/5/5	-
5	BME	H	605	-	-	0/1/1/1	-
3	HEZ	E	603	-	-	3/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 96 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	605	BME	O1-C1-C2-S2
5	A	607	BME	O1-C1-C2-S2
5	B	605	BME	O1-C1-C2-S2
5	B	606	BME	O1-C1-C2-S2
5	C	603	BME	O1-C1-C2-S2

There are no ring outliers.

10 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	602	HEZ	1	0
6	J	601	TAM	1	0
3	C	601	HEZ	1	0
3	M	601	HEZ	1	0
5	E	606	BME	1	0
5	E	605	BME	1	0
5	E	608	BME	1	0
5	H	604	BME	1	0
5	A	606	BME	2	0
5	C	603	BME	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.52	0 100 100	34, 57, 90, 138	0
1	B	523/548 (95%)	-0.48	0 100 100	32, 54, 94, 131	0
1	E	524/548 (95%)	-0.48	3 (0%) 85 76	32, 57, 97, 145	0
1	F	524/548 (95%)	-0.38	1 (0%) 92 87	34, 68, 115, 136	0
1	H	524/548 (95%)	-0.42	0 100 100	33, 64, 100, 160	0
1	J	524/548 (95%)	-0.40	0 100 100	30, 64, 110, 158	0
1	M	524/548 (95%)	0.17	37 (7%) 23 16	35, 78, 162, 219	0
2	C	525/548 (95%)	-0.33	2 (0%) 89 81	31, 63, 120, 155	0
2	D	525/548 (95%)	-0.16	9 (1%) 69 53	33, 67, 142, 187	0
2	G	525/548 (95%)	-0.49	1 (0%) 92 87	31, 58, 102, 141	0
2	I	525/548 (95%)	-0.44	0 100 100	32, 66, 106, 127	0
2	K	525/548 (95%)	-0.07	15 (2%) 54 38	34, 78, 182, 293	0
2	L	525/548 (95%)	-0.25	1 (0%) 92 87	35, 80, 143, 175	0
2	N	524/548 (95%)	-0.42	1 (0%) 92 87	34, 64, 108, 129	0
All	All	7341/7672 (95%)	-0.33	70 (0%) 79 66	30, 64, 131, 293	0

The worst 5 of 70 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	299	THR	5.5
1	M	223	ALA	5.3
1	M	250	ILE	4.7
1	M	292	ILE	4.4
2	D	237	LEU	4.4

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	SEP	H	43	10/11	0.58	0.13	117,132,157,162	0
1	SEP	F	43	10/11	0.59	0.16	95,125,141,151	0
1	SEP	M	43	10/11	0.61	0.14	102,129,154,159	0
1	SEP	E	43	10/11	0.71	0.19	121,127,141,144	0
1	SEP	J	43	10/11	0.71	0.15	121,136,148,152	0
1	SEP	B	43	10/11	0.71	0.13	97,117,144,153	0
1	SEP	A	43	10/11	0.77	0.11	106,126,137,141	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BME	H	605	4/4	0.70	0.14	100,110,112,114	0
6	TAM	J	601	11/11	0.71	0.19	105,126,144,153	0
5	BME	N	603	4/4	0.73	0.17	105,106,107,118	0
5	BME	B	605	4/4	0.73	0.14	94,99,102,105	0
5	BME	A	607	4/4	0.76	0.20	99,106,107,111	0
3	HEZ	C	602	8/8	0.80	0.19	90,114,122,122	0
5	BME	J	605	4/4	0.82	0.25	94,101,101,104	0
6	TAM	G	601	11/11	0.83	0.17	77,131,140,142	0
5	BME	I	605	4/4	0.83	0.17	94,99,104,105	0
5	BME	G	606	4/4	0.84	0.13	59,73,82,99	0
5	BME	G	607	4/4	0.84	0.22	112,112,112,119	0
3	HEZ	B	602	8/8	0.85	0.25	73,99,101,101	0
5	BME	I	604	4/4	0.86	0.14	104,108,111,112	0
3	HEZ	H	602	8/8	0.87	0.21	91,113,128,129	0
5	BME	E	606	4/4	0.87	0.14	58,71,73,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	BME	E	608	4/4	0.87	0.19	75,86,86,93	0
5	BME	B	606	4/4	0.88	0.20	73,89,98,99	0
3	HEZ	I	603	8/8	0.88	0.18	72,77,108,116	0
3	HEZ	D	602	8/8	0.89	0.15	72,82,88,90	0
4	MG	G	603	1/1	0.89	0.09	74,74,74,74	0
3	HEZ	F	601	8/8	0.90	0.15	59,66,75,76	0
4	MG	D	603	1/1	0.91	0.10	89,89,89,89	0
4	MG	E	604	1/1	0.91	0.10	81,81,81,81	0
5	BME	C	606	4/4	0.91	0.13	89,97,101,108	0
5	BME	D	604	4/4	0.91	0.15	54,58,61,69	0
5	BME	D	605	4/4	0.91	0.17	70,91,95,106	0
4	MG	F	603	1/1	0.91	0.07	61,61,61,61	0
3	HEZ	E	603	8/8	0.91	0.15	74,82,85,87	0
4	MG	A	603	1/1	0.91	0.07	76,76,76,76	0
5	BME	A	606	4/4	0.92	0.20	57,58,58,61	0
3	HEZ	A	601	8/8	0.92	0.13	58,64,73,74	0
5	BME	E	605	4/4	0.92	0.11	61,80,84,85	0
5	BME	J	604	4/4	0.92	0.16	73,93,106,130	0
3	HEZ	A	602	8/8	0.92	0.16	74,77,93,96	0
3	HEZ	I	602	8/8	0.92	0.14	44,53,88,91	0
5	BME	C	605	4/4	0.92	0.13	74,82,93,97	0
6	TAM	I	601	11/11	0.92	0.18	70,85,114,121	0
4	MG	H	603	1/1	0.92	0.07	82,82,82,82	0
3	HEZ	F	602	8/8	0.93	0.14	60,67,85,90	0
5	BME	E	607	4/4	0.93	0.15	42,46,55,80	0
3	HEZ	E	601	8/8	0.93	0.14	46,63,85,90	0
5	BME	G	604	4/4	0.93	0.10	48,56,58,69	0
3	HEZ	J	602	8/8	0.93	0.12	55,64,69,70	0
5	BME	A	604	4/4	0.94	0.14	66,75,81,89	0
5	BME	H	604	4/4	0.94	0.15	53,54,55,59	0
3	HEZ	G	602	8/8	0.94	0.12	50,55,61,63	0
3	HEZ	H	601	8/8	0.94	0.13	64,69,76,79	0
5	BME	B	603	4/4	0.94	0.15	54,65,71,73	0
5	BME	J	603	4/4	0.94	0.13	73,73,76,78	0
3	HEZ	L	601	8/8	0.95	0.11	50,59,79,85	0
3	HEZ	M	601	8/8	0.95	0.11	47,54,75,77	0
5	BME	C	604	4/4	0.95	0.21	47,54,61,71	0
3	HEZ	C	601	8/8	0.95	0.09	45,49,56,63	0
5	BME	G	605	4/4	0.95	0.11	39,47,55,79	0
5	BME	K	602	4/4	0.95	0.15	61,62,63,66	0
5	BME	L	602	4/4	0.95	0.15	55,62,67,78	0
5	BME	M	602	4/4	0.95	0.19	59,61,61,73	0

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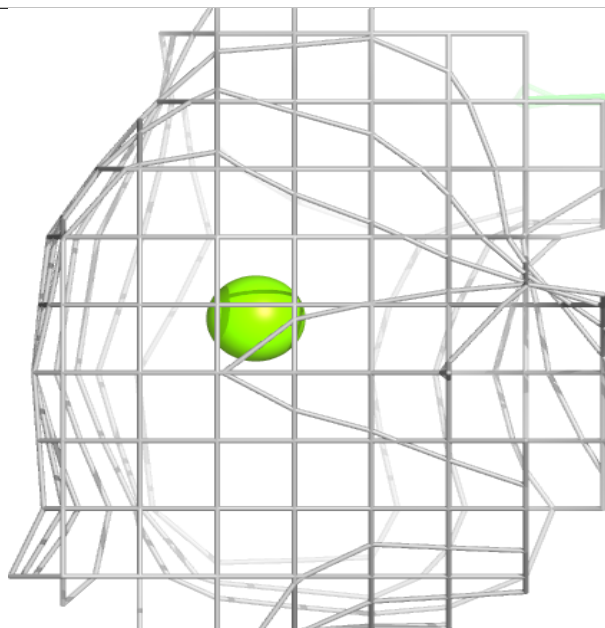
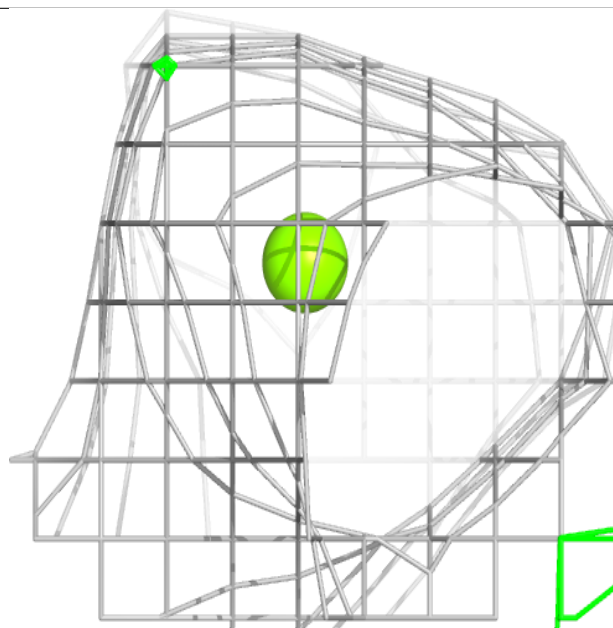
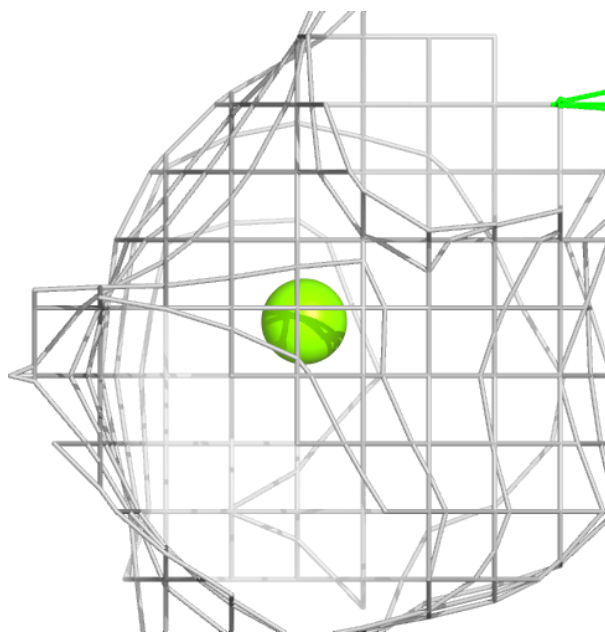
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	BME	A	605	4/4	0.95	0.13	44,50,51,57	0
3	HEZ	B	601	8/8	0.95	0.09	45,47,58,68	0
3	HEZ	E	602	8/8	0.95	0.12	44,50,56,64	0
3	HEZ	D	601	8/8	0.95	0.10	51,60,81,82	0
3	HEZ	N	601	8/8	0.96	0.09	45,48,65,66	0
3	HEZ	K	601	8/8	0.96	0.10	44,45,57,60	0
5	BME	N	604	4/4	0.96	0.12	57,61,62,65	0
5	BME	F	604	4/4	0.97	0.09	50,52,53,63	0
5	BME	B	604	4/4	0.97	0.13	58,62,63,64	0
5	BME	C	603	4/4	0.98	0.07	66,76,77,80	0
4	MG	N	602	1/1	0.98	0.05	80,80,80,80	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.

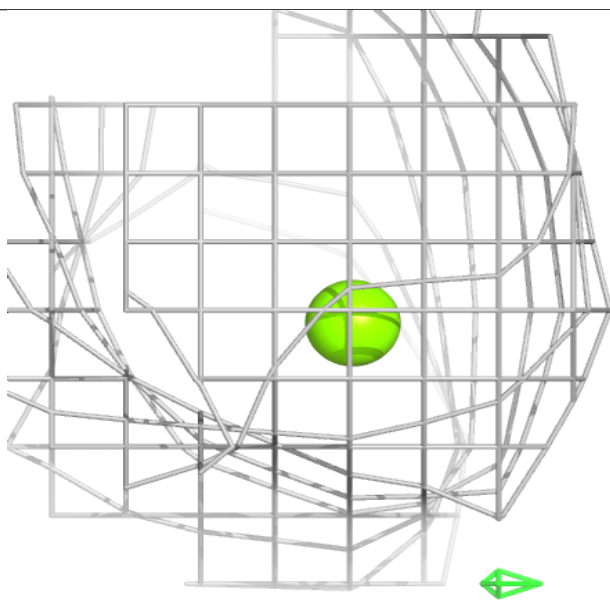
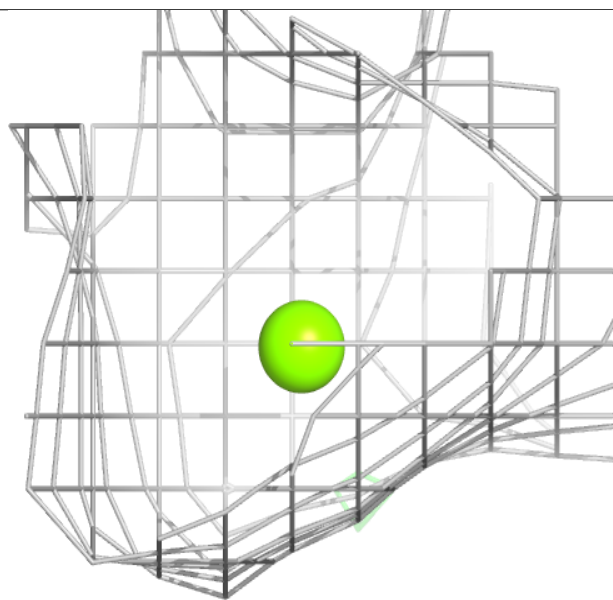
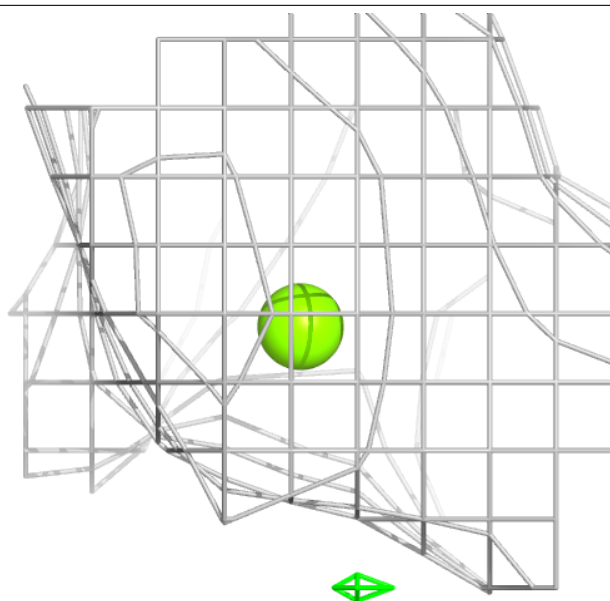
Electron density around MG G 603:

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and green (positive)



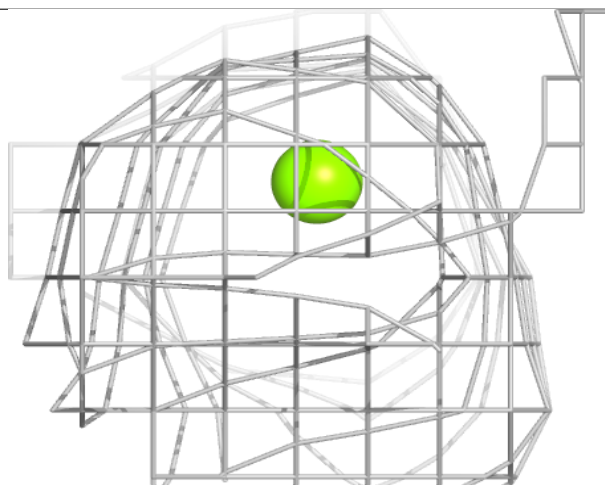
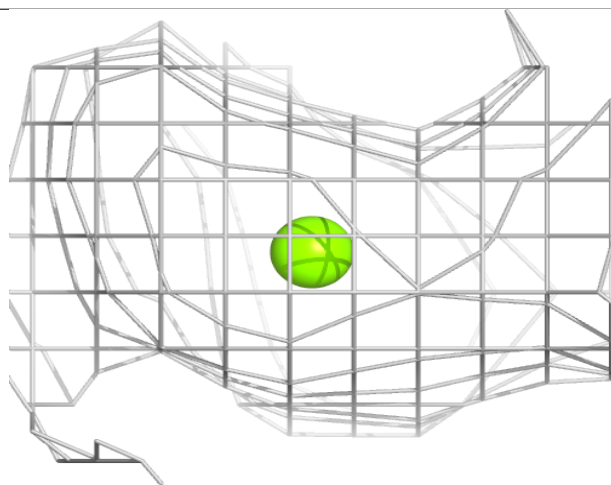
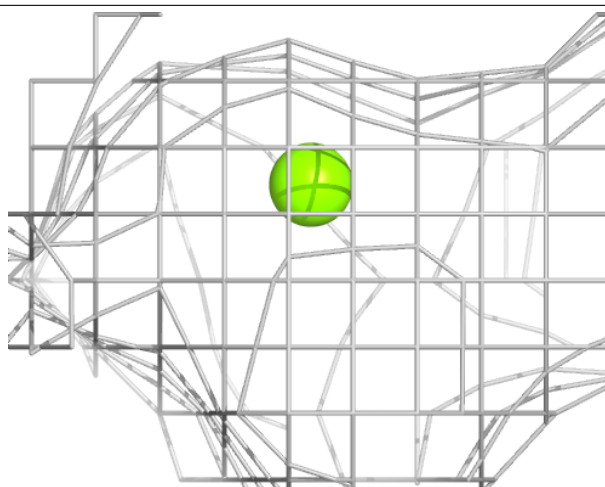
Electron density around MG D 603:

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



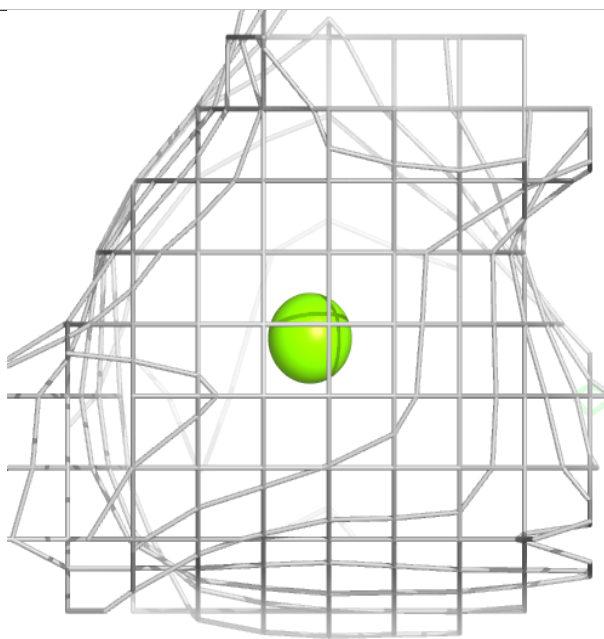
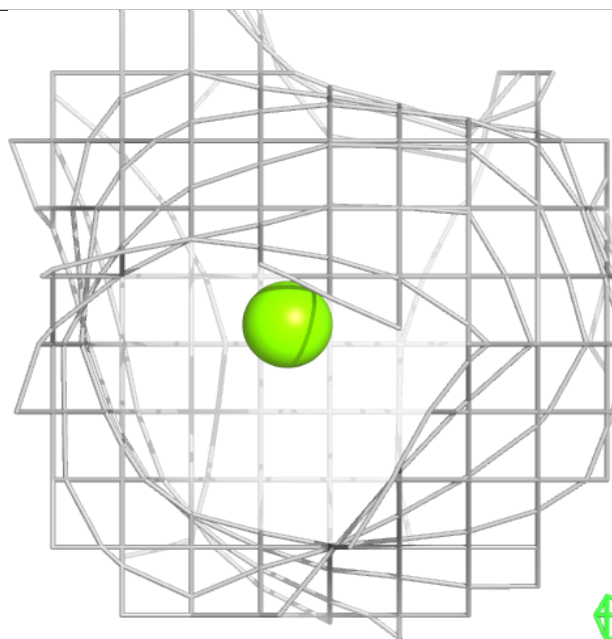
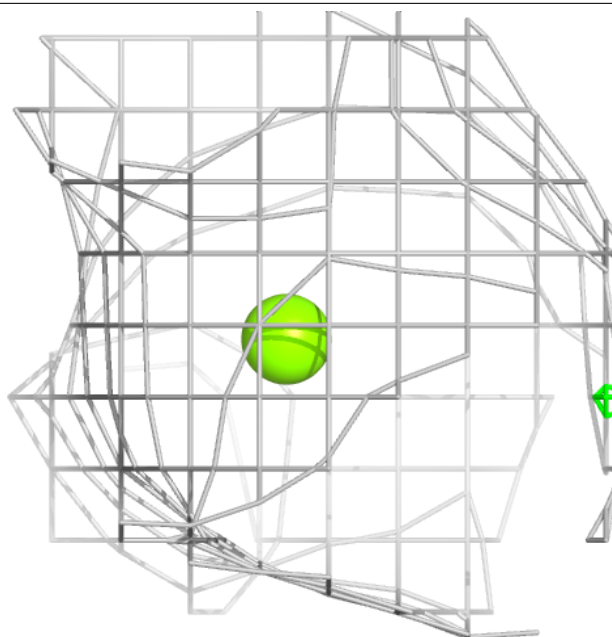
Electron density around MG E 604:

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



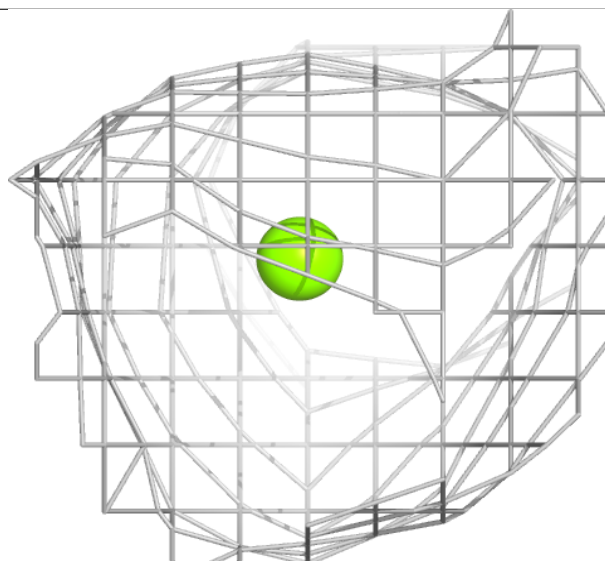
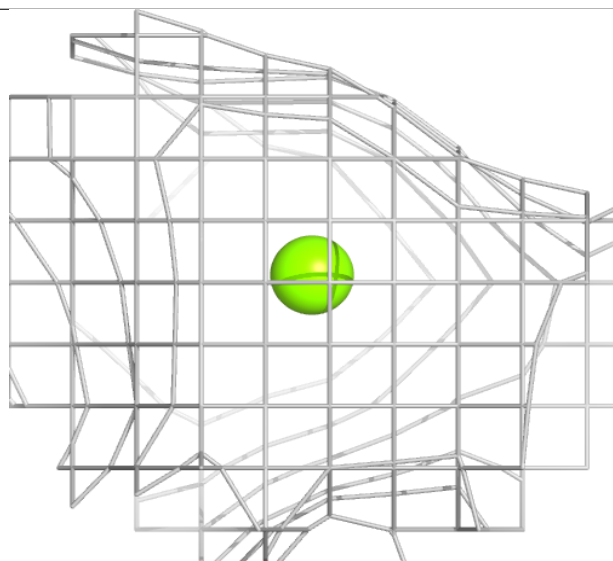
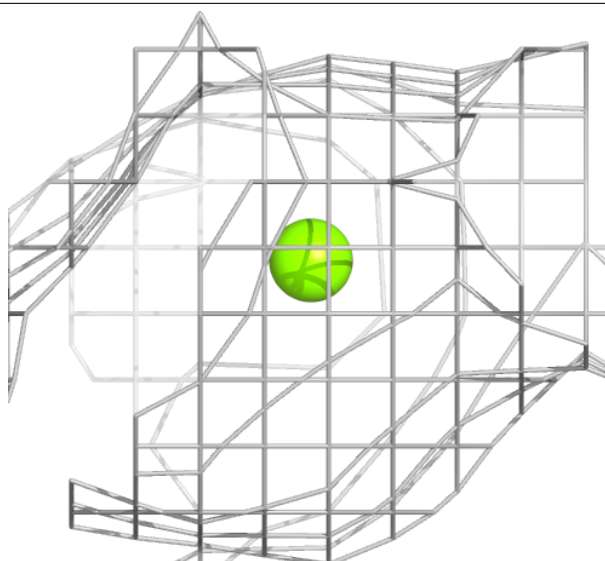
Electron density around MG F 603:

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



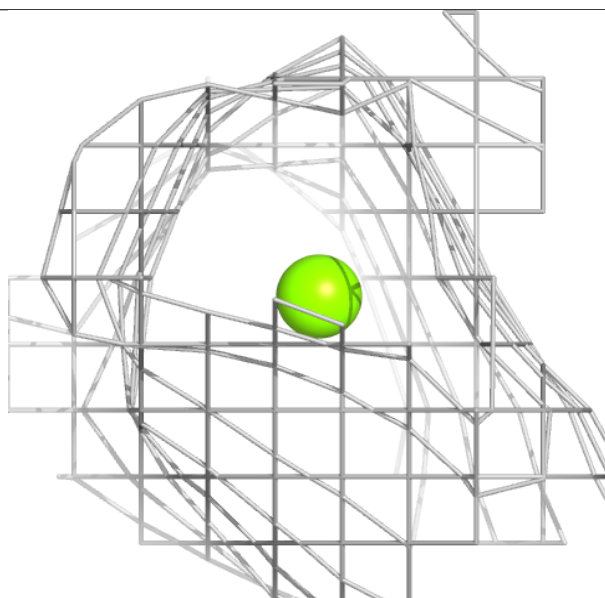
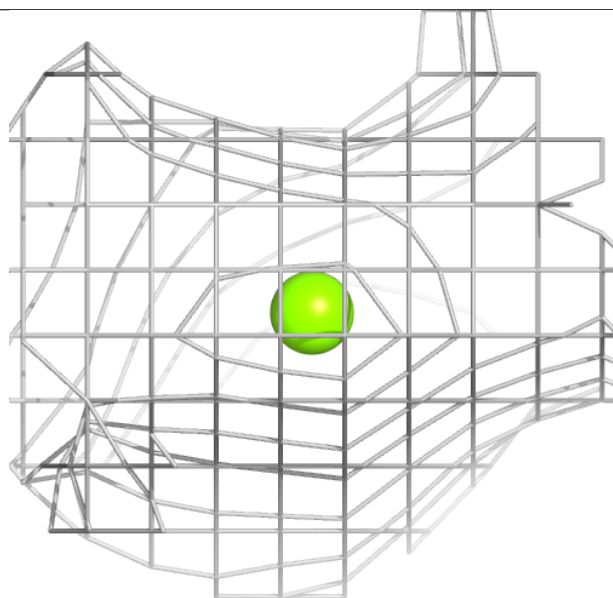
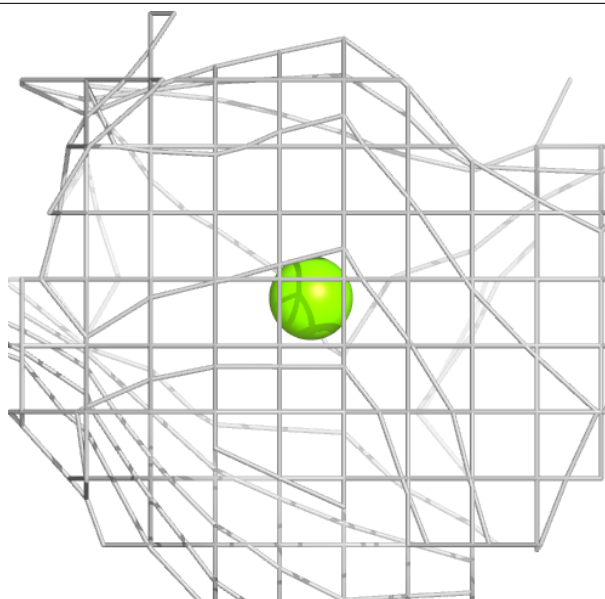
Electron density around MG A 603:

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



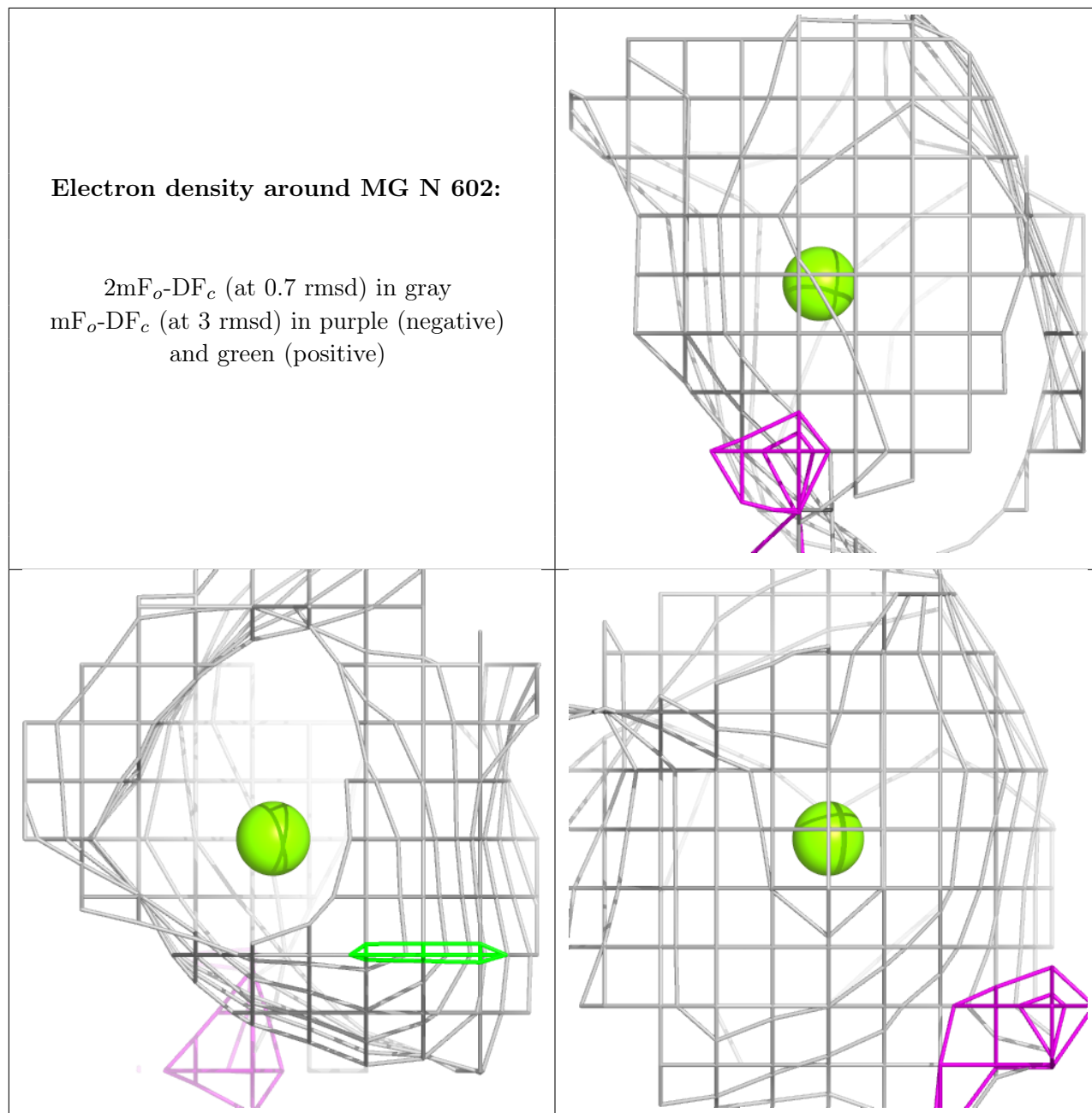
Electron density around MG H 603:

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



Electron density around MG N 602:

$2mF_o-DF_c$ (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.