



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:14 AM UTC

PDB ID : 8IU7 / pdb_00008iu7
Title : Structure of Staphylococcus aureus NrnA (Pde2) in complex with Mg2+
Authors : Cheng, K.; Wang, Y.
Deposited on : 2023-03-23
Resolution : 1.86 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

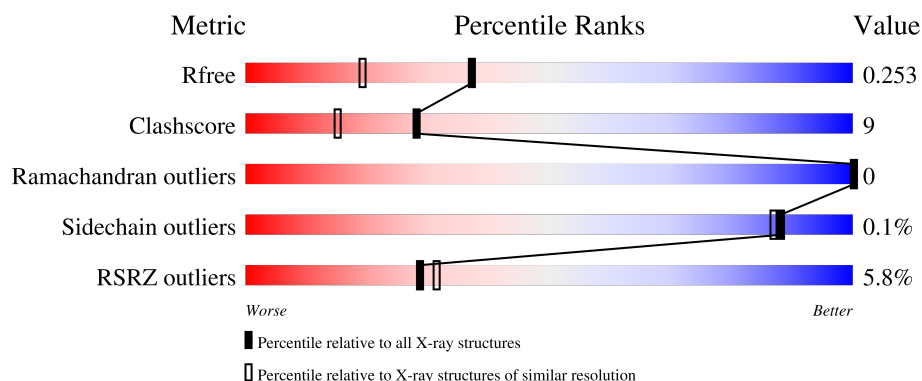
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	333	7% 83% 13% .
1	B	333	2% 84% 13% .
1	C	333	5% 78% 18% .
1	D	333	8% 84% 12% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10313 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 Bifunctional oligoribonuclease and PAP phosphatase NrnA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	0	0
			2531	1596	427	497	11			
1	C	320	Total	C	N	O	S	0	0	0
			2531	1596	427	497	11			
1	D	320	Total	C	N	O	S	0	0	0
			2530	1595	428	496	11			
1	B	323	Total	C	N	O	S	0	0	0
			2551	1606	431	503	11			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A266CBU5
A	-18	GLY	-	expression tag	UNP A0A266CBU5
A	-17	SER	-	expression tag	UNP A0A266CBU5
A	-16	SER	-	expression tag	UNP A0A266CBU5
A	-15	HIS	-	expression tag	UNP A0A266CBU5
A	-14	HIS	-	expression tag	UNP A0A266CBU5
A	-13	HIS	-	expression tag	UNP A0A266CBU5
A	-12	HIS	-	expression tag	UNP A0A266CBU5
A	-11	HIS	-	expression tag	UNP A0A266CBU5
A	-10	HIS	-	expression tag	UNP A0A266CBU5
A	-9	SER	-	expression tag	UNP A0A266CBU5
A	-8	SER	-	expression tag	UNP A0A266CBU5
A	-7	GLU	-	expression tag	UNP A0A266CBU5
A	-6	ASN	-	expression tag	UNP A0A266CBU5
A	-5	LEU	-	expression tag	UNP A0A266CBU5
A	-4	TYR	-	expression tag	UNP A0A266CBU5
A	-3	PHE	-	expression tag	UNP A0A266CBU5
A	-2	GLN	-	expression tag	UNP A0A266CBU5
A	-1	GLY	-	expression tag	UNP A0A266CBU5
A	0	HIS	-	expression tag	UNP A0A266CBU5
C	-19	MET	-	initiating methionine	UNP A0A266CBU5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	GLY	-	expression tag	UNP A0A266CBU5
C	-17	SER	-	expression tag	UNP A0A266CBU5
C	-16	SER	-	expression tag	UNP A0A266CBU5
C	-15	HIS	-	expression tag	UNP A0A266CBU5
C	-14	HIS	-	expression tag	UNP A0A266CBU5
C	-13	HIS	-	expression tag	UNP A0A266CBU5
C	-12	HIS	-	expression tag	UNP A0A266CBU5
C	-11	HIS	-	expression tag	UNP A0A266CBU5
C	-10	HIS	-	expression tag	UNP A0A266CBU5
C	-9	SER	-	expression tag	UNP A0A266CBU5
C	-8	SER	-	expression tag	UNP A0A266CBU5
C	-7	GLU	-	expression tag	UNP A0A266CBU5
C	-6	ASN	-	expression tag	UNP A0A266CBU5
C	-5	LEU	-	expression tag	UNP A0A266CBU5
C	-4	TYR	-	expression tag	UNP A0A266CBU5
C	-3	PHE	-	expression tag	UNP A0A266CBU5
C	-2	GLN	-	expression tag	UNP A0A266CBU5
C	-1	GLY	-	expression tag	UNP A0A266CBU5
C	0	HIS	-	expression tag	UNP A0A266CBU5
D	-19	MET	-	initiating methionine	UNP A0A266CBU5
D	-18	GLY	-	expression tag	UNP A0A266CBU5
D	-17	SER	-	expression tag	UNP A0A266CBU5
D	-16	SER	-	expression tag	UNP A0A266CBU5
D	-15	HIS	-	expression tag	UNP A0A266CBU5
D	-14	HIS	-	expression tag	UNP A0A266CBU5
D	-13	HIS	-	expression tag	UNP A0A266CBU5
D	-12	HIS	-	expression tag	UNP A0A266CBU5
D	-11	HIS	-	expression tag	UNP A0A266CBU5
D	-10	HIS	-	expression tag	UNP A0A266CBU5
D	-9	SER	-	expression tag	UNP A0A266CBU5
D	-8	SER	-	expression tag	UNP A0A266CBU5
D	-7	GLU	-	expression tag	UNP A0A266CBU5
D	-6	ASN	-	expression tag	UNP A0A266CBU5
D	-5	LEU	-	expression tag	UNP A0A266CBU5
D	-4	TYR	-	expression tag	UNP A0A266CBU5
D	-3	PHE	-	expression tag	UNP A0A266CBU5
D	-2	GLN	-	expression tag	UNP A0A266CBU5
D	-1	GLY	-	expression tag	UNP A0A266CBU5
D	0	HIS	-	expression tag	UNP A0A266CBU5
B	-19	MET	-	initiating methionine	UNP A0A266CBU5
B	-18	GLY	-	expression tag	UNP A0A266CBU5
B	-17	SER	-	expression tag	UNP A0A266CBU5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP A0A266CBU5
B	-15	HIS	-	expression tag	UNP A0A266CBU5
B	-14	HIS	-	expression tag	UNP A0A266CBU5
B	-13	HIS	-	expression tag	UNP A0A266CBU5
B	-12	HIS	-	expression tag	UNP A0A266CBU5
B	-11	HIS	-	expression tag	UNP A0A266CBU5
B	-10	HIS	-	expression tag	UNP A0A266CBU5
B	-9	SER	-	expression tag	UNP A0A266CBU5
B	-8	SER	-	expression tag	UNP A0A266CBU5
B	-7	GLU	-	expression tag	UNP A0A266CBU5
B	-6	ASN	-	expression tag	UNP A0A266CBU5
B	-5	LEU	-	expression tag	UNP A0A266CBU5
B	-4	TYR	-	expression tag	UNP A0A266CBU5
B	-3	PHE	-	expression tag	UNP A0A266CBU5
B	-2	GLN	-	expression tag	UNP A0A266CBU5
B	-1	GLY	-	expression tag	UNP A0A266CBU5
B	0	HIS	-	expression tag	UNP A0A266CBU5

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	0	0
2	C	2	Total Mg 2 2	0	0
2	D	2	Total Mg 2 2	0	0
2	B	2	Total Mg 2 2	0	0

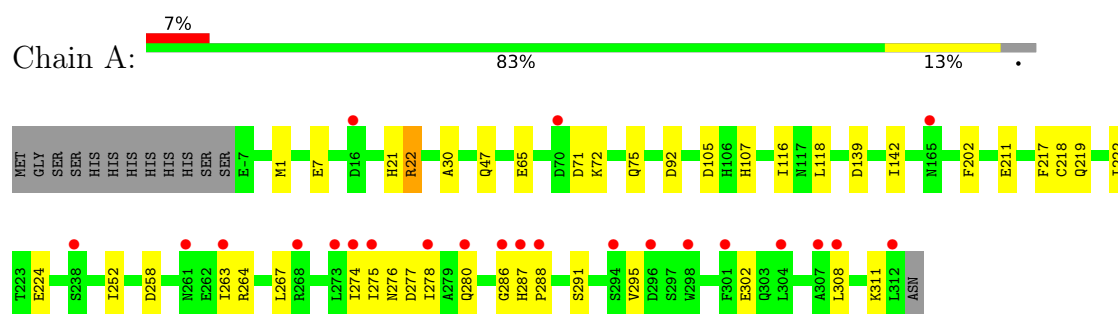
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	55	Total O 55 55	0	0
3	C	26	Total O 26 26	0	0
3	D	26	Total O 26 26	0	0
3	B	55	Total O 55 55	0	0

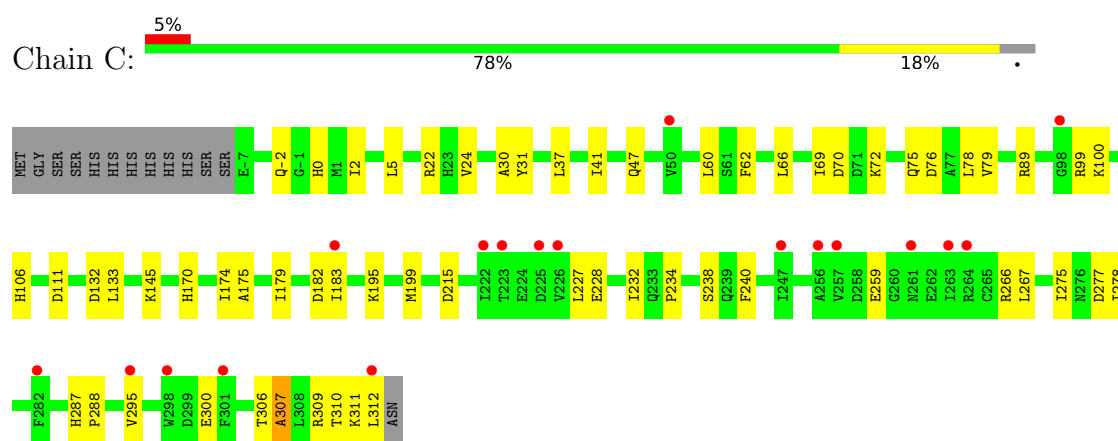
3 Residue-property plots [i](#)

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

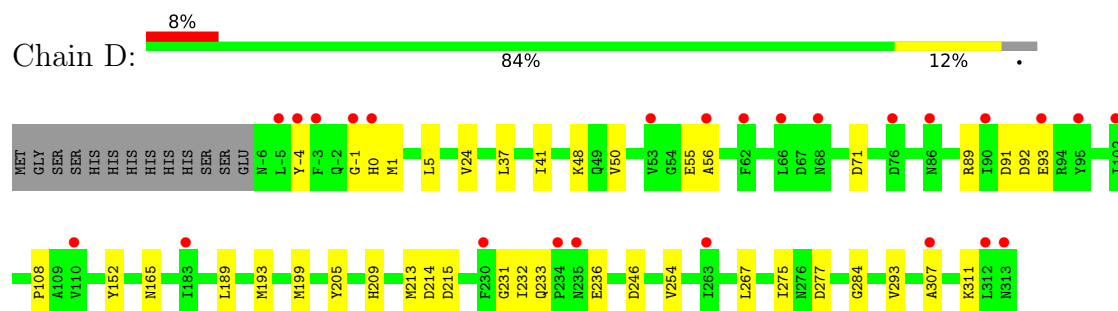
- Molecule 1: Bifunctional oligoribonuclease and PAP phosphatase NrnA



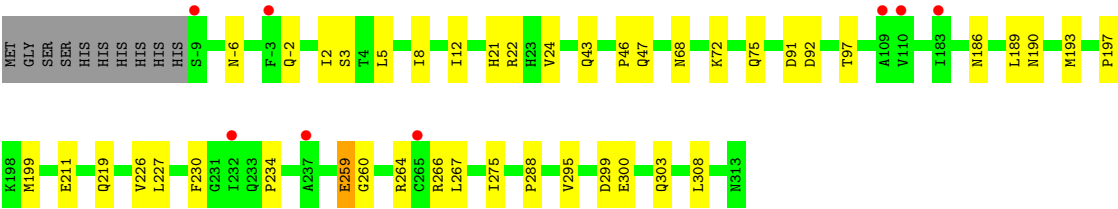
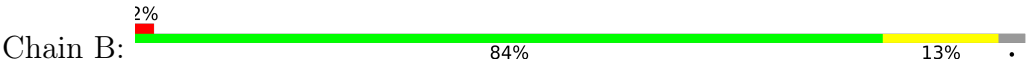
- Molecule 1: Bifunctional oligoribonuclease and PAP phosphatase NrnA



- Molecule 1: Bifunctional oligoribonuclease and PAP phosphatase NrnA



- Molecule 1: Bifunctional oligoribonuclease and PAP phosphatase NrnA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.91Å 119.67Å 119.57Å 90.00° 91.37° 90.00°	Depositor
Resolution (Å)	38.32 – 1.86 38.32 – 1.86	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.32-1.86) 99.8 (38.32-1.86)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 1.85Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.227 , 0.254 0.227 , 0.253	Depositor DCC
R_{free} test set	5965 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	46.4	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 31.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.002 for -h,-l,-k 0.000 for -h,l,k 0.028 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10313	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.54	0/2579	0.75	0/3490
1	B	0.66	1/2599 (0.0%)	0.73	2/3517 (0.1%)
1	C	0.53	1/2579 (0.0%)	0.69	1/3490 (0.0%)
1	D	0.55	2/2578 (0.1%)	0.71	0/3489
All	All	0.57	4/10335 (0.0%)	0.72	3/13986 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	197	PRO	N-CD	-20.76	1.18	1.47
1	D	307	ALA	C-O	6.07	1.31	1.24
1	C	307	ALA	C-O	5.99	1.31	1.24
1	D	108	PRO	N-CD	-5.66	1.39	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	259	GLU	N-CA-C	-6.05	101.53	110.48
1	B	197	PRO	N-CD-CG	5.49	111.43	103.20
1	C	183	ILE	N-CA-C	-5.13	102.23	109.21

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	22	ARG	Sidechain
1	A	264	ARG	Sidechain
1	B	266	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	2531	0	2458	42	0
1	B	2551	0	2474	38	0
1	C	2531	0	2458	53	0
1	D	2530	0	2458	44	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	55	0	0	3	0
3	B	55	0	0	14	0
3	C	26	0	0	15	0
3	D	26	0	0	13	0
All	All	10313	0	9848	177	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 9.

All (177) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:LEU:CD1	1:A:308:LEU:HD11	1.78	1.13
1:A:278:ILE:HD11	1:A:311:LYS:HE3	1.26	1.10
1:B:260:GLY:N	3:B:502:HOH:O	1.84	1.09
1:C:228:GLU:N	3:C:501:HOH:O	1.84	1.08
1:D:199:MET:HE2	1:D:199:MET:HA	1.37	1.03
1:A:276:ASN:OD1	1:A:291:SER:OG	1.78	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:LEU:HD11	1:A:308:LEU:HD11	1.44	1.00
1:C:227:LEU:C	3:C:503:HOH:O	2.03	0.99
1:D:1:MET:N	3:D:501:HOH:O	1.92	0.97
1:B:47:GLN:OE1	1:B:47:GLN:N	1.95	0.97
1:C:227:LEU:HB3	3:C:503:HOH:O	1.64	0.95
1:D:165:ASN:HB2	3:D:503:HOH:O	1.67	0.94
1:B:227:LEU:O	3:B:501:HOH:O	1.84	0.94
1:D:199:MET:HE1	1:D:232:ILE:CD1	1.99	0.93
1:A:302:GLU:O	3:A:501:HOH:O	1.88	0.92
1:B:299:ASP:O	3:B:503:HOH:O	1.87	0.92
1:D:199:MET:HE1	1:D:232:ILE:CG1	2.03	0.89
1:C:227:LEU:C	3:C:501:HOH:O	2.13	0.88
1:D:199:MET:HE1	1:D:232:ILE:HG13	1.53	0.87
1:B:227:LEU:C	3:B:501:HOH:O	2.17	0.86
1:A:267:LEU:HD12	1:A:308:LEU:HD11	1.56	0.85
1:A:278:ILE:CD1	1:A:311:LYS:HE3	2.06	0.84
1:C:295:VAL:HG13	1:C:300:GLU:HB3	1.59	0.84
1:D:-1:GLY:N	3:D:501:HOH:O	2.11	0.80
1:D:152:TYR:OH	3:D:502:HOH:O	1.98	0.79
1:A:267:LEU:CD1	1:A:308:LEU:CD1	2.61	0.79
1:D:231:GLY:O	1:D:232:ILE:HD13	1.83	0.78
1:B:43:GLN:OE1	3:B:505:HOH:O	2.02	0.78
1:D:199:MET:HE1	1:D:232:ILE:HD11	1.65	0.77
1:C:215:ASP:O	1:C:312:LEU:HD22	1.83	0.77
1:B:186:ASN:HD21	1:B:190:ASN:HD21	1.32	0.77
1:B:3:SER:OG	3:B:504:HOH:O	2.01	0.77
1:D:48:LYS:NZ	3:D:504:HOH:O	2.04	0.76
1:C:227:LEU:O	3:C:503:HOH:O	1.98	0.76
1:B:199:MET:HA	1:B:199:MET:HE2	1.66	0.75
1:D:199:MET:CE	1:D:232:ILE:HD11	2.16	0.75
1:D:214:ASP:OD1	3:D:506:HOH:O	2.07	0.73
1:A:278:ILE:HD11	1:A:311:LYS:CE	2.14	0.73
1:D:55:GLU:O	3:D:505:HOH:O	2.06	0.72
1:D:199:MET:HA	1:D:199:MET:CE	2.17	0.72
1:A:275:ILE:HD12	1:A:275:ILE:C	2.15	0.71
1:A:211:GLU:OE1	1:A:219:GLN:NE2	2.22	0.71
1:A:274:ILE:HG22	1:A:277:ASP:OD1	1.91	0.71
1:C:227:LEU:CA	3:C:503:HOH:O	2.36	0.70
1:D:267:LEU:HB3	1:D:275:ILE:HD13	1.73	0.70
1:B:259:GLU:CA	3:B:502:HOH:O	2.40	0.69
1:C:106:HIS:O	3:C:505:HOH:O	2.09	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:MET:CE	1:D:232:ILE:CD1	2.71	0.68
1:C:47:GLN:H	1:C:47:GLN:CD	2.01	0.68
1:A:277:ASP:HA	1:A:280:GLN:NE2	2.09	0.67
1:D:165:ASN:CB	3:D:503:HOH:O	2.31	0.67
1:B:47:GLN:H	1:B:47:GLN:CD	2.02	0.66
1:D:-1:GLY:C	3:D:501:HOH:O	2.39	0.65
1:D:189:LEU:O	1:D:193:MET:HG3	1.97	0.65
1:A:65:GLU:O	3:A:502:HOH:O	2.15	0.65
1:A:72:LYS:NZ	1:A:75:GLN:HG3	2.12	0.64
1:D:56:ALA:C	3:D:505:HOH:O	2.42	0.63
1:C:37:LEU:O	1:C:41:ILE:HG13	1.98	0.63
1:B:234:PRO:HB3	1:B:259:GLU:HG2	1.81	0.62
1:C:5:LEU:HD22	1:C:133:LEU:HD12	1.81	0.62
1:D:165:ASN:ND2	3:D:503:HOH:O	2.01	0.61
1:A:22:ARG:HG3	1:A:30:ALA:HB1	1.82	0.61
1:B:264:ARG:HH11	1:B:264:ARG:HG3	1.65	0.61
1:B:186:ASN:ND2	1:B:190:ASN:ND2	2.48	0.61
1:B:186:ASN:HD21	1:B:190:ASN:ND2	1.98	0.61
1:A:275:ILE:HD12	1:A:276:ASN:N	2.15	0.61
1:C:309:ARG:HA	1:C:312:LEU:HD12	1.82	0.60
1:D:232:ILE:HG23	1:D:236:GLU:HB2	1.83	0.60
1:C:145:LYS:HE2	1:C:182:ASP:O	2.01	0.60
1:C:199:MET:HA	1:C:199:MET:HE2	1.81	0.60
1:A:267:LEU:HD12	1:A:308:LEU:CD1	2.28	0.60
1:B:295:VAL:HG12	1:B:300:GLU:OE2	2.01	0.60
1:C:170:HIS:CE1	1:C:174:ILE:HD11	2.37	0.60
1:A:1:MET:SD	1:A:118:LEU:HD11	2.42	0.59
1:B:230:PHE:N	3:B:501:HOH:O	2.28	0.59
1:D:254:VAL:HG23	1:D:267:LEU:HD12	1.85	0.59
1:A:278:ILE:HD12	1:A:278:ILE:N	2.18	0.59
1:B:226:VAL:O	3:B:501:HOH:O	2.17	0.59
1:A:224:GLU:HG3	1:A:258:ASP:CG	2.28	0.58
1:C:266:ARG:HH11	1:C:266:ARG:HG3	1.68	0.58
1:C:278:ILE:HD11	1:C:311:LYS:HG2	1.85	0.58
1:C:199:MET:HE1	1:C:232:ILE:HG22	1.86	0.58
1:B:259:GLU:HB3	3:B:502:HOH:O	2.04	0.57
1:C:266:ARG:HG3	1:C:266:ARG:NH1	2.19	0.57
1:C:234:PRO:HG2	1:C:259:GLU:HG2	1.87	0.56
1:D:232:ILE:HG23	1:D:236:GLU:OE1	2.05	0.56
1:B:24:VAL:HG13	1:B:91:ASP:HA	1.86	0.56
1:A:105:ASP:OD1	1:A:107:HIS:HD2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:GLN:NE2	1:A:47:GLN:HA	2.20	0.56
1:C:22:ARG:HH21	1:C:66:LEU:HD11	1.71	0.56
1:A:276:ASN:HB2	1:A:288:PRO:HA	1.87	0.56
1:C:228:GLU:CA	3:C:501:HOH:O	2.42	0.56
1:A:72:LYS:HZ1	1:A:75:GLN:HG3	1.71	0.55
1:A:21:HIS:CE1	1:A:92:ASP:HB3	2.43	0.54
1:C:62:PHE:N	3:C:507:HOH:O	2.25	0.54
1:B:259:GLU:CB	3:B:502:HOH:O	2.56	0.54
1:C:111:ASP:OD2	3:C:506:HOH:O	2.19	0.53
1:B:259:GLU:C	3:B:502:HOH:O	2.33	0.53
1:C:-2:GLN:O	1:C:2:ILE:HG13	2.09	0.52
1:C:70:ASP:N	3:C:504:HOH:O	2.03	0.52
1:D:41:ILE:HG22	1:D:50:VAL:HG21	1.91	0.52
1:B:275:ILE:HG13	1:B:288:PRO:O	2.10	0.52
1:C:295:VAL:CG1	1:C:300:GLU:HB3	2.34	0.51
1:B:2:ILE:HA	1:B:5:LEU:HD12	1.92	0.51
1:D:-4:TYR:HD1	1:D:5:LEU:HD11	1.76	0.51
1:C:132:ASP:OD1	1:C:170:HIS:HE1	1.94	0.51
1:B:21:HIS:CD2	1:B:92:ASP:HB3	2.45	0.50
1:D:231:GLY:C	1:D:232:ILE:HD13	2.37	0.50
1:D:214:ASP:CG	3:D:506:HOH:O	2.53	0.50
1:B:8:ILE:O	1:B:12:ILE:HG13	2.11	0.50
1:C:277:ASP:OD1	1:C:311:LYS:NZ	2.45	0.49
1:A:278:ILE:CD1	1:A:278:ILE:N	2.76	0.49
1:C:69:ILE:HB	3:C:504:HOH:O	2.12	0.49
1:D:92:ASP:C	1:D:93:GLU:HG2	2.37	0.49
1:D:205:TYR:CD1	1:D:209:HIS:CE1	3.01	0.49
1:D:213:MET:HB2	1:D:215:ASP:OD1	2.13	0.48
1:A:7:GLU:HG2	1:A:116:ILE:CD1	2.43	0.48
1:A:287:HIS:O	1:A:291:SER:OG	2.30	0.48
1:A:7:GLU:HG2	1:A:116:ILE:HD13	1.95	0.48
1:D:37:LEU:O	1:D:41:ILE:HD12	2.13	0.48
1:B:186:ASN:ND2	1:B:190:ASN:HD21	2.02	0.48
1:D:71:ASP:N	1:D:71:ASP:OD1	2.47	0.48
1:B:72:LYS:O	1:B:75:GLN:HG3	2.14	0.48
1:C:72:LYS:O	1:C:75:GLN:HG3	2.14	0.48
1:A:275:ILE:C	1:A:275:ILE:CD1	2.85	0.47
1:C:24:VAL:O	1:C:89:ARG:NH2	2.47	0.47
1:D:277:ASP:OD2	1:D:311:LYS:NZ	2.45	0.47
1:C:227:LEU:CB	3:C:503:HOH:O	2.33	0.47
1:B:46:PRO:N	1:B:47:GLN:OE1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ASP:HB3	1:A:142:ILE:HD12	1.97	0.46
1:D:232:ILE:CG2	1:D:233:GLN:N	2.78	0.46
1:B:68:ASN:HA	3:B:521:HOH:O	2.15	0.46
1:A:277:ASP:OD1	1:A:277:ASP:N	2.47	0.46
1:D:232:ILE:CG2	1:D:236:GLU:HB2	2.45	0.46
1:A:286:GLY:HA3	3:A:526:HOH:O	2.16	0.46
1:D:199:MET:HE3	1:D:232:ILE:HD11	1.94	0.46
1:A:277:ASP:HA	1:A:280:GLN:HE21	1.78	0.46
1:A:211:GLU:O	1:A:218:CYS:HA	2.15	0.46
1:D:284:GLY:HA3	1:D:293:VAL:HG12	1.98	0.46
1:C:195:LYS:NZ	1:C:240:PHE:HE1	2.14	0.45
1:C:175:ALA:O	1:C:179:ILE:HG13	2.16	0.45
1:D:24:VAL:HG22	1:D:89:ARG:O	2.16	0.45
1:C:0:HIS:ND1	3:C:509:HOH:O	2.33	0.45
1:B:264:ARG:HG3	1:B:264:ARG:NH1	2.30	0.45
1:C:78:LEU:HD13	1:C:100:LYS:HB3	1.99	0.44
1:D:232:ILE:HG22	1:D:233:GLN:N	2.32	0.44
1:C:278:ILE:HD13	1:C:307:ALA:C	2.42	0.44
1:C:76:ASP:HA	1:C:99:ARG:HB2	2.00	0.44
1:C:227:LEU:CB	3:C:501:HOH:O	2.65	0.43
1:A:263:ILE:HB	1:A:295:VAL:HG23	2.00	0.43
1:C:78:LEU:HD12	1:C:79:VAL:N	2.33	0.43
1:C:259:GLU:OE1	1:C:259:GLU:O	2.35	0.43
1:B:267:LEU:HD23	1:B:308:LEU:HD21	2.00	0.43
1:C:259:GLU:O	1:C:259:GLU:CD	2.61	0.43
1:C:31:TYR:CD1	1:C:60:LEU:HD23	2.54	0.43
1:B:303:GLN:HG2	3:B:503:HOH:O	2.18	0.43
1:C:267:LEU:HB3	1:C:275:ILE:HD13	2.00	0.43
1:A:202:PHE:HZ	1:A:222:ILE:HG13	1.84	0.43
1:B:22:ARG:HH11	1:B:22:ARG:HD2	1.71	0.42
1:A:71:ASP:N	1:A:71:ASP:OD1	2.52	0.42
1:D:0:HIS:N	3:D:501:HOH:O	2.50	0.42
1:B:97:THR:O	1:B:97:THR:HG22	2.18	0.42
1:C:287:HIS:CG	1:C:288:PRO:HD2	2.55	0.42
1:D:205:TYR:CE1	1:D:209:HIS:CE1	3.08	0.42
1:A:258:ASP:OD1	1:A:258:ASP:C	2.62	0.41
1:C:266:ARG:HH11	1:C:266:ARG:CG	2.32	0.41
1:C:306:THR:O	1:C:310:THR:HG23	2.19	0.41
1:D:91:ASP:OD1	1:D:92:ASP:N	2.49	0.41
1:B:211:GLU:CD	1:B:219:GLN:HE21	2.29	0.41
1:C:199:MET:CE	1:C:232:ILE:HG22	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:PHE:HD1	1:A:252:ILE:HG22	1.86	0.41
1:B:-6:ASN:O	1:B:-2:GLN:HG3	2.20	0.41
1:C:22:ARG:HB2	1:C:30:ALA:HB1	2.03	0.41
1:C:238:SER:HB3	1:C:266:ARG:NH1	2.36	0.41
1:B:189:LEU:O	1:B:193:MET:HG3	2.20	0.40
1:A:280:GLN:HE21	1:A:280:GLN:HB2	1.61	0.40
1:C:47:GLN:OE1	1:C:47:GLN:N	2.49	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	318/333 (96%)	308 (97%)	10 (3%)	0	100	100
1	B	321/333 (96%)	315 (98%)	6 (2%)	0	100	100
1	C	318/333 (96%)	311 (98%)	7 (2%)	0	100	100
1	D	318/333 (96%)	309 (97%)	9 (3%)	0	100	100
All	All	1275/1332 (96%)	1243 (98%)	32 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	278/290 (96%)	278 (100%)	0	100	100
1	B	281/290 (97%)	281 (100%)	0	100	100
1	C	278/290 (96%)	278 (100%)	0	100	100
1	D	278/290 (96%)	277 (100%)	1 (0%)	84	82
All	All	1115/1160 (96%)	1114 (100%)	1 (0%)	88	87

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	246	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	47	GLN
1	A	75	GLN
1	A	107	HIS
1	A	136	HIS
1	A	138	ASN
1	A	181	HIS
1	A	186	ASN
1	A	280	GLN
1	C	15	ASN
1	C	170	HIS
1	C	280	GLN
1	C	289	ASN
1	C	303	GLN
1	D	6	ASN
1	D	136	HIS
1	D	181	HIS
1	D	186	ASN
1	D	190	ASN
1	D	229	GLN
1	D	233	GLN
1	B	6	ASN
1	B	21	HIS
1	B	186	ASN
1	B	209	HIS
1	B	219	GLN

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Mol	Chain	Res	Type
1	B	233	GLN
1	B	261	ASN
1	B	303	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	320/333 (96%)	0.74	23 (7%) 21 23	38, 55, 70, 78	0
1	B	323/333 (96%)	0.49	8 (2%) 58 62	39, 52, 67, 77	0
1	C	320/333 (96%)	0.81	18 (5%) 30 33	45, 60, 72, 77	0
1	D	320/333 (96%)	0.79	25 (7%) 19 20	44, 58, 73, 80	0
All	All	1283/1332 (96%)	0.71	74 (5%) 29 31	38, 56, 71, 80	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	312	LEU	5.4
1	B	265	CYS	5.0
1	A	301	PHE	4.6
1	D	-5	LEU	4.4
1	A	274	ILE	4.4
1	A	296	ASP	4.2
1	C	298	TRP	3.9
1	A	286	GLY	3.8
1	A	298	TRP	3.7
1	A	275	ILE	3.6
1	D	93	GLU	3.3
1	A	287	HIS	3.3
1	D	-4	TYR	3.2
1	A	304	LEU	3.2
1	C	301	PHE	3.2
1	C	183	ILE	3.1
1	D	110	VAL	3.1
1	C	226	VAL	3.0
1	C	222	ILE	3.0
1	D	183	ILE	3.0
1	D	76	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	-1	GLY	2.9
1	A	263	ILE	2.9
1	C	312	LEU	2.8
1	D	90	ILE	2.8
1	D	53	VAL	2.8
1	C	223	THR	2.7
1	D	102	ILE	2.7
1	B	232	ILE	2.7
1	D	-3	PHE	2.6
1	A	308	LEU	2.6
1	D	86	ASN	2.6
1	C	50	VAL	2.6
1	B	-3	PHE	2.5
1	C	263	ILE	2.5
1	D	307	ALA	2.5
1	A	288	PRO	2.5
1	A	307	ALA	2.4
1	C	295	VAL	2.4
1	A	294	SER	2.4
1	C	261	ASN	2.4
1	C	247	ILE	2.4
1	A	278	ILE	2.3
1	A	273	LEU	2.3
1	D	56	ALA	2.3
1	A	70	ASP	2.3
1	C	225	ASP	2.3
1	C	264	ARG	2.2
1	D	312	LEU	2.2
1	C	256	ALA	2.2
1	D	0	HIS	2.2
1	D	68	ASN	2.2
1	B	-9	SER	2.2
1	D	263	ILE	2.2
1	A	280	GLN	2.2
1	B	110	VAL	2.2
1	D	234	PRO	2.2
1	A	165	ASN	2.1
1	D	230	PHE	2.1
1	D	313	ASN	2.1
1	C	98	GLY	2.1
1	D	66	LEU	2.1
1	A	261	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	95	TYR	2.1
1	B	183	ILE	2.1
1	A	16	ASP	2.1
1	D	62	PHE	2.1
1	A	238	SER	2.1
1	C	257	VAL	2.1
1	D	235	ASN	2.1
1	B	237	ALA	2.1
1	C	282	PHE	2.0
1	B	109	ALA	2.0
1	A	268	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

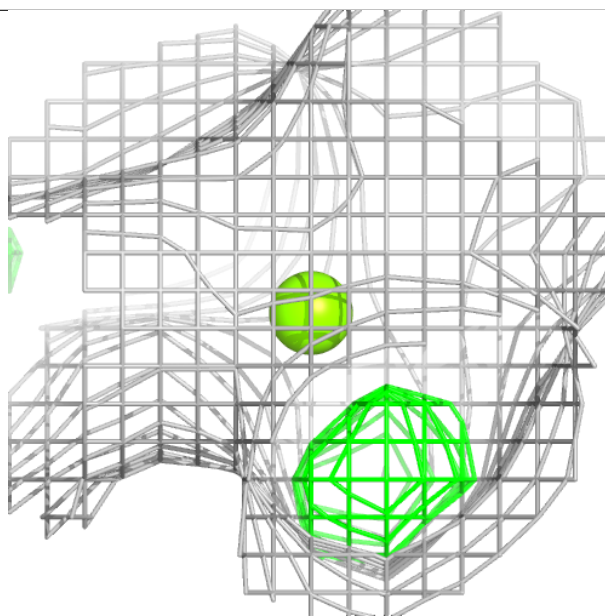
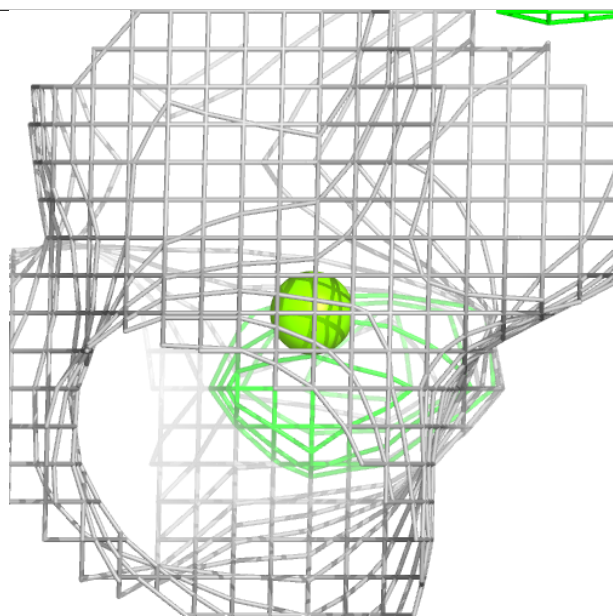
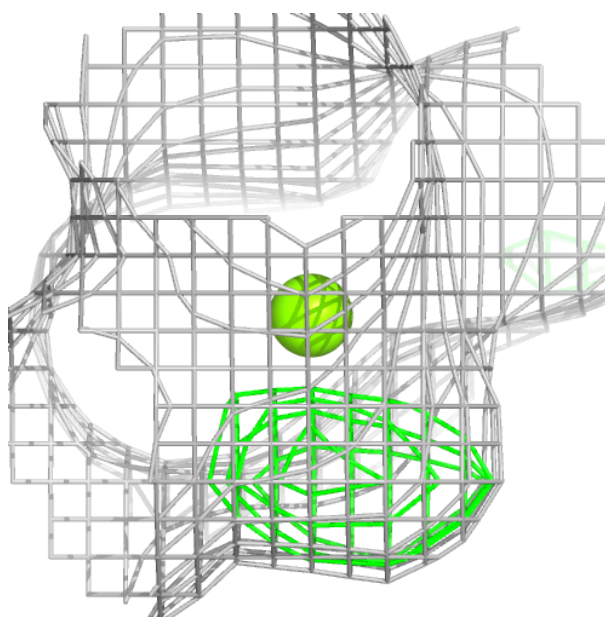
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	D	401	1/1	0.81	0.11	63,63,63,63	0
2	MG	C	402	1/1	0.86	0.14	61,61,61,61	0
2	MG	D	402	1/1	0.88	0.08	58,58,58,58	0
2	MG	A	402	1/1	0.90	0.09	46,46,46,46	0
2	MG	B	401	1/1	0.91	0.07	64,64,64,64	0
2	MG	B	402	1/1	0.91	0.06	48,48,48,48	0
2	MG	C	401	1/1	0.94	0.06	53,53,53,53	0
2	MG	A	401	1/1	0.94	0.06	39,39,39,39	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.

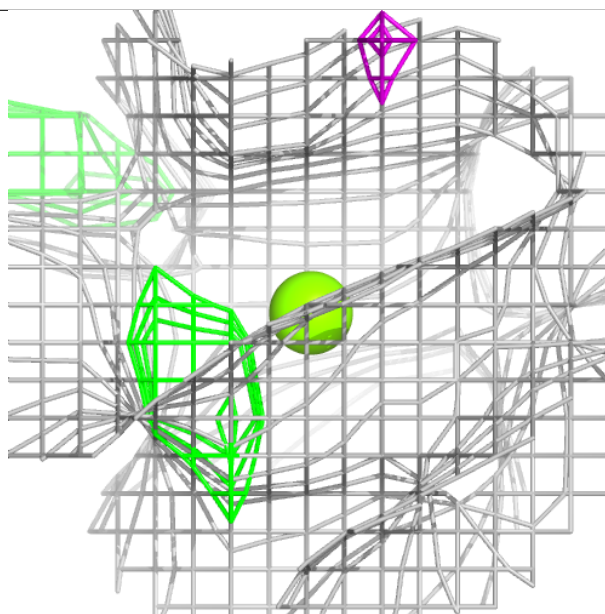
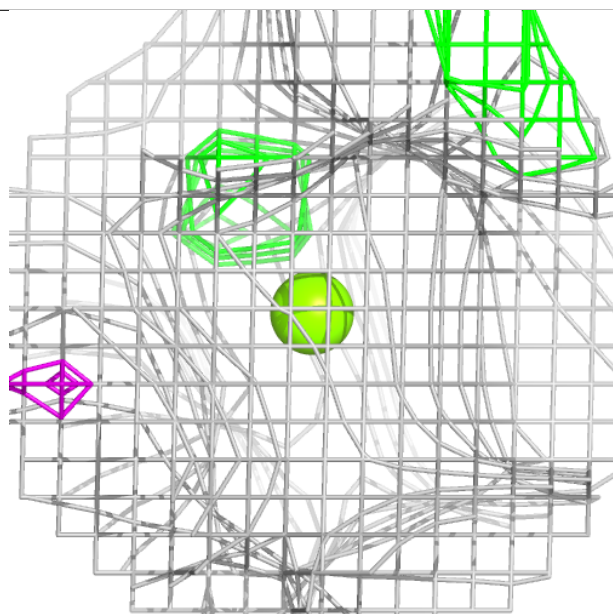
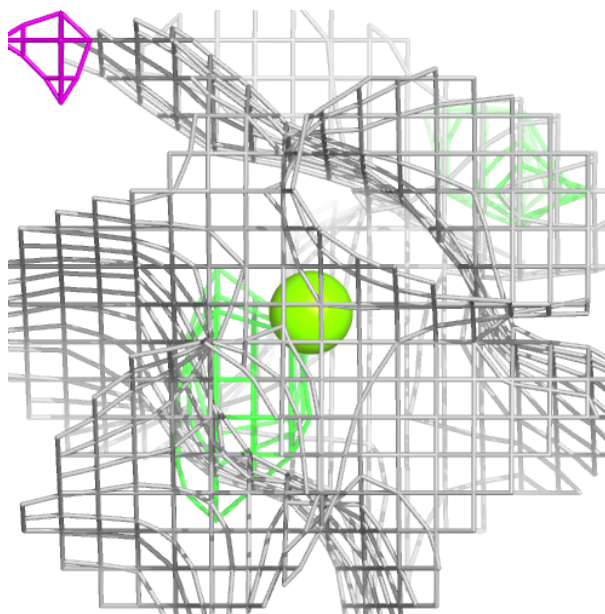
Electron density around MG D 401:

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



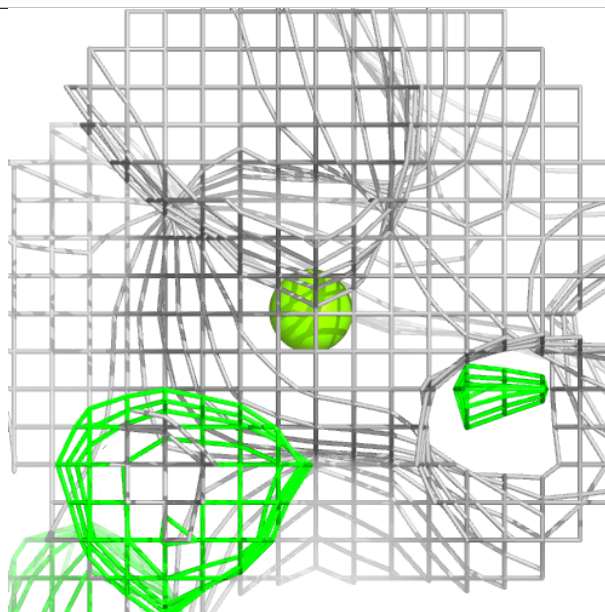
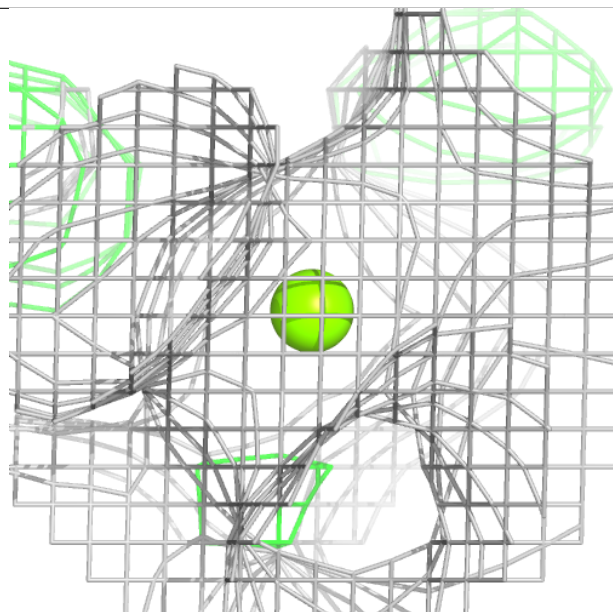
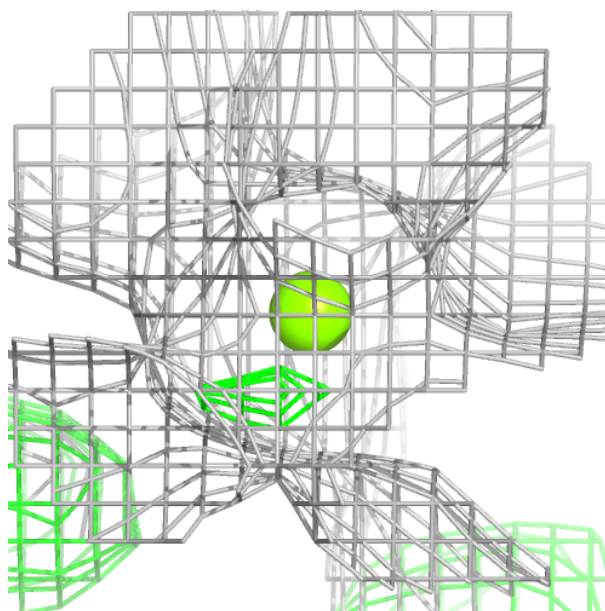
Electron density around MG C 402:

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



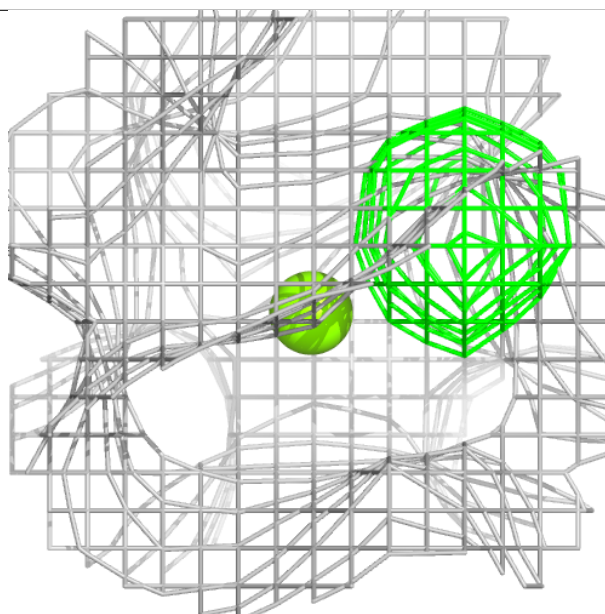
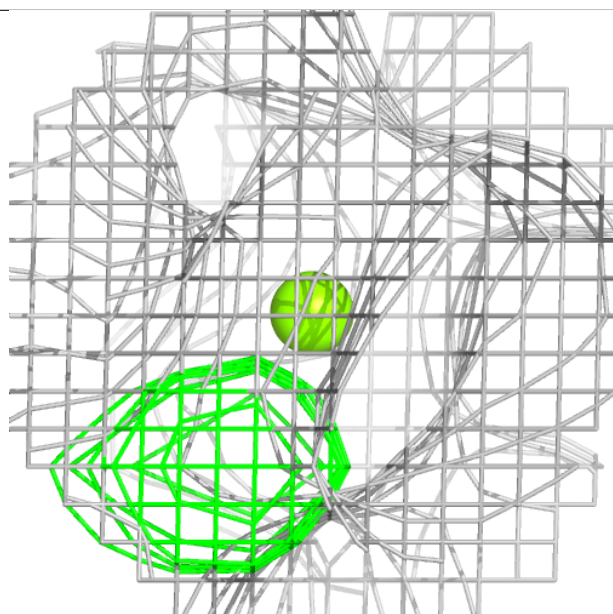
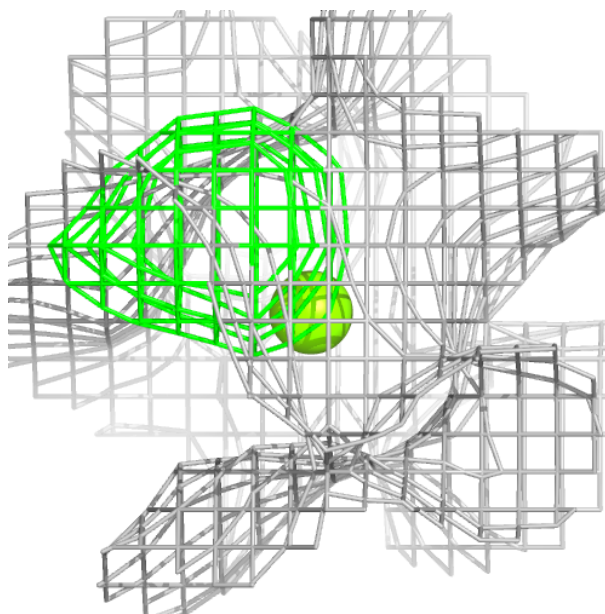
Electron density around MG D 402:

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



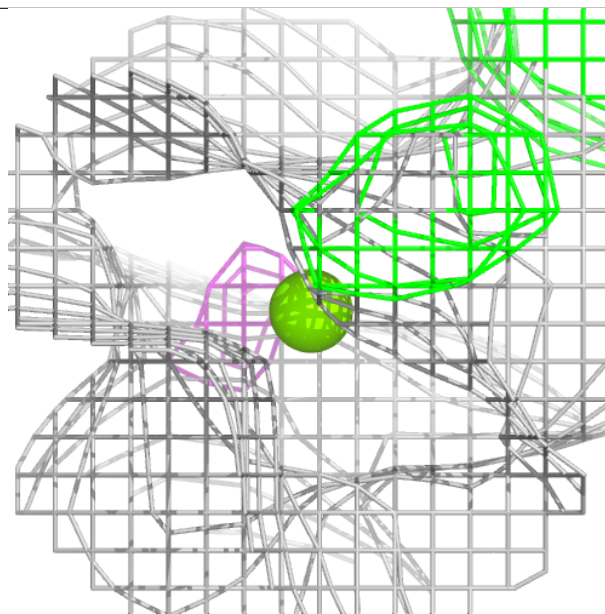
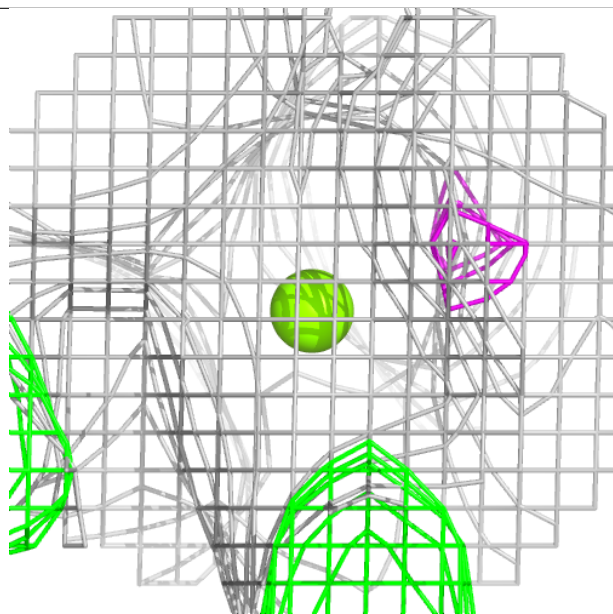
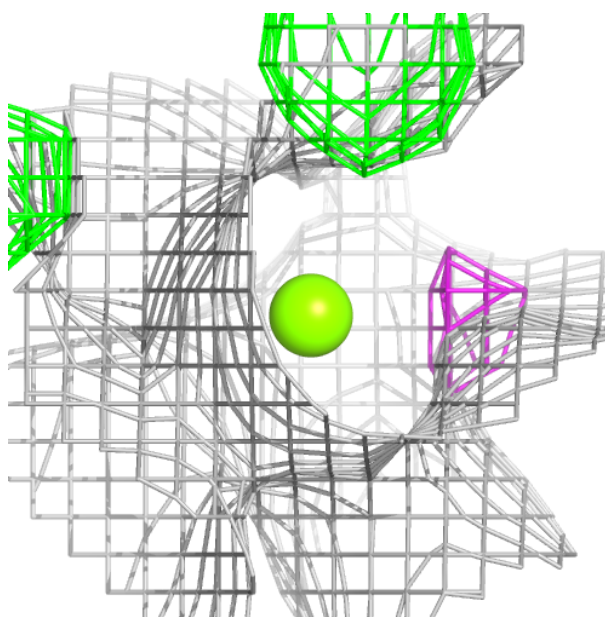
Electron density around MG A 402:

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



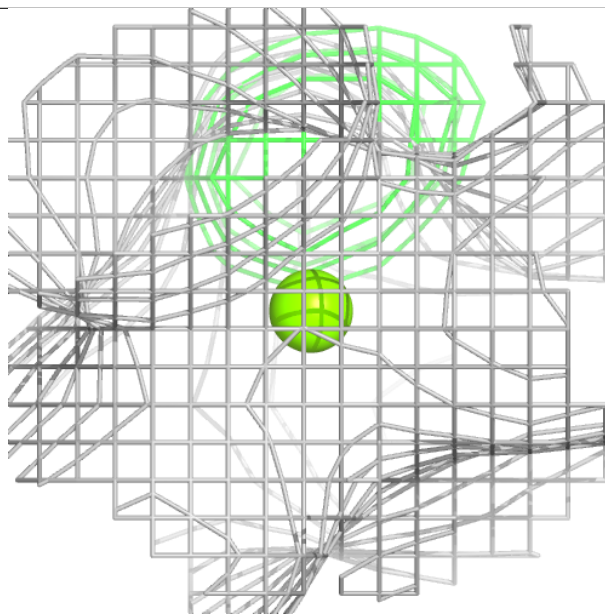
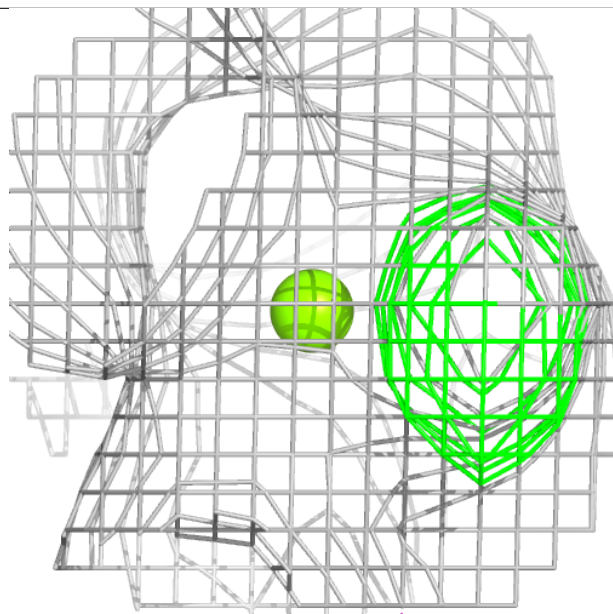
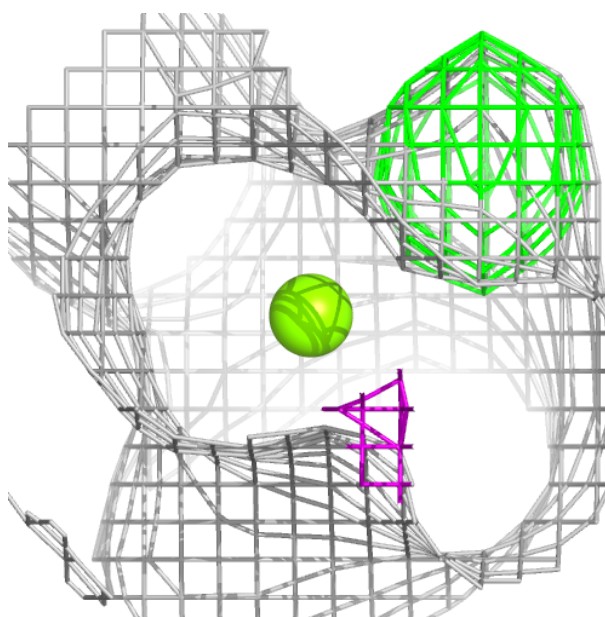
Electron density around MG B 401:

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



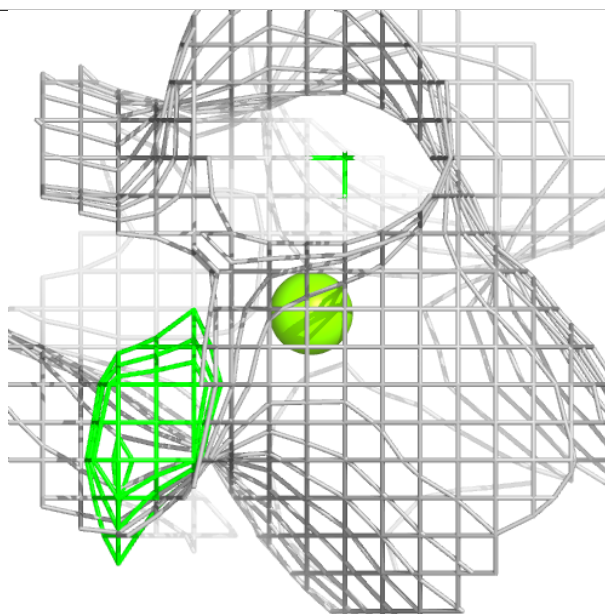
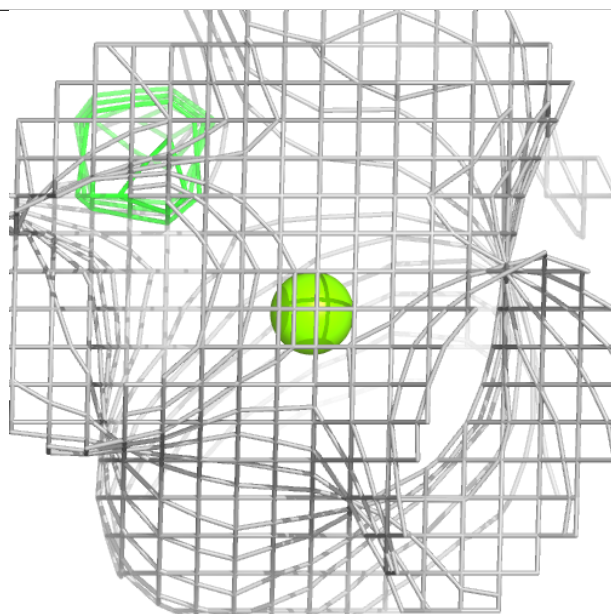
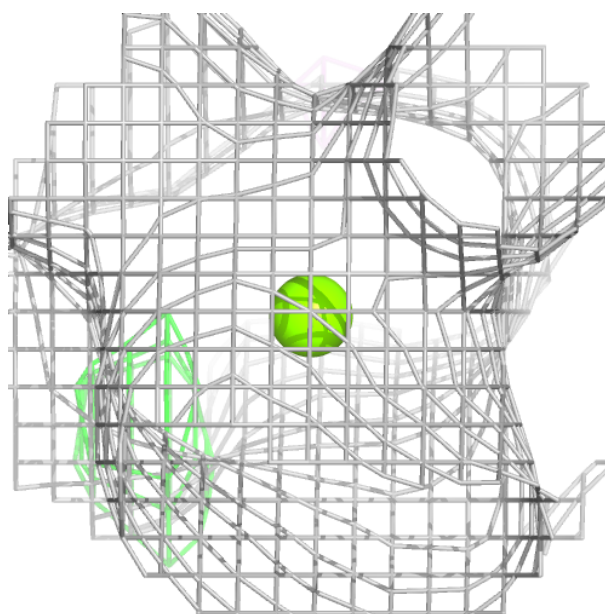
Electron density around MG B 402:

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



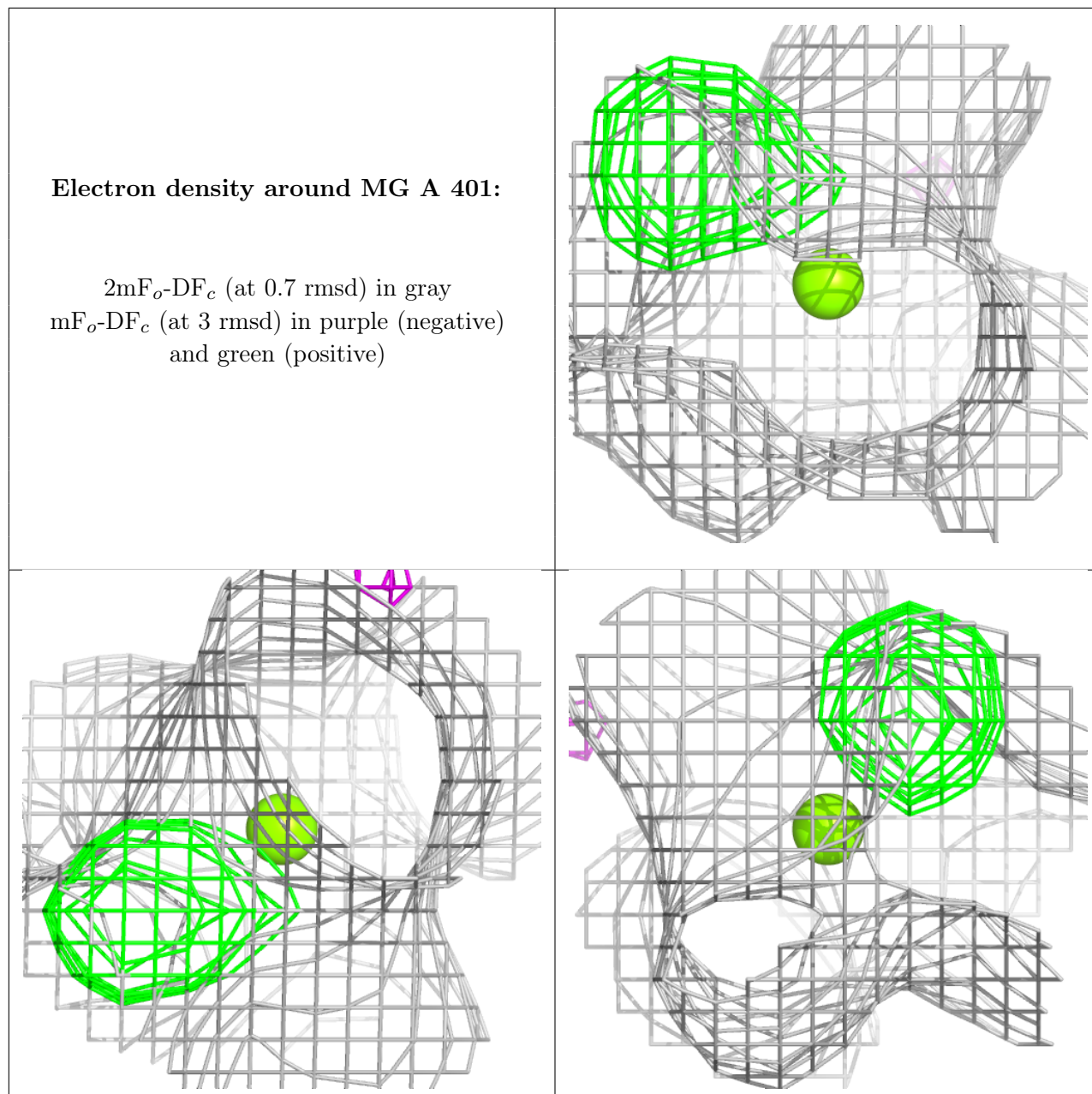
Electron density around MG C 401:

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



Electron density around MG A 401:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.